Supporting Information for:

The C2 hydroxyl group governs the difference in hydrolysis rates of methyl-α-D-*glycero*-D-guloseptanoside and methyl-β-D-*glycero*-D-guloseptanoside

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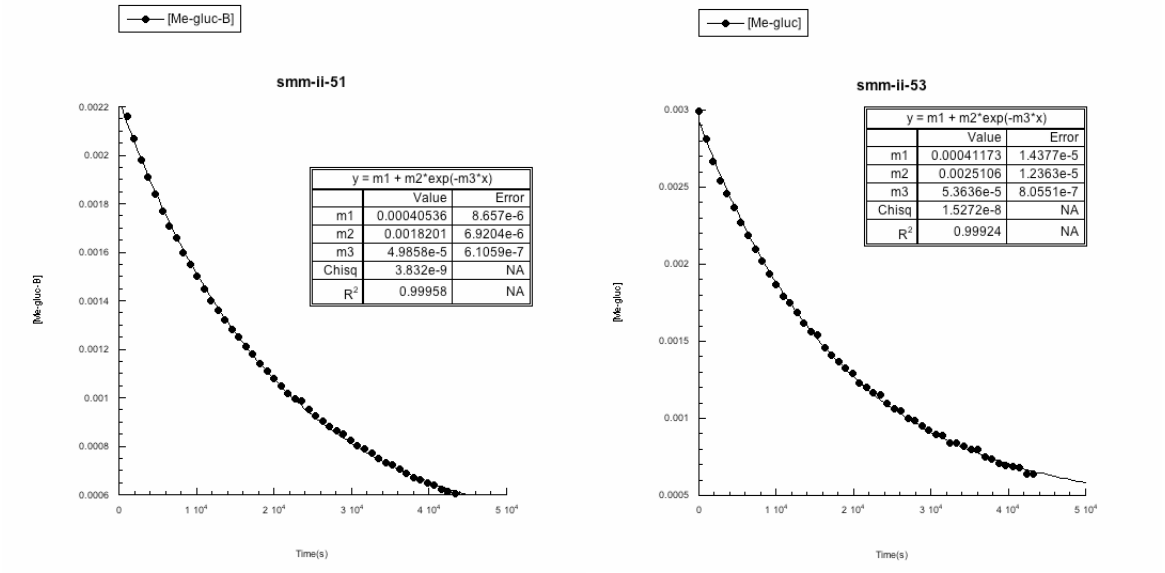
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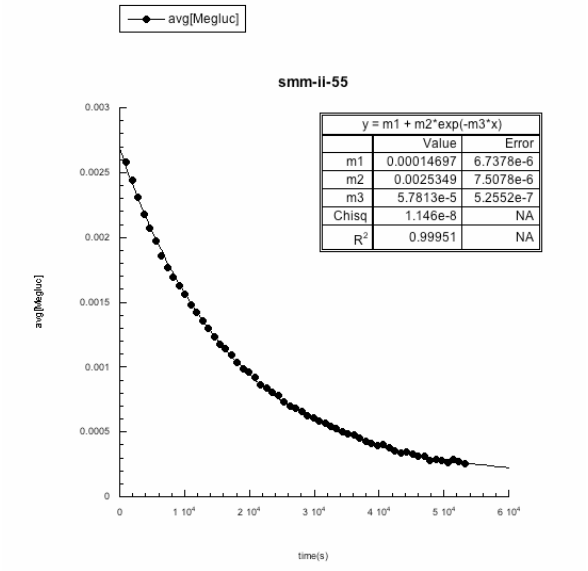
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Section 1: Experimental Hydrolysis Determination: Plots of Concentration vs. Time





Section 2: Conformational Analysis of Septanoside compounds 1, 2, and 3.

A conformational analysis for compounds **1**, **2**, and **3** was carried out in MOE using the procedures described in the manuscript. Below, the full conformational distribution for each compound, including absolute and relative energies at the MMFF94x and B3LYP/6-31+G** (methanol, SMD) levels of theory, and conformational assignment. Standard nomenclature calls for the ring members above the plane to be listed first. In the following assignments, we will be

designating in order around the ring, consecutively (i.e. 1-2-3-4-5-6-O) in order to make visualization of each conformation more feasible.

Compound **1:**

Compound 1	**E(B3LYP)**	***E*(rel) B3LYP**	***E*(MMFF)**	***E*(rel) MMFF**	**Assignment**
21	-841.5214614	0.0	58.356495	6.0	$^{3,4}TC_{5,6}$
34	-841.5214613	0.0	59.522537	7.2	$^{3,4}TC_{5,6}$
32	-841.5208971	0.4	59.44194	7.1	$^{3,4}TC_{5,6}$
46	-841.5205093	0.6	60.839783	8.5	$^{3,4}TC_{5,6}$
71	-841.5204069	0.7	62.331081	10.0	$^{3,4}TC_{5,6}$
49	-841.5203859	0.7	61.194084	8.8	$^{3,4}TC_{5,6}$
63	-841.5203537	0.7	60.499176	9.6	$^{5,6}TC_{O,1}$
58	-841.5201137	0.8	61.74498	9.4	$^{5,6}TC_{O,1}$
16	-841.5199376	1.0	57.548069	5.2	$^{3,4}TC_{5,6}$
47	-841.5199363	1.0	60.858459	8.5	$_{1,2}TC^{3,4}$
36	-841.5196942	1.1	59.907711	7.5	$^{3,4}TC_{5,6}$
72	-841.5196935	1.1	62.350105	10.0	$_{4,5}TC^{6,O}$
61	-841.5195708	1.2	61.879505	9.5	$^{5,6}TC_{O,1}$
70	-841.5195236	1.2	60.850582	10.0	$_{4,5}TC^{6,O}$
19	-841.5193457	1.3	58.133255	5.8	$^{5,6}TC_{O,1}$
2	-841.5193284	1.3	54.079979	1.7	$^{3,4}TC_{5,6}$
40	-841.5187692	1.7	60.420303	8.1	$^{5,6}TC_{O,1}$
28	-841.5180241	2.2	57.38052	6.5	$^{3,4}TC_{5,6}$
59	-841.5174429	2.5	60.296074	9.4	$_{1,2}TC^{3,4}$
54	-841.5169334	2.8	61.467812	9.1	$_{1,2}TC^{3,4}$
37	-841.516542	3.1	60.006794	7.6	$_{3,4}TB^{5,6}$
6	-841.5164359	3.2	55.690693	3.3	$^{3,4}TC_{5,6}$
18	-841.5162835	3.2	57.746937	5.4	$^{3,4}TC_{5,6}$
10	-841.5160798	3.4	57.084854	4.7	$^{3,4}TC_{5,6}$
24	-841.5157089	3.6	58.521881	6.2	$^{3,4}TC_{5,6}$
1	-841.5151889	3.9	52.362373	0.0	$^{3,4}TC_{5,6}$
30	-841.5150656	4.0	58.952492	6.6	$^{3,4}TC_{5,6}$
3	-841.5149476	4.1	53.454048	2.6	$^{3,4}TC_{5,6}$
68	-841.5142289	4.5	60.779083	9.9	chair
15	-841.5141242	4.6	57.489922	5.1	$^{3,4}TC_{5,6}$
67	-841.5140851	4.6	62.212257	9.8	$^{3,4}TC_{5,6}$
8	-841.5138137	4.8	56.631092	4.3	$^{1,2}TC_{3,4}$
43	-841.5136425	4.9	60.584717	8.2	$_{3,4}TC^{5,6}$

29	-841.5132118	5.2	57.425285	6.5	$^{1,2}TC_{3,4}$
26	-841.5131356	5.2	58.755711	6.4	$^{3,4}TC_{5,6}$
53	-841.5130682	5.3	61.461033	9.1	$_{4,5}TC^{6,O}$
38	-841.5122891	5.8	58.619335	7.7	$^{3,4}TC_{5,6}$
4	-841.5122642	5.8	55.161549	2.8	$^{3,4}TC_{5,6}$
64	-841.5122304	5.8	60.526527	9.6	$_{3,4}TB^{5,6}$
48	-841.5119698	6.0	59.489136	8.6	$^{3,4}TC_{5,6}$
65	-841.5118599	6.0	62.096462	9.7	$_{3,4}TB^{5,6}$
45	-841.5116677	6.1	60.810429	8.4	$^{1,2}TC_{3,4}$
7	-841.5116666	6.1	55.777058	3.4	$^{1,2}TC_{3,4}$
42	-841.5114951	6.3	59.068504	8.2	$^{1,2}TC_{3,4}$
17	-841.5114291	6.3	56.224918	5.3	$^{1,2}TC_{3,4}$
25	-841.5112549	6.4	57.149853	6.3	$^{1,2}TC_{3,4}$
50	-841.5109449	6.6	61.234451	8.9	$_{2,3}TC^{4,5}$
39	-841.5109437	6.6	60.266273	7.9	$^{3,4}TC_{5,6}$
52	-841.5107943	6.7	59.891853	9.0	$^{1,2}TC_{3,4}$
33	-841.5106902	6.8	59.486206	7.1	$^{1,2}TC_{3,4}$
14	-841.5105839	6.8	57.487705	5.1	$^{1,2}TC_{3,4}$
11	-841.5101107	7.1	57.15094	4.8	$^{1,2}TC_{3,4}$
22	-841.5100462	7.2	58.35931	6.0	$_{1,2}TB^{3,4}$
51	-841.5100458	7.2	61.278347	8.9	$_{1,2}TB^{3,4}$
13	-841.5093799	7.6	57.372566	5.0	$^{4,5}TC_{6,O}$
5	-841.5086528	8.0	55.587868	3.2	$^{1,2}TC_{3,4}$
35	-841.5082493	8.3	59.686497	7.3	$^{5,6}TC_{O,1}$
60	-841.5081565	8.3	61.845676	9.5	$^{1,2}TC_{3,4}$
12	-841.5079784	8.5	57.309208	4.9	$_{1,2}TC^{3,4}$
20	-841.5078907	8.5	58.147911	5.8	$^{3,4}TC_{5,6}$
27	-841.5077516	8.6	58.835258	6.5	$_{1,2}TC^{3,4}$
9	-841.5077297	8.6	57.053219	4.7	$^{4,5}TC_{6,O}$
41	-841.5073059	8.9	60.518158	8.2	$^{1,2}TC_{3,4}$
56	-841.5072633	8.9	61.679554	9.3	boat
66	-841.506878	9.2	62.183464	9.8	$^{4,5}TC_{6,O}$
44	-841.5061518	9.6	60.74678	8.4	$_{1,2}TC^{3,4}$
69	-841.5055753	10.0	62.316761	10.0	$^{5,6}TC_{O,1}$
23	-841.5051593	10.2	58.499886	6.1	$^{5,6}TC_{O,1}$
57	-841.5048652	10.4	61.732384	9.4	boat
55	-841.5011415	12.8	61.533955	9.2	$^{4,5}TC_{6,O}$
31	-841.4999898	13.5	59.153934	6.8	$^{4,5}TC_{6,O}$
62	-841.4965443	15.6	61.894444	9.5	boat

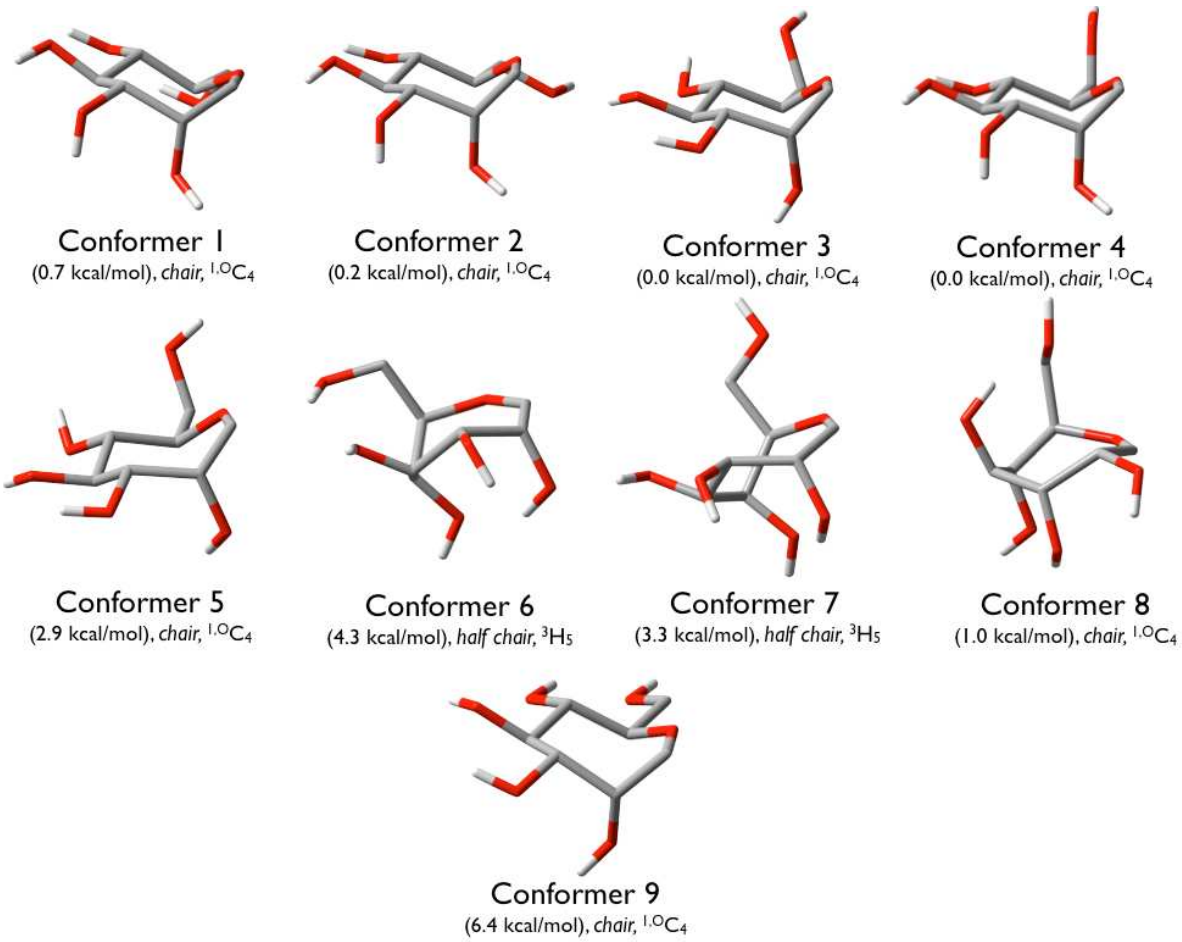
Compound **2**

Compound 2	***E*(B3LYP)**	***E*(rel) B3LYP**	***E*(MMFF)**	***E*(rel) MMFF**	**Assignment**
61	-841.5160984	0.0	58.6404	6.2	$^{3,4}TC_{5,6}$
5	-841.5160981	0.0	54.287563	1.9	$_{4,5}TC^{6,O}$
31	-841.5157148	0.2	56.601971	4.2	$_{4,5}TC^{6,O}$
48	-841.5152044	0.6	58.009708	5.6	$_{4,5}TC^{6,O}$
11	-841.51514	0.6	55.152416	2.7	$_{4,5}TC^{6,O}$
62	-841.5147088	0.9	60.699013	8.3	$_{4,5}TC^{6,O}$
52	-841.5143756	1.1	60.40414	8.0	$_{4,5}TB^{6,O}$
24	-841.514297	1.1	58.559731	6.1	$_{4,5}TC^{6,O}$
13	-841.5139054	1.4	56.536404	4.1	$_{4,5}TC^{6,O}$
1	-841.5139037	1.4	52.556458	0.1	$_{4,5}TC^{6,O}$
89	-841.5138417	1.4	59.105129	6.7	$^{3,4}TC_{5,6}$
82	-841.5136187	1.6	61.900265	9.5	$_{4,5}TC^{6,O}$
21	-841.5135897	1.6	58.267292	5.9	$_{1,2}TC^{3,4}$
29	-841.5133962	1.7	57.763477	5.4	$_{4,5}TC^{6,O}$
33	-841.5131745	1.8	59.377655	7.0	$^{5,6}TC_{O,1}$
53	-841.5131395	1.9	56.747173	4.3	$_{1,2}TC^{3,4}$
6	-841.5131204	1.9	54.947071	2.5	$^{3,4}TC_{5,6}$
77	-841.5130903	1.9	61.718948	9.3	$^{3,4}TC_{5,6}$
26	-841.5129886	2.0	56.771011	4.4	$_{1,2}TC^{3,4}$
44	-841.5129787	2.0	60.057034	7.6	$_{4,5}TC^{6,O}$
19	-841.5128943	2.0	57.412506	5.0	$_{4,5}TC^{6,O}$
49	-841.5127369	2.1	60.335159	7.9	$_{4,5}TC^{6,O}$
56	-841.5125612	2.2	60.637516	8.2	$^{6,O}TC_{1,2}$
63	-841.512349	2.4	60.183277	7.8	$_{4,5}TC^{6,O}$
78	-841.5123427	2.4	58.97353	6.6	chair
72	-841.5123425	2.4	61.503372	9.1	$_{4,5}TC^{6,O}$
97	-841.5121205	2.5	62.467682	10.1	boat
22	-841.5119805	2.6	57.3326	4.9	$_{4,5}TC^{6,O}$
87	-841.5119573	2.6	59.372414	7.0	$_{4,5}TC^{6,O}$
8	-841.5117369	2.7	53.432076	1.0	$_{4,5}TC^{6,O}$
9	-841.5117369	2.7	53.432076	1.0	$_{4,5}TC^{6,O}$
27	-841.5116909	2.8	58.673759	6.3	$^{1,2}TC_{3,4}$
45	-841.5116909	2.8	57.339619	4.9	$^{6,O}TC_{1,2}$
17	-841.5116633	2.8	57.793388	5.4	$^{3,4}TC_{5,6}$
4	-841.5114953	2.9	54.837387	2.4	$_{4,5}TC^{6,O}$

25	-841.5112769	3.0	58.635315	6.2	$_{2,3}TC^{4,5}$
84	-841.5112386	3.0	61.818768	9.4	$_{2,3}TC^{4,5}$
73	-841.5112104	3.1	58.979759	6.6	$_{1,2}TC^{3,4}$
91	-841.5111987	3.1	59.432476	7.0	$_{2,3}TC^{4,5}$
2	-841.5111266	3.1	52.411179	0.0	$_{3,4}TC^{5,6}$
69	-841.5110057	3.2	59.168282	6.8	$_{1,2}TC^{3,4}$
32	-841.5108134	3.3	58.173859	5.8	$_{3,4}TC^{5,6}$
71	-841.5105806	3.5	60.478989	8.1	$_{4,5}TC^{6,O}$
14	-841.5104671	3.5	57.069588	4.7	$_{4,5}TC^{6,O}$
59	-841.510436	3.6	59.536961	7.1	$^{3,4}TC_{5,6}$
38	-841.5102504	3.7	59.939327	7.5	$_{4,5}TC^{6,O}$
10	-841.5102438	3.7	55.09277	2.7	$_{4,5}TC^{6,O}$
40	-841.5102208	3.7	59.894714	7.5	$^{3,4}TC_{5,6}$
64	-841.510054	3.8	60.424591	8.0	$^{O,1}TC_{2,3}$
39	-841.5098512	3.9	58.955879	6.5	$_{3,4}TC^{5,6}$
67	-841.5098182	3.9	61.280827	8.9	$_{3,4}TC^{5,6}$
65	-841.509705	4.0	60.242779	7.8	$_{3,4}TC^{5,6}$
35	-841.5096727	4.0	59.555695	7.1	$_{1,2}TC^{3,4}$
58	-841.5096442	4.1	60.663502	8.3	$^{1,2}TC_{3,4}$
81	-841.5096437	4.1	60.272144	7.9	$^{3,4}TC_{5,6}$
68	-841.509599	4.1	60.852425	8.4	$^{3,4}TC_{5,6}$
54	-841.5095729	4.1	59.785522	7.4	$_{6,O}TC^{1,2}$
46	-841.5095728	4.1	60.017902	7.6	chair
94	-841.5094871	4.1	59.219501	6.8	$^{1,2}TC_{3,4}$
57	-841.5094801	4.2	60.642879	8.2	$^{1,2}TC_{3,4}$
95	-841.5094413	4.2	58.625576	6.2	$^{3,4}TC_{5,6}$
86	-841.5094387	4.2	59.362972	7.0	$_{1,2}TC^{3,4}$
42	-841.5093901	4.2	59.902748	7.5	$^{3,4}TC_{5,6}$
16	-841.5092931	4.3	55.019474	2.6	chair
75	-841.5092774	4.3	60.761963	8.4	$_{6,O}TC^{1,2}$
98	-841.5092292	4.3	62.04443	9.6	$_{6,O}TC^{1,2}$
15	-841.5092224	4.3	55.465443	3.1	$_{4,5}TC^{6,O}$
41	-841.5091913	4.3	57.280369	4.9	$^{1,2}TC_{3,4}$
47	-841.5091819	4.3	60.314548	7.9	boat
23	-841.5090436	4.4	54.821857	2.4	$_{1,2}TC^{3,4}$
30	-841.509042	4.4	58.575199	6.2	chair
43	-841.5090011	4.5	57.875404	5.5	$^{5,6}TC_{O,1}$
34	-841.508799	4.6	58.442787	6.0	$^{3,4}TC_{5,6}$
79	-841.5084782	4.8	61.795567	9.4	chair
36	-841.50836	4.9	57.233089	4.8	boat
60	-841.5082273	4.9	58.578892	6.2	$^{1,2}TC_{3,4}$

7	-841.50814	5.0	55.396698	3.0	$^{3,4}TC_{5,6}$
92	-841.5081196	5.0	61.033756	8.6	$^{1,2}TC_{3,4}$
12	-841.5081084	5.0	56.093372	3.7	$^{3,4}TC_{5,6}$
3	-841.5078351	5.2	52.727547	0.3	chair
96	-841.5077929	5.2	61.416332	9.0	$^{6,O}TB_{1,2}$
88	-841.5077131	5.3	61.410625	9.0	$^{6,O}TC_{1,2}$
74	-841.507418	5.4	60.750778	8.3	boat
55	-841.5073772	5.5	57.753006	5.3	chair
85	-841.5073713	5.5	61.86985	9.5	$^{6,O}TC_{1,2}$
50	-841.5073123	5.5	58.17506	5.8	$_{1,2}TB^{3,4}$
76	-841.5072175	5.6	61.64135	9.2	$_{1,2}TC^{3,4}$
93	-841.5070286	5.7	62.116375	9.7	boat
28	-841.5069184	5.8	57.687714	5.3	boat
51	-841.5069071	5.8	60.383522	8.0	$^{5,6}TC_{O,1}$
83	-841.506648	5.9	61.927094	9.5	boat
90	-841.5064876	6.0	62.190716	9.8	$_{1,2}TC^{3,4}$
70	-841.5064709	6.0	58.10231	5.7	chair
20	-841.5063965	6.1	57.46867	5.1	$^{1,2}TC_{3,4}$
37	-841.5063066	6.1	57.007629	4.6	$^{5,6}TC_{O,1}$
66	-841.5060938	6.3	58.693588	6.3	boat
18	-841.5058906	6.4	55.210739	2.8	chair
80	-841.5044628	7.3	59.641983	7.2	$^{5,6}TC_{O,1}$

Compound **3:**


Conformer 1
(0.7 kcal/mol), chair, $^{1,O}C_4$
Conformer 2
(0.2 kcal/mol), chair, $^{1,O}C_4$
Conformer 3
(0.0 kcal/mol), chair, $^{1,O}C_4$
Conformer 4
(0.0 kcal/mol), chair, $^{1,O}C_4$
Conformer 5
(2.9 kcal/mol), chair, $^{1,O}C_4$
Conformer 6
(4.3 kcal/mol), half chair, $^{3}H_5$
Conformer 7
(3.3 kcal/mol), half chair, $^{3}H_5$
Conformer 8
(1.0 kcal/mol), chair, $^{1,O}C_4$
Conformer 9
(6.4 kcal/mol), chair, $^{1,O}C_4$

Section 3: Hartree-Fock Potential Energy Surfaces

Several computational studies have previously investigated glycosidic hydrolysis, with mixed reports of success isolating discrete transistion states for the bond cleavage process.[i] We have had success isolating transition states for exocyclic bond cleavage using the Hartree-Fock (HF) methodology, although at higher levels of theory (MP2, DFT methods) that include electron correlation, the discrete transition state disappears. This disappearance is caused by a destabilization of the dissociated complex, whose energy is increased due to more accurate treatment of electron correlation. Potential energy surfaces obtained using the HF-optimized geometries in implicit methanol are compared at several methodologies, including HF, B3LYP, MP2, and M06-2X, each utilizing a 6-311+G** basis set. As reported in the manuscript, transition states were connected to their associated minima via intrinsic reaction coordinates. A vibrational frequency analysis confirmed each HF-optimized stationary point as either a minimum or saddle point, and results were used for thermal and vibrational corrections to the free energy with frequencies scaled by a factor of 0.904.

The transition state for dissociation of methanol in the anti orientation from compound **1** is characterized by a C–O bond length of 2.00 Å (**Figure S1**). The barrier for dissocation of methanol is calculated to be 4.8 kcal/mol with the HF methodology, and 6.0 and 6.5 kcal/mol for the MP2 and M06-2X methodologies, respectively. The B3LYP methodology completely underestimates the energy of the transition state, and is further lowered in energy by the HF–derived corrections to the free energy. It is important to note that out of the four methods, HF is the only method to predict a transition state for C–O bond cleavage with a stable oxenium ion-methanol product complex. B3LYP, MP2, and M06-2X all predict an asymptotic dissocation of methanol.

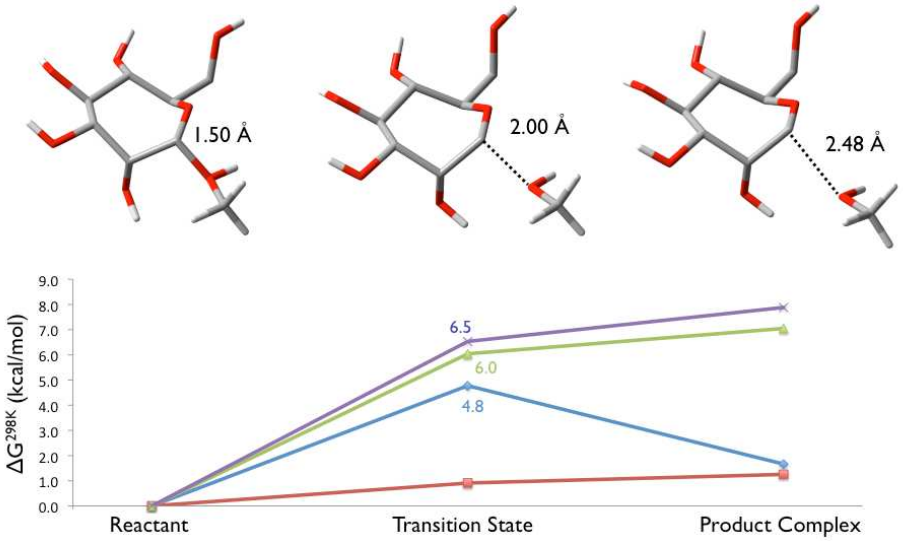


Figure S1: Free energy surface (ΔG, kcal/mol, 298K) for dissociation of methanol (anti orientation) from compound **1** at the HF (blue diamond), B3LYP (red square), MP2 (green triangle), and M06-2X (purple X) level of theory with a 6-311+G** basis set in implicit methanol. Geometries and zero point and thermal energy corrections are from the HF/6-31+G** optimizations carried out in implicit methanol.

The anti orientation of methanol has a relatively small barrier for dissociation, although it is predicted that the gauche orientation should be favored, due to the anti-periplanar relationship between lone pairs on the methanol and the C1-O bond in the ring.[ii] This is indicated by the slightly shorter equilibrium bond between the methanol oxygen and anomeric carbon; in the anti orientation this bond is 1.50 Å, while in the gauche orientation it is decreased to 1.47 Å. In addition, the C1-O(methanol) bond is increased slightly to 2.04 Å at the transition state. HF optimizations on the gauche orientation suggest that the barrier for dissocation of methanol will be significantly higher than for the anti orientation (**Figure S2**).

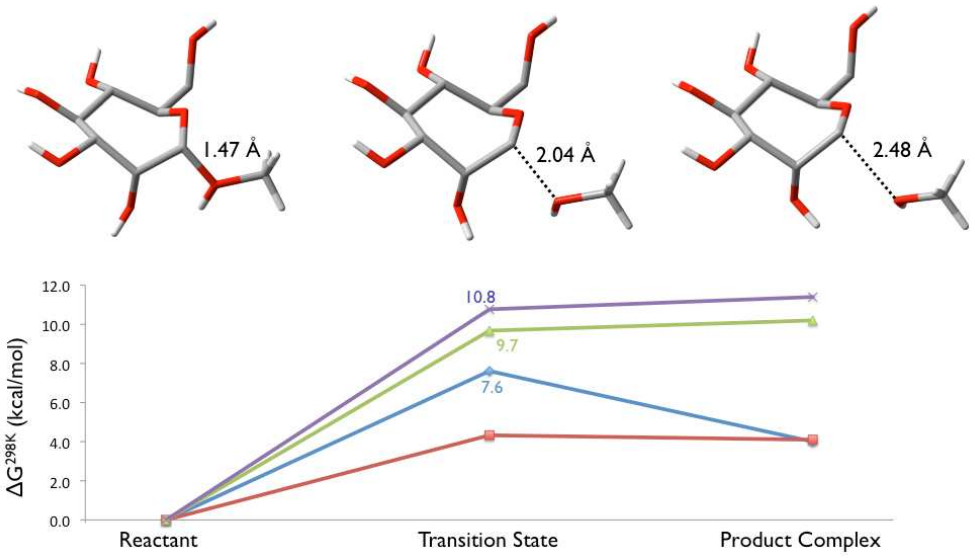


Figure S2: Free energy surface (Δ*G*, kcal/mol, 298K) for dissociation of methanol (gauche orientation) from compound **1** at the HF (blue diamond), B3LYP (red square), MP2 (green triangle), and M06-2X (purple X) level of theory with a 6-311+G** basis set in implicit methanol. Geometries and zero point and thermal energy corrections are from the HF/6-31+G** optimizations carried out in implicit methanol.

While the HF optimizations suggest the gauche orientation is favored, compound **1** is roughly 2.5-3 kcal/mol lower in energy with methanol in the gauche orientation rather than anti orientation, the transition state for dissocation of methanol from the gauche orientation is also higher in energy. (**Figure S3**) This difference in energy ranges from 0.2 kcal/mol (HF method) to 1.0 kcal/mol (MP2, M06-2X).

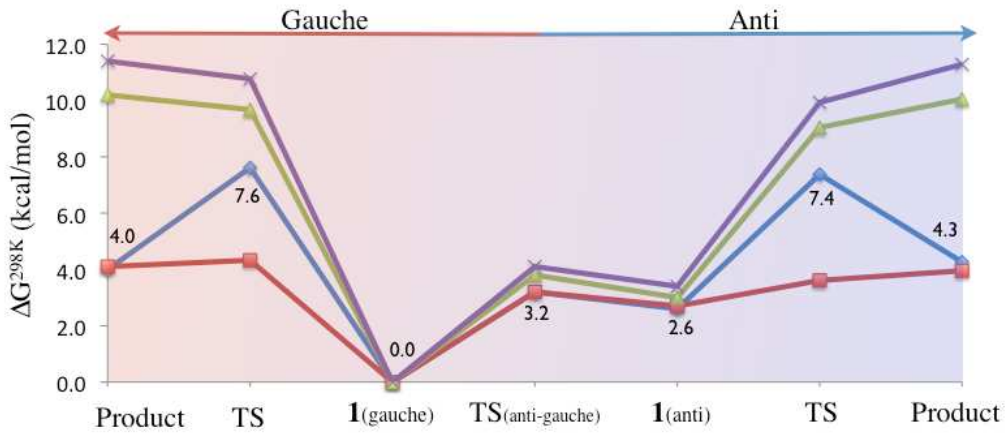


Figure S3: Free energy surface (Δ*G*, kcal/mol, 298K) for dissociation of methanol from compound **1** at the HF (blue diamond, values in figure), B3LYP (red square), MP2 (green triangle), and M06-2X (purple X) level of theory with a 6-311+G** basis set in implicit methanol. Dissociation via the gauche orientation of methanol proceeds to the left of the graph, while dissociation via the anti orientation proceeds via the right side. The transition state for interconversion of anti and gauche orientations of methanol at a C–O bond length of 1.5 Å is labeled TS(anti-gauche) at the center of the graph. Geometries and zero point and thermal energy corrections are from the HF/6-31+G** optimizations carried out in implicit methanol.

In order for the lower energy gauche orientation of methanol to dissociate from the lower barrier anti- orientation, the septanoside must be able to interchange between methanol orientations at some point along the potential energy surface. An examination of the geometries from the relaxed potential energy surface scans does not reveal any intersections at distances relevant to the exocyclic bond cleavage. However, the two structures only differ by rotation of the methanol unit. A transition state for the interchange between gauche and anti orientations of methanol obtained at the HF level of theory indicates that around the equilibrium C-O bond distance of 1.5 Å, the two orientations are separated by a barrier of only 3 kcal/mol. (**Figure S3**) These results suggest that the two orientations can interchange rapidly, and therefore dissociation of methanol from the anti- orientation is chemically feasible.

A second set of identical calculations were carried out on the β anomer, and suggest that compound **2** is roughly 3 kcal/mol higher in energy than compound **1**. The transition state for

dissociation of methanol is predicted to be roughly the same absolute energy as for compound **1**. The equilibrium C1-O(MeOH) bond length is 1.50 Å, the same length as the anti orientation for compound **1.** The transition state bond length for compound **2** is characterized by a slightly longer C-O(MeOH) bond of 2.04 Å than for compound **1**. (**Figure S4**) An investigation of the interactions along the potential energy surface reveal that no hydroxyl groups are close enough to methanol on the β face of the ring, resulting in a lack of interactions between the methanol and the ring for the β anomer (**Figure S4**).

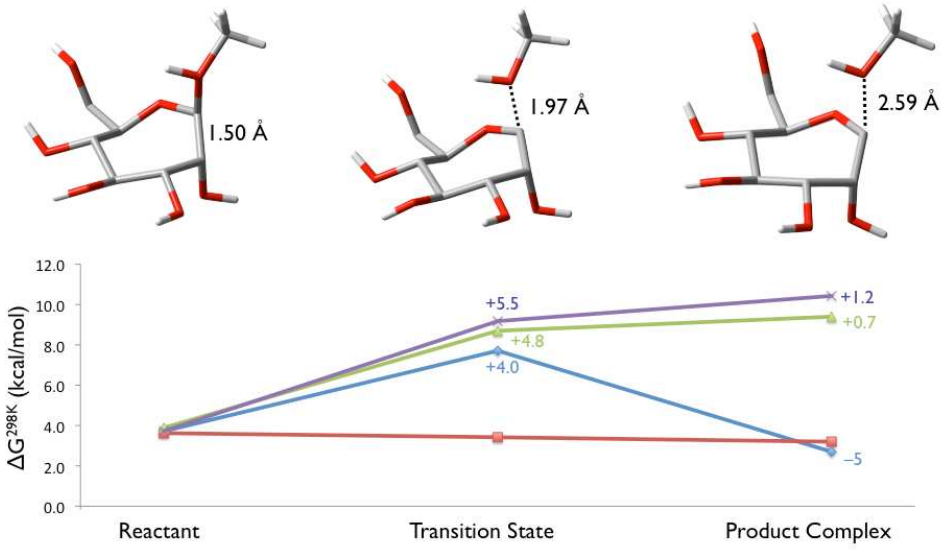


Figure S4: Free energy surface (Δ*G*, kcal/mol, 298K) for dissociation of methanol (gauche orientation) from compound **2** at the HF (blue diamond), B3LYP (red square), MP2 (green triangle), and M06-2X (purple X) level of theory with a 6-311+G** basis set in implicit methanol. Geometries and zero point and thermal energy corrections are from the HF/6-31+G** optimizations carried out in implicit methanol.

Section 4: Ring contraction for β anomer of Compound 3-2

The relaxed potential energy surface scan of compound **3-2** results in an opening of the septanose ring, and reformation of a 6-membered ring (Figure S5). This result appears to be an artifact of the calculation, rather than of scientific relevance, and is mainly attributed to the axial orientation of the C1 proton being unable to interchange to equatorial, resulting in a severely distorted ring.

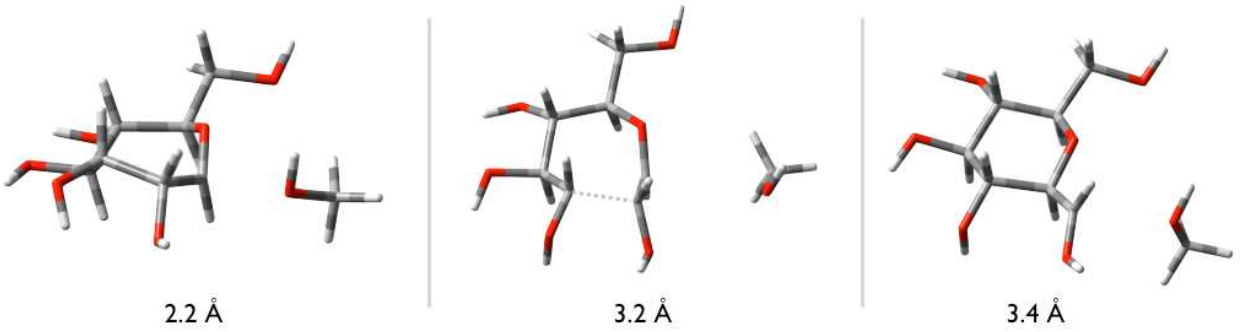


Figure S5: Three geometries around the ring rearrangement of compound 3-2, illustrating the axial orientation of the C1 proton, with cleavage of the C2-C3 bond (3.2 Å structure), and the reforming C1-C3 bond (3.4 Å structure).

Section 5: MP2 Potential Energy Surfaces on the B3LYP/6-31+G* optimized geometries

Potential energy surface scans were carried out at several levels of theory. Csonka *et al* previously identified the M05-2X and M06-2X methodologies as being successful at distinguishing conformational energetics of carbohydrates, and were calibrated against MP2 results.[iii] Our own work suggests that the density functional methods all follow similar trends of asymptotic dissociation, with the only discrepancy being a variation in the overall magnitude of the energy change. Single-point (SP) energy calculations on the HF-optimized geometries reported above reveal that the M06-2X and MP2 SP calculations follow similar trends, with

neither method locating a transition state for exocyclic bond cleavage. Similarly, MP2 SP calculations on the B3LYP-optimized geometries follow the same trend as the M06-2X SP values, although the MP2 results are consistently 2 kcal/mol lower in energy for the dissociated complex. Potential energy surfaces at the MP2/6-311+G**//B3LYP/6-31+G** in methanol (SMD) are presented in Figure S6, S7 and S8 to illustrate this point.

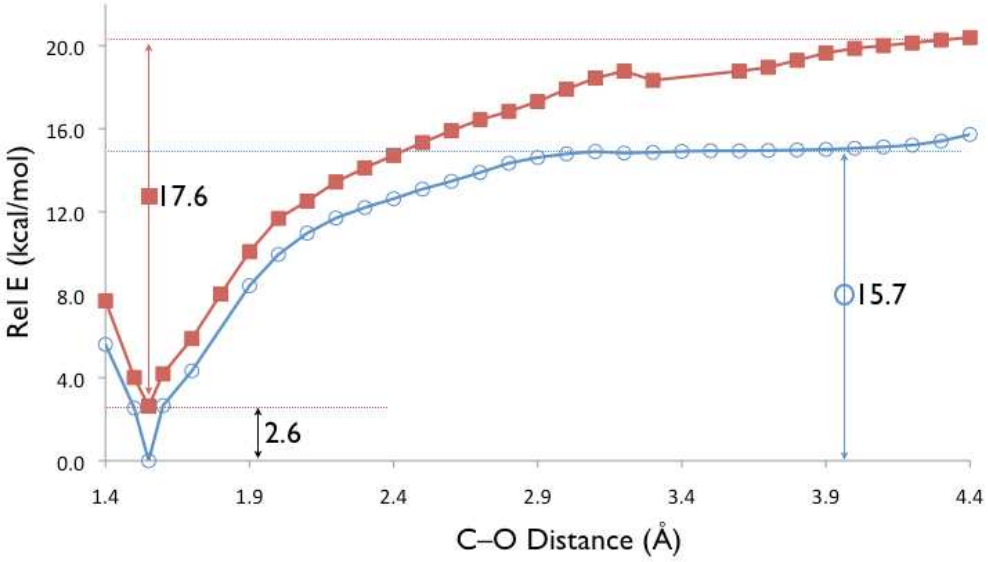


Figure S6: Potential Energy Surface for the hydrolysis of α (open circles) and β anomers (closed squares) derived from compound **3-1**. Energies are determined at the MP2/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

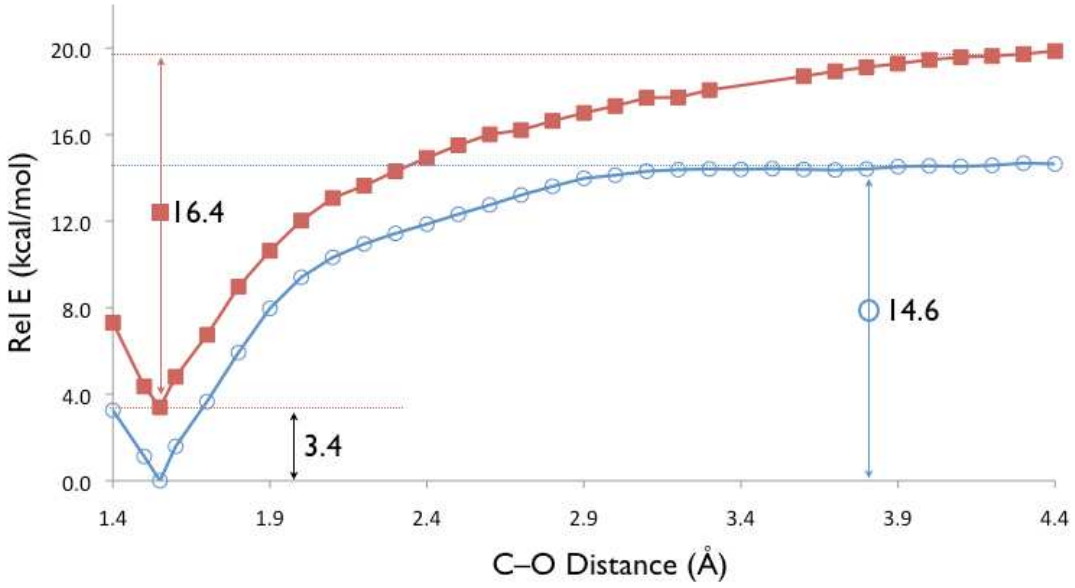


Figure S7: Potential Energy Surface for the hydrolysis of α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the MP2/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

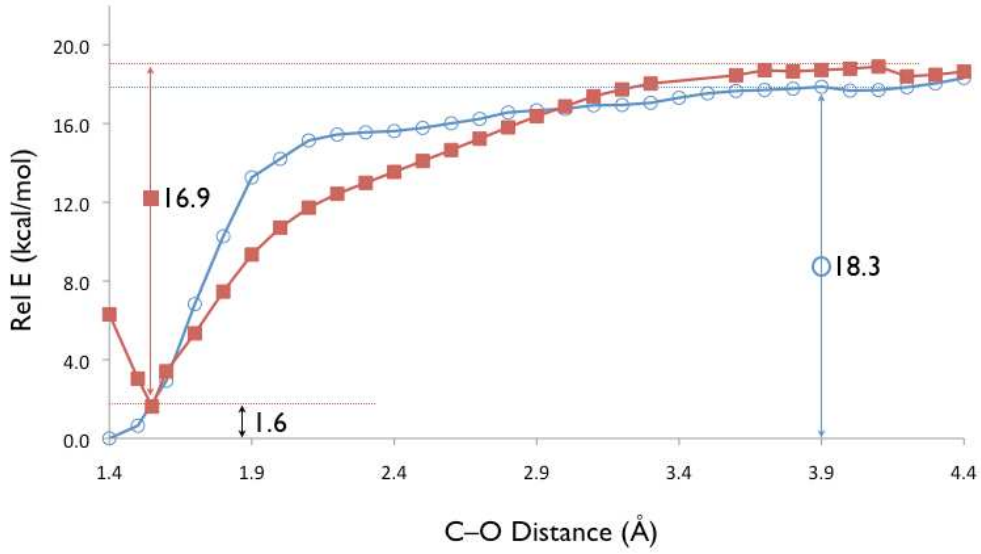


Figure S8: Potential Energy Surface for the hydrolysis of α (open circles) and β anomers (closed squares) derived from compound **3-7**. Energies are determined at the MP2/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

Section 6: Deoxy-analogue relative energetics from relaxed potential energy surface scans and septanoside hydrolysis energies relative to the infinitely separated reference state as well as interacting (3+MeOH) product complex.

Potential energy surfaces for the deoxy analogues reported in the manuscript are reported here (Figure S9 through S13). Surfaces reported in this section were calculated at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory in implicit methanol. In addition to the potential energy surfaces, the dissociation energies relative to infinitely separated products 3 + MeOH, as well as dissociation energies relative to the identified product complex are tabulated in Table S6.1. Set 1 (ΔE Inf. Sep.) is the dissociation energy from **1**(α) or **2**(β) to the infinitely separated reference energy for **3** and MeOH. The second set (ΔE Prod. Complex) are the values already presented in the manuscript, which is the dissociation energy relative to the product complex (interacting **3** and MeOH). The final set of numbers ($\Delta\Delta E$(α– β)) is the difference in dissociation energy between **1**(α) and **2**(β) for each of the state, illustrating that in the infinitely separated reference, β hydrolysis would have a lower barrier, while relative to the hydrogen bonded product complex, α hydrolysis is favored unless you get rid of the C2 hydroxyl (numbers marked in red) at which point you get the same behavior between reference states.

Table S6.1: Dissociation Energy[a] for Septanoside Compound **3** and its deoxy variants relative to infinitely separated products **3** and MeOH, as well as relative to the dissociated product complex described in the manuscript.

	Δ***E*(Inf. Separated)**		Δ***E*(Prod. Complex)**		ΔΔ***E***(α– β)	
	1(α)	**2**(β)	**1**(α)	**2**(β)	(Inf. Sep.)	(P.C.)
Conf. 3–1	22.3	19.9	16.5	18.7	2.4	–2.2
Conf. 3–3	21.5	19.1	17.6	19.8	2.4	–2.2
Conf. 3–7	21.3	20.2	20	20.1	1.1	–0.1
2-deoxy	17.2	14.4	17.6	14.8	2.8	2.8
3-deoxy	20	17	16	17.3	3	–1.3
4-deoxy	20.4	17.2	16.2	17.4	3.2	–1.2
5-deoxy	19.1	17.8	14.4	17.2	1.3	–2.8
7-deoxy	21	17.2	16.3	17.4	3.8	–1.1

[a] Energies reported in units of kcal/mol at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory in implicit (SMD) methanol.

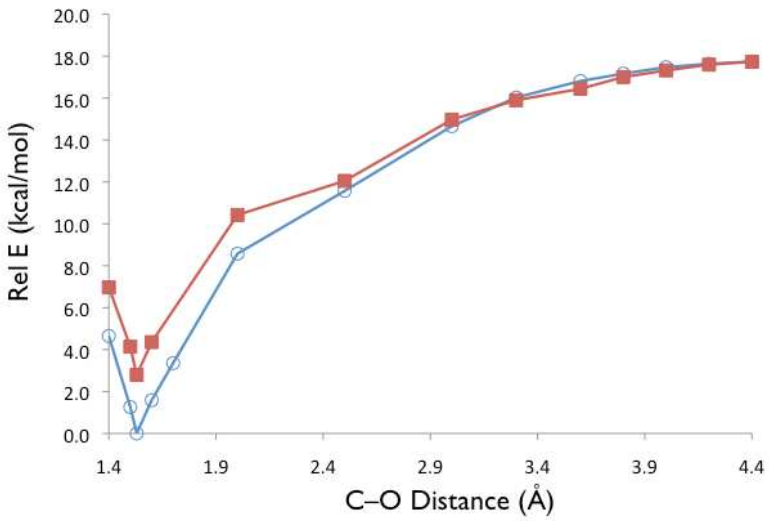


Figure S9: Potential Energy Surface for the hydrolysis of 2-deoxy analogue α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

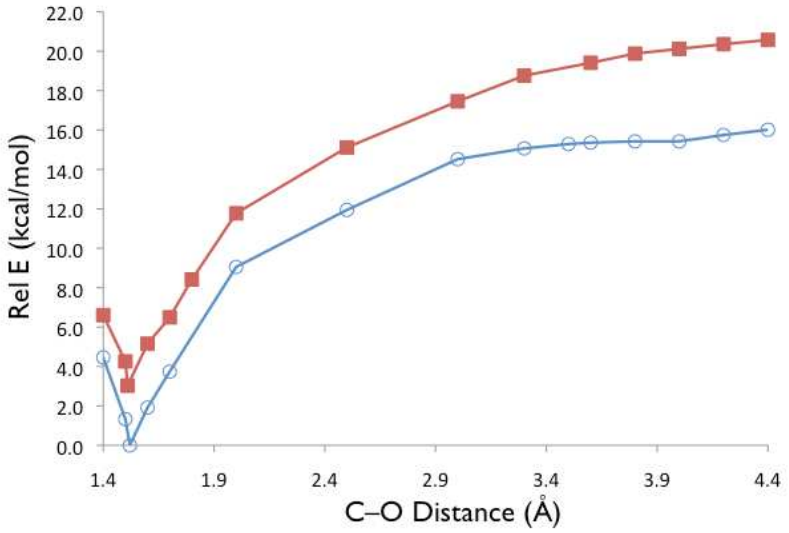


Figure S10: Potential Energy Surface for the hydrolysis of 3-deoxy analogue α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

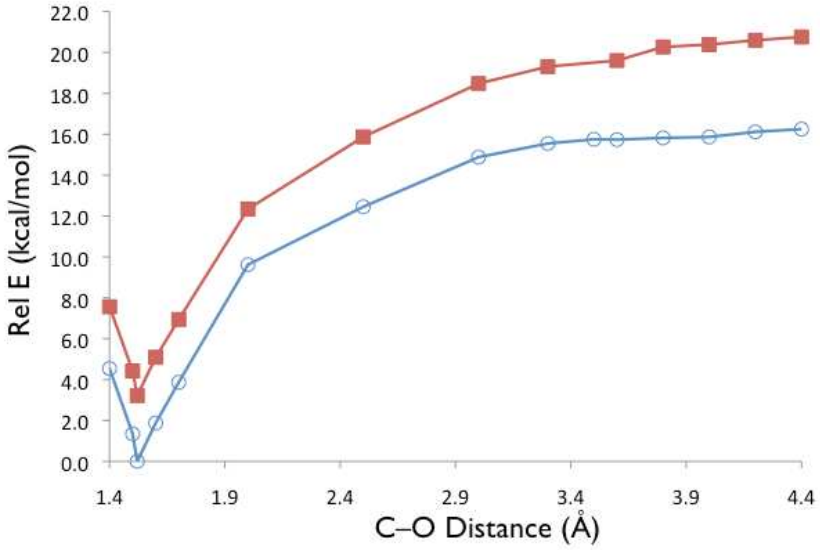


Figure S11: Potential Energy Surface for the hydrolysis of 4-deoxy analogue α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

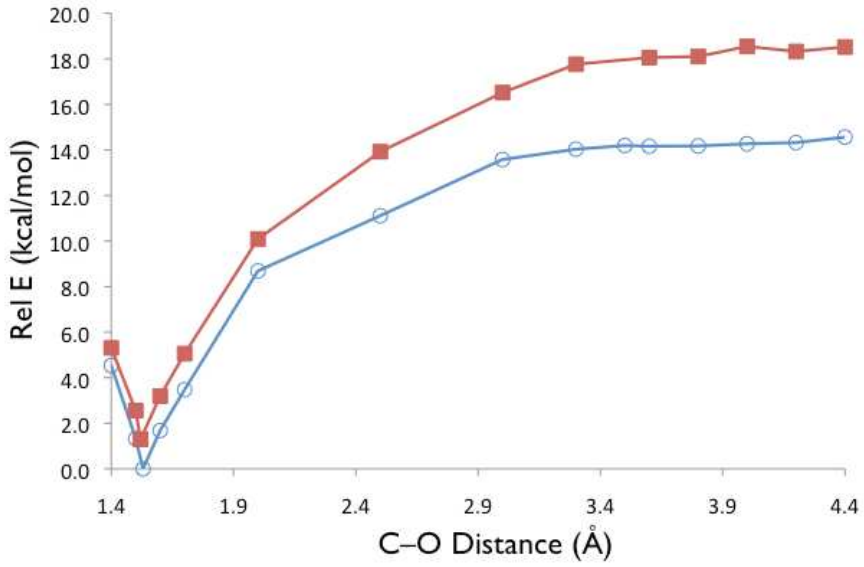


Figure S12: Potential Energy Surface for the hydrolysis of 5-deoxy analogue α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

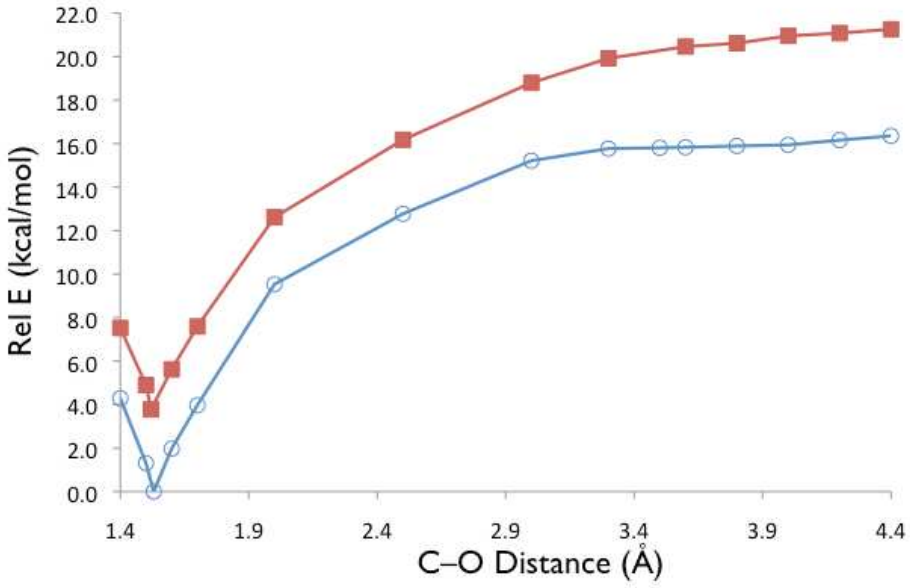


Figure S13: Potential Energy Surface for the hydrolysis of 7-deoxy analogue α (open circles) and β anomers (closed squares) derived from compound **3-3**. Energies are determined at the M06-2X/6-311+G**//B3LYP/6-31+G** level of theory using SMD-methanol for both single point

energies and the geometry optimization. The missing points for the β-anomer at 3.4–3.5 Å are due to a systematic failure in the SCRF routine when defining the solute cavity.

Section 7: Absolute Energies for Relaxed PES Scans.

All energies presented here are bottom-of the-well energies in units of kcal/mol calculated at the M06-2X/6-311+G level of theory in implicit (SMD) methanol using the geometries obtained via a B3LYP/6-31+G** relaxed potential energy surface of the C1–O(methoxy) distance. Frequencies were not evaluated as the relaxed scan does not optimize to a stationary point.**

7.1: Energies for relaxed PES scans of 3-1, 3-3, and 3-7.

Oxocarbenium Compound **3**, Conformer 1

	Compound 1(alpha)		Compound 2 (beta)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-841.5146490	-841.3920823	-841.5033103	-841.3887476
1.5	-841.5151950	-841.3964903	-841.5100357	-841.3940815
1.6	-841.5128020	-841.3958276	-841.5112682	-841.393319
1.7	-841.5087700	-841.3928729	-841.510351	-841.390421
1.8	-841.5050030	-841.3895358	-841.5088018	-841.3870008
1.9	-841.5019800	-841.3863483	-841.5072401	-841.3837073
2	-841.4994950	-841.3837602	-841.5059076	-841.3808876
2.1	-841.4976000	-841.3817735	-841.5049385	-841.3792853
2.2	-841.4962080	-841.3803509	-841.5037737	-841.3775128
2.3	-841.4950700	-841.3794953	-841.5027017	-841.3763466
2.4	-841.4941530	-841.3788638	-841.5016793	-841.3753346
2.5	-841.4935000	-841.3781397	-841.5007544	-841.3742174
2.6	-841.4931540	-841.377464	-841.4999073	-841.3731519
2.7	-841.4930010	-841.3766061	-841.4991343	-841.3720465
2.8	-841.4929800	-841.3756456	-841.4984282	-841.3711723
2.9	-841.4930290	-841.3749439	-841.497845	-841.3700938
3	-841.4930800	-841.3743796	-841.4973448	-841.3689096
3.1	-841.4931410	-841.3739799	-841.4969684	-841.3678881
3.2	-841.4931480	-841.3738341	-841.4966512	-841.3671942
3.3	-841.4931320	-841.3736535	-841.4966311	-841.3676176
3.4	-841.4932650	-841.3735515	*SCRF Failure*	*SCRF Failure*
3.5	-841.4932310	-841.3736196	-841.4964632	*SCRF Failure*
3.6	-841.4931130	-841.3735656	-841.4963353	-841.3667509
3.7	-841.4929290	-841.3734849	-841.4961981	-841.3664453
3.8	-841.4926930	-841.3733606	-841.4959882	-841.3659663

3.9	-841.4932820	-841.3732036	-841.4958792	-841.3655516
4	-841.4932470	-841.373112	-841.4957764	-841.3652915
4.1	-841.4931810	-841.3730516	-841.4957245	-841.3651426
4.2	-841.4931520	-841.3729819	-841.4956955	-841.365023
4.3	-841.4930950	-841.372688	-841.4956764	-841.3649252
4.4	-841.4930527	-841.3722026	-841.4956415	-841.3648358

Oxocarbenium Compound **3**, Conformer 3

	Compound 1(alpha)		Compound 2 (beta)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-841.508677	-841.3950705	-841.5050671	-841.3910403
1.5	-841.514838	-841.3997892	-841.5105962	-841.3951134
1.6	-841.515546	-841.398638	-841.511171	-841.3937896
1.7	-841.51403	-841.395155	-841.5097626	-841.3903859
1.8	-841.512382	-841.3915879	-841.5079955	-841.3866522
1.9	-841.510768	-841.3883688	-841.5071769	-841.3839255
2	-841.509446	-841.3858531	-841.506101	-841.3814895
2.1	-841.508597	-841.3839817	-841.5051077	-841.3795384
2.2	-841.50777	-841.382754	-841.5042905	-841.3785917
2.3	-841.506984	-841.3819103	-841.5034489	-841.3773437
2.4	-841.506275	-841.3812475	-841.5026619	-841.3764067
2.5	-841.505576	-841.3805338	-841.5017079	-841.3755392
2.6	-841.504928	-841.3797546	-841.5009253	-841.3745802
2.7	-841.504353	-841.378793	-841.5002377	-841.3742038
2.8	-841.503919	-841.3779574	-841.4997621	-841.3730841
2.9	-841.503561	-841.37718	-841.4993958	-841.3722622
3	-841.503665	-841.3764798	-841.498667	-841.3712866
3.1	-841.50373	-841.3760137	-841.4983593	-841.3705972
3.2	-841.503947	-841.3757021	-841.4983321	-841.3703465
3.3	-841.504166	-841.375524	-841.4980244	-841.3696266
3.4	-841.504408	-841.3754559	*SCRF Failure*	*SCRF Failure*
3.5	-841.504477	-841.3753699	-841.498067	*SCRF Failure*
3.6	-841.504526	-841.3754617	-841.4977614	-841.3685409
3.7	-841.504742	-841.375726	-841.4975622	-841.3681393
3.8	-841.504849	-841.3755348	-841.4974357	-841.3679837
3.9	-841.504846	-841.3753143	-841.4972694	-841.3677729
4	-841.50479	-841.3751886	-841.4971181	-841.36756
4.1	-841.504723	-841.3751985	-841.4970039	-841.3673537
4.2	-841.504627	-841.37517	-841.4969669	-841.3672675

4.3	-841.504537	-841.3750307	-841.4969206	-841.3671688
4.4	-841.5043295	-841.3750419	-841.4968391	-841.367004

Oxocarbenium Compound **3**, Conformer 7

	Compound 1(alpha)		Compound 2 (beta)	
	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-841.5128102	-841.3972821	-841.5016011	-841.3881886
1.5	-841.5129138	-841.3958928	-841.5076735	-841.3928319
1.6	-841.5103922	-841.3914587	-841.5086076	-841.3917115
1.7	-841.5062719	-841.3849486	-841.5075994	-841.3883618
1.8	-841.5027817	-841.3796211	-841.506154	-841.384872
1.9	-841.4999551	-841.3753594	-841.5048569	-841.3817242
2	-841.5004515	-841.3739146	-841.5038191	-841.3791418
2.1	-841.4994959	-841.3723579	-841.5028772	-841.3770716
2.2	-841.4989973	-841.3717083	-841.5020074	-841.3756512
2.3	-841.4986781	-841.3715608	-841.5011391	-841.3746261
2.4	-841.4983346	-841.371559	-841.5002504	-841.3737519
2.5	-841.4979462	-841.3713607	-841.4994145	-841.372814
2.6	-841.4975162	-841.3708645	-841.4985574	-841.3717568
2.7	-841.4972207	-841.3701788	-841.4977145	-841.3705835
2.8	-841.4969632	-841.3692813	-841.4969806	-841.3694103
2.9	-841.4968872	-841.3686642	-841.4963251	-841.368254
3	-841.4968912	-841.3680926	-841.4957638	-841.3671704
3.1	-841.4968614	-841.3674589	-841.4952404	-841.3661326
3.2	-841.4969289	-841.367083	-841.4948251	-841.365394
3.3	-841.4969804	-841.3667432	-841.4944455	-841.3648379
3.4	-841.4969296	-841.3663568	*SCRF Failure*	*SCRF Failure*
3.5	-841.4970588	-841.3658988	-841.4941538	*SCRF Failure*
3.6	-841.4970717	-841.3656891	-841.4938951	-841.3639504
3.7	-841.497058	-841.3656549	-841.4937576	-841.3634672
3.8	-841.4969735	-841.3656891	-841.4936479	-841.3635366
3.9	-841.4967772	-841.3656819	-841.4935266	-841.3633518
4	-841.4965729	-841.3664516	-841.493409	-841.3632953
4.1	-841.4964073	-841.3666727	-841.4933259	-841.3631724
4.2	-841.4961445	-841.3666655	-841.4933796	-841.3640107
4.3	-841.4958065	-841.3666008	-841.49337	-841.3639381
4.4	-841.4952983	-841.3663171	-841.4932663	-841.3637253

7.2: Energies for Relaxed PES Scans of Model Systems. Energies are bottom-of the-well energies in units of kcal/mol calculated at the M06-2X/6-311+G level of theory in implicit (SMD) methanol using the geometries obtained via a B3LYP/6-31+G** relaxed potential energy surface of the C1–O(methoxy) distance.**

Bare Septanoside Compound 9

	Compound 7 (alpha)		Compound 8 (beta)	
C–O Dist	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-465.3889738	-465.2719957	-465.3856515	-465.2684093
1.5	-465.3961364	-465.2778085	-465.3922875	-465.273671
1.6	-465.398163	-465.2779145	-465.3940506	-465.2736345
1.7	-465.3981652	-465.2759576	-465.3941471	-465.2718982
1.8	-465.3977989	-465.2738238	-465.3939129	-465.2700416
1.9	-465.3974202	-465.271899	-465.3937805	-465.2685005
2	-465.3971524	-465.2703605	-465.3937738	-465.2673829
2.1	-465.3970166	-465.2693679	-465.393937	-465.2667758
2.2	-465.3969188	-465.2689189	-465.3941123	-465.2665306
2.3	-465.3967065	-465.2686192	-465.3942182	-465.2664748
2.4	-465.3963896	-465.2682781	-465.3942351	-465.2664409
2.5	-465.396008	-465.267779	-465.3941368	-465.2661893
2.6	-465.3956122	-465.267118	-465.3939816	-465.2656741
2.7	-465.3951641	-465.2663071	-465.3937312	-465.2650001
2.8	-465.3946841	-465.2653745	-465.3933531	-465.2644672
2.9	-465.3941955	-465.2643988	-465.3929932	-465.2635131
3	-465.3937825	-465.2635514	-465.3928203	-465.2627201
3.1	-465.3934314	-465.2628801	-465.3926144	-465.2620049
3.2	-465.3931462	-465.2622897	-465.3924542	-465.2614065
3.3	-465.3929069	-465.2616917	-465.3924936	-465.2614324
3.4	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*
3.5	-465.3927005	*SCRF Failure*	-465.3923782	*SCRF Failure*
3.6	-465.3924579	-465.2606774	-465.3922769	-465.2607619
3.7	-465.392295	-465.2604075	-465.392057	-465.2602563
3.8	-465.3921551	-465.2601698	-465.3919798	-465.2601274
3.9	-465.3920131	-465.2599537	-465.391851	-465.2596274
4	-465.3918622	-465.2597555	-465.3917467	-465.2593414
4.1	-465.3917724	-465.2596099	-465.3916418	-465.2591413
4.2	-465.3916866	-465.2594612	-465.3915513	-465.2590435
4.3	-465.3916279	-465.2593348	-465.391538	-465.2589437

4.4	-465.3915841	-465.2592508	-465.3914702	-465.2588428

Bare Septanoside Compound 9, C2-OH

	Compound 7 (alpha)		Compound 8 (beta)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-540.6168416	-540.4998702	-540.6074518	-540.4905013
1.5	-540.6215645	-540.5036524	-540.6137238	-540.4951801
1.6	-540.621826	-540.5023344	-540.615229	-540.4947645
1.7	-540.6204291	-540.4992447	-540.614808	-540.4924042
1.8	-540.6186482	-540.4959457	-540.6140063	-540.4898459
1.9	-540.6171402	-540.4929383	-540.613213	-540.4873147
2	-540.6158595	-540.4903248	-540.6126492	-540.4854059
2.1	-540.6147678	-540.4882385	-540.6122386	-540.4840912
2.2	-540.613764	-540.4867066	-540.6118114	-540.4831828
2.3	-540.6127633	-540.4855624	-540.6111577	-540.4823878
2.4	-540.6117812	-540.4846077	-540.6105542	-540.4815487
2.5	-540.6108347	-540.4837065	-540.6099799	-540.4810326
2.6	-540.6099336	-540.4826349	-540.6094528	-540.4803062
2.7	-540.6091547	-540.4814994	-540.6089137	-540.4799302
2.8	-540.6084906	-540.4804041	-540.6084736	-540.4791773
2.9	-540.6080149	-540.4794441	-540.6079761	-540.4780748
3	-540.6076382	-540.4786888	-540.6075902	-540.4772968
3.1	-540.6073773	-540.4780821	-540.6073911	-540.4770439
3.2	-540.6071774	-540.4775831	-540.6072537	-540.4769009
3.3	-540.6071364	-540.4772436	-540.6071446	-540.4763672
3.4	-540.6071202	-540.4769686	*SCRF Failure*	*SCRF Failure*
3.5	-540.6071104	-540.4767514	-540.6070402	*SCRF Failure*
3.6	-540.607312	-540.4762537	-540.6069104	-540.4756609
3.7	-540.6073123	-540.4760709	-540.6068508	-540.4756911
3.8	-540.6072726	-540.4759961	-540.6067173	-540.4753451
3.9	-540.6072172	-540.4758935	-540.6065616	-540.4750302
4	-540.6071206	-540.4758863	-540.6064146	-540.4748075
4.1	-540.607023	-540.4757426	-540.6063092	-540.4745186
4.2	-540.6069378	-540.475603	-540.6062496	-540.4743579
4.3	-540.6068277	-540.4754674	-540.6061823	-540.474184
4.4	-540.6068282	-540.4752577	-540.6060914	-540.4740323

Bare Septanoside Compound 9, C7-OH

	Compound 7 (alpha)		Compound 8 (beta)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-540.6131876	-540.4960637	-540.6090257	-540.4920105
1.5	-540.6195858	-540.5011868	-540.6151932	-540.496813
1.6	-540.6210013	-540.5008281	-540.6167151	-540.4967884
1.7	-540.6205291	-540.4984121	-540.616795	-540.4948144
1.8	-540.6196935	-540.4957708	-540.6162523	-540.4924295
1.9	-540.6190143	-540.4935266	-540.6159302	-540.4906935
2	-540.618469	-540.4916801	-540.6158145	-540.4894458
2.1	-540.6181897	-540.490545	-540.6158033	-540.4887207
2.2	-540.6179925	-540.4899762	-540.6157827	-540.4884138
2.3	-540.6177253	-540.4895734	-540.6160165	-540.488347
2.4	-540.6173805	-540.4891292	-540.6158875	-540.488284
2.5	-540.6170145	-540.4886633	-540.6155742	-540.4877689
2.6	-540.6166554	-540.4880639	-540.6153199	-540.4872883
2.7	-540.6162058	-540.4872709	-540.6151084	-540.4867939
2.8	-540.6157055	-540.4864484	-540.6147682	-540.4860275
2.9	-540.6152733	-540.4856096	-540.6144081	-540.485078
3	-540.6148545	-540.4847569	-540.614131	-540.4843646
3.1	-540.61447	-540.4838822	-540.6138815	-540.4837427
3.2	-540.6141705	-540.4831952	-540.6138481	-540.4835593
3.3	-540.6139487	-540.4827351	-540.613759	-540.4831196
3.4	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*
3.5	-540.6137798	*SCRF Failure*	-540.6136555	*SCRF Failure*
3.6	-540.613467	-540.4817204	-540.6135104	-540.4822638
3.7	-540.6132953	-540.4814322	-540.613369	-540.4818886
3.8	-540.6132795	-540.4813741	-540.6132267	-540.4817848
3.9	-540.6131304	-540.4810622	-540.6130767	-540.4813798
4	-540.6129242	-540.4807352	-540.6129086	-540.4809878
4.1	-540.6127098	-540.4803844	-540.6127802	-540.4807147
4.2	-540.6127884	-540.4805376	-540.6126949	-540.4804273
4.3	-540.612719	-540.4804027	-540.6127714	-540.4801588
4.4	-540.612628	-540.4802272	-540.6127534	-540.4800704

Acyclic Oxocarbenium Ion **6**

	Symmetrical (no alpha/beta equivalents)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-309.3159756	-309.2396702
1.5	-309.3233046	-309.2457146
1.6	-309.325162	-309.245855

1.7	-309.3249487	-309.2435686
1.8	-309.3241746	-309.2412226
1.9	-309.3234491	-309.2391902
2	-309.3229765	-309.2376335
2.1	-309.3227018	-309.2366407
2.2	-309.3224423	-309.236122
2.3	-309.3221974	-309.2360194
2.4	-309.3217818	-309.2356512
2.5	-309.321258	-309.2351783
2.6	-309.3207003	-309.2344862
2.7	-309.3201566	-309.2335509
2.8	-309.3196039	-309.2326122
2.9	-309.3190269	-309.2316445
3	-309.3185216	-309.2307201
3.1	-309.3181109	-309.2298941
3.2	-309.3177548	-309.2291879
3.3	-309.3174789	-309.2286484
3.4	*SCRF Failure*	*SCRF Failure*
3.5	-309.3172636	*SCRF Failure*
3.6	-309.3168916	-309.2274421
3.7	-309.3168194	-309.2268202
3.8	-309.3167648	-309.2267337
3.9	-309.3165709	-309.2264834
4	-309.3165088	-309.2263717
4.1	-309.3164714	-309.2262323
4.2	-309.3164534	-309.2261116
4.3	-309.3163804	-309.2260102
4.4	-309.3164471	-309.2260604

Acyclic oxocarbenium **6**, C2-OH

	Compound **4** (alpha equivalent)		Compound **5** (beta equivalent)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-384.5334185	-384.4574622	-384.5391522	-384.4613321
1.5	-384.5401603	-384.4628564	-384.5448869	-384.4663561
1.6	-384.5414551	-384.4624136	-384.545799	-384.4657923
1.7	-384.5404988	-384.4596882	-384.5446711	-384.4630653
1.8	-384.5394018	-384.4565129	-384.5429695	-384.4600204
1.9	-384.5383046	-384.4540043	-384.5417333	-384.4574286
2	-384.5374237	-384.4520772	-384.5405303	-384.4551031
2.1	-384.5367155	-384.4506805	-384.5397006	-384.4533657
2.2	-384.5360636	-384.4498561	-384.5389573	-384.4522033

2.3	-384.5354567	-384.4494544	-384.5381654	-384.4512737
2.4	-384.5347954	-384.4490055	-384.5373522	-384.4503883
2.5	-384.5340247	-384.4484094	-384.5365344	-384.4495077
2.6	-384.5335376	-384.4483253	-384.5356882	-384.4484973
2.7	-384.533066	-384.4477144	-384.534871	-384.4473008
2.8	-384.532707	-384.4471892	-384.5341382	-384.4461986
2.9	-384.5329341	-384.4469148	-384.5334576	-384.4450971
3	-384.5331196	-384.4467652	-384.5328562	-384.4441151
3.1	-384.5335156	-384.4465946	-384.5323699	-384.4433008
3.2	-384.5338418	-384.4463241	-384.5319441	-384.4424239
3.3	-384.5341754	-384.4462921	-384.5315749	-384.4417045
3.4	-384.5346087	-384.446251	*SCRF Failure*	*SCRF Failure*
3.5	-384.5349771	-384.4462625	-384.5313653	*SCRF Failure*
3.6	-384.535356	-384.4463526	-384.5310192	-384.4408143
3.7	-384.5356513	-384.4462968	-384.530817	-384.4404932
3.8	-384.5358377	-384.4461957	-384.5306385	-384.4402273
3.9	-384.535963	-384.4460908	-384.5305568	-384.4400342
4	-384.5360393	-384.4459273	-384.5304428	-384.4398853
4.1	-384.5360393	-384.445795	-384.5303686	-384.4396916
4.2	-384.5360993	-384.4455979	-384.5302482	-384.4394572
4.3	-384.5360726	-384.4454363	-384.530172	-384.4393941
4.4	-384.5359274	-384.4452318	-384.530116	-384.4393297

Acyclic oxocarbenium **6**, C6-OH

	Compound **4** (alpha equivalent)		Compound **5** (beta equivalent)	
C–O Dist.	B3LYP/6-31+G**	M06-2X/6-311+G**	B3LYP/6-31+G**	M06-2X/6-311+G**
1.4	-384.5504473	-384.473915	-384.5497839	-384.4733457
1.5	-384.5573632	-384.4795809	-384.5567294	-384.4788387
1.6	-384.5587822	-384.4792896	-384.5583082	-384.4785168
1.7	-384.5580114	-384.476718	-384.5574228	-384.4759537
1.8	-384.5566232	-384.4736895	-384.5560221	-384.4729137
1.9	-384.5554136	-384.4710221	-384.5547638	-384.4703802
2	-384.5546292	-384.4690917	-384.5539512	-384.4682858
2.1	-384.5541603	-384.467829	-384.5533489	-384.4667898
2.2	-384.5537705	-384.4671192	-384.552894	-384.4659448
2.3	-384.5533475	-384.466672	-384.5523931	-384.4654696
2.4	-384.5528881	-384.4662608	-384.5517923	-384.4649794
2.5	-384.5523478	-384.4656596	-384.5511758	-384.4640368
2.6	-384.5517899	-384.464827	-384.5505413	-384.4641901
2.7	-384.5512376	-384.4639346	-384.5499416	-384.463933
2.8	-384.5506464	-384.4629327	-384.5493476	-384.4639373

2.9	-384.550306	-384.4623848	-384.5489999	-384.4638515
3	-384.5498477	-384.461499	-384.5486343	-384.4634996
3.1	-384.549465	-384.460434	-384.5482569	-384.4632108
3.2	-384.5491712	-384.4597136	-384.5479746	-384.4631988
3.3	-384.5489195	-384.4591463	-384.5478162	-384.4631645
3.4	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*	*SCRF Failure*
3.5	-384.5487322	*SCRF Failure*	-384.5476589	-384.4632513
3.6	-384.548567	-384.4584751	*SCRF Failure*	-384.4632322
3.7	-384.5484184	-384.4581539	*SCRF Failure*	-384.4634003
3.8	-384.5482644	-384.457825	-384.547264	-384.4633614
3.9	-384.5480867	-384.4574528	-384.5548521	-384.4632515
4	-384.5479585	-384.4571617	-384.5548956	-384.4631821
4.1	-384.5478718	-384.4569443	-384.5550692	-384.4633491
4.2	-384.5478395	-384.4568412	-384.5550479	-384.4632514
4.3	-384.5476676	-384.4566756	-384.5549119	-384.4631666
4.4	-384.5477375	-384.4567684	-384.554782	-384.4628482

7.3: Energies for Single Variations in Hydroxyl Group Positions (Scheme 1D, Table 1 in manuscript). Energies are bottom-of the-well energies in units of kcal/mol calculated at the M06-2X/6-311+G level of theory in implicit (SMD) methanol using the geometries obtained via a B3LYP/6-31+G** relaxed potential energy surface of the C1–O(methoxy) distance.**

Single hydroxyl additions

	2-OH		3-OH		4-OH		5-OH		7-OH	
C–O Dist.	10 (!)	11 (")	13 (!)	14 (")	16 (!)	17 (")	19 (!)	20 (")	22 (!)	23 (")
1.4	-540.6168416	-540.4998702	-540.5008943	-540.4967571	-540.5024029	-540.4976019	-540.4997514	-540.4961889	-540.4910546	-540.4870614
1.5	-540.6215645	-540.5036524	-540.505752	-540.4993434	-540.5072073	-540.5025795	-540.5043784	-540.4988045	-540.4960807	-540.4918443
1.6	-540.621826	-540.5023344	-540.5052408	-540.5003971	-540.5067622	-540.5024048	-540.5037451	-540.4972265	-540.4956167	-540.491707
1.7	-540.6204291	-540.4992447	-540.5027619	-540.498731	-540.5044417	-540.5004492	-540.5012269	-540.4952477	-540.4930401	-540.4899017
2	-540.6158595	-540.4903248	-540.4961813	-540.4939505	-540.4979192	-540.4951058	-540.493974	-540.4898534	-540.4860376	-540.4839533
2.5	-540.6108347	-540.4837065	-540.492742	-540.4928049	-540.4947568	-540.493676	-540.4899964	-540.4885211	-540.4827483	-540.4822426
3	-540.6076382	-540.4786888	-540.4884291	-540.4892348	-540.4905976	-540.4899982	-540.4855648	-540.4850283	-540.4789631	-540.4786298
3.3	-540.6071364	-540.4772436	-540.4865963	-540.4875188	-540.4888543	-540.488369	-540.4838342	-540.4831645	-540.4770341	-540.4774108
3.6	-540.607312	-540.4762537	-540.4854252	-540.4863889	-540.4877437	-540.4873297	-540.4832673	-540.4824255	-540.4761571	-540.4767107
3.8	-540.6072726	-540.4759961	-540.4850248	-540.4860271	-540.48731	-540.4869767	-540.4827962	-540.4820959	-540.4760329	-540.4763903
4	-540.6071206	-540.4758863	-540.4846283	-540.4858852	-540.4868674	-540.4864286	-540.4831794	-540.481674	-540.4754108	-540.4756093
4.4	-540.6068282	-540.4752577	-540.4841195	-540.4855398	-540.4868879	-540.4860867	-540.4823048	-540.481165	-540.4750356	-540.4745514

Single deoxy structures

	2-deoxy		3-deoxy		4-deoxy		5-deoxy		7-deoxy	
C–O Dist.	!	"	!	"	!	"	!	"	!	"
1.4	-766.1748986	-766.1711983	-766.1700046	-766.1665851	-766.1673571	-766.1625361	-766.1685586	-766.1673251	-766.172178	-766.1670341
1.5	-766.1803023	-766.1757128	-766.1750077	-766.1703272	-766.1724468	-766.1675353	-766.1736671	-766.1717146	-766.1769358	-766.1712124
1.6	-766.179776	-766.1753629	-766.1740682	-766.168904	-766.1716017	-766.1664829	-766.1731093	-766.1707001	-766.1758756	-766.1700612
1.7	-766.1769576	*SCRF Failure*	-766.1711546	-766.1667658	-766.1684223	-766.1635254	-766.1702513	-766.1677323	-766.1726903	-766.1669228
2	-766.0506968	-766.1656962	-766.1626938	-766.1583548	-766.1592594	-766.154919	-766.1619442	-766.1597053	-766.1638295	-766.1589172
2.5	-766.1686419	-766.1631061	-766.1580779	-766.1530233	-766.1547439	-766.1492954	-766.1580809	-766.1536029	-766.1586668	-766.1532397
3	-766.1638684	-766.1584464	-766.153973	-766.1493013	-766.1508771	-766.1451449	-766.1541485	-766.1494696	-766.1547712	-766.1490663
3.3	-766.1589458	-766.1569713	-766.1531048	-766.1472185	-766.1498115	-766.1438193	-766.1534269	-766.1474821	-766.153888	-766.147275
3.6	-766.156765	*SCRF Failure*	-766.1527499	*SCRF Failure*	-766.1494863	*SCRF Failure*	-766.1531678	*SCRF Failure*	-766.1538264	*SCRF Failure*
3.8	-766.155517	-766.1561051	-766.1526378	-766.146184	-766.1495128	-766.1433467	-766.1532182	-766.1470159	-766.1537889	-766.1464146
4	-766.1549475	-766.1552091	-766.1525337	-766.1454412	-766.1493763	-766.1422897	-766.1531984	-766.1469461	-766.1536936	-766.146164
4.2	-766.1544625	-766.1547056	-766.1525355	-766.1450527	-766.1493025	-766.1421011	-766.1530487	-766.1462362	-766.1536132	-766.1456249
4.4	-766.1542044	-766.1542689	-766.1520209	-766.1446774	-766.1489043	-766.1417645	-766.1529644	-766.1465864	-766.1532647	-766.1454262

7.4: Energies for fluoro substitutions at the C2-position on the septanoside compound 9. Energies are bottom-of the-well energies in units of kcal/mol calculated at the M06-2X/6-311+G level of theory in implicit (SMD) methanol using the geometries obtained via a B3LYP/6-31+G** relaxed potential energy surface of the C1–O(methoxy) distance.**

C2-F Substitution

C–O Dist.	alpha	beta
1.4	-564.5086743	-564.5053221
1.5	-564.5145401	-564.5096469
1.6	-564.5139619	-564.5086891
1.7	-564.511304	-564.5058787
1.8	-564.507667	-564.5027868
1.9	-564.5048452	-564.4999705
2	-564.5022408	-564.4975762
2.1	-564.5000856	-564.4956543
2.2	-564.4983795	-564.4942391
2.3	-564.497019	-564.4930451
2.4	-564.4957519	-564.4919073
2.5	-564.4945345	-564.4911889
2.6	-564.493263	-564.4903564
2.7	-564.4919407	-564.489834
2.8	-564.4905689	-564.4891079
2.9	-564.4888917	-564.4880745
3	-564.4878022	-564.4873087
3.1	-564.4868626	-564.4870131
3.2	-564.4862439	-564.4869865
3.3	-564.4857255	-564.4864364
3.4	-564.4853132	-564.485779
3.5	-564.4849707	-564.4857266
3.6	-564.4843364	-564.4854255
3.7	-564.4841501	-564.4851079
3.8	-564.484034	-564.484867
3.9	-564.4839582	-564.4845731
4	-564.4839325	-564.4844019
4.1	-564.4839214	-564.4842353
4.2	-564.4838256	-564.484105
4.3	-564.4837516	-564.4839134

4.4	-564.4836502	-564.4838512

7.5: Comparison of energetics for Gauche/Anti orientation of the C1-MeOH group. Energies are bottom-of the-well energies in units of kcal/mol calculated at the B3LYP/6-311+G level of theory in implicit (SMD) methanol using the geometries obtained via a B3LYP/6-31+G** relaxed potential energy surface of the C1–O(methoxy) distance.**

	Compound **1** (alpha)		Compound **2** (beta)	
C–O Dist.	Gauche (MeOH)	Anti (MeOH)	Gauche (MeOH)	Anti (MeOH)
1.4	-841.4015679	-841.3950705	-841.3910403	-841.3901237
1.5	-841.404737	-841.3997892	-841.3951134	-841.3953066
1.6	-841.4027774	-841.398638	-841.3937896	-841.3944007
1.7	-841.3988051	-841.395155	-841.3903859	-841.3912831
1.8	-841.3945509	-841.3915879	-841.3866522	-841.3878308
1.9	-841.3907327	-841.3883688	-841.3839255	-841.3850823
2	-841.3873585	-841.3858531	-841.3814895	-841.382432
2.1	-841.3845701	-841.3839817	-841.3795384	-841.3804692
2.2	-841.3823531	-841.382754	-841.3785917	-841.378786
2.3	-841.3806453	-841.3819103	-841.3773437	-841.3776377
2.4	-841.379485	-841.3812475	-841.3764067	-841.3767459
2.5	-841.3782148	-841.3805338	-841.3755392	-841.3758378
2.6	-841.3767869	-841.3797546	-841.3745802	-841.375155
2.7	-841.3753719	-841.378793	-841.3742038	-841.3741668
2.8	-841.3739948	-841.3779574	-841.3730841	-841.373265
2.9	-841.3728291	-841.37718	-841.3722622	-841.3719307
3	-841.3721068	-841.3764798	-841.3712866	#N/A
3.1	-841.3713324	-841.3760137	-841.3705972	-841.3702985
3.2	-841.3709194	-841.3757021	-841.3703465	-841.3695255
3.3	-841.3705574	-841.375524	-841.3696266	-841.3689962
3.4	-841.3702022	-841.3754559	#N/A	#N/A
3.5	-841.3698439	-841.3753699	#N/A	#N/A
3.6	-841.3693546	-841.3754617	-841.3685409	-841.3671456
3.7	-841.3692538	-841.375726	-841.3681393	-841.3668779
3.8	-841.3693808	-841.3755348	-841.3679837	-841.3667538
3.9	-841.369221	-841.3753143	-841.3677729	-841.366505
4	-841.3690937	-841.3751886	-841.36756	-841.3662689
4.1	-841.3689482	-841.3751985	-841.3673537	-841.3661125
4.2	-841.3687392	-841.37517	-841.3672675	-841.3660757

4.3	-841.3684683	-841.3750307	-841.3671688	-841.3660047
4.4	-841.3682383	-841.3750419	-841.367004	-841.3659566

7.6: Absolute energies determined using geometries calculated at the HF/6-31+G level of theory. Energies are reported as free energies in units of kcal/mol calculated at the specified level of theory in implicit (SMD) methanol with the thermal and entropic correction to the free energy obtained from the HF/6-31+G** optimized geometries.**

Compound 1			Single Points Δ*G*(298K)			
Stationary Pt.	Gcorr (HF)	Imag Freq?	HF	B3LYP	MP2	M06-2X
RC Gauche	0.220613	no	-836.7486143	-841.4984955	-839.3194545	-841.181035
RC Anti	0.220425	no	-836.7444926	-841.4941591	-839.3146415	-841.1756865
TS Anti-Gauche	0.22068	-93.0985	-836.7439327	-841.4934823	-839.3134509	-841.1745708
TS Gauche	0.21778	-215.1892	-836.7364833	-841.4916003	-839.3040347	-841.1638752
TS Anti	0.217555	-204.0271	-836.7368836	-841.4927099	-839.3050129	-841.1652767
PC Gauche	0.213556	no	-836.7422794	-841.4919717	-839.303262	-841.1628126
PC Anti	0.214595	no	-836.7418424	-841.4921618	-839.3034069	-841.1631216

Compound 2			Single Points Δ*G*(298K)			
Stationary Pt.	Gcorr (HF)	Imag Freq?	HF	B3LYP	MP2	M06-2X
RC Gauche	0.221981	no	-836.7385644	-841.4883846	-839.3084383	-841.1697443
TS Gauche	0.217956	-213.0501	-836.7322017	-841.4887066	-839.3007787	-841.1610579
PC Gauche	0.212706	no	-836.7401687	-841.4890108	-839.2996507	-841.1590573

Section 8: Cartesian Coordinates for Relaxed PES Scans of the C1-O(MeOH) using the B3LYP/6-31+G methodology and HF/6-31+G** stationary points.**

8.1: Geometries for Relaxed PES Scans of 3-1, 3-3, and 3-7

Oxocarbenium Compound 3, Conformer 1

Scan Point for comp3_1_alpha_1.4Å

C	-1.14105700	1.41428500	0.06129100
C	0.29082900	1.83098200	-0.33293500
C	1.41297600	0.92886000	0.21093000
C	-1.61707400	0.04610800	-0.43556500
C	1.55798000	-0.36674400	-0.61827800
C	-0.72808700	-1.12427600	0.00700400
H	-1.21822300	1.42186500	1.15769400
H	0.36806800	1.87245500	-1.42474500
H	-1.64108300	0.05088700	-1.53502300
H	2.34969300	1.48163100	0.06770900
H	1.99356500	-0.11138600	-1.59131600
H	-0.41752500	-1.02942700	1.05098500
O	1.19198900	0.68091800	1.59300900
H	2.03479100	0.65763200	2.06916300
O	0.50421500	3.17314700	0.11057400
H	0.52272900	3.18002800	1.08237300
O	-2.07037100	2.34605400	-0.49549500
H	-1.80072900	3.24105800	-0.23561800
O	-2.93167000	-0.20044500	0.07032400
H	-3.48909100	0.56149400	-0.15484800
C	-1.38883300	-2.49652600	-0.19637700
H	-1.83130900	-2.55681900	-1.20063400
H	-0.61472500	-3.26586500	-0.12174800
O	-2.34306100	-2.78219500	0.81409500
H	-3.03518200	-2.10283600	0.75357100
O	0.43905100	-1.13385600	-0.87329000
C	3.93285000	-1.07471300	-0.21597700
H	4.11640100	-1.29191400	-1.26794900
H	4.18507000	-0.05155100	0.05129600
H	4.40053700	-1.79321000	0.45316000
O	2.45888000	-1.21612900	0.03512000
H	2.16724000	-2.15185300	-0.06931900

Scan Point for comp3_1_alpha_1.5Å

C	-1.24327600	1.34919800	0.04147600
C	0.16134600	1.87013700	-0.32032600
C	1.33228800	1.03586600	0.23040900
C	-1.60249300	-0.05251600	-0.46358400
C	1.56155000	-0.24508300	-0.59141400
C	-0.66049200	-1.15947900	0.03292700
H	-1.34752800	1.35170600	1.13548700
H	0.25273100	1.93374600	-1.40975000
H	-1.57744500	-0.05814300	-1.56331900
H	2.23525000	1.64370200	0.09506800
H	2.01394600	-0.00511100	-1.55793200
H	-0.39126700	-1.02432200	1.08312200
O	1.10913200	0.77789500	1.60988400
H	1.95456800	0.73572300	2.08054500
O	0.27951900	3.21420900	0.14715000
H	0.28433700	3.20549600	1.11911000
O	-2.22665500	2.20624400	-0.54100300
H	-2.06456800	3.11436600	-0.24098800
O	-2.91827800	-0.38310300	-0.01337100
H	-3.50730900	0.35345700	-0.24354600
C	-1.22658300	-2.57352100	-0.16900700
H	-1.63134600	-2.67522700	-1.18553400
H	-0.40815000	-3.29089100	-0.05717100
O	-2.19297000	-2.90289700	0.81531400
H	-2.92760500	-2.27472900	0.71681100
O	0.54046800	-1.12130500	-0.80658200
C	4.02842400	-0.96344600	-0.36556900
H	4.05677800	-1.41045300	-1.35885100
H	4.30485000	0.08783400	-0.37544600
H	4.61505100	-1.52058300	0.36239700
O	2.62254200	-1.01445600	0.13822000
H	2.32306000	-1.94618900	0.23363600

Scan Point for comp3_1_alpha_1.6Å

C	-1.28375900	1.32095600	0.04590800
C	0.10222300	1.88613300	-0.32695500
C	1.29929300	1.07962400	0.21541600
C	-1.60617700	-0.09096200	-0.45717100
C	1.53886200	-0.19030300	-0.61278000
C	-0.63299400	-1.17363100	0.03058300
H	-1.37896900	1.32069500	1.14052000

H	0.18192700	1.95655200	-1.41678500
H	-1.58933100	-0.09484600	-1.55712100
H	2.19103500	1.70211900	0.07249700
H	2.03590800	0.02614400	-1.56093800
H	-0.35656800	-1.03491700	1.07776300
O	1.08137600	0.82215300	1.59445500
H	1.93055900	0.74548000	2.05436700
O	0.18726500	3.22958400	0.14538400
H	0.20379700	3.21699100	1.11721700
O	-2.29837400	2.14505900	-0.52955100
H	-2.16797200	3.05742600	-0.22736400
O	-2.90727800	-0.45997400	0.00328700
H	-3.51867200	0.26035800	-0.22054500
C	-1.15590500	-2.60279200	-0.17958300
H	-1.56371900	-2.70852300	-1.19437000
H	-0.31505400	-3.29533500	-0.07877300
O	-2.10468500	-2.96837700	0.80821700
H	-2.86008800	-2.36392600	0.71901400
O	0.56339200	-1.09018200	-0.81917000
C	4.06857600	-0.89766300	-0.36682000
H	4.07624100	-1.35416800	-1.35659300
H	4.33472600	0.15650800	-0.39987300
H	4.69813500	-1.43591500	0.34006100
O	2.69184200	-0.95932000	0.18675200
H	2.40903600	-1.89436200	0.28433700

Scan Point for comp3_1_alpha_1.7Å

C	-1.33922100	1.27912100	0.05607600
C	0.01995200	1.89818800	-0.33073200
C	1.25096400	1.13003800	0.19777700
C	-1.61024900	-0.14027000	-0.45634000
C	1.51764600	-0.12053500	-0.64327800
C	-0.59472300	-1.18926900	0.01865100
H	-1.42104500	1.26769800	1.15149200
H	0.08473600	1.97473200	-1.42120100
H	-1.59963900	-0.13473900	-1.55639200
H	2.11816800	1.78330400	0.04956500
H	2.05699100	0.08297200	-1.56957200
H	-0.30733800	-1.04413400	1.06160000
O	1.04962100	0.86179700	1.57575100
H	1.90609400	0.75772800	2.01708000
O	0.06333200	3.24098600	0.14499600
H	0.10015600	3.22715900	1.11633800

O	-2.39115300	2.06720400	-0.50076500
H	-2.28974800	2.98255300	-0.19611200
O	-2.89177800	-0.56496900	0.00809500
H	-3.53269400	0.13267700	-0.20513800
C	-1.06637600	-2.63574000	-0.19220600
H	-1.49539600	-2.75086900	-1.19691100
H	-0.19901800	-3.29752200	-0.11630200
O	-1.97525300	-3.04016300	0.81778700
H	-2.75902800	-2.47049700	0.74533600
O	0.59468300	-1.05092300	-0.84341600
C	4.12329000	-0.80019600	-0.35511000
H	4.12278800	-1.25494200	-1.34633900
H	4.38097500	0.25644200	-0.39513400
H	4.78365100	-1.32915700	0.33154000
O	2.76776300	-0.87602600	0.22645900
H	2.50493600	-1.81468000	0.32986200

Scan Point for comp3_1_alpha_1.8Å

C	-1.36449100	1.26347100	0.06530200
C	-0.01811700	1.90490100	-0.33190100
C	1.22840200	1.14721400	0.18203800
C	-1.61918100	-0.15785900	-0.45282800
C	1.48789700	-0.08915900	-0.67454800
C	-0.58860700	-1.19598100	0.01370300
H	-1.43588000	1.24546400	1.16121300
H	0.03534700	1.98637400	-1.42275100
H	-1.61426800	-0.14630900	-1.55295700
H	2.08827000	1.80871300	0.02959700
H	2.06150700	0.09075000	-1.58402900
H	-0.29159200	-1.04899200	1.05330300
O	1.04018700	0.86732600	1.55800900
H	1.90069400	0.72239600	1.98027500
O	0.01309600	3.24460500	0.14899500
H	0.06412000	3.22839700	1.11970900
O	-2.43292600	2.03746500	-0.47863900
H	-2.34654100	2.95199000	-0.16689500
O	-2.89006900	-0.60448500	0.01688800
H	-3.54335900	0.08366100	-0.18979500
C	-1.03567300	-2.64916400	-0.20205400
H	-1.47321500	-2.76629700	-1.20271200
H	-0.15534500	-3.29519300	-0.13881300
O	-1.92586600	-3.07370000	0.81580100
H	-2.72360300	-2.52282700	0.75102100

O	0.59644000	-1.03270400	-0.85791800
C	4.16859000	-0.74805900	-0.34431600
H	4.16889500	-1.20615200	-1.33474300
H	4.40834500	0.31293800	-0.39612900
H	4.85919300	-1.25735500	0.32861900
O	2.83085400	-0.84505700	0.25555200
H	2.59078500	-1.78733800	0.36320100

Scan Point for comp3_1_alpha_1.9Å

C	-1.38341600	1.25342300	0.07506400
C	-0.04911900	1.91247300	-0.33606300
C	1.20967500	1.15917300	0.16100200
C	-1.62729800	-0.16889900	-0.44829200
C	1.45819300	-0.06613400	-0.70677500
C	-0.58835400	-1.20224400	0.01085700
H	-1.44141800	1.22935000	1.17146900
H	-0.00965800	1.99890300	-1.42719800
H	-1.62774800	-0.15189500	-1.54850400
H	2.06582000	1.82410800	0.00361700
H	2.06313800	0.08660200	-1.60041100
H	-0.28422700	-1.05621500	1.04820900
O	1.03251200	0.86812300	1.53503300
H	1.89482600	0.68141700	1.93739400
O	-0.02153500	3.24833200	0.15136100
H	0.04426800	3.22836400	1.12116900
O	-2.46791700	2.01499000	-0.45346900
H	-2.40330400	2.92473000	-0.12340700
O	-2.89002100	-0.63055200	0.02615100
H	-3.54946800	0.05591100	-0.16658500
C	-1.02048600	-2.65850500	-0.21360800
H	-1.46703700	-2.77199500	-1.21057600
H	-0.13169000	-3.29414600	-0.16488700
O	-1.89476200	-3.09991100	0.81010300
H	-2.70268600	-2.56331400	0.75360600
O	0.59597000	-1.02406600	-0.86603700
C	4.21736100	-0.70893000	-0.32893900
H	4.21904000	-1.17653800	-1.31569300
H	4.44233800	0.35485800	-0.39800000
H	4.93238200	-1.19749800	0.33511000
O	2.89381400	-0.81849200	0.28466300
H	2.67160600	-1.76217500	0.40277800

Scan Point for comp3_1_alpha_2.0Å

C	-1.39902800	1.24612700	0.08546300
C	-0.07727300	1.91995800	-0.34224300
C	1.19313300	1.16836700	0.13247900
C	-1.63554400	-0.17602100	-0.44376500
C	1.42980800	-0.05049600	-0.74037500
C	-0.59185800	-1.20807000	0.00839800
H	-1.44091400	1.21541400	1.18227600
H	-0.05500400	2.01361200	-1.43328200
H	-1.64081000	-0.15363500	-1.54400700
H	2.04531800	1.83546700	-0.03548200
H	2.06567400	0.07164100	-1.61690600
H	-0.28119700	-1.06389500	1.04386600
O	1.03354900	0.86961700	1.50607300
H	1.89690700	0.63256700	1.87962600
O	-0.04746900	3.25064600	0.15517100
H	0.03664200	3.22393500	1.12346300
O	-2.49917500	1.99740900	-0.42445100
H	-2.45745200	2.89907500	-0.06989800
O	-2.89201400	-0.64847500	0.03440700
H	-3.55380300	0.04073500	-0.14041100
C	-1.01693600	-2.66522500	-0.22398400
H	-1.47295300	-2.77318500	-1.21717700
H	-0.12372500	-3.29539300	-0.18919400
O	-1.87786000	-3.11817000	0.80524700
H	-2.69211900	-2.59048800	0.75737400
O	0.59384100	-1.02236700	-0.87210100
C	4.26798900	-0.68184200	-0.31175500
H	4.27596100	-1.19319600	-1.27732500
H	4.47052500	0.38205100	-0.43506200
H	5.00737900	-1.12143200	0.36114500
O	2.95737300	-0.79185100	0.31647900
H	2.75186200	-1.73453700	0.45908200

Scan Point for comp3_1_alpha_2.1Å

C	-1.41113900	1.24202500	0.09538700
C	-0.09966800	1.92804000	-0.34661200
C	1.18174700	1.17328600	0.09843500
C	-1.64731000	-0.17920400	-0.43859500
C	1.39657900	-0.03889300	-0.78363200
C	-0.59970000	-1.21161000	0.00414200

H	-1.43725600	1.20453400	1.19234400
H	-0.09669200	2.03671600	-1.43645500
H	-1.66038300	-0.15280800	-1.53875200
H	2.03227800	1.83930400	-0.08223900
H	2.05360600	0.05609200	-1.64783800
H	-0.27684800	-1.06785300	1.03588400
O	1.04572700	0.86733000	1.47237100
H	1.91045300	0.59038700	1.81625000
O	-0.06368800	3.24974300	0.17015000
H	0.03798100	3.20865200	1.13634500
O	-2.52286200	1.98841400	-0.39548800
H	-2.49527300	2.88226500	-0.02052000
O	-2.89772000	-0.65798800	0.04712300
H	-3.56146800	0.03310900	-0.11277000
C	-1.02082200	-2.66954600	-0.23021000
H	-1.48716500	-2.77514100	-1.21875100
H	-0.12432700	-3.29549700	-0.20764000
O	-1.86800200	-3.12921400	0.80671100
H	-2.68737300	-2.60895800	0.76707900
O	0.58173600	-1.02150100	-0.88678100
C	4.32416200	-0.65276800	-0.27679800
H	4.36431800	-1.17506700	-1.23641000
H	4.50004500	0.41440700	-0.41518500
H	5.07172500	-1.06030500	0.40826700
O	3.01078200	-0.78961600	0.33026400
H	2.82550100	-1.73516300	0.47290600

Scan Point for comp3_1_alpha_2.2Å

C	-1.41902600	1.24456900	0.09955800
C	-0.10808200	1.93438300	-0.33960700
C	1.17438000	1.16320500	0.07691600
C	-1.65806900	-0.17390200	-0.44336300
C	1.36192800	-0.03965900	-0.81880400
C	-0.61759700	-1.21239000	0.00448600
H	-1.44355500	1.19873800	1.19622200
H	-0.11493900	2.06691800	-1.42666700
H	-1.66360800	-0.14405800	-1.54355600
H	2.02855200	1.82269400	-0.10943100
H	2.03365500	0.03341800	-1.67325800
H	-0.28694400	-1.06348200	1.03290200
O	1.05669700	0.84066600	1.44865200
H	1.92223200	0.53461800	1.76692300
O	-0.05900800	3.24337700	0.20437700

H	0.04907500	3.18207800	1.16880700
O	-2.53035100	1.99535900	-0.38438200
H	-2.50750500	2.88388000	0.00333800
O	-2.91303400	-0.64943800	0.03161800
H	-3.57242500	0.04604400	-0.12802900
C	-1.04462200	-2.66961500	-0.22069800
H	-1.51146800	-2.78060000	-1.20826900
H	-0.15077000	-3.29912700	-0.19264200
O	-1.89348600	-3.11593800	0.82043700
H	-2.71271500	-2.59604600	0.77352000
O	0.56517900	-1.03129000	-0.89240000
C	4.38721500	-0.63486400	-0.26709200
H	4.44713900	-1.17548700	-1.21598100
H	4.53622100	0.43303500	-0.43089400
H	5.14746200	-1.00542200	0.42585100
O	3.07709300	-0.79154300	0.33570100
H	2.91812400	-1.73710900	0.50076900

Scan Point for comp3_1_alpha_2.3Å

C	-1.42922100	1.24559500	0.10838100
C	-0.12126400	1.93830400	-0.33472900
C	1.16449500	1.15483700	0.04946500
C	-1.67100900	-0.16915900	-0.44479100
C	1.33192600	-0.04171500	-0.85490200
C	-0.63360900	-1.21276200	0.00014600
H	-1.44832200	1.19135100	1.20492000
H	-0.14275200	2.08931700	-1.41884500
H	-1.67483200	-0.13322500	-1.54485500
H	2.01761900	1.81233600	-0.14640500
H	2.02390600	0.00873600	-1.69480300
H	-0.29169000	-1.06091900	1.02447200
O	1.07373600	0.81451700	1.41904000
H	1.94418400	0.48881200	1.70583300
O	-0.05724900	3.23709500	0.22968300
H	0.06254700	3.16023700	1.19158500
O	-2.54267900	2.00009900	-0.36412800
H	-2.52377600	2.88268200	0.03706400
O	-2.92731600	-0.64479000	0.02493100
H	-3.58330300	0.05610300	-0.12560600
C	-1.06679300	-2.66907200	-0.21693700
H	-1.54018500	-2.78316700	-1.20089800
H	-0.17507500	-3.30159100	-0.19054000
O	-1.91073300	-3.10550100	0.83220200

H	-2.72998400	-2.58562900	0.78508300
O	0.54830300	-1.03916000	-0.90544500
C	4.44651000	-0.61627100	-0.25424600
H	4.51460600	-1.16698700	-1.19726600
H	4.57764600	0.45160000	-0.43391700
H	5.21960000	-0.96287000	0.43757000
O	3.14263600	-0.78671400	0.35187200
H	3.01000900	-1.72971200	0.54703000

Scan Point for comp3_1_alpha_2.4Å

C	-1.44152700	1.24019700	0.13083800
C	-0.15267300	1.94567100	-0.34592300
C	1.14983200	1.16562700	-0.01086700
C	-1.68767700	-0.17174100	-0.42769300
C	1.29868400	-0.03148600	-0.91439200
C	-0.63925900	-1.21638100	-0.01230700
H	-1.42998500	1.17846300	1.22721300
H	-0.21115600	2.10749600	-1.42654200
H	-1.71522000	-0.12802900	-1.52729600
H	1.99293500	1.82805400	-0.23246400
H	2.00400300	-0.00426100	-1.74480600
H	-0.27549100	-1.07309300	1.00598700
O	1.10795800	0.81558400	1.35804900
H	1.98259300	0.45942700	1.59646000
O	-0.07622000	3.23779200	0.23105400
H	0.07942200	3.15080200	1.18691600
O	-2.57332900	1.98917300	-0.30637100
H	-2.55908100	2.86346400	0.11283800
O	-2.93052500	-0.65757300	0.06623400
H	-3.58954900	0.04700900	-0.05090500
C	-1.07349400	-2.67150600	-0.23703000
H	-1.57436900	-2.77317300	-1.20857800
H	-0.17909700	-3.30058400	-0.24504200
O	-1.88589500	-3.12498800	0.82901400
H	-2.71068000	-2.61241800	0.80839300
O	0.52983500	-1.03689100	-0.93697700
C	4.50705300	-0.59588600	-0.18667600
H	4.61295200	-1.15122200	-1.12383900
H	4.63522800	0.47180700	-0.37083900
H	5.26160000	-0.93015900	0.53141000
O	3.18422200	-0.77397400	0.37147800
H	3.06187700	-1.71354200	0.58555300

Scan Point for comp3_1_alpha_2.5Å

C	1.45721300	-1.23075700	0.14612900
C	0.18479300	-1.95084500	-0.35214300
C	-1.13157400	-1.17859200	-0.05003300
C	1.70152900	0.17970800	-0.41684700
C	-1.27103000	0.01329500	-0.95873600
C	0.63939100	1.21959000	-0.02504700
H	1.42288700	-1.16247500	1.24160300
H	0.26754500	-2.11943800	-1.43009700
H	1.74897900	0.13034900	-1.51558100
H	-1.96491000	-1.84891100	-0.28484800
H	-1.98575700	-0.00348100	-1.78225700
H	0.25913800	1.08003300	0.98781800
O	-1.12331800	-0.81492200	1.31594400
H	-2.00130300	-0.44457000	1.52421900
O	0.10588600	-3.23787700	0.23427300
H	-0.07030800	-3.14425600	1.18589500
O	2.60389100	-1.97216000	-0.26410100
H	2.59317300	-2.84144300	0.16556900
O	2.93053400	0.67944000	0.09694300
H	3.59695700	-0.02123700	-0.00027700
C	1.06694000	2.67619900	-0.25355400
H	1.59101400	2.77279900	-1.21321900
H	0.16785000	3.29745000	-0.28916500
O	1.84913400	3.14585900	0.82766100
H	2.68083400	2.64442500	0.82883300
O	-0.51810700	1.02784300	-0.96441300
C	-4.55487000	0.56476200	-0.15046800
H	-4.67761500	1.13085800	-1.07939100
H	-4.66329800	-0.50226200	-0.35100700
H	-5.31416100	0.87244600	0.57471500
O	-3.23255700	0.75971200	0.39967500
H	-3.12908200	1.69639800	0.63351900

Scan Point for comp3_1_alpha_2.6Å

C	1.36352500	1.30985300	-0.17327800
C	0.05665600	1.93310500	0.36333900
C	-1.20426400	1.05159300	0.13016200
C	1.74263000	-0.06586000	0.40137600
C	-1.20857400	-0.14157800	1.04465300

C	0.76084000	-1.19369200	0.04211200
H	1.29343600	1.21561200	-1.26512200
H	0.16669100	2.13104800	1.43420100
H	1.81649600	0.00163400	1.49774300
H	-2.07748700	1.65446700	0.40207300
H	-1.90478300	-0.19628800	1.88256400
H	0.34461000	-1.08619500	-0.96022000
O	-1.23294800	0.67305200	-1.23158700
H	-2.06888500	0.18526100	-1.37511100
O	-0.15124000	3.19495600	-0.24433000
H	-0.34283600	3.06640200	-1.18907100
O	2.45949200	2.15068200	0.17803000
H	2.34874000	3.01512300	-0.24764700
O	2.99408100	-0.47103800	-0.14105400
H	3.60270900	0.28404400	-0.07417900
C	1.31184200	-2.60968800	0.25754000
H	1.86733400	-2.66221200	1.20296900
H	0.46807700	-3.30254700	0.31464800
O	2.10055800	-3.01322500	-0.84555100
H	2.88526100	-2.44135700	-0.87066700
O	-0.38851700	-1.09917000	1.00908800
C	-4.60276700	-0.63006800	0.00986300
H	-4.91556700	-1.16716500	0.91082500
H	-4.62257900	0.44455900	0.19898600
H	-5.28081400	-0.86180100	-0.81732900
O	-3.24399500	-0.97057300	-0.34453000
H	-3.19917300	-1.92004700	-0.53980600

Scan Point for comp3_1_alpha_2.7Å

C	1.35607200	1.31545500	-0.19146900
C	0.05754500	1.93032500	0.37317400
C	-1.20084800	1.03648000	0.17363100
C	1.76064700	-0.05124700	0.38732000
C	-1.17693300	-0.15391600	1.09145000
C	0.78380900	-1.19170500	0.05525100
H	1.26011100	1.21070000	-1.28036300
H	0.19180400	2.13430000	1.43999300
H	1.85500200	0.02683700	1.48134200
H	-2.07303700	1.63366700	0.46113100
H	-1.87528800	-0.22733200	1.92685800
H	0.34544300	-1.09409100	-0.93854600
O	-1.25849900	0.64529100	-1.18395200
H	-2.09594800	0.14908400	-1.30241100

O	-0.17543200	3.18740900	-0.23465800
H	-0.38856600	3.05398500	-1.17406600
O	2.45173600	2.16998800	0.12521900
H	2.31973000	3.03037600	-0.30252200
O	3.00559900	-0.44901900	-0.17485800
H	3.60545700	0.31491700	-0.13290400
C	1.35133200	-2.60164400	0.26874500
H	1.92348000	-2.64422100	1.20467800
H	0.51452900	-3.30120200	0.34412700
O	2.12385200	-3.00392500	-0.84604100
H	2.90388700	-2.42660200	-0.88712000
O	-0.35140100	-1.10447400	1.04156000
C	-4.64967900	-0.62785900	-0.03389700
H	-4.98404400	-1.17212400	0.85506000
H	-4.65727100	0.44425000	0.17029200
H	-5.31919500	-0.83828300	-0.87373000
O	-3.29061800	-0.98328800	-0.36953800
H	-3.25964500	-1.92545500	-0.59890500

Scan Point for comp3_1_alpha_2.8Å

C	1.34384500	1.32108000	-0.21920100
C	0.06264900	1.93030200	0.38854400
C	-1.19247300	1.02086500	0.24510000
C	1.78047900	-0.03501900	0.36208200
C	-1.12374300	-0.16204500	1.16952100
C	0.80748600	-1.19035400	0.06974200
H	1.20748100	1.20281200	-1.30239300
H	0.23474800	2.14686600	1.44710400
H	1.90296100	0.05658800	1.45224400
H	-2.05965700	1.61188200	0.55960500
H	-1.79737200	-0.24283200	2.02460600
H	0.33418400	-1.10485300	-0.90900100
O	-1.29723600	0.61428000	-1.10473000
H	-2.13659900	0.10839500	-1.18405100
O	-0.20713100	3.17774300	-0.22302400
H	-0.45189300	3.03240600	-1.15287500
O	2.44335600	2.18858500	0.04554600
H	2.29201000	3.03852600	-0.39655600
O	3.01508400	-0.42435500	-0.22755500
H	3.59915200	0.35303100	-0.22754100
C	1.39667100	-2.59251400	0.27625000
H	1.99186100	-2.62343700	1.19812600
H	0.56984500	-3.30076400	0.37647700

O	2.14555200	-2.99223300	-0.85531000
H	2.91791300	-2.40664700	-0.91894200
O	-0.29810500	-1.10955700	1.09146900
C	-4.71975300	-0.63096300	-0.15444100
H	-5.18674200	-1.25611700	0.61297000
H	-4.73462500	0.41116500	0.16869700
H	-5.26787800	-0.72510000	-1.09718700
O	-3.33336000	-0.99773700	-0.33355000
H	-3.29163400	-1.92384800	-0.61963000

Scan Point for comp3_1_alpha_2.9Å

C	1.33427300	1.32857400	-0.23244700
C	0.05797300	1.92860100	0.39407900
C	-1.18817800	1.00263200	0.29040300
C	1.79595000	-0.01902000	0.34960700
C	-1.08562600	-0.17680400	1.21543400
C	0.83242900	-1.18756500	0.07827700
H	1.17982700	1.20234000	-1.31241700
H	0.24847300	2.16132600	1.44605500
H	1.93247900	0.08011100	1.43754700
H	-2.05299100	1.58591300	0.62530100
H	-1.74878100	-0.26871500	2.07788900
H	0.33785700	-1.11000500	-0.89068700
O	-1.32474600	0.58556600	-1.05290600
H	-2.16737400	0.07818800	-1.11059300
O	-0.24291500	3.16294400	-0.22984200
H	-0.50470500	2.99902000	-1.15206300
O	2.42924600	2.20919000	0.00772500
H	2.26575000	3.05119900	-0.44502200
O	3.02696300	-0.39600700	-0.25494000
H	3.59780400	0.39097500	-0.27468800
C	1.44157700	-2.58238900	0.27627600
H	2.05044100	-2.60621700	1.18935300
H	0.62461500	-3.30031300	0.38848700
O	2.17831800	-2.97282000	-0.86637800
H	2.94273200	-2.37815600	-0.94114000
O	-0.25505000	-1.11782100	1.12089900
C	-4.76778100	-0.63509500	-0.19553100
H	-5.25618400	-1.26507600	0.55445500
H	-4.78052500	0.40310900	0.14008400
H	-5.29731900	-0.71329600	-1.15031800
O	-3.38110400	-1.01266200	-0.34729800
H	-3.34148300	-1.93112700	-0.65691200

Scan Point for comp3_1_alpha_3.0Å

C	1.32354300	1.33665300	-0.24535000
C	0.05122400	1.92898500	0.39735400
C	-1.18444500	0.98523100	0.33228800
C	1.80883700	-0.00368600	0.33533400
C	-1.04548100	-0.18441500	1.26381600
C	0.85342400	-1.18420800	0.08706500
H	1.15344300	1.20389500	-1.32219200
H	0.25853100	2.17854100	1.44244400
H	1.96245100	0.10198900	1.42058400
H	-2.04882000	1.56085400	0.68164300
H	-1.68993200	-0.27932900	2.14014100
H	0.33808900	-1.11513900	-0.87179800
O	-1.34696900	0.55003400	-1.00177400
H	-2.19157900	0.03961000	-1.03962400
O	-0.27913800	3.14947600	-0.23859500
H	-0.55608700	2.96757900	-1.15313100
O	2.41400500	2.22860300	-0.02601500
H	2.24242400	3.06259000	-0.49024000
O	3.03343300	-0.37032100	-0.28785600
H	3.59476600	0.42301900	-0.32205000
C	1.48031200	-2.57201000	0.27836400
H	2.10402100	-2.58786800	1.18151400
H	0.67242100	-3.29781900	0.40519700
O	2.20236800	-2.95736700	-0.87522800
H	2.95921000	-2.35497100	-0.96368200
O	-0.21305200	-1.12144900	1.15205400
C	-4.80312600	-0.63367400	-0.23549900
H	-5.31914600	-1.26492000	0.49460300
H	-4.80488700	0.39985200	0.11461100
H	-5.31321400	-0.68915400	-1.20240900
O	-3.42045000	-1.03422100	-0.36018000
H	-3.38899800	-1.94401700	-0.69507900

Scan Point for comp3_1_alpha_3.1Å

C	1.30474400	1.34913700	-0.25931900
C	0.03484000	1.92418400	0.40512000
C	-1.18395900	0.95604600	0.37678500
C	1.82520200	0.02020900	0.31799100

C	-0.99924300	-0.20181100	1.31270900
C	0.88574800	-1.17819900	0.09555400
H	1.11483800	1.20722600	-1.33160100
H	0.25957600	2.18924700	1.44286800
H	1.99921100	0.13342900	1.39958000
H	-2.05090500	1.51819000	0.74158600
H	-1.62192000	-0.30338500	2.20411000
H	0.34854300	-1.12237700	-0.85222400
O	-1.37091200	0.50084500	-0.94718600
H	-2.21816600	-0.01015500	-0.96577000
O	-0.33320200	3.13112700	-0.23588200
H	-0.62610600	2.93453500	-1.14243300
O	2.38428800	2.26033400	-0.06719600
H	2.19875700	3.08285700	-0.54603700
O	3.04257700	-0.32851400	-0.32873500
H	3.58916000	0.47428300	-0.37897900
C	1.53979000	-2.55416000	0.28075000
H	2.18179800	-2.55522700	1.17115300
H	0.74674400	-3.29264000	0.42746700
O	2.24473200	-2.93299500	-0.88527200
H	2.98927500	-2.31837000	-0.99175700
O	-0.15792100	-1.12823300	1.18319100
C	-4.84738600	-0.63839700	-0.29282700
H	-5.42097300	-1.29323800	0.37035700
H	-4.85055800	0.37625600	0.10883700
H	-5.29588700	-0.63302700	-1.29141800
O	-3.46780200	-1.06347100	-0.35275300
H	-3.43588600	-1.96241600	-0.71566400

Scan Point for comp3_1_alpha_3.2Å

C	1.26243100	1.36711700	-0.27888600
C	0.00022200	1.90963100	0.42674800
C	-1.18787400	0.90258500	0.44320300
C	1.84768900	0.06194100	0.28973400
C	-0.93661800	-0.23633500	1.38711600
C	0.93633900	-1.16642700	0.12063100
H	1.03440900	1.20484800	-1.34055700
H	0.25276900	2.18977100	1.45396200
H	2.06875200	0.19353700	1.36031600
H	-2.06278700	1.43849100	0.82796400
H	-1.53005500	-0.34717000	2.29741400
H	0.35944200	-1.13846500	-0.80465900
O	-1.39584400	0.42844900	-0.87066800

H	-2.24321900	-0.08720100	-0.86960900
O	-0.42584600	3.10031800	-0.20797400
H	-0.74227500	2.89008400	-1.10360800
O	2.31804700	2.31464700	-0.14087200
H	2.08988600	3.12263900	-0.62600400
O	3.04241500	-0.26002700	-0.41155000
H	3.56835700	0.55440100	-0.48821000
C	1.64120500	-2.51910500	0.28827700
H	2.33410400	-2.48731400	1.13896100
H	0.88211600	-3.28017000	0.48923700
O	2.29043800	-2.89166700	-0.91211900
H	3.00666200	-2.25462500	-1.06875200
O	-0.06576700	-1.13394500	1.24706400
C	-4.88545200	-0.66530500	-0.42028100
H	-5.52748500	-1.28957200	0.20872400
H	-4.92522700	0.36585000	-0.06577500
H	-5.22621800	-0.70620900	-1.45962900
O	-3.50875900	-1.09297400	-0.31296200
H	-3.44435700	-2.01191600	-0.61638500

Scan Point for comp3_1_alpha_3.3Å

C	1.23755200	1.37891500	-0.29061100
C	-0.02402600	1.89848400	0.43310800
C	-1.18895800	0.86511400	0.47988600
C	1.85944500	0.08986100	0.27588900
C	-0.89374900	-0.25906600	1.42936300
C	0.97031200	-1.15795700	0.12978700
H	0.99542800	1.20511700	-1.34719100
H	0.24113800	2.19091100	1.45371700
H	2.09600000	0.23283000	1.34156700
H	-2.06764300	1.38512000	0.87737900
H	-1.46645000	-0.37560100	2.35239100
H	0.37328400	-1.14615900	-0.78286500
O	-1.41187800	0.37351600	-0.82466900
H	-2.26408100	-0.13720300	-0.81474700
O	-0.48849400	3.07524300	-0.20051200
H	-0.81304100	2.85362000	-1.09044400
O	2.27564300	2.34864400	-0.17571400
H	2.02421900	3.14867300	-0.66244700
O	3.04810000	-0.21175700	-0.44456000
H	3.55920700	0.61116400	-0.52974300
C	1.70683100	-2.49490800	0.28637600
H	2.41720000	-2.44566300	1.12169600

H	0.96899500	-3.27166900	0.50501100
O	2.33812800	-2.85696700	-0.92693900
H	3.03515800	-2.20353400	-1.10163100
O	-0.00888100	-1.14045700	1.27678400
C	-4.91572900	-0.67222500	-0.44901700
H	-5.57341200	-1.29650300	0.16351700
H	-4.94430000	0.35380900	-0.07872200
H	-5.24575300	-0.69169000	-1.49240100
O	-3.54711200	-1.12174000	-0.33287200
H	-3.49008000	-2.03438200	-0.65592100

Scan Point for comp3_1_alpha_3.4Å

C	1.20530500	1.39457800	-0.29966700
C	-0.05889000	1.87932600	0.44261100
C	-1.19374200	0.81487300	0.51468000
C	1.87195400	0.12720400	0.26422000
C	-0.85151700	-0.30018600	1.46053400
C	1.01720000	-1.14591000	0.13163700
H	0.95213100	1.20781600	-1.35147200
H	0.21446100	2.18199300	1.45812100
H	2.11586100	0.28028600	1.32692700
H	-2.07724400	1.31330900	0.92831400
H	-1.40830800	-0.43582500	2.39102000
H	0.40643800	-1.15234200	-0.77198800
O	-1.43145200	0.30961300	-0.78170400
H	-2.28917000	-0.19423400	-0.76577800
O	-0.56695000	3.04034600	-0.18643200
H	-0.90094600	2.80654900	-1.06966600
O	2.21580700	2.39547200	-0.20605100
H	1.93075400	3.18654800	-0.68889400
O	3.06072200	-0.14299800	-0.46823300
H	3.54838400	0.69302500	-0.56064900
C	1.79401900	-2.46105000	0.27911000
H	2.51396300	-2.38986200	1.10468400
H	1.08170900	-3.25796900	0.50898300
O	2.41862300	-2.80770100	-0.94217700
H	3.09378100	-2.13469400	-1.12814100
O	0.05476900	-1.15658900	1.29282200
C	-4.95372700	-0.68136500	-0.46682300
H	-5.62374200	-1.30254600	0.13543200
H	-4.96349100	0.33927600	-0.08076200
H	-5.28279300	-0.67863200	-1.51061500
O	-3.59451900	-1.15865900	-0.35577500

H	-3.55139300	-2.06338600	-0.70291200

Scan Point for comp3_1_alpha_3.5Å

C	1.08730300	1.43890900	-0.30361100
C	-0.18407600	1.81505100	0.48526900
C	-1.22402600	0.66261600	0.58833500
C	1.87886400	0.23432500	0.23462300
C	-0.76432000	-0.43478700	1.50320500
C	1.13736300	-1.10873900	0.11395800
H	0.81413600	1.23074200	-1.34686400
H	0.09906200	2.13662300	1.49224300
H	2.13349000	0.40231800	1.29298900
H	-2.13068200	1.08283700	1.03670700
H	-1.28484600	-0.63648300	2.44312400
H	0.51121100	-1.16822100	-0.77759700
O	-1.46568400	0.14632800	-0.70307400
H	-2.31483200	-0.37451800	-0.67379600
O	-0.80807800	2.93032700	-0.12287900
H	-1.15833600	2.66255600	-0.99006300
O	2.01073700	2.52301500	-0.24377300
H	1.63772600	3.28748600	-0.70926300
O	3.06950500	0.07741800	-0.52666600
H	3.47545300	0.95600600	-0.62084800
C	2.02888800	-2.35058500	0.24828700
H	2.74907500	-2.21653300	1.06589300
H	1.39116500	-3.20605700	0.48731300
O	2.66670600	-2.64385200	-0.97945800
H	3.28476500	-1.92017900	-1.17241900
O	0.20407000	-1.21013900	1.29491600
C	-4.95320400	-0.71967900	-0.59883900
H	-5.73630900	-1.28452100	-0.08410100
H	-4.95478600	0.31000800	-0.23756500
H	-5.13427700	-0.72726800	-1.67847600
O	-3.65227700	-1.26900000	-0.28950500
H	-3.62260300	-2.19024500	-0.59112100

Scan Point for comp3_1_alpha_3.6Å

C	1.07246000	1.44160200	-0.31086000
C	-0.19484200	1.80858900	0.49061300
C	-1.21546000	0.64115700	0.62354800

C	1.88714500	0.24851700	0.22055400
C	-0.71788400	-0.43349200	1.54509000
C	1.15684800	-1.10253700	0.11994700
H	0.78854100	1.22518300	-1.34935900
H	0.09755800	2.14807700	1.48908900
H	2.15790500	0.42486900	1.27349200
H	-2.12066000	1.05138600	1.08427900
H	-1.21008900	-0.62272700	2.50278800
H	0.51190200	-1.17077300	-0.75734800
O	-1.47131300	0.10882700	-0.65809600
H	-2.32508100	-0.40506100	-0.62404600
O	-0.84480100	2.90491500	-0.12397400
H	-1.20654200	2.61713200	-0.98000400
O	1.98394700	2.53671200	-0.26768800
H	1.60365800	3.29013100	-0.74514300
O	3.06614200	0.10109600	-0.56013500
H	3.46011700	0.98380200	-0.66605300
C	2.06054100	-2.33683900	0.24084800
H	2.79155400	-2.19769500	1.04791600
H	1.43308300	-3.19742500	0.48884700
O	2.68251600	-2.62494700	-0.99625900
H	3.29092500	-1.89576100	-1.19896600
O	0.25196300	-1.20295900	1.32313000
C	-4.97601200	-0.71459100	-0.62661400
H	-5.77452400	-1.26874400	-0.12409200
H	-4.96654900	0.31381800	-0.26176700
H	-5.14342900	-0.71572200	-1.70850300
O	-3.68846300	-1.28509400	-0.30165100
H	-3.66506500	-2.20332500	-0.61251500

Scan Point for comp3_1_alpha_3.7Å

C	1.05204900	1.44454700	-0.31992900
C	-0.20898000	1.79486400	0.49992800
C	-1.20870100	0.61191000	0.65774300
C	1.89586300	0.26722400	0.20177500
C	-0.67062200	-0.43935800	1.58291000
C	1.18316800	-1.09472100	0.12556700
H	0.75511600	1.21974600	-1.35278800
H	0.09432400	2.14539800	1.49139300
H	2.18517900	0.45497900	1.24777500
H	-2.11248700	1.01045500	1.13141600
H	-1.13573800	-0.61984000	2.55586500
H	0.52016100	-1.17832800	-0.73673100

O	-1.47829500	0.06423300	-0.61420000
H	-2.33760100	-0.44028400	-0.57514200
O	-0.88583000	2.87690400	-0.11043600
H	-1.25835300	2.57772800	-0.95785100
O	1.94603100	2.55454900	-0.29470000
H	1.54689100	3.30002400	-0.76924500
O	3.06119700	0.13255000	-0.60126500
H	3.44130100	1.01988600	-0.71801700
C	2.10505000	-2.31640100	0.23542600
H	2.84679300	-2.16577200	1.03051500
H	1.49291600	-3.18452200	0.49537000
O	2.71120700	-2.59953400	-1.01064900
H	3.30613100	-1.86252300	-1.22504100
O	0.30748300	-1.19504700	1.35052800
C	-5.00300700	-0.71261000	-0.65873000
H	-5.81803400	-1.25518500	-0.17026000
H	-4.98543000	0.31564500	-0.29374400
H	-5.15188200	-0.71150000	-1.74335800
O	-3.73017400	-1.30121900	-0.31085700
H	-3.71115400	-2.21812600	-0.62565900

Scan Point for comp3_1_alpha_3.8Å

C	1.00434600	1.44744700	-0.33728100
C	-0.23189200	1.77208900	0.52918300
C	-1.19942300	0.56750800	0.71926700
C	1.89673800	0.30222800	0.17363000
C	-0.61086100	-0.46503200	1.63543800
C	1.22113100	-1.08043500	0.13351300
H	0.67248200	1.19833700	-1.35377500
H	0.10024300	2.12678300	1.51005700
H	2.20921400	0.51419600	1.20842400
H	-2.09876300	0.94817700	1.21535300
H	-1.04650100	-0.65288000	2.62068200
H	0.53700900	-1.19304900	-0.70886300
O	-1.48997300	0.00434300	-0.54102100
H	-2.35353500	-0.49299100	-0.49207300
O	-0.95282800	2.84108900	-0.05306300
H	-1.34790500	2.53777800	-0.88876000
O	1.86689100	2.58171000	-0.36569900
H	1.41378300	3.31872200	-0.80390100
O	3.04366000	0.18787100	-0.65844800
H	3.38938900	1.08404300	-0.80864900
C	2.18105500	-2.27377300	0.22682000

H	2.94174300	-2.09343300	0.99719500
H	1.60311000	-3.15661300	0.51364700
O	2.75665200	-2.55124500	-1.03483500
H	3.32323500	-1.79923700	-1.27306600
O	0.38229700	-1.19417300	1.38287200
C	-4.99573900	-0.72429300	-0.75563800
H	-5.86004000	-1.26162800	-0.35388900
H	-5.00198000	0.30047700	-0.38047000
H	-5.03767000	-0.71242700	-1.84970300
O	-3.76881600	-1.33086900	-0.29268400
H	-3.73899200	-2.25050800	-0.59878300

Scan Point for comp3_1_alpha_3.9Å

C	0.93467900	1.45847200	-0.33723500
C	-0.29010900	1.72524400	0.56200000
C	-1.19504400	0.47768800	0.77770400
C	1.89247400	0.35910700	0.15188800
C	-0.54118700	-0.53514700	1.67483100
C	1.28645400	-1.05544000	0.13149800
H	0.58893200	1.19121400	-1.34443500
H	0.05424000	2.09570100	1.53267100
H	2.22209700	0.59010400	1.17710500
H	-2.09845400	0.81579900	1.29618800
H	-0.95189300	-0.75671200	2.66376900
H	0.58946100	-1.20707300	-0.69429100
O	-1.49138700	-0.10466300	-0.47341500
H	-2.36527600	-0.58438300	-0.42314800
O	-1.07463300	2.76121600	0.00115200
H	-1.47198200	2.44304800	-0.82790700
O	1.74057000	2.63269300	-0.38939600
H	1.23157500	3.35218900	-0.79416800
O	3.01942600	0.29649800	-0.71247400
H	3.32117300	1.20697200	-0.87148400
C	2.31259600	-2.19471200	0.20094900
H	3.09029900	-1.96320100	0.94006100
H	1.79553100	-3.10510400	0.51621500
O	2.85603000	-2.45121200	-1.07947500
H	3.36946500	-1.66992100	-1.34296500
O	0.48149600	-1.21269500	1.39781200
C	-4.97969000	-0.72514300	-0.84717400
H	-5.89270700	-1.22131400	-0.50462100
H	-4.97836000	0.30825500	-0.49656900
H	-4.93464300	-0.73997100	-1.94115600

O	-3.81743600	-1.36225700	-0.27249600
H	-3.80302900	-2.29266000	-0.54569600

Scan Point for comp3_1_alpha_4.0Å

C	0.88692900	1.46220900	-0.33420200
C	-0.33275400	1.68972200	0.58317600
C	-1.18502100	0.40987300	0.82445900
C	1.89248600	0.39930200	0.14082400
C	-0.47463100	-0.57225000	1.71439100
C	1.33211900	-1.03426800	0.13388300
H	0.53335500	1.17617700	-1.33349300
H	0.01112400	2.08685800	1.54346600
H	2.23182100	0.64335800	1.15966900
H	-2.09009000	0.71572200	1.35957100
H	-0.85524900	-0.79890800	2.71386900
H	0.61691800	-1.20760300	-0.67176300
O	-1.48467500	-0.18928700	-0.41801100
H	-2.37403700	-0.64112400	-0.37463400
O	-1.16675600	2.68652300	0.02250200
H	-1.56149300	2.34133700	-0.79686300
O	1.64826700	2.66435700	-0.40628900
H	1.11186700	3.35853000	-0.81975700
O	3.00548100	0.37389900	-0.74327500
H	3.27621600	1.29366200	-0.90462300
C	2.39226800	-2.14275400	0.17069500
H	3.18546900	-1.89111300	0.88608800
H	1.91130300	-3.06848400	0.49827600
O	2.90258200	-2.37950100	-1.12733300
H	3.38674400	-1.58369500	-1.40247500
O	0.56707900	-1.21277200	1.42147000
C	-4.97517400	-0.71566800	-0.89067000
H	-5.90858800	-1.19924900	-0.58719200
H	-4.96913400	0.31383300	-0.52875500
H	-4.88969000	-0.71990500	-1.98233500
O	-3.84629300	-1.37930600	-0.28074400
H	-3.83934900	-2.30769600	-0.56094800

Scan Point for comp3_1_alpha_4.1Å

C	0.84832200	1.46592700	-0.33473400
C	-0.36342300	1.66384500	0.60077000

C	-1.17242300	0.35962600	0.86708100
C	1.89077400	0.42992100	0.12161400
C	-0.41286200	-0.58822800	1.75399000
C	1.36539300	-1.01734200	0.13570800
H	0.48494400	1.16951100	-1.32745500
H	-0.01855300	2.08192100	1.55179100
H	2.24765600	0.68719000	1.13116900
H	-2.07661500	0.64275500	1.41574800
H	-0.75941000	-0.80504800	2.76773200
H	0.63359300	-1.21373300	-0.64938500
O	-1.47690800	-0.25655600	-0.36580000
H	-2.37221700	-0.69522900	-0.32194700
O	-1.23755400	2.62701400	0.04291000
H	-1.63205100	2.25996900	-0.76694900
O	1.57723400	2.68729300	-0.42072200
H	1.02025200	3.36517900	-0.83401400
O	2.98312100	0.42711200	-0.78825800
H	3.23531700	1.35164000	-0.95175200
C	2.45103700	-2.10096300	0.15110700
H	3.25686400	-1.82838300	0.84431700
H	1.99928700	-3.03533600	0.49534500
O	2.93230900	-2.33392500	-1.15871100
H	3.39360800	-1.53047900	-1.45024000
O	0.64005600	-1.20197200	1.44525900
C	-4.96765900	-0.70779700	-0.93174300
H	-5.92039900	-1.17744500	-0.66902900
H	-4.95742500	0.31752300	-0.55807200
H	-4.84102300	-0.70161600	-2.01948500
O	-3.87457400	-1.39809800	-0.28823200
H	-3.87825000	-2.32527900	-0.57209900

Scan Point for comp3_1_alpha_4.2Å

C	0.80221300	1.46811000	-0.32931000
C	-0.40185400	1.62327100	0.62448000
C	-1.16205800	0.29406600	0.91111500
C	1.88610900	0.46578800	0.10618300
C	-0.35029900	-0.62376700	1.78378800
C	1.40629100	-0.99668900	0.12526000
H	0.43337000	1.16401900	-1.31777900
H	-0.05677600	2.05471700	1.56951800
H	2.25151800	0.73124600	1.11076400
H	-2.06157400	0.55145600	1.47917500
H	-0.66294900	-0.84678700	2.80713200

H	0.66711000	-1.21251200	-0.64760200
O	-1.47579700	-0.34210200	-0.30980900
H	-2.37773800	-0.76454000	-0.26310100
O	-1.31791500	2.55439800	0.07907500
H	-1.71528800	2.17015800	-0.72129500
O	1.49000000	2.71266600	-0.42176700
H	0.90755800	3.37278900	-0.82848500
O	2.96182900	0.50098200	-0.82226900
H	3.17741900	1.43393900	-0.99068800
C	2.52417600	-2.04706800	0.12055900
H	3.33090000	-1.75234800	0.80369200
H	2.10562900	-2.99541900	0.46817700
O	2.99389800	-2.26280200	-1.19617200
H	3.43025800	-1.44712300	-1.49168600
O	0.71341000	-1.20372300	1.44961200
C	-4.93994700	-0.68667400	-1.00135900
H	-5.92872000	-1.11017100	-0.80053100
H	-4.91151200	0.34281400	-0.64033000
H	-4.73953300	-0.70240100	-2.07800500
O	-3.92528400	-1.41269400	-0.27462900
H	-3.95857900	-2.34585900	-0.53559000

Scan Point for comp3_1_alpha_4.3Å

C	0.77356300	1.46509800	-0.33905500
C	-0.41192600	1.60689000	0.64045200
C	-1.14602100	0.26688200	0.95082500
C	1.88347900	0.48363100	0.07791600
C	-0.29563200	-0.61651300	1.82358100
C	1.42656000	-0.98529400	0.12910500
H	0.38780800	1.15091200	-1.31800600
H	-0.05154900	2.04664400	1.57605300
H	2.27071900	0.76758800	1.06890000
H	-2.03889200	0.51456400	1.53313200
H	-0.57730000	-0.82026900	2.85996300
H	0.67072400	-1.22251800	-0.62080300
O	-1.46942500	-0.38911700	-0.25705600
H	-2.37977400	-0.79099600	-0.21451500
O	-1.35160800	2.52437300	0.11312200
H	-1.76054200	2.13395800	-0.67837400
O	1.44038200	2.71931400	-0.45212100
H	0.83952800	3.36824000	-0.84988300
O	2.93333700	0.52451200	-0.87923600
H	3.13203000	1.45886200	-1.06019900

C	2.55852700	-2.01997100	0.11328900
H	3.37337400	-1.70701600	0.77870400
H	2.15981800	-2.97035300	0.47842400
O	3.00654500	-2.24330700	-1.20957700
H	3.42524200	-1.42500500	-1.52279600
O	0.77251100	-1.17964600	1.47586500
C	-4.94580200	-0.68813700	-1.03232700
H	-5.94132800	-1.10443500	-0.84972400
H	-4.91506900	0.33920000	-0.66527300
H	-4.72946100	-0.69898800	-2.10605900
O	-3.94913500	-1.42602300	-0.29457900
H	-3.98265900	-2.35674700	-0.56360600

Scan Point for comp3_1_alpha_4.4Å

C	0.73418800	1.46046300	-0.35016100
C	-0.42302000	1.59315100	0.66461300
C	-1.12714000	0.24158400	1.00009800
C	1.87447600	0.50476100	0.04314300
C	-0.23626300	-0.60783100	1.86741600
C	1.44922000	-0.97168700	0.13464800
H	0.32444100	1.12837700	-1.31339800
H	-0.04039100	2.04234100	1.58689700
H	2.28962900	0.81387000	1.01477900
H	-2.01340000	0.47573500	1.59798300
H	-0.48513300	-0.79341000	2.91572000
H	0.67871300	-1.24001500	-0.58916100
O	-1.45819300	-0.43154400	-0.19614700
H	-2.37491400	-0.81609000	-0.16015400
O	-1.38947500	2.49639200	0.16227200
H	-1.81220500	2.10117400	-0.61955400
O	1.37585600	2.72426900	-0.49784300
H	0.75300000	3.35675900	-0.88814400
O	2.88971400	0.54900300	-0.95049400
H	3.05587900	1.48374200	-1.16031400
C	2.60225900	-1.98247600	0.11060600
H	3.42602300	-1.63837100	0.74913000
H	2.23336800	-2.93330100	0.50481000
O	3.02239600	-2.22390900	-1.21814200
H	3.41633300	-1.40420900	-1.55856800
O	0.83557500	-1.15287200	1.50343000
C	-4.94408300	-0.70482500	-1.06902500
H	-5.94325300	-1.11912800	-0.90137900
H	-4.91600300	0.32111800	-0.69772700

H	-4.71434500	-0.71157200	-2.14009900
O	-3.95942600	-1.44756100	-0.32185600
H	-3.98715100	-2.37607600	-0.59860800

Scan Point for comp3_1_alpha_4.5Å

C	0.63152300	1.45775400	-0.31993500
C	-0.50283300	1.50262700	0.72610100
C	-1.11073100	0.10639600	1.06316300
C	1.84234900	0.57620500	0.02858500
C	-0.14545700	-0.70060400	1.89149600
C	1.52081100	-0.92621300	0.11512600
H	0.21903400	1.10681400	-1.27503300
H	-0.12559600	1.96695000	1.64284000
H	2.26863300	0.90314000	0.98991900
H	-1.99270400	0.27694400	1.68888500
H	-0.35842100	-0.92353300	2.94020100
H	0.75470200	-1.24236200	-0.59395300
O	-1.43320900	-0.58053700	-0.12820300
H	-2.36178800	-0.93556500	-0.10698300
O	-1.53855000	2.34536500	0.25683000
H	-1.94617700	1.93622800	-0.52571700
O	1.18055600	2.76445100	-0.47202600
H	0.49661800	3.36074100	-0.81463900
O	2.81958600	0.69338600	-0.99754500
H	2.91452200	1.63774300	-1.20871000
C	2.74214100	-1.85200300	0.05192700
H	3.56098000	-1.44691700	0.66022200
H	2.45686100	-2.82603000	0.45882500
O	3.13251500	-2.06533100	-1.29095500
H	3.45251600	-1.21936600	-1.64432500
O	0.95145700	-1.16596200	1.49392100
C	-4.84082400	-0.66926900	-1.17322500
H	-5.87426200	-1.02315500	-1.10637100
H	-4.78956100	0.35376900	-0.79600400
H	-4.50705400	-0.69178100	-2.21625500
O	-3.98002400	-1.46732900	-0.33521700
H	-4.04881800	-2.39533200	-0.60676800

Scan Point for comp3_1_beta_1.4Å

C	-0.26776000	1.59114200	-0.15060500

C	1.22463000	1.27012200	0.00388600
C	1.58246500	0.05618400	0.87490800
C	-1.12371200	0.42957300	-0.66899600
C	1.17591900	-1.32749400	0.31508700
C	-1.25917100	-0.70862200	0.36065800
H	-0.67386900	1.91465600	0.81726600
H	1.64420400	1.10685400	-0.99301200
H	-0.69366700	0.02867700	-1.59847600
H	2.67646400	0.04807800	0.93363800
H	1.67678200	-2.10557200	0.90143300
H	-1.29276800	-0.30278600	1.37601200
O	1.03137100	0.21388600	2.17660900
H	1.62947200	-0.17823000	2.83027100
O	1.90143900	2.42388100	0.51363400
H	1.63077500	2.55590200	1.43741400
O	-0.42400900	2.64943800	-1.10604400
H	-0.04259900	3.45898700	-0.73308700
O	-2.44657200	0.91297600	-0.93652900
H	-2.35998800	1.79020400	-1.34615900
C	-2.50719900	-1.57980700	0.14444600
H	-2.60735900	-1.84930500	-0.91506600
H	-2.38250900	-2.49753200	0.72436500
O	-3.69353700	-0.95204200	0.62757700
H	-3.79567700	-0.12273700	0.13016600
O	-0.17070000	-1.66724200	0.28184400
C	3.02308400	-1.90968800	-1.27897200
H	3.68741300	-1.18333300	-0.81948600
H	3.12479400	-2.90767200	-0.85388900
H	3.10607000	-1.90233900	-2.36286600
O	1.62830600	-1.43700800	-1.00527400
H	0.97255100	-1.93341400	-1.54553200

Scan Point for comp3_1_beta_1.5Å

C	-0.25379300	1.58837800	-0.15717300
C	1.23537500	1.25658300	0.00710500
C	1.57897200	0.04832700	0.89216900
C	-1.11780400	0.42968500	-0.66955300
C	1.14228500	-1.33258800	0.36445700
C	-1.27455100	-0.69534400	0.36998700
H	-0.66192300	1.92450500	0.80553000
H	1.65823700	1.08082500	-0.98570300
H	-0.68625000	0.01421100	-1.59163400
H	2.67239100	0.02040200	0.94755100

H	1.66299300	-2.12940300	0.90152800
H	-1.31707700	-0.28024200	1.38107400
O	1.03191500	0.23233000	2.19305300
H	1.62496900	-0.16001500	2.85135600
O	1.91939400	2.40765000	0.51172800
H	1.64272400	2.55110800	1.43204100
O	-0.39654000	2.63827200	-1.12361700
H	-0.01283700	3.44923700	-0.75623000
O	-2.43427200	0.92249200	-0.94922900
H	-2.33685300	1.79508500	-1.36633000
C	-2.52175700	-1.56520200	0.14618600
H	-2.60821500	-1.84527900	-0.91178100
H	-2.40736900	-2.47717600	0.73712300
O	-3.71145800	-0.92855200	0.60749500
H	-3.80499200	-0.10394600	0.10070500
O	-0.18564200	-1.66166200	0.32221000
C	3.01650800	-1.92854900	-1.29113000
H	3.68336400	-1.20558000	-0.82882800
H	3.10980500	-2.92335100	-0.85587600
H	3.12785500	-1.93709000	-2.37322000
O	1.63171900	-1.43681500	-1.04961200
H	0.98083800	-1.97076300	-1.55581700

Scan Point for comp3_1_beta_1.6Å

C	-0.24831500	1.58923900	-0.16943500
C	1.24128600	1.25855900	-0.00839100
C	1.58900300	0.06470200	0.89388000
C	-1.11416700	0.42379300	-0.66396500
C	1.11805900	-1.32088200	0.42511800
C	-1.28734000	-0.67811100	0.39618900
H	-0.65260200	1.93906100	0.78997500
H	1.65906200	1.06753100	-1.00003600
H	-0.67865000	-0.01251400	-1.57438900
H	2.68267300	0.01713200	0.92385500
H	1.66302000	-2.12593400	0.92060200
H	-1.34714700	-0.24366500	1.39828700
O	1.07123300	0.28808200	2.20167400
H	1.67188100	-0.09819600	2.85701400
O	1.92847700	2.41436400	0.47916900
H	1.66157300	2.56332500	1.40161100
O	-0.39420900	2.62493700	-1.15028200
H	-0.01218600	3.44208400	-0.79513100
O	-2.42705000	0.91464800	-0.96057500

H	-2.32410400	1.78101000	-1.38939600
C	-2.52405400	-1.56142300	0.16632300
H	-2.58630300	-1.86337900	-0.88735600
H	-2.41425800	-2.46043800	0.77752200
O	-3.72630300	-0.92465700	0.59104600
H	-3.81636200	-0.11119200	0.06601800
O	-0.19085000	-1.64328900	0.39673500
C	2.98429400	-2.00762700	-1.30813800
H	3.68093100	-1.32911400	-0.82098300
H	3.02453000	-3.01332200	-0.88908700
H	3.12611400	-2.00882600	-2.38758500
O	1.63211900	-1.44593300	-1.08488400
H	0.96189400	-1.97827900	-1.56347700

Scan Point for comp3_1_beta_1.7Å

C	-0.23500000	1.58760500	-0.17491700
C	1.25172700	1.24624000	-0.00965700
C	1.58842500	0.05990800	0.90616600
C	-1.10790900	0.42398300	-0.66237100
C	1.08433500	-1.32268900	0.47881900
C	-1.30627100	-0.66096600	0.40976700
H	-0.63851000	1.94904900	0.78050400
H	1.66809500	1.04006600	-0.99844300
H	-0.66799700	-0.02902400	-1.56222400
H	2.68061100	-0.00954500	0.92808100
H	1.64291400	-2.14412900	0.92704900
H	-1.37778900	-0.21525000	1.40593900
O	1.08368800	0.31263800	2.21507000
H	1.67988100	-0.07859100	2.87192800
O	1.94896800	2.39956400	0.46760900
H	1.68481300	2.55788000	1.38932100
O	-0.37104000	2.61467100	-1.16569000
H	0.01598200	3.43259700	-0.81782600
O	-2.41344500	0.92184500	-0.97622400
H	-2.29883600	1.78149600	-1.41560100
C	-2.53977900	-1.54604300	0.17020600
H	-2.58561400	-1.85888600	-0.88105200
H	-2.44012400	-2.43857200	0.79245700
O	-3.74654300	-0.90298400	0.56974300
H	-3.82994400	-0.09674300	0.03274700
O	-0.20869000	-1.63069900	0.44712600
C	2.97536500	-2.03254600	-1.32147000
H	3.67396700	-1.35158100	-0.83931400

H	3.01426300	-3.03141300	-0.88471200
H	3.13972200	-2.05872400	-2.39842900
O	1.63295400	-1.46063700	-1.12429900
H	0.96608000	-2.01677900	-1.57635800

Scan Point for comp3_1_beta_1.8Å

C	-0.23319800	1.58532700	-0.17980400
C	1.25219800	1.24049300	-0.00839300
C	1.58243800	0.06205500	0.91993000
C	-1.10651100	0.41976700	-0.66338600
C	1.05817700	-1.31921400	0.52854000
C	-1.32244900	-0.65237500	0.41712600
H	-0.63905800	1.95505000	0.77136300
H	1.66947700	1.02223300	-0.99397200
H	-0.65904600	-0.04495000	-1.55332200
H	2.67326900	-0.02092400	0.93910700
H	1.62872700	-2.15333000	0.93406600
H	-1.40278100	-0.20015400	1.40947800
O	1.08348300	0.33610500	2.22814000
H	1.67746500	-0.05341900	2.88840600
O	1.95364800	2.39357500	0.46107400
H	1.68792000	2.56111200	1.38074100
O	-0.36343200	2.60416600	-1.17936700
H	0.00733700	3.42930100	-0.83117500
O	-2.40721300	0.91751800	-0.99400400
H	-2.28522800	1.77525500	-1.43550600
C	-2.54999300	-1.54332700	0.16978400
H	-2.58256500	-1.86371500	-0.87955800
H	-2.45505600	-2.43082600	0.79985300
O	-3.76158300	-0.89929800	0.55081500
H	-3.84347900	-0.09968200	0.00385600
O	-0.21953700	-1.62067000	0.47987100
C	2.99967300	-2.02879200	-1.32097200
H	3.68901000	-1.29228500	-0.91140500
H	3.07531200	-2.98133700	-0.79276200
H	3.16758200	-2.15816500	-2.39087200
O	1.65273700	-1.47544700	-1.16323100
H	1.00429500	-2.07535200	-1.58164300

Scan Point for comp3_1_beta_1.9Å

C	-0.23400700	1.58267900	-0.19328200
C	1.25020300	1.24003000	-0.00541400
C	1.57514900	0.07426100	0.94109800
C	-1.10393700	0.41056900	-0.66828800
C	1.03900300	-1.30813500	0.58647700
C	-1.33469700	-0.64401300	0.42599200
H	-0.64763300	1.96675600	0.74878900
H	1.67496200	1.00715700	-0.98416800
H	-0.64687500	-0.06865700	-1.54545400
H	2.66487000	-0.01766600	0.96080600
H	1.62152700	-2.15093700	0.95348800
H	-1.42393300	-0.18029600	1.41209500
O	1.07703200	0.37011400	2.24613600
H	1.67292100	-0.00660100	2.91243200
O	1.94870500	2.39763500	0.45528100
H	1.66958800	2.58233700	1.36771800
O	-0.35592400	2.58527700	-1.20980300
H	-0.00348600	3.42063300	-0.86739700
O	-2.40061000	0.90280800	-1.01911300
H	-2.27327700	1.75458700	-1.47083600
C	-2.55495300	-1.54408300	0.17648500
H	-2.57482900	-1.87714000	-0.86906700
H	-2.46300600	-2.42310600	0.81869300
O	-3.77179100	-0.89908200	0.53675500
H	-3.85453700	-0.11018600	-0.02537300
O	-0.22483600	-1.60832700	0.51660300
C	3.01791700	-2.04727800	-1.32711000
H	3.71206600	-1.30457300	-0.93597600
H	3.09177100	-2.98396600	-0.76935800
H	3.20177000	-2.21508200	-2.39000300
O	1.67960400	-1.48340200	-1.19366700
H	1.03259000	-2.09761200	-1.58966800

Scan Point for comp3_1_beta_2.0Å

C	-0.24307700	1.57742700	-0.21143500
C	1.23979200	1.24573300	0.01005500
C	1.55462100	0.09059800	0.97490000
C	-1.09780100	0.39036100	-0.68009100
C	1.02403000	-1.29579700	0.64149900
C	-1.34194800	-0.64560900	0.42843600
H	-0.67713400	1.97824600	0.71382500
H	1.68371300	1.00291200	-0.95738600
H	-0.62088500	-0.10238200	-1.53912500

H	2.64368000	-0.00073800	1.00871700
H	1.62198600	-2.14317000	0.96993400
H	-1.43559300	-0.17078800	1.40865200
O	1.03918500	0.39790700	2.27174600
H	1.63482500	0.04012600	2.94890300
O	1.92698700	2.40818700	0.47299100
H	1.61817000	2.61198200	1.37158000
O	-0.35140200	2.55703100	-1.25191900
H	-0.12191000	3.42677100	-0.89276900
O	-2.38963800	0.86782900	-1.06376900
H	-2.25481900	1.71590000	-1.52132500
C	-2.55696500	-1.55300200	0.18283700
H	-2.56807000	-1.90199200	-0.85744000
H	-2.46870700	-2.42132800	0.83991900
O	-3.77609200	-0.90246100	0.52361500
H	-3.85881100	-0.12656000	-0.05638300
O	-0.22458200	-1.60485100	0.53885000
C	3.06655300	-2.03915000	-1.33007800
H	3.76214100	-1.29683600	-0.93942300
H	3.13395000	-2.96890800	-0.75842700
H	3.27241200	-2.22628900	-2.38654800
O	1.73437900	-1.46824800	-1.22013100
H	1.09311800	-2.08347400	-1.62049800

Scan Point for comp3_1_beta_2.1Å

C	-0.20855400	1.56308400	-0.19021200
C	1.25728100	1.17999500	0.06433400
C	1.50792300	0.01301400	1.03360800
C	-1.09257900	0.41368300	-0.69294900
C	0.95192100	-1.35176500	0.66571700
C	-1.38332000	-0.63485500	0.39149100
H	-0.65054700	1.96858400	0.72985200
H	1.71616400	0.92473900	-0.89258900
H	-0.61973700	-0.07695800	-1.55512300
H	2.59173500	-0.10824000	1.11121300
H	1.53240400	-2.22813800	0.94548200
H	-1.47178500	-0.18044700	1.38139900
O	0.94554800	0.32395300	2.31037600
H	1.48119500	-0.08592400	3.00812800
O	1.96911600	2.31981800	0.54525000
H	1.64139300	2.53861000	1.43350600
O	-0.25717600	2.55658000	-1.22051600
H	0.11195600	3.38340000	-0.87475400

O	-2.36596200	0.93547100	-1.08064900
H	-2.20467500	1.77365000	-1.54661400
C	-2.61730800	-1.50563100	0.11337700
H	-2.62692400	-1.83038200	-0.93457500
H	-2.55764400	-2.39085400	0.75091400
O	-3.82171500	-0.83149200	0.45893900
H	-3.88521300	-0.04505600	-0.10898900
O	-0.28828900	-1.62657600	0.49283100
C	3.17365400	-1.85103500	-1.33622500
H	3.73926100	-0.96307000	-1.05335200
H	3.40246000	-2.67960800	-0.65917100
H	3.41401400	-2.12983300	-2.36558100
O	1.76924100	-1.50097900	-1.26294100
H	1.24571500	-2.24362000	-1.61090300

Scan Point for comp3_1_beta_2.2Å

C	-0.21162500	1.55764900	-0.21735400
C	1.25000300	1.18659700	0.08003200
C	1.48145200	0.03902200	1.07803500
C	-1.08122100	0.39149600	-0.70787300
C	0.93638900	-1.33242400	0.72613500
C	-1.39105200	-0.63026800	0.39645500
H	-0.67518000	1.98689800	0.68079800
H	1.73258100	0.91284200	-0.85987600
H	-0.58790400	-0.11977000	-1.54623100
H	2.56304000	-0.07789000	1.18501300
H	1.53197100	-2.20669000	0.97911500
H	-1.48968300	-0.15681600	1.37629800
O	0.88523000	0.37016500	2.33487200
H	1.40631200	-0.02317200	3.05292200
O	1.94666200	2.33667000	0.55623800
H	1.59579300	2.57383600	1.43084700
O	-0.24023700	2.52133500	-1.27605600
H	0.07856900	3.37088900	-0.93600700
O	-2.34771700	0.89657400	-1.13609800
H	-2.17901200	1.72431700	-1.61816000
C	-2.61897100	-1.50956200	0.12024300
H	-2.61508300	-1.85497600	-0.92094500
H	-2.56570300	-2.38145300	0.77645100
O	-3.82746500	-0.82949000	0.43759900
H	-3.88829500	-0.05796000	-0.15074100
O	-0.29123000	-1.61699100	0.52829400
C	3.21997100	-1.86908900	-1.32891400

H	3.79251900	-0.98360000	-1.05050700
H	3.43414300	-2.68877300	-0.63552500
H	3.48007200	-2.16721900	-2.34876400
O	1.82231900	-1.50336100	-1.28033200
H	1.29569600	-2.25020900	-1.61137700

Scan Point for comp3_1_beta_2.3Å

C	-0.23888000	1.54954200	-0.21246600
C	1.21830400	1.18405400	0.11461900
C	1.43583700	0.03247400	1.11284300
C	-1.09350900	0.38205800	-0.72465800
C	0.91750500	-1.33980300	0.73147700
C	-1.40428200	-0.65207400	0.36759600
H	-0.72338900	1.97257600	0.67775200
H	1.72145300	0.91512000	-0.81580400
H	-0.58646800	-0.11828300	-1.56152800
H	2.51540800	-0.07298000	1.24746800
H	1.52914400	-2.21323400	0.94512500
H	-1.50112100	-0.19317800	1.35426300
O	0.80191000	0.34475800	2.35578600
H	1.31408600	-0.04207300	3.08389800
O	1.89935500	2.33542700	0.60851500
H	1.52650900	2.57457900	1.47349000
O	-0.24944000	2.51673400	-1.26759500
H	0.07602400	3.36156900	-0.92177400
O	-2.35953700	0.87933500	-1.16141500
H	-2.19409500	1.70760800	-1.64333700
C	-2.62701500	-1.53477500	0.08287400
H	-2.62226800	-1.87043300	-0.96129700
H	-2.57042300	-2.41210500	0.73152300
O	-3.83664600	-0.86044200	0.40737200
H	-3.90313900	-0.08672100	-0.17737700
O	-0.29339200	-1.63355600	0.48274900
C	3.36624700	-1.75372600	-1.27500300
H	3.87190600	-0.83768900	-0.96657000
H	3.58053800	-2.55628600	-0.56117800
H	3.71398000	-2.04458600	-2.27119900
O	1.95253100	-1.46344700	-1.31875100
H	1.48836500	-2.24085600	-1.67043700

Scan Point for comp3_1_beta_2.4Å

C	-0.23936000	1.54206100	-0.23355900
C	1.21109800	1.18309600	0.13112800
C	1.40200800	0.04976300	1.15778500
C	-1.08532100	0.36406400	-0.73810000
C	0.89868300	-1.32790300	0.78118200
C	-1.41478100	-0.65214900	0.36595900
H	-0.74176800	1.98406000	0.63682100
H	1.73373200	0.89423600	-0.78233600
H	-0.56475900	-0.15062700	-1.55774200
H	2.47693300	-0.05018800	1.32790700
H	1.52496500	-2.19700200	0.96960900
H	-1.52458500	-0.18020200	1.34492100
O	0.72793800	0.38474000	2.37345400
H	1.21542900	0.01058000	3.12466700
O	1.88378200	2.34024100	0.61973200
H	1.48619500	2.60237300	1.46686800
O	-0.22806400	2.48604300	-1.30966400
H	0.01343600	3.35780400	-0.96283300
O	-2.34374200	0.85313000	-1.20373400
H	-2.16899900	1.67652700	-1.69124900
C	-2.63176000	-1.54028500	0.07506800
H	-2.61279800	-1.88795200	-0.96490500
H	-2.58344500	-2.40967800	0.73499300
O	-3.84534300	-0.86212500	0.37550900
H	-3.90498000	-0.09588300	-0.21982200
O	-0.30072800	-1.62977800	0.50686400
C	3.42932800	-1.74561400	-1.24883000
H	3.91992500	-0.82706900	-0.92271700
H	3.62808500	-2.54656800	-0.52816600
H	3.81641100	-2.03404000	-2.23166300
O	2.01838900	-1.46405200	-1.33724300
H	1.56901200	-2.25016000	-1.68749100

Scan Point for comp3_1_beta_2.5Å

C	-0.27342000	1.53709700	-0.27987800
C	1.17997800	1.22404500	0.11665400
C	1.36775500	0.14346800	1.20130600
C	-1.08707500	0.32340700	-0.75407500
C	0.91621900	-1.25864600	0.85573600
C	-1.40686500	-0.66733400	0.37639400
H	-0.79708000	1.99646300	0.56828100
H	1.72147600	0.90008300	-0.77377800

H	-0.54668000	-0.20375500	-1.55286400
H	2.43809600	0.08207200	1.41288300
H	1.57681400	-2.10263400	1.04206600
H	-1.54545800	-0.17034300	1.33896100
O	0.64010400	0.51535500	2.37350300
H	1.08737600	0.15720800	3.15680600
O	1.82503900	2.41316900	0.56119900
H	1.40299900	2.71395000	1.38324300
O	-0.26893800	2.44460100	-1.38648800
H	-0.08615500	3.33841500	-1.06055300
O	-2.35174400	0.76856500	-1.24503000
H	-2.19145900	1.58111800	-1.75534900
C	-2.59192600	-1.59929000	0.09271100
H	-2.54839100	-1.97303900	-0.93740600
H	-2.52795800	-2.44887900	0.77665300
O	-3.82798300	-0.94810900	0.35924700
H	-3.89995000	-0.19801900	-0.25494900
O	-0.26347700	-1.60531000	0.56199300
C	3.50640800	-1.83544900	-1.18089600
H	4.04744400	-0.95777200	-0.82261600
H	3.61945600	-2.65534000	-0.46254200
H	3.91755700	-2.14130300	-2.14913800
O	2.12585600	-1.45259400	-1.32352100
H	1.63461700	-2.20742300	-1.68463400

Scan Point for comp3_1_beta_2.6Å

C	-0.28836400	1.53032800	-0.30194400
C	1.16205600	1.23017500	0.11676100
C	1.33501900	0.18207100	1.23658900
C	-1.09259600	0.30454900	-0.76218300
C	0.90026600	-1.22895100	0.91121600
C	-1.42046400	-0.67019600	0.38003300
H	-0.82268200	2.00370600	0.53156000
H	1.71351400	0.87950400	-0.75770900
H	-0.54198200	-0.23372900	-1.54683200
H	2.40152800	0.13213400	1.46956100
H	1.57448500	-2.06321100	1.09454900
H	-1.57926100	-0.15977100	1.33238900
O	0.58290100	0.58144500	2.38286700
H	1.01549800	0.24414600	3.18362700
O	1.80201500	2.43111800	0.53395400
H	1.36913500	2.75731800	1.34059100
O	-0.27444700	2.41637400	-1.42530000

H	-0.10226500	3.31739400	-1.11355800
O	-2.35488500	0.73481500	-1.27138500
H	-2.19437100	1.53577900	-1.79952200
C	-2.58754000	-1.62307100	0.09156300
H	-2.51756400	-2.01607700	-0.92999800
H	-2.52643000	-2.45806700	0.79356900
O	-3.83678200	-0.98346900	0.32000000
H	-3.90652500	-0.24709200	-0.31084300
O	-0.26673600	-1.59156100	0.59653600
C	3.59491300	-1.82761500	-1.14597700
H	4.10699100	-0.93638300	-0.77802300
H	3.71260800	-2.64177600	-0.42164200
H	4.03866300	-2.12707600	-2.10220600
O	2.21015000	-1.47844200	-1.32081400
H	1.74118300	-2.25277600	-1.66872400

Scan Point for comp3_1_beta_2.7Å

C	-0.30856600	1.52154200	-0.36191200
C	1.13693900	1.27064800	0.10761000
C	1.29717500	0.27620700	1.27822100
C	-1.08851200	0.26328100	-0.77527000
C	0.90842700	-1.15516800	0.98529900
C	-1.41553500	-0.67101200	0.40062400
H	-0.86887500	2.03209100	0.43176000
H	1.71922100	0.89353100	-0.73562400
H	-0.51951200	-0.29964900	-1.52912600
H	2.35639600	0.26105200	1.54660900
H	1.61259500	-1.96405200	1.17274800
H	-1.59665900	-0.12861100	1.33087100
O	0.49954100	0.70821700	2.37952100
H	0.91459800	0.42088000	3.20854800
O	1.74008500	2.50181900	0.48763700
H	1.28401500	2.85093400	1.27190900
O	-0.27956000	2.34152600	-1.53411400
H	-0.09262000	3.25666000	-1.27696400
O	-2.35046300	0.65111200	-1.31769100
H	-2.19288400	1.41393800	-1.89998700
C	-2.55592100	-1.66170200	0.13334900
H	-2.45519000	-2.09994300	-0.86705200
H	-2.49252900	-2.46152500	0.87516600
O	-3.82264000	-1.04020900	0.30632200
H	-3.89732800	-0.33854800	-0.36223400
O	-0.24077300	-1.55764400	0.66056500

C	3.64962100	-1.90613500	-1.07720600
H	4.18058300	-1.02978300	-0.69965500
H	3.70934100	-2.71337100	-0.33798300
H	4.12126000	-2.23564000	-2.01030100
O	2.28834800	-1.50653200	-1.30868400
H	1.79951100	-2.27023700	-1.65142600

Scan Point for comp3_1_beta_2.8Å

C	-0.31618600	1.51447200	-0.37289600
C	1.12413100	1.27071400	0.11900800
C	1.26391600	0.29070800	1.30630200
C	-1.09456100	0.25284400	-0.78085400
C	0.89531600	-1.14284100	1.00310300
C	-1.42595000	-0.67736500	0.39729200
H	-0.88577600	2.03526500	0.40737000
H	1.71887600	0.88126900	-0.71026400
H	-0.52239700	-0.31403000	-1.52928400
H	2.31701200	0.28491300	1.59824600
H	1.61411000	-1.94443200	1.16848900
H	-1.61382500	-0.13320500	1.32494000
O	0.43921900	0.73061300	2.38290400
H	0.83612900	0.45291400	3.22402300
O	1.72175400	2.50596800	0.49170300
H	1.25352000	2.86664300	1.26348400
O	-0.27219500	2.31862100	-1.55535300
H	-0.09752900	3.23882200	-1.30817900
O	-2.35392200	0.63788700	-1.33044200
H	-2.19073100	1.38536100	-1.93074700
C	-2.55727500	-1.67725800	0.12640800
H	-2.44293800	-2.12312900	-0.86916300
H	-2.49698700	-2.47049200	0.87559400
O	-3.82921100	-1.06203900	0.28059800
H	-3.90217000	-0.36831400	-0.39634100
O	-0.24373400	-1.55553700	0.66103900
C	3.71386400	-1.88381000	-1.01221400
H	4.21896200	-0.99948300	-0.61767000
H	3.71980500	-2.67335900	-0.25147200
H	4.25221600	-2.23526100	-1.90028100
O	2.37428600	-1.48929400	-1.34904900
H	1.91262900	-2.25802200	-1.71683700

Scan Point for comp3_1_beta_2.9Å

C	-0.37451200	1.50949500	-0.39598100
C	1.06549400	1.31490300	0.11973400
C	1.20984200	0.36130300	1.32970000
C	-1.10968700	0.21877700	-0.79367100
C	0.90624000	-1.08611700	1.02528600
C	-1.42104500	-0.70925500	0.39222200
H	-0.96926000	2.02600900	0.36821100
H	1.68130600	0.92292200	-0.69343200
H	-0.51223400	-0.33838600	-1.52970400
H	2.25479400	0.39911300	1.64765200
H	1.66191800	-1.85548500	1.18018300
H	-1.63128500	-0.16341100	1.31369900
O	0.34130700	0.78552600	2.37604500
H	0.72403100	0.53039700	3.23078200
O	1.62741000	2.57161600	0.47209400
H	1.13353400	2.94385100	1.22187200
O	-0.33727000	2.29466000	-1.59096300
H	-0.18309200	3.22221000	-1.35775900
O	-2.37609200	0.55518000	-1.35799200
H	-2.23130800	1.28915900	-1.97894600
C	-2.51599200	-1.74891000	0.12274600
H	-2.38188600	-2.19769900	-0.86892700
H	-2.43301300	-2.53465500	0.87764400
O	-3.80845200	-1.17531800	0.26617600
H	-3.90459000	-0.49534900	-0.42159500
O	-0.20909300	-1.54464800	0.66724800
C	3.86889600	-1.84711200	-0.93044200
H	4.35162000	-0.95408000	-0.52699200
H	3.84081500	-2.62267400	-0.15559100
H	4.45106500	-2.21254900	-1.78471300
O	2.54612100	-1.46187600	-1.33683100
H	2.10071700	-2.23901600	-1.70617000

Scan Point for comp3_1_beta_3.0Å

C	-0.47279900	1.49490700	-0.48336100
C	0.96629800	1.43379200	0.06607900
C	1.13694600	0.59249700	1.35459300
C	-1.11015600	0.13243600	-0.80627700
C	0.96388900	-0.88849500	1.13089800
C	-1.37155800	-0.74656300	0.42892700
H	-1.11647300	2.01869100	0.23459700

H	1.62021700	1.01312800	-0.70278500
H	-0.46169800	-0.42193600	-1.50021700
H	2.16206900	0.73848300	1.70477900
H	1.78152400	-1.57992000	1.33297900
H	-1.64813600	-0.16715700	1.31128400
O	0.19500300	1.01572000	2.33323200
H	0.54225600	0.81081400	3.21617400
O	1.44824900	2.74696200	0.31234000
H	0.90100400	3.16977400	0.99497600
O	-0.46408500	2.19891700	-1.72836300
H	-0.35542900	3.14636400	-1.55663300
O	-2.38937400	0.33927900	-1.40114600
H	-2.28423000	1.01315200	-2.09351100
C	-2.36642000	-1.89094100	0.20276100
H	-2.17059100	-2.38593900	-0.75605800
H	-2.23695100	-2.61988600	1.00644600
O	-3.70668900	-1.42398500	0.28487500
H	-3.84389500	-0.79784800	-0.44570100
O	-0.09866300	-1.45850100	0.77529500
C	4.00289900	-1.91990000	-0.83420000
H	4.49475000	-1.02706900	-0.44131500
H	3.96885000	-2.68602300	-0.05008700
H	4.58172200	-2.30097100	-1.68408300
O	2.68359000	-1.52647900	-1.24304500
H	2.22616500	-2.30537100	-1.59287500

Scan Point for comp3_1_beta_3.1Å

C	-0.51925000	1.48877200	-0.45913600
C	0.91766500	1.42285300	0.09621100
C	1.08097000	0.56167700	1.37343100
C	-1.15169900	0.13223900	-0.81504200
C	0.92548300	-0.91428300	1.11386000
C	-1.40679100	-0.78209900	0.39522000
H	-1.16777500	1.99518400	0.26677400
H	1.57696900	1.01560000	-0.67527100
H	-0.50364000	-0.40061500	-1.52595600
H	2.10081500	0.70989500	1.73786600
H	1.75105900	-1.60166200	1.29862500
H	-1.69496900	-0.22970000	1.29096800
O	0.12396800	0.95893700	2.34757600
H	0.46284100	0.74018800	3.23038100
O	1.39512100	2.73298900	0.36518500
H	0.84247500	3.14588700	1.04968000

O	-0.50800600	2.21842300	-1.68916100
H	-0.40087400	3.16222000	-1.49759800
O	-2.43426800	0.35045000	-1.39871200
H	-2.33339500	1.03851400	-2.07758100
C	-2.38342200	-1.93493900	0.13335700
H	-2.17535800	-2.40026900	-0.83766400
H	-2.24593000	-2.68342800	0.91752100
O	-3.73122300	-1.49183400	0.22130900
H	-3.87788600	-0.85442800	-0.49751100
O	-0.12498100	-1.48617700	0.72819700
C	4.24946600	-1.78253500	-0.81716800
H	4.72067100	-0.88963300	-0.39963400
H	4.23731300	-2.57137100	-0.05529300
H	4.83394900	-2.12332900	-1.68019900
O	2.91846600	-1.41017500	-1.20823200
H	2.48657700	-2.18408000	-1.59880400

Scan Point for comp3_1_beta_3.2Å

C	-0.53915900	1.47587000	-0.48464300
C	0.88930300	1.43797100	0.09462800
C	1.04226100	0.60307700	1.39043400
C	-1.14954900	0.10522000	-0.82461100
C	0.90848100	-0.87931600	1.15667300
C	-1.41330400	-0.78907900	0.39870400
H	-1.20529000	1.98792900	0.22108200
H	1.56575400	1.02433800	-0.65839300
H	-0.48373200	-0.43303700	-1.51474500
H	2.05428000	0.77055000	1.76810600
H	1.73903000	-1.55301700	1.36765400
H	-1.72242000	-0.22336600	1.27903000
O	0.06506300	1.00696200	2.34153700
H	0.39226300	0.80905300	3.23361500
O	1.34672400	2.75868000	0.34617400
H	0.77825100	3.17760000	1.01384200
O	-0.51676100	2.18225900	-1.72801700
H	-0.42387100	3.13073300	-1.55280600
O	-2.42498300	0.29663100	-1.43279800
H	-2.32133400	0.97292700	-2.12297700
C	-2.37188900	-1.95842700	0.14342700
H	-2.14268600	-2.43951100	-0.81507600
H	-2.23824000	-2.69020900	0.94385700
O	-3.72607000	-1.53010200	0.20141600
H	-3.86862500	-0.90824700	-0.53171000

O	-0.12881200	-1.47112500	0.76543500
C	4.33856200	-1.75984900	-0.77849400
H	4.79260700	-0.85338400	-0.37130600
H	4.32360400	-2.53380000	-0.00155200
H	4.94057500	-2.11032800	-1.62544300
O	3.00963800	-1.41122400	-1.19751700
H	2.59320700	-2.19768100	-1.57971000

Scan Point for comp3_1_beta_3.3Å

C	-0.44217300	1.40840900	-0.69241300
C	0.93283800	1.51208200	0.00050700
C	0.97222600	0.91343800	1.43263300
C	-1.00679800	-0.01515900	-0.84109400
C	0.90425200	-0.59013100	1.40774000
C	-1.35507600	-0.69766400	0.49293800
H	-1.17235000	2.01500600	-0.14236200
H	1.67829000	0.99449800	-0.61030200
H	-0.28303000	-0.64511300	-1.37790000
H	1.93810700	1.17673100	1.87218300
H	1.75645100	-1.19081600	1.73178400
H	-1.73475300	-0.00146000	1.24156400
O	-0.10262500	1.44307500	2.19476900
H	0.10302700	1.35618200	3.13955400
O	1.34775000	2.86775800	0.05873600
H	0.73296600	3.36959600	0.61982700
O	-0.32296800	1.89482100	-2.03134200
H	-0.24226000	2.86027900	-2.00910100
O	-2.23322700	0.04080900	-1.56720900
H	-2.09427300	0.62048600	-2.33497200
C	-2.27636900	-1.91735000	0.37095900
H	-1.97406900	-2.54457700	-0.47637200
H	-2.18842000	-2.50231600	1.28974100
O	-3.63673700	-1.51828900	0.26612500
H	-3.73360400	-1.01958000	-0.56229900
O	-0.08532800	-1.27442200	1.04698200
C	4.01531400	-2.08066100	-0.59423300
H	4.39233500	-1.16613800	-0.13021000
H	3.99265500	-2.87898000	0.15759500
H	4.69040400	-2.37021000	-1.40869500
O	2.69936900	-1.78893300	-1.08834200
H	2.34337000	-2.58992600	-1.50000900

Scan Point for comp3_1_beta_3.5Å

C	-0.50260500	1.36261000	-0.75093300
C	0.83939800	1.56686800	-0.01683600
C	0.85565400	1.03604900	1.44224400
C	-0.99090000	-0.09299000	-0.85214100
C	0.86251600	-0.46863500	1.48540500
C	-1.35385000	-0.73152500	0.49964000
H	-1.28129300	1.95559400	-0.25526200
H	1.63119000	1.06073600	-0.57682700
H	-0.21794300	-0.70898600	-1.33373800
H	1.79071200	1.36751100	1.90186300
H	1.73069600	-1.01017000	1.86630100
H	-1.79433700	-0.02246200	1.20141800
O	-0.27106400	1.54426900	2.14146400
H	-0.09603600	1.51060700	3.09576400
O	1.18496100	2.94306100	-0.00788900
H	0.52616500	3.43785300	0.50766000
O	-0.35845800	1.79367000	-2.10626700
H	-0.32569000	2.76198900	-2.12643000
O	-2.19120000	-0.13205100	-1.62173000
H	-2.05284600	0.41873200	-2.41058400
C	-2.20916000	-2.00055400	0.40333600
H	-1.84573200	-2.64911700	-0.40292400
H	-2.12622600	-2.53840700	1.35092200
O	-3.58272000	-1.67600600	0.23348500
H	-3.67364000	-1.22069400	-0.62021400
O	-0.07845600	-1.21770900	1.12329500
C	4.23173300	-1.96196100	-0.48060300
H	4.54616100	-1.00944400	-0.04740300
H	4.22080900	-2.72559100	0.30668900
H	4.94958800	-2.25340500	-1.25693200
O	2.92201600	-1.75999700	-1.03269800
H	2.62106600	-2.59580900	-1.41824700

Scan Point for comp3_1_beta_3.6Å

C	-0.46264300	1.38967600	-0.69615800
C	0.89761800	1.48418800	0.02758600
C	0.89866200	0.88944900	1.46244900
C	-1.03736900	-0.02918900	-0.85420600
C	0.83142900	-0.61319600	1.42927800
C	-1.41048800	-0.71352100	0.47198800

H	-1.19933300	2.00473300	-0.16454000
H	1.65217800	0.95834400	-0.56535600
H	-0.31048800	-0.66358300	-1.38154700
H	1.85389400	1.15106600	1.92579500
H	1.67993000	-1.21634000	1.75917100
H	-1.79989800	-0.01880000	1.21687800
O	-0.19337200	1.42227300	2.19613700
H	-0.01202900	1.33506800	3.14591500
O	1.32292600	2.83606400	0.08998600
H	0.69784300	3.34686100	0.63128000
O	-0.30786100	1.87011400	-2.03358900
H	-0.21495900	2.83456800	-2.01270900
O	-2.25220900	0.03769800	-1.59825900
H	-2.09092600	0.59850500	-2.37544500
C	-2.33197100	-1.93082400	0.33087900
H	-2.01634500	-2.55636000	-0.51282200
H	-2.26134500	-2.51861400	1.24932200
O	-3.68934700	-1.52826000	0.20377100
H	-3.77175800	-1.03035800	-0.62666000
O	-0.14965000	-1.29544100	1.04320000
C	4.21094500	-1.85850200	-0.43856100
H	4.33071200	-0.88576900	0.04441500
H	4.17320700	-2.63844100	0.33184000
H	5.07368100	-2.03960400	-1.09099300
O	2.99024300	-1.80660200	-1.19279700
H	2.87269300	-2.65653200	-1.64166900

Scan Point for comp3_1_beta_3.7Å

C	-0.48711300	1.38706100	-0.68799200
C	0.87186100	1.48256300	0.03809700
C	0.87187000	0.87810000	1.46926600
C	-1.05557300	-0.03300900	-0.85813000
C	0.81569200	-0.62441100	1.42254900
C	-1.42434000	-0.73205500	0.46156300
H	-1.22708300	1.99443600	-0.15214900
H	1.62981700	0.96360800	-0.55666700
H	-0.32678000	-0.65897000	-1.39275300
H	1.82383900	1.14249700	1.93778000
H	1.66986000	-1.22414600	1.74467200
H	-1.81965200	-0.04706600	1.21238500
O	-0.22599400	1.39849900	2.20286000
H	-0.04755200	1.30492700	3.15259500
O	1.29111800	2.83568100	0.11043000

H	0.66299900	3.33965400	0.65462000
O	-0.33355000	1.87904200	-2.02139000
H	-0.24572000	2.84379600	-1.99267200
O	-2.27195900	0.03535300	-1.59958600
H	-2.11565800	0.60645500	-2.37022900
C	-2.33682900	-1.95461100	0.30765400
H	-2.01674100	-2.56862600	-0.54286600
H	-2.26181900	-2.55189900	1.21958600
O	-3.69713200	-1.56066000	0.18492300
H	-3.78328600	-1.05464100	-0.64021100
O	-0.15962100	-1.31018900	1.02821200
C	4.29707600	-1.77908300	-0.39509400
H	4.33236400	-0.81598700	0.11963300
H	4.25161600	-2.58132800	0.35169500
H	5.21079700	-1.89431400	-0.99054500
O	3.12845500	-1.77031400	-1.22848900
H	3.09661600	-2.60503500	-1.71803500

Scan Point for comp3_1_beta_3.8Å

C	-0.50599800	1.38504800	-0.66966400
C	0.84861000	1.45804500	0.06743800
C	0.82955800	0.83343400	1.49012400
C	-1.08511500	-0.02748300	-0.86712900
C	0.76918300	-0.66741700	1.41763200
C	-1.46334200	-0.75080300	0.43666400
H	-1.24446300	1.98957400	-0.12861600
H	1.60699500	0.94068400	-0.52841600
H	-0.35998200	-0.64829600	-1.41273400
H	1.77732200	1.08697200	1.97301100
H	1.62045600	-1.27498900	1.73251700
H	-1.86257000	-0.08000300	1.19817200
O	-0.27411300	1.34771000	2.21909900
H	-0.10492300	1.24177600	3.16922800
O	1.27901500	2.80595900	0.16298800
H	0.64795600	3.30836800	0.70517700
O	-0.34001900	1.89775900	-1.99387100
H	-0.25304700	2.86202600	-1.94979500
O	-2.29965100	0.06490700	-1.60887600
H	-2.13607400	0.64553800	-2.37074000
C	-2.37702700	-1.96801100	0.25105900
H	-2.05506200	-2.56129900	-0.61340500
H	-2.30580400	-2.58794000	1.14803400
O	-3.73661600	-1.56981100	0.13373500

H	-3.82073800	-1.04725500	-0.68115700
O	-0.20396100	-1.34304300	1.00088700
C	4.47961100	-1.68326700	-0.38738500
H	4.47565000	-0.74204500	0.16760900
H	4.46613400	-2.51668700	0.32575200
H	5.39621600	-1.73713700	-0.98719000
O	3.30935300	-1.68542100	-1.21887500
H	3.30699300	-2.50103300	-1.74057100

Scan Point for comp3_1_beta_3.9Å

C	-0.46501800	1.37991700	-0.62874400
C	0.87094600	1.36290700	0.14620100
C	0.78317400	0.68668700	1.54275800
C	-1.11643700	0.00785500	-0.88418000
C	0.65110800	-0.80514300	1.41299800
C	-1.55910300	-0.74021200	0.38473500
H	-1.18455300	2.00823400	-0.08919400
H	1.62290100	0.83469500	-0.44818800
H	-0.41621000	-0.63307900	-1.43903300
H	1.72888200	0.87525700	2.05876900
H	1.46192000	-1.46624900	1.72540100
H	-1.93848100	-0.07691600	1.16270300
O	-0.31434400	1.22624500	2.26299700
H	-0.16867400	1.09099200	3.21324800
O	1.35665600	2.68503100	0.30568600
H	0.71833800	3.20145400	0.82534400
O	-0.23655100	1.91999100	-1.93302500
H	-0.13908500	2.88173200	-1.86597700
O	-2.30838700	0.19467500	-1.64426000
H	-2.08656200	0.76348300	-2.40032500
C	-2.52880400	-1.90121400	0.13492300
H	-2.21964300	-2.47442300	-0.74753300
H	-2.50501700	-2.55983700	1.00661300
O	-3.86514800	-1.43271700	0.01036100
H	-3.91336600	-0.88917900	-0.79338000
O	-0.34415400	-1.41588700	0.95102800
C	4.72626400	-1.60445800	-0.43432800
H	4.67422500	-0.85237200	0.35660500
H	4.86868700	-2.59262800	0.02027500
H	5.58106400	-1.37894200	-1.08333500
O	3.48891500	-1.53691400	-1.16019800
H	3.52690100	-2.17364700	-1.88888400

Scan Point for comp3_1_beta_4.0Å

C	-0.49724400	1.38159600	-0.61005700
C	0.83827300	1.35821000	0.16584200
C	0.75163000	0.65716700	1.55062200
C	-1.14231000	0.01138300	-0.89068900
C	0.63072200	-0.83223800	1.38983900
C	-1.58015700	-0.76160400	0.36500400
H	-1.22034900	1.99653900	-0.06007500
H	1.59365200	0.84363300	-0.43593900
H	-0.43941300	-0.61584300	-1.45787500
H	1.69521800	0.84204300	2.07190900
H	1.44810200	-1.49317500	1.68495100
H	-1.96127400	-0.11422300	1.15537600
O	-0.35055600	1.17778500	2.27712700
H	-0.21002000	1.02047000	3.22477900
O	1.31676900	2.67972300	0.34885900
H	0.67700300	3.18180000	0.88064400
O	-0.27112700	1.94605100	-1.90432900
H	-0.18427500	2.90753100	-1.82114600
O	-2.33584600	0.20670400	-1.64592300
H	-2.11999000	0.79951500	-2.38514700
C	-2.54486000	-1.92239400	0.09605800
H	-2.23591700	-2.47693600	-0.79821400
H	-2.51461900	-2.59762300	0.95478200
O	-3.88410200	-1.45865100	-0.01465600
H	-3.93933400	-0.90233300	-0.80906000
O	-0.36044500	-1.44086400	0.91635800
C	4.88277900	-1.53179300	-0.42936800
H	4.82697100	-0.78013100	0.36169900
H	5.02567900	-2.51985400	0.02533800
H	5.73913800	-1.30453100	-1.07573300
O	3.64753000	-1.46640500	-1.15902000
H	3.68864300	-2.10358900	-1.88712900

Scan Point for comp3_1_beta_4.1Å

C	-0.49929200	1.37803000	-0.59724700
C	0.83155900	1.33535400	0.18574300
C	0.73110800	0.61983900	1.56235900
C	-1.15425500	0.01646800	-0.89550900
C	0.59525300	-0.86640100	1.38573600

C	-1.60895200	-0.76285100	0.35029600
H	-1.22033400	1.99330400	-0.04499300
H	1.58655300	0.82152500	-0.41727200
H	-0.45267900	-0.61256000	-1.46241200
H	1.67392800	0.78944200	2.09015100
H	1.40413100	-1.53891700	1.67785900
H	-1.98760800	-0.11821300	1.14407600
O	-0.36949900	1.14404000	2.28868300
H	-0.23612700	0.97470500	3.23532100
O	1.31928100	2.65085100	0.38659000
H	0.68078500	3.15135700	0.92137200
O	-0.26132500	1.95401900	-1.88426500
H	-0.17469400	2.91468000	-1.79202400
O	-2.33935000	0.22966000	-1.65909800
H	-2.11248100	0.83211700	-2.38725600
C	-2.58511900	-1.91027200	0.06561700
H	-2.27662900	-2.46141700	-0.83086700
H	-2.56817300	-2.59235800	0.91933700
O	-3.91788900	-1.42965400	-0.05035600
H	-3.96170400	-0.86823300	-0.84184500
O	-0.40017400	-1.46012300	0.90239000
C	4.97569200	-1.48626100	-0.42074500
H	4.90436600	-0.73537500	0.36982300
H	5.11531200	-2.47387700	0.03596100
H	5.84141100	-1.25542900	-1.05326100
O	3.75197300	-1.42572000	-1.17009100
H	3.80384100	-2.06877100	-1.89229100

Scan Point for comp3_1_beta_4.2Å

C	-0.50318900	1.38050400	-0.56977100
C	0.82677800	1.30388500	0.21229700
C	0.71501000	0.56125800	1.57373800
C	-1.17229000	0.03323100	-0.89888300
C	0.55872500	-0.91904600	1.36812400
C	-1.64120300	-0.76577400	0.32907700
H	-1.21749300	1.99111600	-0.00409700
H	1.57576200	0.79348600	-0.40114200
H	-0.47533600	-0.59238100	-1.47536900
H	1.65900400	0.70775200	2.10614100
H	1.35703100	-1.60852600	1.64924200
H	-2.01494100	-0.13292700	1.13458900
O	-0.37993400	1.08615300	2.30817900
H	-0.25328100	0.89324500	3.25124500

O	1.33144300	2.60837000	0.44244900
H	0.70398200	3.10172200	0.99672000
O	-0.25804700	1.98261000	-1.84333200
H	-0.17614100	2.94166400	-1.73254800
O	-2.35120200	0.27507700	-1.66334200
H	-2.11555400	0.89629900	-2.37279100
C	-2.63110500	-1.89472400	0.01818700
H	-2.32702000	-2.43178200	-0.88819200
H	-2.62512800	-2.59383300	0.85823500
O	-3.95688600	-1.39406500	-0.09145700
H	-3.99155400	-0.81760300	-0.87248700
O	-0.44384600	-1.48946800	0.87155300
C	5.07930800	-1.43139000	-0.42842100
H	4.99681400	-0.68638100	0.36661600
H	5.22182400	-2.42107300	0.02289200
H	5.94846000	-1.19075100	-1.05255600
O	3.86101600	-1.37402000	-1.18684100
H	3.92102100	-2.01495300	-1.91025800

Scan Point for comp3_1_beta_4.3Å

C	-0.55788100	1.37487500	-0.59011600
C	0.77202200	1.34343200	0.19513400
C	0.67542900	0.61841000	1.56692000
C	-1.19228700	0.00652700	-0.90234900
C	0.56354700	-0.86794200	1.37796500
C	-1.63810400	-0.79161600	0.33480500
H	-1.28872400	1.97447400	-0.03365800
H	1.53455600	0.84265800	-0.40940100
H	-0.48021900	-0.60637800	-1.47387900
H	1.61303200	0.79823600	2.10069700
H	1.38276100	-1.52939800	1.66696600
H	-2.03027400	-0.16078600	1.13311300
O	-0.43636300	1.12314200	2.28956000
H	-0.30998100	0.94332000	3.23525600
O	1.24370700	2.66321500	0.40583900
H	0.60229900	3.15000900	0.94980300
O	-0.32582400	1.96604000	-1.87115700
H	-0.25385500	2.92697800	-1.76976800
O	-2.37924900	0.20908600	-1.66593400
H	-2.16085000	0.82232000	-2.38764000
C	-2.59319000	-1.95323100	0.03587400
H	-2.27120400	-2.49022800	-0.86438000
H	-2.56707600	-2.64293800	0.88321100

O	-3.93415400	-1.49630200	-0.08052600
H	-3.98543400	-0.92707500	-0.86595500
O	-0.41981700	-1.47374000	0.88505500
C	5.22233500	-1.40180900	-0.38979300
H	5.13298800	-0.65756300	0.40523700
H	5.36859300	-2.39079000	0.06183100
H	6.09242000	-1.15627900	-1.01076500
O	4.00647500	-1.35088200	-1.15244700
H	4.07154800	-1.99291600	-1.87443400

Scan Point for comp3_1_beta_4.4Å

C	-0.59252100	1.37202800	-0.59533300
C	0.73661000	1.35729700	0.19193800
C	0.64397600	0.63764500	1.56673300
C	-1.21039400	-0.00464000	-0.90496400
C	0.55394600	-0.85059700	1.38137500
C	-1.64610300	-0.80763800	0.33269200
H	-1.33095200	1.96472900	-0.04156700
H	1.50495700	0.86109400	-0.40899300
H	-0.49066100	-0.60895800	-1.47602300
H	1.57688000	0.83236400	2.10350400
H	1.38229900	-1.49923700	1.67374800
H	-2.04901100	-0.18167800	1.12948900
O	-0.47710800	1.13090700	2.28256800
H	-0.35373700	0.95358300	3.22914200
O	1.19572900	2.68240700	0.39688800
H	0.55050300	3.16548800	0.93964300
O	-0.36496700	1.96211000	-1.87759800
H	-0.29858900	2.92360900	-1.77764100
O	-2.40020900	0.18164100	-1.66830500
H	-2.18863800	0.79039600	-2.39572000
C	-2.58305500	-1.98375900	0.03309400
H	-2.25120400	-2.51615800	-0.86631300
H	-2.54803200	-2.67257800	0.88080700
O	-3.93062800	-1.54755800	-0.08575500
H	-3.98870600	-0.97775900	-0.87032100
O	-0.41883700	-1.47134300	0.88603800
C	5.34097400	-1.36837200	-0.36625500
H	5.24056800	-0.62769500	0.43078500
H	5.49076800	-2.35783600	0.08313500
H	6.21398100	-1.11460500	-0.97980700
O	4.13040600	-1.32336200	-1.13763200
H	4.20387400	-1.96495300	-1.85918200

Scan Point for comp3_1_beta_4.5Å

C	-0.63552600	1.37139300	-0.59546800
C	0.69551200	1.37321400	0.18893400
C	0.61316400	0.65303000	1.56393600
C	-1.23354200	-0.01367500	-0.90741800
C	0.54930400	-0.83620900	1.37579000
C	-1.65181000	-0.82878400	0.32847900
H	-1.38119500	1.95189700	-0.03862800
H	1.46861600	0.88609900	-0.41325800
H	-0.50659500	-0.60403900	-1.48387900
H	1.54201800	0.86324200	2.10178200
H	1.38960700	-1.47050800	1.66583800
H	-2.06441600	-0.21264300	1.12797500
O	-0.51634200	1.12858900	2.27805500
H	-0.39238700	0.95120100	3.22453700
O	1.13954800	2.70373700	0.39246300
H	0.49291300	3.17830700	0.94106700
O	-0.41908800	1.96753200	-1.87672300
H	-0.36089400	2.92923500	-1.77364200
O	-2.42944100	0.15639300	-1.66503100
H	-2.23032600	0.76783700	-2.39361700
C	-2.56868900	-2.01997400	0.02678900
H	-2.22964400	-2.54330000	-0.87525000
H	-2.52013600	-2.71120500	0.87186100
O	-3.92373900	-1.60628500	-0.08739100
H	-3.99231500	-1.03190100	-0.86780600
O	-0.41199800	-1.47254200	0.87774000
C	5.47511700	-1.32766200	-0.34908000
H	5.37002900	-0.58885900	0.44910200
H	5.62931800	-2.31708700	0.09888500
H	6.34763000	-1.06845300	-0.96109900
O	4.26527700	-1.28747000	-1.12178100
H	4.34286000	-1.92745400	-1.84430200

<u>Oxocarbenium Compound 3, Conformer 3</u>

Scan Point for comp3_3_alpha_1.4Å

C	-1.12899300	1.43566900	0.14845200
C	0.20964800	1.73556500	-0.54696900

C	1.40722200	0.95607800	0.01133600
C	-1.68713000	0.01868400	-0.03628900
C	1.47762700	-0.44920300	-0.62715100
C	-0.69557700	-1.09896000	0.34717300
H	-1.01619700	1.62579100	1.22241800
H	0.11728800	1.51582100	-1.62014900
H	-1.97178500	-0.11593700	-1.08565300
H	2.30358800	1.49311000	-0.31503600
H	1.85355800	-0.35901000	-1.65163900
H	-0.20982000	-0.88282500	1.30294500
O	1.35826500	0.91377800	1.43276800
H	2.25217200	1.01943300	1.78875000
O	0.52733300	3.12026900	-0.37165700
H	-0.28762200	3.62406200	-0.53317800
O	-2.05140100	2.38746500	-0.40395900
H	-2.84287200	2.40382000	0.15479400
O	-2.85322600	-0.03394200	0.79749900
H	-3.48655900	-0.65997800	0.41581400
C	-1.32777200	-2.47555500	0.45669000
H	-0.53387400	-3.21082700	0.63495700
H	-2.00643800	-2.48563500	1.31711500
O	-2.03606800	-2.77937000	-0.75158100
H	-2.41418900	-3.66690900	-0.66932800
O	0.30271000	-1.17623700	-0.71613500
O	2.37908000	-1.23560000	0.10014700
H	2.19289200	-2.18857500	-0.05674400
C	3.84473000	-0.95251400	-0.01002500
H	4.10801400	-0.95537300	-1.06739700
H	4.00793700	0.01168800	0.46410300
H	4.32184000	-1.75813600	0.54226500

Scan Point for comp3_3_alpha_1.5Å

C	-1.16236100	1.41661300	0.15163300
C	0.16777500	1.74810200	-0.54602500
C	1.38119400	0.98311900	0.00116800
C	-1.69184700	-0.01113300	-0.04031900
C	1.45244400	-0.41211200	-0.64558900
C	-0.68385000	-1.11062700	0.35318000
H	-1.05082600	1.60285300	1.22646800
H	0.07406200	1.53559600	-1.62065400
H	-1.96458600	-0.15041800	-1.09223100
H	2.26893700	1.52704400	-0.33721500
H	1.85706500	-0.34633400	-1.65843600

H	-0.20261900	-0.88292500	1.30813800
O	1.34548300	0.94321200	1.42156500
H	2.24501300	1.04089000	1.76622700
O	0.46307000	3.13514600	-0.35940500
H	-0.35938400	3.62783200	-0.51700600
O	-2.10464900	2.35161300	-0.39415500
H	-2.89813900	2.34374900	0.16196200
O	-2.86272900	-0.08844700	0.78379100
H	-3.48494200	-0.71855900	0.39061600
C	-1.28958900	-2.49868100	0.45986400
H	-0.48223600	-3.21929300	0.63728500
H	-1.96758700	-2.52189900	1.32040000
O	-1.99144500	-2.81273300	-0.74913600
H	-2.35311500	-3.70734700	-0.66939000
O	0.32283200	-1.17665200	-0.70728300
O	2.45342800	-1.21401200	0.13222100
H	2.29525400	-2.16351500	-0.06041900
C	3.89499200	-0.88412300	-0.02475500
H	4.13308800	-0.86235000	-1.08825900
H	4.04431300	0.07892200	0.45716500
H	4.42524300	-1.67620600	0.49962500

Scan Point for comp3_3_alpha_1.6Å

C	-1.20478200	1.38629600	0.16052700
C	0.10513100	1.76164200	-0.55369300
C	1.34682400	1.02676100	-0.02375600
C	-1.69532100	-0.05482000	-0.03834600
C	1.43167100	-0.36315600	-0.67291600
C	-0.65827600	-1.12748900	0.35176400
H	-1.08258500	1.56512500	1.23543800
H	0.00259800	1.55118200	-1.62793000
H	-1.96646400	-0.19712800	-1.09022700
H	2.21850900	1.58505100	-0.38015700
H	1.87528500	-0.32512200	-1.66898300
H	-0.17724600	-0.88802800	1.30353200
O	1.33204600	0.99537500	1.39573600
H	2.23813900	1.09140300	1.72371000
O	0.36439600	3.15420800	-0.36310000
H	-0.47274700	3.62583700	-0.50739600
O	-2.18220800	2.29717500	-0.36171500
H	-2.96896100	2.25329200	0.20262400
O	-2.85981600	-0.16966400	0.78898600
H	-3.46997300	-0.80815100	0.39044000

C	-1.22169000	-2.53287900	0.45405900
H	-0.39211900	-3.23045600	0.62055500
H	-1.89031900	-2.57991700	1.32085700
O	-1.92394500	-2.85972100	-0.75067700
H	-2.25484900	-3.76658300	-0.67539300
O	0.35058900	-1.16487700	-0.71336000
O	2.52711600	-1.16857500	0.17047000
H	2.39279900	-2.11529400	-0.04359000
C	3.94764400	-0.80412800	-0.01380200
H	4.17424000	-0.77384900	-1.08019000
H	4.08271600	0.16408100	0.46340500
H	4.51834900	-1.57616500	0.49957400

Scan Point for comp3_3_alpha_1.7Å

C	-1.24296300	1.36140900	0.16679700
C	0.05076800	1.77435200	-0.55551400
C	1.31282900	1.06075500	-0.03921400
C	-1.69724200	-0.09099900	-0.03823300
C	1.40877900	-0.32031900	-0.69872400
C	-0.63827100	-1.14097200	0.35347800
H	-1.11697700	1.53617100	1.24202700
H	-0.05658400	1.56958000	-1.63036400
H	-1.96340400	-0.23668100	-1.09089300
H	2.17200300	1.63258100	-0.40412900
H	1.88401100	-0.30241500	-1.67939000
H	-0.15848100	-0.89123900	1.30262500
O	1.30935800	1.02830200	1.37862500
H	2.22074300	1.10728100	1.69632200
O	0.28302600	3.16943800	-0.35546600
H	-0.56092600	3.62841400	-0.49986700
O	-2.24948900	2.24678000	-0.34156800
H	-3.04211100	2.14672400	0.20793900
O	-2.85807100	-0.23639900	0.78771000
H	-3.45455700	-0.88524400	0.38514300
C	-1.16686300	-2.55941700	0.45067800
H	-0.31960900	-3.23770300	0.60721200
H	-1.82638100	-2.62532100	1.32320200
O	-1.87067400	-2.89567400	-0.74986500
H	-2.17322700	-3.81283800	-0.67986900
O	0.37583500	-1.15580800	-0.71368300
O	2.60519600	-1.13082000	0.19663800
H	2.49580200	-2.07238000	-0.04552600
C	4.00355200	-0.72636300	-0.01060100

H	4.21619200	-0.67693100	-1.07981700
H	4.12169900	0.24253200	0.47136400
H	4.61683100	-1.47975600	0.48289200

Scan Point for comp3_3_alpha_1.8Å

C	-1.28302600	1.34542100	0.15788000
C	0.01755600	1.78964800	-0.53200200
C	1.27670300	1.07765900	-0.00580000
C	-1.69819200	-0.11775600	-0.06022600
C	1.38490500	-0.28140700	-0.69662300
C	-0.63449500	-1.14928000	0.37056900
H	-1.18935400	1.52257400	1.23601300
H	-0.06897200	1.60217100	-1.61192800
H	-1.92492700	-0.26969300	-1.12122400
H	2.14012000	1.66142700	-0.34072800
H	1.87561300	-0.26673300	-1.66874300
H	-0.17603500	-0.88162800	1.32415300
O	1.23414600	1.01549700	1.40851900
H	2.13501700	0.90933500	1.74841400
O	0.22940400	3.18278700	-0.30392900
H	-0.60967900	3.63834700	-0.48288200
O	-2.29469100	2.20659000	-0.37892500
H	-3.10685300	2.07258700	0.13377400
O	-2.88188100	-0.28711300	0.72543800
H	-3.44844000	-0.95114500	0.30468000
C	-1.14142700	-2.57446300	0.46444500
H	-0.28608900	-3.23907300	0.63518700
H	-1.81012400	-2.64514800	1.32959100
O	-1.82507100	-2.92533400	-0.74287900
H	-2.11712000	-3.84585500	-0.67167400
O	0.40970000	-1.16003400	-0.67560600
O	2.71886900	-1.07250800	0.21699700
H	2.61540200	-2.01744900	-0.00891800
C	4.08549900	-0.64518000	-0.09158600
H	4.26367200	-0.70859300	-1.16683700
H	4.18260000	0.37868800	0.26629100
H	4.75622200	-1.30673200	0.45797300

Scan Point for comp3_3_alpha_1.9Å

C	-1.31303200	1.32977000	0.15889000

C	-0.02072100	1.80455600	-0.52382300
C	1.24596600	1.09589900	-0.01296000
C	-1.69978200	-0.13985600	-0.06922100
C	1.35930200	-0.25243400	-0.71075800
C	-0.63155500	-1.16056900	0.37772000
H	-1.22902800	1.50451300	1.23840400
H	-0.10729900	1.63407300	-1.60653800
H	-1.91292900	-0.29375900	-1.13304500
H	2.10810800	1.68367500	-0.34648500
H	1.88636200	-0.26533900	-1.66314000
H	-0.18594500	-0.88509500	1.33498900
O	1.20705200	1.01831900	1.39900200
H	2.07845600	0.73532400	1.71715600
O	0.17476600	3.19572400	-0.27183300
H	-0.66012100	3.64977700	-0.47285100
O	-2.34075600	2.17084000	-0.37946200
H	-3.15070200	2.01706300	0.13151000
O	-2.88803600	-0.33059200	0.70379300
H	-3.44345400	-0.99731300	0.27278600
C	-1.12117300	-2.59252100	0.46063800
H	-0.25770200	-3.24688500	0.62953800
H	-1.79011100	-2.67643200	1.32456300
O	-1.79669000	-2.94608500	-0.75012700
H	-2.07613700	-3.87095300	-0.68552800
O	0.43506800	-1.16493800	-0.65299500
O	2.80883300	-0.98951300	0.27187800
H	2.69233100	-1.95033100	0.14378500
C	4.15310600	-0.60647200	-0.14153900
H	4.29012700	-0.79821700	-1.20844800
H	4.26448900	0.45382000	0.07895200
H	4.85899100	-1.19420200	0.44861200

Scan Point for comp3_3_alpha_2.0Å

C	-0.03131800	1.81067700	-0.51831600
C	1.23545400	1.09035700	-0.02207900
C	-1.70795100	-0.14129900	-0.08003300
C	1.32702800	-0.25219400	-0.72887100
C	-0.64556000	-1.16161200	0.38660200
H	-1.24174000	1.49406700	1.24052300
H	-0.12162700	1.65808400	-1.60348000
H	-1.89888700	-0.29345800	-1.14796500
H	2.09941100	1.67178800	-0.36197800
H	1.87786200	-0.29246400	-1.66635400

H	-0.20132800	-0.87948400	1.34187100
O	1.20640000	1.00469000	1.38976700
H	2.06891700	0.68399300	1.69671800
O	0.17055800	3.19544600	-0.24318000
H	-0.66757600	3.65347200	-0.42015400
O	-2.34893100	2.17442600	-0.37538300
H	-3.16130800	2.02365800	0.13223100
O	-2.90759200	-0.33779700	0.67037200
H	-3.44965900	-1.01016300	0.23063900
C	-1.13477800	-2.59189100	0.47162600
H	-0.27310800	-3.24670200	0.64819100
H	-1.80790100	-2.66974600	1.33264300
O	-1.80487300	-2.94504100	-0.74108100
H	-2.08362600	-3.87034700	-0.67769700
O	0.43285200	-1.17523300	-0.63977600
O	2.88102300	-0.97863500	0.29942000
H	2.77324000	-1.94078200	0.19225300
C	4.19893400	-0.58748700	-0.16995200
H	4.31002200	-0.80866100	-1.23471900
H	4.29423700	0.48288000	0.01187500
H	4.94553700	-1.13241200	0.41255100

Scan Point for comp3_3_alpha_2.1Å

C	1.41213700	-1.26669900	0.15193000
C	0.14011300	-1.82532700	-0.50701900
C	-1.16134200	-1.16607600	-0.01633900
C	1.70714500	0.22328100	-0.09795700
C	-1.31745600	0.16837400	-0.71883300
C	0.60298900	1.18275100	0.40145400
H	1.35430300	-1.43132000	1.23474400
H	0.21471600	-1.68347900	-1.59501300
H	1.86121600	0.38663200	-1.17011000
H	-1.99376100	-1.78962000	-0.35998800
H	-1.90778800	0.21214300	-1.63152600
H	0.19267100	0.86952800	1.36207300
O	-1.14802200	-1.06821000	1.39473400
H	-2.00585700	-0.70461200	1.67122300
O	0.01140000	-3.21369400	-0.21044800
H	0.86526300	-3.63407900	-0.40410700
O	2.47360300	-2.05448100	-0.39677600
H	3.28383200	-1.86094400	0.09940000
O	2.91076200	0.48753600	0.62318000
H	3.40984400	1.18058500	0.16520300
C	1.01387200	2.63700000	0.48317300

H	0.12237100	3.24293400	0.68498900
H	1.70243700	2.74538200	1.32853900
O	1.63344800	3.03122200	-0.74290600
H	1.87309000	3.96725100	-0.67640300
O	-0.50183900	1.14740800	-0.60298900
O	-3.01059200	0.73639500	0.38599400
H	-2.87716400	1.68878900	0.53324700
C	-4.27778600	0.52787700	-0.28463900
H	-4.31354000	1.08105200	-1.22711900
H	-4.36578100	-0.54323200	-0.46886200
H	-5.08397100	0.85648800	0.37677400

Scan Point for comp3_3_alpha_2.2Å

C	1.42110300	-1.26696900	0.15955000
C	0.15517100	-1.83025300	-0.50736600
C	-1.15082700	-1.16111000	-0.04095300
C	1.71869600	0.22168200	-0.09813000
C	-1.28695600	0.16918700	-0.75116100
C	0.61482100	1.18377600	0.39864400
H	1.35310000	-1.42361400	1.24295700
H	0.24374600	-1.70169400	-1.59604200
H	1.87419700	0.38090800	-1.17069400
H	-1.98097800	-1.78177200	-0.39474700
H	-1.90242100	0.23584200	-1.64584400
H	0.19592700	0.86825900	1.35464200
O	-1.16132400	-1.04993300	1.36859700
H	-2.01902900	-0.66622200	1.62082100
O	0.01734100	-3.21371300	-0.19510700
H	0.86914700	-3.64172300	-0.38095100
O	2.48670300	-2.05869300	-0.37410200
H	3.29139300	-1.86737200	0.13186600
O	2.91965400	0.48941000	0.62457900
H	3.42120500	1.17877200	0.16368600
C	1.02425000	2.63759900	0.48298800
H	0.13138300	3.24304800	0.68012400
H	1.70712000	2.74458400	1.33318800
O	1.65115500	3.03184700	-0.73877800
H	1.88701600	3.96885100	-0.67219600
O	-0.48994100	1.15161900	-0.61161700
O	-3.07208700	0.73097100	0.40543100
H	-2.95037600	1.68342100	0.55669500
C	-4.33075100	0.51175200	-0.27074900
H	-4.36805300	1.06297000	-1.21495700

H	-4.40803400	-0.56005800	-0.45791700
H	-5.15038300	0.82974400	0.38039600

Scan Point for comp3_3_alpha_2.3Å

C	1.43337700	-1.26102200	0.17275600
C	0.18288700	-1.83472600	-0.51421800
C	-1.13434300	-1.16467700	-0.08064700
C	1.72957400	0.22685400	-0.09273900
C	-1.25795600	0.16379700	-0.79404200
C	0.61761200	1.18748200	0.39029500
H	1.34397400	-1.40781600	1.25590500
H	0.29276600	-1.71649300	-1.60220600
H	1.89568100	0.38067000	-1.16446800
H	-1.95536600	-1.78754600	-0.45135400
H	-1.89518800	0.25030000	-1.67202600
H	0.18624200	0.87054500	1.34023600
O	-1.17989500	-1.04276400	1.32706500
H	-2.03723100	-0.63544000	1.54707800
O	0.04120000	-3.21479500	-0.19092900
H	0.89531200	-3.64424500	-0.36243400
O	2.51222100	-2.05316100	-0.33178300
H	3.30163800	-1.86736200	0.19967300
O	2.92022700	0.50488100	0.64161800
H	3.42602100	1.19092800	0.18036900
C	1.01904800	2.64296700	0.47672700
H	0.12134400	3.24454600	0.66338000
H	1.69156600	2.75320700	1.33476200
O	1.65763900	3.03755800	-0.73834400
H	1.88623700	3.97641400	-0.67211000
O	-0.48119000	1.15220600	-0.63104700
O	-3.12634600	0.71064100	0.43073500
H	-3.01134900	1.66090100	0.59557400
C	-4.38794000	0.49090700	-0.23529000
H	-4.43807600	1.05128000	-1.17393500
H	-4.45895700	-0.57908400	-0.43635000
H	-5.20901500	0.79317700	0.42233600

Scan Point for comp3_3_alpha_2.4Å

C	1.43477800	-1.26687500	0.18314300
C	0.19065300	-1.83893600	-0.51639400

C	-1.12776300	-1.15352400	-0.11087300
C	1.74164300	0.21785700	-0.08954500
C	-1.22853000	0.17294700	-0.82897600
C	0.63344800	1.18768200	0.38485700
H	1.33000000	-1.40478500	1.26605500
H	0.31815800	-1.73373200	-1.60382300
H	1.91449700	0.36569500	-1.16103700
H	-1.94757400	-1.77128700	-0.49247000
H	-1.88009300	0.27947900	-1.69454400
H	0.18946900	0.87284700	1.32962100
O	-1.19903000	-1.01677500	1.29438200
H	-2.05403800	-0.58940400	1.48991700
O	0.03208500	-3.21377800	-0.18019700
H	0.88036600	-3.65575200	-0.34853100
O	2.51605700	-2.06769100	-0.30103300
H	3.30013800	-1.87922900	0.23747100
O	2.92882100	0.49318800	0.65041700
H	3.44236400	1.17283700	0.18818300
C	1.04269500	2.64036600	0.47371300
H	0.14702500	3.24744500	0.65190800
H	1.70742500	2.74626500	1.33837300
O	1.69507800	3.02962100	-0.73531100
H	1.92442300	3.96838400	-0.66999100
O	-0.46206200	1.16087200	-0.64459200
O	-3.18444700	0.71339700	0.45254600
H	-3.07924900	1.66249200	0.62644100
C	-4.44248000	0.48736300	-0.21473600
H	-4.49888500	1.05522600	-1.14882000
H	-4.50197400	-0.58124200	-0.42769500
H	-5.27072900	0.77280800	0.44211500

Scan Point for comp3_3_alpha_2.5Å

C	1.43436000	-1.27369000	0.19443100
C	0.19664500	-1.84167900	-0.51958500
C	-1.12174000	-1.14116500	-0.14084100
C	1.75409300	0.20749600	-0.08385300
C	-1.19922000	0.18466200	-0.86170000
C	0.65120300	1.18836100	0.38061700
H	1.31339600	-1.40383200	1.27662000
H	0.34191800	-1.74667100	-1.60575000
H	1.93455400	0.34922300	-1.15491800
H	-1.94066400	-1.75266400	-0.53408100
H	-1.86071500	0.30881600	-1.71803500

H	0.19434000	0.87807800	1.32077000
O	-1.21792800	-0.99271400	1.26172400
H	-2.07595800	-0.56032100	1.43754400
O	0.02036400	-3.21195100	-0.17473400
H	0.86221000	-3.66645900	-0.34173700
O	2.51731700	-2.08362800	-0.26941400
H	3.29764500	-1.88780400	0.27208600
O	2.93814400	0.47805700	0.66206000
H	3.46089700	1.14982300	0.19853700
C	1.07086700	2.63773600	0.46977800
H	0.17846900	3.25203700	0.63911700
H	1.72859000	2.73975100	1.34026500
O	1.73673900	3.01869900	-0.73420400
H	1.96749700	3.95733600	-0.67188200
O	-0.43998300	1.17062300	-0.65727300
O	-3.24463000	0.71782600	0.47322900
H	-3.15335200	1.66358900	0.66837100
C	-4.50009500	0.48824400	-0.19490400
H	-4.56329900	1.06664000	-1.12233300
H	-4.54873100	-0.57800100	-0.42279900
H	-5.33366200	0.75536900	0.46346000

Scan Point for comp3_3_alpha_2.6Å

C	-1.41857700	1.28980900	0.21087900
C	-0.18850900	1.84081900	-0.52920500
C	1.12515800	1.11682200	-0.18093200
C	-1.76729400	-0.18453100	-0.06896900
C	1.16862200	-0.21024600	-0.90194400
C	-0.67595400	-1.18886300	0.37312200
H	-1.27129300	1.41251200	1.29059400
H	-0.35896000	1.75162600	-1.61226900
H	-1.96743700	-0.31718300	-1.13769900
H	1.94640700	1.71530200	-0.58926600
H	1.83359100	-0.35648000	-1.75293800
H	-0.19957700	-0.89346200	1.30855000
O	1.24904600	0.95915800	1.21849900
H	2.10415500	0.50952600	1.37241000
O	0.01799000	3.20666500	-0.18444200
H	-0.81677500	3.67735500	-0.34192700
O	-2.49915300	2.11799400	-0.22462500
H	-3.27064200	1.92909600	0.33186200
O	-2.94299100	-0.44077100	0.69439200
H	-3.48497500	-1.09936900	0.23392200

C	-1.12044300	-2.63120400	0.45649600
H	-0.23682200	-3.26238100	0.60842300
H	-1.76737300	-2.72858200	1.33551800
O	-1.80968000	-2.98970400	-0.74104600
H	-2.05136900	-3.92606800	-0.68639700
O	0.40674800	-1.18689700	-0.67712100
O	3.29154500	-0.74332600	0.50127400
H	3.21535400	-1.68552200	0.71704100
C	4.54806400	-0.50408100	-0.15926300
H	4.62313500	-1.08712300	-1.08313800
H	4.58543700	0.56099900	-0.39508000
H	5.38270900	-0.75634900	0.50384100

Scan Point for comp3_3_alpha_2.7Å

C	1.42467900	-1.28681400	0.22641000
C	0.21171100	-1.84414300	-0.53721900
C	-1.10981600	-1.11869000	-0.22357500
C	1.77729500	0.18644600	-0.05479800
C	-1.13755900	0.20707400	-0.94692600
C	0.67874100	1.19292500	0.36464100
H	1.25412900	-1.40344000	1.30343500
H	0.40559300	-1.76224600	-1.61703600
H	1.99465800	0.31403900	-1.12077400
H	-1.92112000	-1.71811700	-0.65028100
H	-1.79821200	0.35900500	-1.80091900
H	0.18594600	0.90123500	1.29288000
O	-1.27019700	-0.95367900	1.17111800
H	-2.13000500	-0.50157500	1.30066600
O	-0.00263400	-3.20715600	-0.18713100
H	0.83190400	-3.68177300	-0.33323500
O	2.51611500	-2.11493900	-0.18060400
H	3.27602700	-1.91662700	0.38852900
O	2.93966200	0.44807700	0.72632600
H	3.49140900	1.10040900	0.26849400
C	1.12043200	2.63607400	0.44774400
H	0.23432500	3.26669100	0.58678000
H	1.75659500	2.73725500	1.33417300
O	1.82327300	2.99039300	-0.74294700
H	2.05878800	3.92852500	-0.69177200
O	-0.38890300	1.18721000	-0.70259700
O	-3.33920700	0.73108300	0.52554200
H	-3.27013600	1.66720500	0.76724200
C	-4.60377900	0.49480100	-0.11939900

H	-4.69189300	1.08544000	-1.03745600
H	-4.64131800	-0.56814400	-0.36501300
H	-5.43178100	0.73816500	0.55536800

Scan Point for comp3_3_alpha_2.8Å

C	-1.39875800	1.31180700	0.23880600
C	-0.18493000	1.83978500	-0.54371300
C	1.12257100	1.07763600	-0.26065700
C	-1.79546900	-0.14961400	-0.04396800
C	1.10164400	-0.24866100	-0.98207100
C	-0.71981700	-1.18770600	0.35930700
H	-1.20686300	1.41846200	1.31334400
H	-0.40178000	1.77044500	-1.62002500
H	-2.02865900	-0.26709500	-1.10784400
H	1.94007700	1.65611700	-0.70429500
H	1.75368000	-0.42643500	-1.83818800
H	-0.20808600	-0.91176500	1.28239200
O	1.31169300	0.90214300	1.12921100
H	2.16701300	0.43190300	1.23715400
O	0.07254600	3.19424400	-0.18952100
H	-0.75304500	3.69044600	-0.31390500
O	-2.47321900	2.17145600	-0.14654800
H	-3.22741000	1.99623400	0.43744800
O	-2.95451100	-0.38421900	0.75002500
H	-3.52590400	-1.02381200	0.29820300
C	-1.19851500	-2.61908700	0.44379300
H	-0.32746200	-3.27227700	0.57300600
H	-1.82791000	-2.70607900	1.33648200
O	-1.92173400	-2.95263100	-0.74066400
H	-2.17705100	-3.88566600	-0.69156700
O	0.33698800	-1.21016800	-0.71963800
O	3.38858200	-0.77202800	0.54632800
H	3.33167200	-1.70427300	0.80462300
C	4.65493800	-0.52644200	-0.09149800
H	4.74946400	-1.11373300	-1.01119600
H	4.68727100	0.53733100	-0.33443000
H	5.48225700	-0.76648700	0.58525000

Scan Point for comp3_3_alpha_2.9Å

C	1.37769900	1.33300800	-0.24769300

C	0.16140700	1.83708000	0.54615800
C	-1.13105800	1.03924100	0.29414000
C	1.81151500	-0.11718600	0.03839600
C	-1.06684200	-0.28526700	1.01592200
C	0.75591700	-1.18052300	-0.35294100
H	1.17093000	1.42889100	-1.32057000
H	0.39650900	1.78634200	1.61952500
H	2.05576700	-0.22550700	1.10083000
H	-1.95372600	1.59949700	0.75139100
H	-1.71253800	-0.48490100	1.87266600
H	0.22549200	-0.91484900	-1.26866000
O	-1.34572600	0.84881100	-1.09018100
H	-2.19885800	0.36663400	-1.17875500
O	-0.13694200	3.17989000	0.18027800
H	0.67763300	3.69837200	0.28487200
O	2.43474600	2.22067600	0.12143900
H	3.18493700	2.06635000	-0.47332400
O	2.96888000	-0.32855100	-0.76426600
H	3.55664700	-0.95634900	-0.31678700
C	1.26522800	-2.60059900	-0.44609900
H	0.40724200	-3.27222800	-0.56798200
H	1.88655300	-2.67187800	-1.34581000
O	2.00792700	-2.92097700	0.72986100
H	2.28142500	-3.84861900	0.67700800
O	-0.28826200	-1.23001500	0.73813300
O	-3.43837400	-0.80569100	-0.56995100
H	-3.39604700	-1.73382400	-0.84460700
C	-4.69925800	-0.54997100	0.07420300
H	-4.79535700	-1.14045900	0.99179100
H	-4.71962900	0.51284700	0.32258700
H	-5.53262400	-0.77817800	-0.59919900

Scan Point for comp3_3_alpha_3.0Å

C	1.28037400	1.38999200	-0.29400700
C	0.08431800	1.82603400	0.56906800
C	-1.15968200	0.93072400	0.42067200
C	1.83169200	-0.02243100	-0.01462600
C	-0.94503200	-0.36288100	1.16584700
C	0.82960300	-1.16254000	-0.31863200
H	0.99945700	1.44970900	-1.35251000
H	0.39117100	1.81577500	1.62516300
H	2.14988400	-0.09314500	1.03125900
H	-1.98948600	1.44111800	0.92149600

H	-1.51456600	-0.58931400	2.06927200
H	0.21654300	-0.95136000	-1.19564000
O	-1.45302900	0.67967200	-0.93843100
H	-2.28059000	0.13662900	-0.95149300
O	-0.33433100	3.13441100	0.19845200
H	0.44660800	3.71095400	0.23008100
O	2.29290100	2.35660800	-0.00759900
H	3.00085800	2.26418100	-0.66343500
O	2.94776500	-0.16979100	-0.88723200
H	3.59064500	-0.77116500	-0.48035200
C	1.43284800	-2.54380700	-0.42836600
H	0.62234100	-3.28248600	-0.44138000
H	1.96301800	-2.59855900	-1.38570400
O	2.31736300	-2.76672800	0.66963800
H	2.68591500	-3.65899900	0.59025500
O	-0.12846000	-1.26056400	0.84629500
O	-3.45428600	-1.01573000	-0.34327000
H	-3.41434800	-1.84663300	-0.84074700
C	-4.82955300	-0.59720600	-0.24060400
H	-5.41956700	-1.34602400	0.29825100
H	-4.83632600	0.33969900	0.31958500
H	-5.26236000	-0.43070100	-1.23302800

Scan Point for comp3_3_alpha_3.1Å

C	1.23048200	1.41546100	-0.31312100
C	0.04826500	1.81621200	0.58521700
C	-1.16322800	0.87115200	0.49383100
C	1.84105000	0.02727800	-0.03809500
C	-0.87522400	-0.41069400	1.23481900
C	0.87305700	-1.15009500	-0.31058500
H	0.91314900	1.45296600	-1.36238200
H	0.39204100	1.83483800	1.62935600
H	2.18501800	-0.02466100	1.00084700
H	-1.99290200	1.35313500	1.02250500
H	-1.40969700	-0.65969000	2.15387300
H	0.22410300	-0.96218300	-1.16683500
O	-1.49803000	0.59407700	-0.85037900
H	-2.31912400	0.03748600	-0.83010700
O	-0.43609900	3.10108800	0.21073300
H	0.32082600	3.70955600	0.20403700
O	2.21562000	2.42099000	-0.06954000
H	2.92276200	2.32162200	-0.72548800
O	2.94191400	-0.08454700	-0.93433500

H	3.60729500	-0.67361800	-0.54553500
C	1.52285100	-2.50798600	-0.44015900
H	0.73952800	-3.27548200	-0.43355500
H	2.02860300	-2.54205000	-1.41159200
O	2.44340700	-2.69972100	0.63361200
H	2.83588800	-3.58117400	0.54788900
O	-0.04291400	-1.28193900	0.88469700
O	-3.50618200	-1.07924200	-0.26221100
H	-3.41272800	-1.91325000	-0.74742200
C	-4.86888500	-0.62184100	-0.38313100
H	-5.56090800	-1.36027600	0.03468500
H	-4.94261800	0.30633900	0.18686900
H	-5.12317300	-0.42614100	-1.43041300

Scan Point for comp3_3_alpha_3.2Å

C	1.18651100	1.43860000	-0.31653700
C	0.00723000	1.79728100	0.60205300
C	-1.17127500	0.81026400	0.52860900
C	1.85380400	0.07294200	-0.05813900
C	-0.82583200	-0.46079700	1.26290900
C	0.92594300	-1.14077400	-0.30881000
H	0.84896100	1.46538200	-1.35986100
H	0.36638200	1.82730000	1.64064000
H	2.22795500	0.03318600	0.97069700
H	-2.00916400	1.26191900	1.07109100
H	-1.34130800	-0.73260000	2.18653100
H	0.25763400	-0.98004800	-1.15579800
O	-1.51765500	0.52012700	-0.80956200
H	-2.34044500	-0.03617600	-0.78111600
O	-0.52858600	3.06465900	0.23744000
H	0.20462500	3.70124800	0.22333000
O	2.14134300	2.47711300	-0.09064200
H	2.85095000	2.38433400	-0.74521300
O	2.93212800	0.00597400	-0.98634100
H	3.64660800	-0.52990000	-0.60907800
C	1.61933200	-2.47666700	-0.44278500
H	0.85948000	-3.26743900	-0.44018700
H	2.12635300	-2.49093200	-1.41408100
O	2.54361200	-2.64571900	0.63147400
H	2.95264900	-3.51993500	0.54955900
O	0.03205700	-1.30130600	0.90014700
O	-3.55387300	-1.12571200	-0.27191400
H	-3.46483700	-1.95623700	-0.76386100

C	-4.90460200	-0.64125300	-0.42024000
H	-5.61896900	-1.36700200	-0.01805800
H	-4.97198300	0.28709200	0.15027300
H	-5.13376900	-0.43887200	-1.47206100

Scan Point for comp3_3_alpha_3.3Å

C	1.16403100	1.44885200	-0.32656200
C	-0.00617400	1.79208200	0.60993900
C	-1.16570000	0.78058500	0.56405000
C	1.85934500	0.09600200	-0.07266600
C	-0.78256000	-0.47917300	1.29954400
C	0.94948200	-1.13563900	-0.30183000
H	0.80808100	1.46383900	-1.36409900
H	0.36983300	1.83715800	1.64194500
H	2.25165900	0.06802700	0.94976500
H	-2.00250700	1.21882700	1.11912600
H	-1.27690900	-0.75501000	2.23353800
H	0.26230700	-0.98975100	-1.13632900
O	-1.53014600	0.47539200	-0.76566000
H	-2.35589000	-0.07805900	-0.72803900
O	-0.57579300	3.04466200	0.24604000
H	0.13240500	3.70842500	0.25980400
O	2.10646100	2.50331000	-0.12350100
H	2.81564200	2.40449300	-0.77781900
O	2.92314900	0.04370800	-1.01846300
H	3.65753500	-0.46783000	-0.64602000
C	1.66324000	-2.45993000	-0.44477200
H	0.91592900	-3.26246200	-0.43521200
H	2.15950200	-2.46472300	-1.42174000
O	2.60150800	-2.61587300	0.61916200
H	3.01666200	-3.48715900	0.53702400
O	0.08167200	-1.30736400	0.92423900
O	-3.59406700	-1.15116700	-0.29226300
H	-3.50823100	-1.97378500	-0.79782500
C	-4.93696100	-0.64864200	-0.44808400
H	-5.66309500	-1.36750400	-0.05453900
H	-4.99698000	0.27759600	0.12665500
H	-5.15642000	-0.43825100	-1.50038500

Scan Point for comp3_3_alpha_3.4Å

C	1.13759900	1.46051500	-0.33246900
C	-0.02852200	1.77838900	0.61755500
C	-1.16247800	0.73714700	0.59625100
C	1.86863700	0.12674900	-0.08085700
C	-0.73849600	-0.51307100	1.32670400
C	0.98506800	-1.12603100	-0.29968900
H	0.76853000	1.46170900	-1.36567100
H	0.36079500	1.83969700	1.64394300
H	2.27003000	0.11051200	0.93832700
H	-1.99982600	1.15661500	1.16472500
H	-1.21549500	-0.80262300	2.26555700
H	0.28231000	-0.99470100	-1.12362300
O	-1.54392000	0.41583500	-0.72495100
H	-2.37535800	-0.12970900	-0.67718500
O	-0.63625200	3.01330700	0.25456400
H	0.05305300	3.69679300	0.25701300
O	2.05567500	2.53929600	-0.14574500
H	2.76494900	2.44870700	-0.80125000
O	2.92564800	0.09816100	-1.03507200
H	3.67680300	-0.39026300	-0.66521000
C	1.72757000	-2.43299500	-0.45637900
H	0.99890800	-3.25238600	-0.44505900
H	2.21511900	-2.42063900	-1.43768900
O	2.67834800	-2.57282400	0.59854800
H	3.11067800	-3.43508800	0.51036300
O	0.13895900	-1.32072100	0.93777700
O	-3.64857900	-1.17542600	-0.30200700
H	-3.56628600	-1.99530100	-0.81252900
C	-4.98224300	-0.65438200	-0.47212600
H	-5.72200700	-1.36359400	-0.08636400
H	-5.03584900	0.27238100	0.10236800
H	-5.18818400	-0.44105500	-1.52656500

Scan Point for comp3_3_alpha_3.5Å

C	1.10228000	1.47250100	-0.33622500
C	-0.06022900	1.75500400	0.62858700
C	-1.16335200	0.68080200	0.62285300
C	1.87684700	0.16369900	-0.08930800
C	-0.69447600	-0.55820900	1.34582100
C	1.02944800	-1.11498300	-0.30050300
H	0.72037300	1.45944000	-1.36476600
H	0.34118900	1.82758800	1.64979400
H	2.28623700	0.16049600	0.92681800

H	-2.00495600	1.07601500	1.20194300
H	-1.15459800	-0.86576600	2.28737800
H	0.31402300	-1.00497100	-1.11676600
O	-1.55357700	0.34430400	-0.69228000
H	-2.39307600	-0.18829200	-0.63976100
O	-0.70854200	2.97176700	0.27443400
H	-0.03701700	3.67270300	0.25696600
O	1.98720100	2.58083300	-0.16289300
H	2.69080800	2.51280200	-0.82714900
O	2.92671000	0.16642400	-1.05159300
H	3.69472600	-0.29946000	-0.68724500
C	1.81201700	-2.39715600	-0.46673900
H	1.11093700	-3.24007400	-0.45156800
H	2.29071700	-2.36627800	-1.45199400
O	2.77557700	-2.50692500	0.58004300
H	3.24200800	-3.35007600	0.48213600
O	0.20255400	-1.33802100	0.94503100
O	-3.70695100	-1.20454400	-0.31467600
H	-3.63563900	-2.02236300	-0.83003200
C	-5.03027700	-0.66003100	-0.48787900
H	-5.78314500	-1.35657500	-0.10410000
H	-5.06945800	0.26729400	0.08683300
H	-5.23045500	-0.44296600	-1.54265400

Scan Point for comp3_3_alpha_3.6Å

C	0.99777200	1.49498300	-0.34235000
C	-0.14745000	1.70056700	0.66135900
C	-1.18207600	0.56103500	0.67653700
C	1.86369500	0.24100200	-0.11603000
C	-0.61908300	-0.64315000	1.38947600
C	1.10090300	-1.09432600	-0.29354600
H	0.58478600	1.45479100	-1.35769300
H	0.28223900	1.78962800	1.67005400
H	2.30100400	0.27182600	0.88806100
H	-2.03529500	0.90277500	1.27217500
H	-1.03857500	-0.97784200	2.34064900
H	0.35989900	-1.04689900	-1.09296300
O	-1.57609800	0.19648000	-0.62922200
H	-2.41080600	-0.34485300	-0.56184200
O	-0.87663900	2.87966600	0.33875600
H	-0.24143000	3.61166100	0.27660900
O	1.81077900	2.66105000	-0.19724100
H	2.45529700	2.67583400	-0.92150700

O	2.88372600	0.30356300	-1.10754900
H	3.67548800	-0.14696100	-0.77498800
C	1.97188400	-2.31727100	-0.46613000
H	1.34566100	-3.21274600	-0.37538100
H	2.38405000	-2.28824200	-1.48108700
O	3.00681700	-2.30839100	0.51726600
H	3.53630000	-3.11280200	0.41307200
O	0.32064800	-1.36258300	0.97310200
O	-3.75038400	-1.30212000	-0.25998100
H	-3.66915300	-2.13478700	-0.74963800
C	-5.00594000	-0.68263000	-0.60618600
H	-5.84227000	-1.33795000	-0.34212000
H	-5.07229600	0.24095500	-0.02800900
H	-5.04392400	-0.44697300	-1.67520900

Scan Point for comp3_3_alpha_3.7Å

C	0.91328200	1.51811600	-0.32134700
C	-0.24929900	1.62244700	0.67774200
C	-1.19383400	0.40877700	0.68145800
C	1.86884700	0.32959200	-0.10161200
C	-0.54809700	-0.76944100	1.36783400
C	1.20661900	-1.05372000	-0.31463200
H	0.51038100	1.45656800	-1.34014600
H	0.16745900	1.73433900	1.68959300
H	2.28884700	0.37517200	0.90933800
H	-2.06559600	0.67879300	1.28661900
H	-0.94917500	-1.16314400	2.30412200
H	0.46775300	-1.04079200	-1.11749500
O	-1.57372200	0.02897500	-0.62468600
H	-2.42370600	-0.48945300	-0.55937600
O	-1.06627600	2.74496000	0.36296900
H	-0.48792400	3.52263300	0.30188600
O	1.63477300	2.74030200	-0.15990700
H	2.29656800	2.79818000	-0.86649900
O	2.89490400	0.48648700	-1.07630900
H	3.70948200	0.07676600	-0.74590400
C	2.16289900	-2.20666200	-0.51314100
H	1.60080000	-3.14583600	-0.44870100
H	2.57653600	-2.12312600	-1.52459500
O	3.18979800	-2.14970300	0.47685400
H	3.76396500	-2.92229900	0.36857100
O	0.44217700	-1.40942900	0.93914700
O	-3.81862000	-1.35239600	-0.26122800

H	-3.79435700	-2.19365400	-0.74231700
C	-5.03744000	-0.65900100	-0.60068400
H	-5.90926600	-1.25581000	-0.31360000
H	-5.03768100	0.27583000	-0.03712800
H	-5.07621400	-0.43837900	-1.67278700

Scan Point for comp3_3_alpha_3.8Å

C	0.87617200	1.52124400	-0.32005600
C	-0.26615500	1.59533500	0.70539500
C	-1.18386600	0.36072100	0.71986100
C	1.86976200	0.35846000	-0.13258100
C	-0.49438100	-0.79917100	1.39462400
C	1.24163200	-1.04393400	-0.31875200
H	0.45084000	1.45341300	-1.32920000
H	0.16991000	1.70994500	1.70887200
H	2.32770000	0.42017700	0.86044900
H	-2.05157200	0.60843800	1.33996200
H	-0.86574000	-1.20221500	2.33923900
H	0.49124400	-1.05791500	-1.11094800
O	-1.57565500	-0.02452900	-0.58098000
H	-2.43166700	-0.53224800	-0.51502400
O	-1.11271200	2.70226400	0.41519000
H	-0.55137900	3.49152500	0.34475000
O	1.57118700	2.76062300	-0.17106000
H	2.20871200	2.84049700	-0.89745300
O	2.85032700	0.54067800	-1.14959600
H	3.70265900	0.20073700	-0.83735000
C	2.22303700	-2.17609900	-0.51789600
H	1.67876400	-3.12599000	-0.45825600
H	2.63909300	-2.08153100	-1.52732000
O	3.24325100	-2.10283600	0.47763600
H	3.82365100	-2.87207000	0.37971700
O	0.50718000	-1.41001800	0.95052600
O	-3.85801500	-1.37376500	-0.27744300
H	-3.83765000	-2.21054900	-0.76641000
C	-5.05149900	-0.65124500	-0.64311200
H	-5.94342700	-1.22724000	-0.37567000
H	-5.04212500	0.28307400	-0.07882200
H	-5.06172700	-0.42925600	-1.71561100

Scan Point for comp3_3_alpha_3.9Å

C	0.84132300	1.52125100	-0.32034800
C	-0.28458100	1.56660900	0.72498500
C	-1.17212600	0.31004500	0.75692400
C	1.86792300	0.38586000	-0.14904800
C	-0.44278000	-0.83404500	1.41769900
C	1.27522700	-1.03339600	-0.32191700
H	0.40034400	1.44110100	-1.32185800
H	0.16636800	1.69197000	1.72058600
H	2.34277900	0.46168900	0.83492700
H	-2.03263300	0.53778700	1.39410900
H	-0.79040900	-1.24991900	2.36587000
H	0.51534500	-1.07136400	-1.10424900
O	-1.58163800	-0.08688500	-0.53516800
H	-2.44684700	-0.57651300	-0.46191200
O	-1.16457900	2.65126100	0.45056400
H	-0.62805000	3.45768300	0.38422400
O	1.50704000	2.77835500	-0.18464000
H	2.13078500	2.87281300	-0.92113200
O	2.82426400	0.59109700	-1.18484800
H	3.69137900	0.27643200	-0.88707600
C	2.28602400	-2.13812600	-0.53031800
H	1.76918800	-3.10260200	-0.46237400
H	2.68794800	-2.03458300	-1.54451100
O	3.31453600	-2.03296600	0.45382200
H	3.91809100	-2.78321700	0.34923100
O	0.56781200	-1.41766600	0.95800500
O	-3.90986200	-1.38716400	-0.28036000
H	-3.88931100	-2.22277900	-0.77131200
C	-5.07227900	-0.63736400	-0.68773000
H	-5.98606100	-1.19391700	-0.45492800
H	-5.06308600	0.29533000	-0.12075800
H	-5.03880600	-0.41316200	-1.75932100

Scan Point for comp3_3_alpha_4.0Å

C	0.78015000	1.52242900	-0.31306400
C	-0.32854900	1.52245100	0.75079300
C	-1.16035000	0.22924200	0.80798600
C	1.85502600	0.43142200	-0.15380700
C	-0.37190100	-0.88512000	1.45217400
C	1.31368800	-1.00895600	-0.32432800
H	0.32608900	1.41953700	-1.30667200
H	0.13418600	1.67456700	1.73725100

H	2.33569800	0.52279400	0.82620100
H	-2.01428800	0.42388300	1.46449400
H	-0.68488800	-1.31773500	2.40502200
H	0.53701300	-1.07186700	-1.08836900
O	-1.58349000	-0.19460400	-0.47129000
H	-2.45767600	-0.66651900	-0.38481800
O	-1.26186600	2.56428300	0.48541400
H	-0.76284300	3.39124100	0.38659000
O	1.39128700	2.80814800	-0.19169300
H	1.98681700	2.93507800	-0.94623000
O	2.79368200	0.67611600	-1.19693000
H	3.67182100	0.38078100	-0.91148800
C	2.36148700	-2.07099900	-0.56618800
H	1.88581900	-3.05619800	-0.49303200
H	2.73217800	-1.94409600	-1.58953900
O	3.41089900	-1.93129700	0.39106300
H	4.05980900	-2.63407000	0.23931900
O	0.65101400	-1.42754400	0.96956500
O	-3.95644500	-1.40942700	-0.24374600
H	-3.93811200	-2.26625000	-0.69676900
C	-5.02946200	-0.61690200	-0.79169700
H	-5.98738700	-1.13202900	-0.66673500
H	-5.04742600	0.32046400	-0.23261100
H	-4.85800300	-0.40639900	-1.85289200

Scan Point for comp3_3_alpha_4.1Å

C	0.73139900	1.52170900	-0.31105100
C	-0.35862400	1.49154000	0.77152200
C	-1.14542100	0.17086600	0.84753200
C	1.84101000	0.46349900	-0.16483800
C	-0.30789700	-0.91042700	1.48785500
C	1.33781300	-0.99256100	-0.32413500
H	0.26346100	1.40032600	-1.29619000
H	0.11562600	1.66435500	1.74910100
H	2.33098100	0.57019300	0.80918900
H	-1.99629000	0.33975400	1.51485000
H	-0.58552500	-1.33973700	2.45310900
H	0.54476200	-1.07871500	-1.06863100
O	-1.57009700	-0.27416600	-0.42376700
H	-2.45326700	-0.72829500	-0.33847800
O	-1.33023500	2.50049700	0.51777300
H	-0.86118500	3.34424600	0.41438000
O	1.30450000	2.82599300	-0.20532500

H	1.89038200	2.96350700	-0.96559800
O	2.76002100	0.73351900	-1.21863400
H	3.64775400	0.45624500	-0.94459300
C	2.41011000	-2.02350500	-0.58973200
H	1.96482500	-3.02249000	-0.51200700
H	2.75795100	-1.88218200	-1.61926000
O	3.47245200	-1.85698900	0.34875500
H	4.13584300	-2.54352600	0.18584700
O	0.72029400	-1.42544000	0.98731500
O	-3.97976600	-1.43145000	-0.26026100
H	-3.97418700	-2.28596000	-0.71784900
C	-5.00847100	-0.60244400	-0.83721200
H	-5.98817000	-1.07994700	-0.73231100
H	-5.00474900	0.33798100	-0.28301400
H	-4.80508200	-0.40353600	-1.89503300

Scan Point for comp3_3_alpha_4.2Å

C	0.67207100	1.51602100	-0.29864100
C	-0.39937600	1.43295100	0.79896300
C	-1.13109900	0.08031900	0.87275800
C	1.82760200	0.50540400	-0.17120700
C	-0.24181800	-0.97018200	1.49481200
C	1.38569900	-0.96985000	-0.33506600
H	0.19648300	1.37880000	-1.27812900
H	0.08173700	1.61568200	1.77160500
H	2.32211400	0.62686300	0.79877300
H	-1.98029900	0.20907300	1.55070700
H	-0.49063400	-1.41741000	2.45985600
H	0.59021800	-1.08651100	-1.07246000
O	-1.55130800	-0.37645800	-0.39634900
H	-2.45324400	-0.79198400	-0.32064600
O	-1.41421900	2.40415300	0.56899900
H	-0.98009700	3.26557800	0.45858500
O	1.19083000	2.84307100	-0.19471200
H	1.77564500	3.00049500	-0.95222500
O	2.72432400	0.82078600	-1.23139000
H	3.62604400	0.58401500	-0.96492000
C	2.49975000	-1.95097000	-0.61713800
H	2.10047900	-2.96946200	-0.54253300
H	2.83161000	-1.78763900	-1.64862800
O	3.56158200	-1.74262800	0.31336000
H	4.25636400	-2.39381300	0.13694700
O	0.80155200	-1.43702500	0.97943200

O	-4.01655400	-1.43581700	-0.28691600
H	-4.03352000	-2.28396900	-0.75585800
C	-5.01570600	-0.56799100	-0.85910200
H	-6.01233900	-1.00859600	-0.75144300
H	-4.97421800	0.37095600	-0.30397000
H	-4.80873800	-0.37494400	-1.91732000

Scan Point for comp3_3_alpha_4.3Å

C	0.60131700	1.50694600	-0.27789000
C	-0.44451800	1.36092700	0.83736500
C	-1.11622300	-0.02380600	0.89634100
C	1.80843700	0.55403800	-0.18489400
C	-0.17192400	-1.04003200	1.49406300
C	1.44223600	-0.94156900	-0.34924600
H	0.11457900	1.35739800	-1.25002700
H	0.04497000	1.54716700	1.80537300
H	2.31949900	0.69678400	0.77331100
H	-1.96256100	0.05519500	1.58522700
H	-0.38930000	-1.51196200	2.45510000
H	0.64940400	-1.09644600	-1.08230800
O	-1.52945600	-0.48307200	-0.37479900
H	-2.44543700	-0.86686500	-0.31347200
O	-1.50293700	2.29245800	0.64137800
H	-1.10532300	3.17013100	0.52060200
O	1.05843800	2.85625700	-0.16835400
H	1.62795000	3.04589400	-0.93026800
O	2.66126300	0.92009600	-1.26533500
H	3.58379800	0.76814800	-1.00915800
C	2.60099900	-1.86667200	-0.64174600
H	2.24994200	-2.90288400	-0.57053400
H	2.91942500	-1.68259700	-1.67397600
O	3.65713300	-1.61449600	0.28424700
H	4.37185200	-2.24524800	0.11294100
O	0.89037000	-1.44530000	0.96616300
O	-4.04536100	-1.45007200	-0.32757400
H	-4.08751000	-2.27818500	-0.82956400
C	-5.00172300	-0.52197100	-0.87812100
H	-6.01800200	-0.91870300	-0.78386600
H	-4.91728800	0.39980500	-0.29965900
H	-4.78320300	-0.31176000	-1.93076000

Scan Point for comp3_3_alpha_4.4Å

C	0.50783000	1.49350900	-0.24266600
C	-0.52270200	1.25985900	0.87242900
C	-1.10011300	-0.16810400	0.91299100
C	1.77317800	0.61726600	-0.18065000
C	-0.08658200	-1.12300600	1.49715200
C	1.49813000	-0.89575200	-0.35913700
H	0.02497700	1.33549700	-1.21529900
H	-0.04326600	1.46544800	1.84168500
H	2.29133700	0.78143400	0.77023800
H	-1.94821800	-0.15466700	1.60382800
H	-0.26294500	-1.61597100	2.45600600
H	0.70559300	-1.09001100	-1.08290200
O	-1.48352700	-0.64721100	-0.36074400
H	-2.41487800	-0.99618800	-0.32404900
O	-1.64108600	2.12191300	0.69218500
H	-1.30224600	3.02622300	0.58939700
O	0.87842200	2.86660200	-0.10382200
H	1.40888400	3.11902600	-0.87531200
O	2.57987800	1.04904700	-1.27211700
H	3.51511400	0.93892700	-1.04231000
C	2.70665600	-1.74391300	-0.68094300
H	2.42240400	-2.80058200	-0.61144000
H	2.99208200	-1.53295700	-1.71778000
O	3.76348700	-1.43197100	0.22575300
H	4.51073700	-2.01943400	0.03951400
O	0.99739100	-1.44809100	0.95790500
O	-4.04319700	-1.47675500	-0.39495100
H	-4.13436600	-2.25594400	-0.96434000
C	-4.91001800	-0.43589200	-0.88907600
H	-5.95501700	-0.76096300	-0.85568400
H	-4.77661500	0.42509100	-0.23171400
H	-4.64279000	-0.15699700	-1.91410900

Scan Point for comp3_3_beta_1.4Å

C	-0.67550700	-1.63236300	-0.17039100
C	-1.75311500	-0.55455900	-0.29357000
C	-1.61997100	0.66572700	0.62734100
C	0.75872600	-1.12847000	-0.37915300
C	-0.44760700	1.63139600	0.36023100
C	1.22899100	-0.19883700	0.76815300
H	-0.73725700	-2.09898100	0.82224200
H	-1.76340800	-0.20437300	-1.33551900

H	0.83489500	-0.59348900	-1.33543800
H	-2.51912800	1.27068000	0.45423000
H	-0.59814400	2.50091500	1.00363500
H	0.79848200	-0.52550100	1.71992600
O	-1.51960200	0.32538900	2.00530800
H	-2.34852700	-0.09839000	2.27694300
O	-3.03567600	-1.11236700	0.01999500
H	-3.14563200	-1.92023900	-0.50642600
O	-1.01551400	-2.59910300	-1.17200700
H	-0.35561100	-3.30945100	-1.13394500
O	1.56061600	-2.31337800	-0.42416000
H	2.41355100	-2.08969000	-0.82892600
C	2.73812000	-0.17450800	0.94295100
H	2.99316800	0.61503700	1.65929600
H	3.06256500	-1.13517200	1.35618200
O	3.36447400	0.06930100	-0.32507000
H	4.32374100	0.09676200	-0.19406000
O	0.85945800	1.19216600	0.54869200
O	-0.57518300	2.13059600	-0.94150800
H	-0.20985300	1.53138400	-1.62966800
C	-0.16060400	3.54601400	-1.21814300
H	-0.36649000	3.69054200	-2.27603600
H	-0.80153400	4.16011500	-0.59020500
H	0.89640200	3.64262800	-0.97675300

Scan Point for comp3_3_beta_1.5Å

C	-0.70491900	-1.61224500	-0.18449300
C	-1.76264400	-0.51281800	-0.29347900
C	-1.60962500	0.68751300	0.64990200
C	0.74196700	-1.13673800	-0.37984700
C	-0.40975300	1.61929500	0.41813600
C	1.23233000	-0.23708000	0.78067800
H	-0.77997100	-2.09330800	0.80022500
H	-1.76103800	-0.14348900	-1.32849000
H	0.83866100	-0.59608100	-1.33023000
H	-2.49220700	1.31713700	0.48343800
H	-0.54910500	2.52482300	1.01028400
H	0.80842000	-0.57803700	1.73003300
O	-1.52316600	0.31949000	2.02281300
H	-2.37125700	-0.06801600	2.28943300
O	-3.05605800	-1.05089000	0.00683700
H	-3.18290200	-1.84363100	-0.53831900
O	-1.05886800	-2.55551700	-1.20295900

H	-0.41966300	-3.28463500	-1.16687700
O	1.51752200	-2.33865000	-0.42945900
H	2.37267900	-2.13470300	-0.83992400
C	2.74297800	-0.22469200	0.93719300
H	3.01212400	0.55020700	1.66423200
H	3.06430900	-1.19454500	1.33090900
O	3.35483400	0.03557000	-0.33379300
H	4.31593200	0.05167900	-0.21478100
O	0.86898300	1.16877000	0.60733800
O	-0.53950400	2.13781600	-0.98339900
H	-0.12005000	1.53584800	-1.63498800
C	-0.09581900	3.53869700	-1.23770500
H	-0.27929200	3.70343700	-2.29746900
H	-0.73280600	4.16573000	-0.61817800
H	0.95914600	3.62329000	-0.98064200

Scan Point for comp3_3_beta_1.6Å

C	-0.64030700	-1.62884300	-0.19789600
C	-1.73610300	-0.56585200	-0.28642200
C	-1.62792300	0.62035600	0.68151000
C	0.78981700	-1.10282400	-0.38893500
C	-0.45409800	1.58449500	0.47814400
C	1.25347500	-0.20857400	0.78553900
H	-0.69528500	-2.12825000	0.77900900
H	-1.74708600	-0.17483900	-1.31269100
H	0.86975700	-0.54973800	-1.33309500
H	-2.52826300	1.22550600	0.52363500
H	-0.62414800	2.51780100	1.01487600
H	0.85240900	-0.58562500	1.73088200
O	-1.53238600	0.22887300	2.04814200
H	-2.38104800	-0.15723500	2.31518800
O	-3.00862800	-1.15697000	0.00255400
H	-3.10219500	-1.94702500	-0.55323100
O	-0.96480300	-2.56640900	-1.23096900
H	-0.31227200	-3.28363100	-1.19770600
O	1.60522500	-2.27700900	-0.44862300
H	2.44781600	-2.04655000	-0.87031900
C	2.76254900	-0.12643600	0.92885400
H	3.00143400	0.64569300	1.66935700
H	3.13219400	-1.08762700	1.30069800
O	3.34849500	0.18673800	-0.34138300
H	4.30872400	0.24910500	-0.22998800
O	0.82105200	1.18890800	0.65769000

O	-0.62633900	2.10643100	-1.02449200
H	-0.11251500	1.54085600	-1.63748600
C	-0.27943200	3.52739900	-1.25911500
H	-0.45233200	3.69788800	-2.32056700
H	-0.96785300	4.10879300	-0.64944300
H	0.76187100	3.69206100	-0.98254600

Scan Point for comp3_3_beta_1.7Å

C	-0.67952000	-1.60525500	-0.21265800
C	-1.74822300	-0.51332300	-0.28371400
C	-1.60987400	0.64850400	0.70937000
C	0.76722800	-1.11941000	-0.39383200
C	-0.40378900	1.57266500	0.53953800
C	1.26143600	-0.26045900	0.79313200
H	-0.74966200	-2.11848200	0.75598300
H	-1.74795100	-0.10156200	-1.30132600
H	0.86955000	-0.55940500	-1.33095800
H	-2.48929700	1.28552000	0.56328600
H	-0.54635100	2.53707700	1.02445600
H	0.86558900	-0.64989600	1.73534000
O	-1.52809500	0.22487400	2.06871400
H	-2.39697200	-0.11309900	2.33602100
O	-3.03552500	-1.07648400	-0.00679800
H	-3.15377600	-1.84641600	-0.58553500
O	-1.02570600	-2.51681100	-1.26120600
H	-0.39042800	-3.24999300	-1.23913600
O	1.54531100	-2.31809000	-0.46054300
H	2.38453600	-2.12152600	-0.90479000
C	2.77223300	-0.19586000	0.91661400
H	3.02788000	0.54338700	1.68460500
H	3.13791900	-1.17428500	1.24498700
O	3.34080400	0.16405400	-0.34796000
H	4.30283800	0.21696600	-0.24794000
O	0.84340300	1.15129800	0.71026300
O	-0.58380000	2.11772500	-1.06062000
H	-0.04766000	1.54794800	-1.64734100
C	-0.20893800	3.52555000	-1.27429400
H	-0.33760100	3.71593600	-2.33952400
H	-0.90711900	4.11932000	-0.68722400
H	0.82404900	3.68149700	-0.96064300

Scan Point for comp3_3_beta_1.8Å

C	-0.68757300	-1.59978200	-0.22062000
C	-1.74721400	-0.49827200	-0.28166500
C	-1.60521100	0.64749300	0.72878800
C	0.76402100	-1.12455000	-0.39428400
C	-0.38408800	1.55199100	0.59367000
C	1.27053600	-0.28955600	0.80375900
H	-0.76472800	-2.12491700	0.74101700
H	-1.73495800	-0.06974700	-1.29183400
H	0.87137300	-0.55377500	-1.32366800
H	-2.47154500	1.30001400	0.58328100
H	-0.51532600	2.54103700	1.02755400
H	0.88153200	-0.69265500	1.74290800
O	-1.54736000	0.20020900	2.08356200
H	-2.45313400	0.09974400	2.41435700
O	-3.04056400	-1.05464000	-0.02396300
H	-3.16816700	-1.80254600	-0.62879900
O	-1.03625200	-2.49425400	-1.28265300
H	-0.40202800	-3.22876700	-1.27224700
O	1.53222700	-2.32835800	-0.47313900
H	2.35892300	-2.14410200	-0.94476000
C	2.78150700	-0.21857600	0.91295800
H	3.04101700	0.49656300	1.70216000
H	3.15606300	-1.20495400	1.20543400
O	3.33027300	0.18709600	-0.34541300
H	4.29239700	0.25152900	-0.25405700
O	0.84604600	1.12744900	0.75421600
O	-0.57467900	2.12262600	-1.10281200
H	-0.01682200	1.55829000	-1.67250600
C	-0.19162600	3.52391500	-1.29060900
H	-0.27162700	3.73574400	-2.35740900
H	-0.91023300	4.11830800	-0.72823400
H	0.82762400	3.68323900	-0.93354900

Scan Point for comp3_3_beta_1.9Å

C	-0.68964500	-1.59749100	-0.22796700
C	-1.74940200	-0.49322900	-0.26479400
C	-1.60585800	0.62772900	0.76698300
C	0.76246900	-1.12198300	-0.40064900
C	-0.37814200	1.52633100	0.64688800
C	1.28060600	-0.30829600	0.80624700
H	-0.76363100	-2.14306000	0.72253000

H	-1.72793300	-0.03612600	-1.26126500
H	0.86462900	-0.53671000	-1.32125700
H	-2.47404300	1.28122700	0.64392900
H	-0.49915600	2.53469100	1.03657900
H	0.89968100	-0.72443100	1.74287000
O	-1.56465600	0.09206000	2.08873200
H	-1.98759500	0.71527000	2.69987400
O	-3.04385800	-1.05386800	-0.03273400
H	-3.17257900	-1.77406300	-0.67007400
O	-1.04272100	-2.46750400	-1.30790300
H	-0.40823800	-3.20197200	-1.31669800
O	1.52796300	-2.32551300	-0.50062500
H	2.33337600	-2.14755000	-1.00944400
C	2.79156400	-0.22720900	0.90099700
H	3.05406600	0.46719500	1.70756600
H	3.17574800	-1.21874800	1.16166300
O	3.32144900	0.21898500	-0.35089100
H	4.28344200	0.29448000	-0.26765400
O	0.84463300	1.10888800	0.78381200
O	-0.59237900	2.13674500	-1.13958800
H	-0.01465800	1.58145400	-1.69567600
C	-0.20729400	3.53390800	-1.30410400
H	-0.26144300	3.77071600	-2.36818900
H	-0.93497800	4.12539600	-0.74925500
H	0.80406800	3.69534500	-0.92352200

Scan Point for comp3_3_beta_2.0Å

C	-1.74922500	-0.48087600	-0.26562300
C	-1.60396400	0.62171900	0.78504600
C	0.75643800	-1.12063300	-0.40740700
C	-0.36497400	1.50372700	0.70270400
C	1.28500900	-0.33804100	0.81521200
H	-0.77535200	-2.15023800	0.70341500
H	-1.71811800	-0.00643400	-1.25330500
H	0.85511200	-0.51208600	-1.31325700
H	-2.46208100	1.28848100	0.66528200
H	-0.47630500	2.52515700	1.05832100
H	0.90568800	-0.76844400	1.74581100
O	-1.57925700	0.06504400	2.09963900
H	-2.00736500	0.67968800	2.71606100
O	-3.04861400	-1.03473600	-0.04803900
H	-3.18066500	-1.74348000	-0.69741800
O	-1.05376500	-2.44625200	-1.33151900

H	-0.42357300	-3.18426400	-1.34956200
O	1.51873400	-2.32220900	-0.53764300
H	2.31563000	-2.13782500	-1.05745700
C	2.79596200	-0.25718300	0.90207600
H	3.06374000	0.41934000	1.72192500
H	3.18081100	-1.25447300	1.13882200
O	3.31587500	0.21601700	-0.34342300
H	4.27800800	0.29462200	-0.26474800
O	0.84699900	1.08263400	0.82324100
O	-0.58688000	2.17126000	-1.16950200
H	-0.00303500	1.62261200	-1.72370900
C	-0.18197200	3.56122700	-1.29833600
H	-0.22972500	3.83720400	-2.35415700
H	-0.89859100	4.15170000	-0.72722100
H	0.83137800	3.70309500	-0.91305600

Scan Point for comp3_3_beta_2.1Å

C	-0.70292700	-1.58658600	-0.26018400
C	-1.75021200	-0.46898400	-0.25859100
C	-1.59976900	0.60881500	0.81692600
C	0.75123600	-1.11362100	-0.42165600
C	-0.35550600	1.48151800	0.76067300
C	1.28625300	-0.36541600	0.81960000
H	-0.78043800	-2.16481900	0.67051400
H	-1.71797700	0.02942500	-1.23395000
H	0.84554100	-0.47791100	-1.30931200
H	-2.45319300	1.28380200	0.71294900
H	-0.45810700	2.51356000	1.08644600
H	0.90282600	-0.80948000	1.74185500
O	-1.57581600	0.02348200	2.11979600
H	-2.00680900	0.62333300	2.74877300
O	-3.05126300	-1.02186500	-0.05130400
H	-3.18973700	-1.71127700	-0.71994600
O	-1.06546100	-2.41198100	-1.37028500
H	-0.43787800	-3.15142000	-1.40838600
O	1.51235600	-2.31013200	-0.58901300
H	2.30531200	-2.11191900	-1.10996600
C	2.79667500	-0.28847200	0.90765400
H	3.06633700	0.36868800	1.74253900
H	3.17822400	-1.29213800	1.12227200
O	3.31579900	0.21075000	-0.32737800
H	4.27814100	0.28645700	-0.24831900

O	0.84975300	1.05931900	0.85355500
O	-0.60651500	2.21181200	-1.19218800
H	-0.03454500	1.64954100	-1.74258500
C	-0.15250100	3.58378400	-1.30062100
H	-0.20627300	3.89253800	-2.34789400
H	-0.83385100	4.19023900	-0.70277600
H	0.87209400	3.68407800	-0.93048400

Scan Point for comp3_3_beta_2.2Å

C	-0.71870900	-1.57018700	-0.28900900
C	-1.75736000	-0.44366900	-0.24768200
C	-1.59617900	0.60296900	0.85745000
C	0.73444200	-1.09367400	-0.44067500
C	-0.34524000	1.46454000	0.82082900
C	1.27098400	-0.39607200	0.82987900
H	-0.79563200	-2.17922800	0.62185100
H	-1.72030700	0.08540400	-1.20651300
H	0.82054900	-0.41630200	-1.29786900
H	-2.44426800	1.28716600	0.77404400
H	-0.43572300	2.50792500	1.11200100
H	0.86806500	-0.85263800	1.73736500
O	-1.57143300	-0.01481100	2.14514100
H	-2.00002900	0.57092900	2.78904000
O	-3.06177300	-0.99104800	-0.05348900
H	-3.20900200	-1.65671100	-0.74410000
O	-1.09259000	-2.35256400	-1.42553600
H	-0.47912400	-3.10155400	-1.48925700
O	1.49784900	-2.27689100	-0.66626900
H	2.31778600	-2.03782000	-1.12591700
C	2.78067100	-0.34676100	0.93440400
H	3.05466700	0.30628600	1.77108800
H	3.14065900	-1.35730800	1.15464900
O	3.32094900	0.13821600	-0.29712300
H	4.28410800	0.19382800	-0.21040200
O	0.85271800	1.03679700	0.88910700
O	-0.62103200	2.26134300	-1.21117500
H	-0.12734100	1.66709200	-1.80091800
C	-0.05156700	3.58596700	-1.31654700
H	-0.10728200	3.92219000	-2.35602200
H	-0.65608100	4.24209900	-0.68848300
H	0.98921100	3.59163300	-0.97770800

Scan Point for comp3_3_beta_2.3Å

C	-0.63607000	-1.59784600	-0.30835800
C	-1.72026300	-0.51802400	-0.23716200
C	-1.60580600	0.49054600	0.90677500
C	0.79498200	-1.05677000	-0.46038600
C	-0.39604400	1.40430700	0.89930000
C	1.31941100	-0.36751100	0.81942200
H	-0.67882600	-2.22953300	0.58920500
H	-1.70145800	0.04617500	-1.17580400
H	0.84789300	-0.36208600	-1.30593800
H	-2.48362400	1.13913700	0.85066600
H	-0.53060400	2.44609700	1.18077300
H	0.96422600	-0.87552300	1.71966000
O	-1.54756100	-0.17230800	2.17071600
H	-1.99553900	0.37314300	2.83661500
O	-3.00202000	-1.12484400	-0.06835300
H	-3.12056200	-1.76787500	-0.78537800
O	-0.98142500	-2.37120700	-1.45961000
H	-0.33089000	-3.08621100	-1.54490100
O	1.60453300	-2.20454200	-0.71143300
H	2.37668100	-1.94125700	-1.23514200
C	2.82456000	-0.22262100	0.89495600
H	3.07470200	0.39214200	1.76746700
H	3.25488500	-1.21901800	1.04133200
O	3.29925900	0.37872300	-0.31110400
H	4.25787600	0.49638900	-0.23838100
O	0.81763100	1.03685700	0.93448800
O	-0.74562200	2.24898300	-1.21122500
H	-0.14784100	1.71923200	-1.76404300
C	-0.34314700	3.63261700	-1.30119300
H	-0.40496600	3.96736700	-2.34153500
H	-1.04315400	4.20858300	-0.69371800
H	0.67710500	3.77174900	-0.92884200

Scan Point for comp3_3_beta_2.4Å

C	-0.56161500	-1.61913500	-0.34357600
C	-1.69436000	-0.59483200	-0.22593700
C	-1.61419700	0.37585200	0.95390100
C	0.84327000	-1.01046600	-0.48474400
C	-0.45638800	1.35378300	0.95568400
C	1.34112500	-0.32867800	0.81026600

H	-0.56923900	-2.28407900	0.53039200
H	-1.71117400	0.00410200	-1.14315200
H	0.86318200	-0.29488600	-1.31445300
H	-2.52753100	0.97565900	0.93771600
H	-0.64160400	2.39137000	1.22509000
H	1.01080600	-0.87086800	1.69976600
O	-1.49283100	-0.32741200	2.19138800
H	-1.96291500	0.16370500	2.88376200
O	-2.94376000	-1.26749800	-0.06682500
H	-3.03647000	-1.89321800	-0.80278500
O	-0.88197600	-2.36543100	-1.51978400
H	-0.21559400	-3.06275600	-1.62426700
O	1.70269700	-2.11520900	-0.76055800
H	2.46699900	-1.80542300	-1.27036700
C	2.83760000	-0.11445900	0.88510500
H	3.06124900	0.49639000	1.76743900
H	3.31403200	-1.09220200	1.01409200
O	3.28082400	0.52740600	-0.31170400
H	4.23157400	0.69562000	-0.23507200
O	0.77192500	1.05071400	0.95698600
O	-0.83887000	2.26582800	-1.23106800
H	-0.13361000	1.81876100	-1.72659300
C	-0.58379300	3.68420700	-1.25553200
H	-0.57839600	4.04486600	-2.28958100
H	-1.39854900	4.16494000	-0.71115300
H	0.37331500	3.92319700	-0.77931100

Scan Point for comp3_3_beta_2.5Å

C	-0.38157800	-1.65816100	-0.38146200
C	-1.61824800	-0.77107100	-0.20018000
C	-1.61038600	0.14530700	1.02610000
C	0.94613800	-0.89215600	-0.51614900
C	-0.57712000	1.25403500	1.02451800
C	1.39204700	-0.20669300	0.79612600
H	-0.30004000	-2.35770000	0.46118800
H	-1.71728400	-0.13375200	-1.08625400
H	0.86861500	-0.14329200	-1.31275400
H	-2.58828800	0.63067500	1.07412500
H	-0.87656100	2.26620300	1.28764600
H	1.13488400	-0.80420600	1.67415400
O	-1.35245300	-0.59941700	2.21603800
H	-1.82052300	-0.18816600	2.95995500
O	-2.78491800	-1.57936700	-0.05153200

H	-2.84608800	-2.15715700	-0.82856500
O	-0.63731600	-2.38283800	-1.58624000
H	0.10943800	-2.98352600	-1.73744500
O	1.91734500	-1.87942000	-0.85602800
H	2.61658100	-1.46842200	-1.38730400
C	2.85619700	0.16997200	0.86125100
H	3.02001000	0.78206700	1.75598600
H	3.43766000	-0.75239000	0.96369500
O	3.21431600	0.88341200	-0.32319700
H	4.14632900	1.13867600	-0.25727900
O	0.67471200	1.09919600	0.98259100
O	-1.15298600	2.21573300	-1.21009900
H	-0.40876800	1.87694900	-1.73249300
C	-1.09402500	3.65467800	-1.20901200
H	-1.16760300	4.03786900	-2.23271500
H	-1.95002100	4.00861600	-0.63121600
H	-0.16610000	4.01370800	-0.75013700

Scan Point for comp3_3_beta_2.6Å

C	-0.29448000	-1.68713800	-0.39688700
C	-1.57197500	-0.86254100	-0.20497400
C	-1.60887700	0.02937700	1.03940000
C	0.99685400	-0.86131400	-0.52608900
C	-0.64273400	1.19610700	1.03545300
C	1.40327400	-0.15172000	0.78589900
H	-0.17936900	-2.38990400	0.43908300
H	-1.69947200	-0.21432900	-1.08066400
H	0.89014000	-0.12104800	-1.32657100
H	-2.61372300	0.45420000	1.10312200
H	-0.99943500	2.19384600	1.28274400
H	1.17481100	-0.75808600	1.66552600
O	-1.29636600	-0.71602200	2.21519800
H	-1.78772100	-0.34717200	2.96672200
O	-2.69721200	-1.72919100	-0.07530300
H	-2.69703900	-2.32896200	-0.83854600
O	-0.51933900	-2.41154600	-1.60775200
H	0.23724000	-3.00237500	-1.74802200
O	2.01417800	-1.80485400	-0.85342800
H	2.69388700	-1.36875900	-1.38968400
C	2.84403800	0.30421600	0.85389600
H	2.97423400	0.92146200	1.75058400
H	3.47244100	-0.58705400	0.95550800
O	3.16427400	1.03747900	-0.32867200

H	4.08189300	1.34061800	-0.26349500
O	0.61261600	1.11607000	0.96655600
O	-1.39413800	2.27428500	-1.20796500
H	-0.76470400	1.91237000	-1.85051500
C	-1.19167600	3.69644800	-1.12649800
H	-1.34965500	4.16422700	-2.10483000
H	-1.92914400	4.08642600	-0.42177000
H	-0.18303200	3.93415400	-0.76945900

Scan Point for comp3_3_beta_2.7Å

C	-0.34623700	-1.63382900	-0.48574100
C	-1.60795600	-0.81747300	-0.17410600
C	-1.58055500	-0.00574400	1.12634200
C	0.95464400	-0.81811000	-0.57210700
C	-0.60963700	1.15741500	1.12365700
C	1.38968000	-0.21986700	0.78688300
H	-0.21866100	-2.41549100	0.27464700
H	-1.77258300	-0.11171800	-0.99755600
H	0.84095800	-0.00827900	-1.30218300
H	-2.57838000	0.41948300	1.26308400
H	-0.95595300	2.16125500	1.36294100
H	1.13096600	-0.86663300	1.62750800
O	-1.22038100	-0.82510700	2.23511300
H	-1.64687700	-0.48200100	3.03677500
O	-2.73100700	-1.68639900	-0.04562100
H	-2.77884100	-2.22951300	-0.84846600
O	-0.62364300	-2.23368500	-1.75285400
H	0.08160000	-2.86855800	-1.95151900
O	1.95303700	-1.73826300	-1.00270800
H	2.67047200	-1.24162400	-1.42744800
C	2.84726800	0.17160900	0.87767800
H	2.99564600	0.77235200	1.78277000
H	3.43509600	-0.74756700	0.97524500
O	3.21321900	0.90078400	-0.29442600
H	4.14910200	1.14137900	-0.22724000
O	0.64119500	1.06464400	1.02654600
O	-1.35390800	2.34200500	-1.18563000
H	-0.71561900	1.96929900	-1.81284100
C	-1.12049100	3.75731900	-1.08811600
H	-1.24123500	4.23899500	-2.06535400
H	-1.86703800	4.15929200	-0.39966400
H	-0.11704800	3.96959400	-0.70098700

Scan Point for comp3_3_beta_2.8Å

C	0.08116700	-1.68667700	-0.48332900
C	-1.33554200	-1.19529500	-0.15754800
C	-1.47674300	-0.43109500	1.16431500
C	1.15206200	-0.58634700	-0.59119400
C	-0.84302900	0.94339500	1.13963000
C	1.44119900	0.12906600	0.74973400
H	0.40163100	-2.40894100	0.27855900
H	-1.66621600	-0.52810300	-0.96324300
H	0.85316100	0.15459800	-1.34047500
H	-2.54498400	-0.28225200	1.34349600
H	-1.43287500	1.82934800	1.36971200
H	1.38157300	-0.55365100	1.59967100
O	-0.87352700	-1.14765500	2.23658300
H	-1.32034600	-0.91609200	3.06677900
O	-2.22364300	-2.30526000	-0.04900500
H	-2.13388800	-2.83483700	-0.85771400
O	-0.05398700	-2.34343900	-1.74481900
H	0.78616000	-2.78258300	-1.94946400
O	2.33924000	-1.25895200	-1.00126200
H	2.88881000	-0.64950900	-1.51735600
C	2.74085200	0.89929500	0.80688100
H	2.76570400	1.47735300	1.73813100
H	3.55877400	0.17085600	0.83303900
O	2.83683100	1.75313700	-0.33334800
H	3.65629800	2.26491700	-0.26544100
O	0.38410300	1.17593600	0.99993700
O	-2.05874300	1.99389000	-1.15351100
H	-1.42818400	1.78468500	-1.85880400
C	-2.11577000	3.42216600	-1.00341000
H	-2.43330800	3.90132200	-1.93695000
H	-2.85501800	3.63408400	-0.22768600
H	-1.14466300	3.83050800	-0.69932400

Scan Point for comp3_3_beta_2.9Å

C	0.46029300	-1.62061700	-0.50284100
C	-1.02437600	-1.45926800	-0.14706000
C	-1.30110600	-0.76534700	1.19359700
C	1.26233400	-0.31014500	-0.60907100
C	-0.99258000	0.71649500	1.17190700

C	1.40793000	0.44134700	0.73523200
H	0.94594600	-2.26409200	0.24209500
H	-1.51040600	-0.86879000	-0.93395400
H	0.79912300	0.35209200	-1.34840800
H	-2.37135900	-0.85996700	1.39529800
H	-1.76770100	1.44746200	1.39850200
H	1.51623600	-0.24257800	1.57896500
O	-0.53173000	-1.34750400	2.23942900
H	-1.01268500	-1.25383600	3.07724700
O	-1.64481700	-2.73760000	-0.04288400
H	-1.47297800	-3.21983900	-0.86758600
O	0.45191700	-2.27363500	-1.77376500
H	1.36662700	-2.49966800	-2.00394100
O	2.56297000	-0.70425200	-1.03767300
H	2.95850700	0.01121900	-1.55888700
C	2.50162600	1.48431800	0.78351800
H	2.40561900	2.04959500	1.71815900
H	3.46197300	0.95729000	0.79705400
O	2.39210900	2.34153200	-0.35264400
H	3.10513500	2.99614200	-0.31302400
O	0.14528200	1.22140800	1.00915100
O	-2.55165200	1.51055400	-1.14083300
H	-1.94478900	1.48273000	-1.89554900
C	-2.95613600	2.87414200	-0.93704000
H	-3.45540900	3.27196600	-1.82861700
H	-3.66431400	2.87820500	-0.10526300
H	-2.10007700	3.51248600	-0.68778600

Scan Point for comp3_3_beta_3.0Å

C	-1.43991800	-0.86140000	-0.55696200
C	-1.72043000	0.59855800	-0.16942300
C	-1.17938700	1.01808400	1.20493000
C	0.04685000	-1.26326000	-0.61981800
C	0.32630700	1.15674900	1.21351300
C	0.76442000	-1.21395200	0.74962400
H	-1.94695200	-1.52713800	0.15302500
H	-1.26783300	1.25782800	-0.92192100
H	0.57760700	-0.62119000	-1.33118700
H	-1.58760500	2.00784100	1.42389100
H	0.79426500	2.11424800	1.44323400
H	0.11316700	-1.52469500	1.56808900
O	-1.54410600	0.07903300	2.20728600
H	-1.59075600	0.53114600	3.06532800

O	-3.12497100	0.82424900	-0.10570000
H	-3.50614400	0.55542900	-0.95699200
O	-2.02506200	-1.00483900	-1.85319300
H	-2.03076100	-1.94726900	-2.08188100
O	0.04502700	-2.61575600	-1.06528700
H	0.86399000	-2.79140400	-1.55234600
C	2.07162000	-1.96902400	0.82881900
H	2.55665700	-1.73158800	1.78318900
H	1.83684000	-3.03956200	0.82071500
O	2.90321000	-1.60873900	-0.27340000
H	3.74274300	-2.08568800	-0.19038400
O	1.14444300	0.21919400	1.05319700
O	0.90552400	2.89256300	-1.16376700
H	0.98751000	2.29486500	-1.92145700
C	2.20273400	3.44077300	-0.87294500
H	2.60773500	3.97961600	-1.73789300
H	2.07501200	4.14637300	-0.04831600
H	2.90882200	2.65638800	-0.57459900

Scan Point for comp3_3_beta_3.1Å

C	1.16579100	-1.21826800	-0.56026000
C	-0.20050000	-1.79649700	-0.15699200
C	-0.70436200	-1.35666200	1.22737300
C	1.24370900	0.32048900	-0.63313400
C	-1.16864400	0.08249800	1.21972000
C	1.04896300	1.01715200	0.73229500
H	1.92837500	-1.56880400	0.14670600
H	-0.94668800	-1.49296400	-0.90262600
H	0.49811100	0.70013100	-1.34070400
H	-1.57650700	-1.97079700	1.46571700
H	-2.20715400	0.33505200	1.43082200
H	1.49201800	0.44996900	1.55150600
O	0.30640000	-1.50361900	2.21528400
H	-0.11507500	-1.64144000	3.07919300
O	-0.12565800	-3.21772800	-0.09714200
H	0.20740000	-3.53113700	-0.95428200
O	1.42023500	-1.76582400	-1.85584900
H	2.33947100	-1.56716500	-2.09471300
O	2.56271500	0.60436900	-1.08568100
H	2.55620600	1.43234400	-1.58928100
C	1.50568200	2.45524400	0.80441600
H	1.16870700	2.88109500	1.75683900
H	2.60155400	2.45175700	0.80093600

O	0.98373300	3.18331900	-0.30468600
H	1.26398100	4.10747300	-0.22306700
O	-0.43255700	1.08183400	1.03725600
O	-3.10995400	0.26895800	-1.18995800
H	-2.56660900	0.59712400	-1.92047200
C	-4.01121400	1.31162500	-0.78889600
H	-4.65995600	1.61145300	-1.62130200
H	-4.63111600	0.91057700	0.01637600
H	-3.46859400	2.19136700	-0.42257500

Scan Point for comp3_3_beta_3.2Å

C	1.10451100	-1.26217700	-0.57431700
C	-0.27854200	-1.77749100	-0.14536900
C	-0.72461300	-1.32400900	1.25276300
C	1.25699700	0.26991300	-0.64284500
C	-1.12255900	0.13342400	1.25672300
C	1.12226600	0.97611900	0.72818700
H	1.86549600	-1.65471000	0.11173900
H	-1.02491500	-1.42259400	-0.86909500
H	0.52066700	0.68542200	-1.33874300
H	-1.61993700	-1.89512300	1.51347800
H	-2.14882800	0.43117800	1.47696100
H	1.56508200	0.39393500	1.53787600
O	0.30583000	-1.52236400	2.20975900
H	-0.09664800	-1.65512300	3.08280800
O	-0.27851400	-3.20049700	-0.10405600
H	0.05971500	-3.51859900	-0.95706800
O	1.29934600	-1.81367400	-1.87753400
H	2.22500700	-1.67475400	-2.13074200
O	2.58013300	0.49165900	-1.12121800
H	2.59721200	1.30286800	-1.65155800
C	1.63133700	2.39876500	0.78023700
H	1.32596600	2.84513800	1.73394700
H	2.72609800	2.36207400	0.75338900
O	1.10591700	3.13333000	-0.32493300
H	1.40494000	4.05181800	-0.25219600
O	-0.34626200	1.09953500	1.06756400
O	-3.13456300	0.41934900	-1.21513600
H	-2.63557200	0.78991600	-1.95763800
C	-4.02630300	1.42920400	-0.71973000
H	-4.72309100	1.75965000	-1.49967100
H	-4.59857400	0.97981300	0.09519700
H	-3.47628700	2.29790200	-0.33815900

Scan Point for comp3_3_beta_3.3Å

C	1.16068800	-1.20283900	-0.60004200
C	-0.18341900	-1.78931000	-0.13981000
C	-0.61538600	-1.36690900	1.27241500
C	1.23461600	0.33537400	-0.66143600
C	-1.08541600	0.06870700	1.29692700
C	1.10022900	1.02579900	0.71765700
H	1.95769800	-1.56076800	0.06364500
H	-0.96497100	-1.46795900	-0.84176200
H	0.46067800	0.71753800	-1.33531800
H	-1.47406100	-1.98365600	1.55178400
H	-2.11925100	0.31341800	1.54532900
H	1.59221900	0.46172600	1.51161100
O	0.44800900	-1.51891900	2.20143400
H	0.07529200	-1.67671300	3.08348900
O	-0.11131100	-3.21074700	-0.10865200
H	0.22028100	-3.50658900	-0.97220400
O	1.34920000	-1.73620600	-1.91172100
H	2.25991200	-1.54957200	-2.18745000
O	2.53219000	0.62604300	-1.17182000
H	2.49493600	1.44019600	-1.69657600
C	1.53884700	2.47179200	0.76697700
H	1.23611300	2.89666000	1.73129900
H	2.63304600	2.49019300	0.71213700
O	0.94922600	3.18560500	-0.31925300
H	1.20400900	4.11742100	-0.24768700
O	-0.36339400	1.07357500	1.09514300
O	-3.23757900	0.27424800	-1.19625300
H	-2.77676000	0.67380700	-1.94831100
C	-4.16517400	1.23548300	-0.67081900
H	-4.89714300	1.53595700	-1.43039300
H	-4.69347300	0.75302500	0.15481300
H	-3.64916900	2.12793900	-0.29663300

Scan Point for comp3_3_beta_3.5Å

C	1.11083700	-1.24702500	-0.63833300
C	-0.24000100	-1.76723300	-0.12162000
C	-0.59176600	-1.32658900	1.30915100
C	1.25631300	0.28520200	-0.69488000

C	-0.99204200	0.13033800	1.34583500
C	1.21693800	0.97158400	0.69190000
H	1.91764100	-1.64990200	-0.01333800
H	-1.03292900	-1.40538700	-0.79135600
H	0.46855700	0.70886000	-1.32749300
H	-1.46752100	-1.90126700	1.62313300
H	-2.00823600	0.42393400	1.61576300
H	1.70127400	0.37511200	1.46634200
O	0.50055300	-1.53399000	2.19184200
H	0.15919200	-1.65895500	3.09174800
O	-0.23884000	-3.18996700	-0.09279100
H	-0.00200000	-3.50332300	-0.98067100
O	1.21222800	-1.77813200	-1.96051400
H	2.10242200	-1.58906200	-2.29566300
O	2.53852800	0.51818600	-1.26783500
H	2.52324300	1.36127900	-1.74651300
C	1.74650700	2.38678800	0.72771200
H	1.49426700	2.83330400	1.69662900
H	2.83826200	2.33157200	0.64911800
O	1.18266100	3.13416700	-0.34932800
H	1.49086000	4.04992700	-0.28126400
O	-0.23027600	1.09889200	1.11655600
O	-3.47828600	0.38780500	-1.10412500
H	-3.04042200	0.75151400	-1.88746500
C	-4.37357100	1.38220900	-0.58339500
H	-5.13554600	1.65679800	-1.32278800
H	-4.86792800	0.94391100	0.28691900
H	-3.83297000	2.28435200	-0.27175800

Scan Point for comp3_3_beta_3.6Å

C	1.10445600	-1.28088100	-0.61930500
C	-0.26924300	-1.74459800	-0.10926600
C	-0.61598100	-1.27237900	1.31319100
C	1.30445000	0.24406400	-0.69742600
C	-0.96865800	0.19675000	1.31988400
C	1.27463300	0.95335100	0.67824200
H	1.89010200	-1.70262800	0.02000200
H	-1.04197400	-1.36166500	-0.79153400
H	0.53844900	0.68543600	-1.34457600
H	-1.51268700	-1.81295400	1.62862200
H	-1.98015700	0.52805200	1.56419000
H	1.72969400	0.35356000	1.46768000
O	0.46240900	-1.50295300	2.20662900

H	0.11087400	-1.60119300	3.10595400
O	-0.32158500	-3.16548600	-0.06245000
H	-0.09079700	-3.49941900	-0.94439100
O	1.19996400	-1.83555700	-1.93224300
H	2.09796600	-1.67816000	-2.26302900
O	2.59968400	0.42263800	-1.25996100
H	2.62130700	1.26168300	-1.74560700
C	1.85132300	2.35024000	0.69588000
H	1.60411400	2.82320500	1.65348700
H	2.94136200	2.25592500	0.63113300
O	1.32582400	3.09635500	-0.40122200
H	1.66473100	4.00212800	-0.34677000
O	-0.17333500	1.13568500	1.08238000
O	-3.62890800	0.42654000	-1.09470300
H	-3.34224600	0.71116200	-1.97471500
C	-4.48381400	1.44211800	-0.54709600
H	-5.36220800	1.60700500	-1.18262300
H	-4.81711100	1.08783000	0.43137100
H	-3.94683000	2.39027400	-0.42125500

Scan Point for comp3_3_beta_3.7Å

C	1.07736300	-1.29656100	-0.63014000
C	-0.29865100	-1.72533900	-0.09723300
C	-0.60443900	-1.24830600	1.33275800
C	1.31332000	0.22282000	-0.71379500
C	-0.91807500	0.22934900	1.34951100
C	1.32991100	0.93264000	0.66168800
H	1.86240400	-1.73682100	-0.00270500
H	-1.07448600	-1.31993800	-0.76351000
H	0.54641200	0.68320000	-1.34644000
H	-1.50837900	-1.76628600	1.66508600
H	-1.91529000	0.58682500	1.61491700
H	1.78867400	0.32189600	1.44067100
O	0.48516700	-1.50865000	2.20382300
H	0.14964200	-1.59616900	3.11041700
O	-0.38761900	-3.14438400	-0.05212500
H	-0.17759800	-3.48268400	-0.93754400
O	1.13932800	-1.85489200	-1.94338000
H	2.03486400	-1.71565200	-2.28902000
O	2.60167100	0.36805100	-1.30148800
H	2.63608200	1.20573000	-1.78876300
C	1.93801600	2.31601100	0.66619300
H	1.72916300	2.79162500	1.63170300

H	3.02341000	2.19751900	0.57035700
O	1.39813800	3.07664500	-0.41359600
H	1.75474800	3.97584700	-0.36406300
O	-0.10430900	1.14850900	1.09743300
O	-3.70780600	0.47290900	-1.06875900
H	-3.44089000	0.75386300	-1.95610800
C	-4.57223400	1.47793700	-0.51654800
H	-5.46823800	1.61504700	-1.13381500
H	-4.87527100	1.13028100	0.47411700
H	-4.05308800	2.43890500	-0.41517100

Scan Point for comp3_3_beta_3.8Å

C	1.14702900	-1.27927900	-0.61080000
C	-0.22860100	-1.73670600	-0.09968700
C	-0.57585300	-1.25003400	1.31810000
C	1.34910500	0.24476900	-0.70393900
C	-0.93249300	0.21748000	1.30128900
C	1.31261900	0.96968600	0.66357700
H	1.93023700	-1.69522300	0.03528000
H	-0.99967300	-1.35819800	-0.78666000
H	0.58693900	0.67977400	-1.35983600
H	-1.47172300	-1.78839000	1.63972100
H	-1.94795700	0.54882800	1.52848900
H	1.76358600	0.37920900	1.46220900
O	0.50282400	-1.46806800	2.21372100
H	0.15164500	-1.55516300	3.11427500
O	-0.28368800	-3.15685400	-0.04040000
H	-0.05582200	-3.49909300	-0.91992600
O	1.24606000	-1.84724500	-1.91774600
H	2.14542500	-1.69447100	-2.24704700
O	2.64742300	0.41625600	-1.26136700
H	2.67188500	1.24962200	-1.75662700
C	1.88796700	2.36714200	0.66765000
H	1.63499800	2.85163900	1.61801200
H	2.97841900	2.27297700	0.61019200
O	1.36810400	3.09940800	-0.44141200
H	1.70812800	4.00537700	-0.39804900
O	-0.13832100	1.15517200	1.05585900
O	-3.83824900	0.42904300	-1.13833600
H	-3.68843200	0.77135900	-2.03177200
C	-4.72328800	1.32737600	-0.45170600
H	-5.68206900	1.41959900	-0.97627800
H	-4.90205500	0.90502800	0.53999300

H	-4.27566100	2.32282400	-0.34143000

Scan Point for comp3_3_beta_3.9Å

C	1.16184000	-1.27630800	-0.60907200
C	-0.21099900	-1.73788400	-0.09369600
C	-0.55661800	-1.24685100	1.32324700
C	1.35846200	0.24821800	-0.70770900
C	-0.92309700	0.21779900	1.29557200
C	1.31821800	0.97868700	0.65685100
H	1.94778200	-1.68718300	0.03692300
H	-0.98511200	-1.36504000	-0.78031400
H	0.59509400	0.67775600	-1.36582300
H	-1.44830200	-1.78883500	1.65046900
H	-1.94256800	0.54304800	1.51415300
H	1.77070600	0.39319300	1.45821200
O	0.52642300	-1.45393500	2.21579100
H	0.17980400	-1.53413500	3.11873100
O	-0.25999700	-3.15793800	-0.02947000
H	-0.03560200	-3.50219700	-0.90911100
O	1.26061300	-1.84810300	-1.91433700
H	2.15899800	-1.69368300	-2.24553500
O	2.65641100	0.42235000	-1.26512500
H	2.67772700	1.25346200	-1.76431100
C	1.88741200	2.37858500	0.65583400
H	1.63198800	2.86560000	1.60427000
H	2.97829800	2.28894400	0.59925900
O	1.36502000	3.10459200	-0.45615300
H	1.70267000	4.01166000	-0.41706600
O	-0.13460700	1.15901300	1.04548200
O	-3.96026800	0.36807300	-1.14634700
H	-3.80642600	0.70841500	-2.03981600
C	-4.73967400	1.33200300	-0.42144300
H	-5.71053300	1.50230100	-0.90264900
H	-4.90794800	0.92134800	0.57701000
H	-4.20859400	2.28742800	-0.33064200

Scan Point for comp3_3_beta_4.0Å

C	1.18368700	-1.27161100	-0.60696900
C	-0.18686900	-1.73881800	-0.08999300
C	-0.53412000	-1.24394300	1.32556200

C	1.37339200	0.25360700	-0.71076300
C	-0.91154400	0.21735500	1.28696600
C	1.32613800	0.98946100	0.65081400
H	1.97153100	-1.67652700	0.04044500
H	-0.96289600	-1.37267100	-0.77796600
H	0.60966200	0.67679700	-1.37255800
H	-1.42161900	-1.79043200	1.65674700
H	-1.93558600	0.53578900	1.49501000
H	1.77983200	0.40940000	1.45536800
O	0.55188700	-1.43927500	2.21678600
H	0.20827900	-1.51277800	3.12142000
O	-0.22829400	-3.15880700	-0.02088900
H	-0.00429900	-3.50482300	-0.89996300
O	1.28534800	-1.84713900	-1.91036500
H	2.18343100	-1.69079500	-2.24146300
O	2.67185100	0.43176300	-1.26565000
H	2.68991100	1.26001900	-1.76967100
C	1.88730900	2.39256300	0.64589800
H	1.62776500	2.88112800	1.59243300
H	2.97877400	2.30912500	0.59115600
O	1.36235000	3.11220700	-0.46903400
H	1.69658200	4.02070400	-0.43356500
O	-0.12910400	1.16275800	1.03376900
O	-4.07393400	0.33575100	-1.15950500
H	-3.92933700	0.70144900	-2.04441600
C	-4.80758000	1.29680600	-0.38538200
H	-5.78670700	1.50573800	-0.83340100
H	-4.95860700	0.86151000	0.60543600
H	-4.25003500	2.23579000	-0.28270200

Scan Point for comp3_3_beta_4.1Å

C	1.19915600	-1.27709800	-0.59238100
C	-0.17721400	-1.73709200	-0.08404600
C	-0.53381000	-1.22817100	1.32450200
C	1.39630900	0.24667700	-0.71042600
C	-0.91207600	0.23143200	1.26241700
C	1.33197800	0.99902700	0.64160500
H	1.97935200	-1.67723900	0.06706000
H	-0.94671300	-1.37562400	-0.78173900
H	0.64595700	0.66503100	-1.39007400
H	-1.42312900	-1.77147900	1.65613500
H	-1.93971400	0.55123700	1.44984100
H	1.77828700	0.42820000	1.45684500

O	0.54729600	-1.41327100	2.22338000
H	0.19982500	-1.47079600	3.12763600
O	-0.22220900	-3.15621900	-0.00266700
H	0.00773200	-3.51058200	-0.87688900
O	1.31315400	-1.86582400	-1.88890900
H	2.21752000	-1.72169000	-2.20828400
O	2.70508800	0.41174500	-1.24527300
H	2.73278000	1.22328200	-1.77503300
C	1.88914600	2.40378600	0.62980200
H	1.62720900	2.89538300	1.57417500
H	2.98090700	2.32368800	0.57651500
O	1.36239700	3.11790000	-0.48780700
H	1.69469100	4.02723000	-0.45577500
O	-0.12774100	1.17426600	1.00574400
O	-4.18225400	0.31970700	-1.20903800
H	-4.06214100	0.73092400	-2.07754300
C	-4.81379000	1.27130000	-0.33910700
H	-5.79297500	1.57719000	-0.72737300
H	-4.95539200	0.77839800	0.62573600
H	-4.18823600	2.16124600	-0.19885900

Scan Point for comp3_3_beta_4.2Å

C	1.20513200	-1.27632700	-0.59389100
C	-0.16990700	-1.73716800	-0.08290100
C	-0.52431000	-1.22836300	1.32616100
C	1.40046600	0.24751400	-0.71328500
C	-0.90365700	0.23111100	1.26569600
C	1.33813600	1.00062500	0.63834500
H	1.98687300	-1.67525400	0.06447300
H	-0.94096100	-1.37642400	-0.77927500
H	0.64833700	0.66466800	-1.39171000
H	-1.41248000	-1.77242600	1.65959500
H	-1.93021500	0.55053800	1.45905300
H	1.78690700	0.43080400	1.45295100
O	0.55862400	-1.41224500	2.22316400
H	0.21280700	-1.47043000	3.12802300
O	-0.21373000	-3.15633900	-0.00119100
H	0.01538600	-3.51068400	-0.87564100
O	1.31740500	-1.86583500	-1.89020600
H	2.22061600	-1.71971200	-2.21194600
O	2.70804400	0.41361200	-1.25078600
H	2.73391300	1.22491200	-1.78100200
C	1.89368900	2.40600300	0.62450700

H	1.63336500	2.89786100	1.56919100
H	2.98541600	2.32707000	0.56880500
O	1.36366000	3.11889300	-0.49231600
H	1.69534000	4.02850600	-0.46180900
O	-0.12088000	1.17445500	1.00629200
O	-4.26241300	0.33385100	-1.25385800
H	-4.17377600	0.79794200	-2.09920300
C	-4.80837800	1.24681400	-0.28951700
H	-5.78970800	1.62069000	-0.60632200
H	-4.92723000	0.69202200	0.64426900
H	-4.13729500	2.09751800	-0.11892600

Scan Point for comp3_3_beta_4.3Å

C	1.21413100	-1.27616300	-0.59719800
C	-0.15904900	-1.73503500	-0.07946500
C	-0.50694200	-1.22358400	1.33032900
C	1.41073600	0.24733800	-0.71871100
C	-0.88516200	0.23622700	1.26844500
C	1.35548700	1.00167500	0.63259200
H	1.99847700	-1.67558000	0.05779000
H	-0.93267800	-1.37471300	-0.77318900
H	0.65573600	0.66492800	-1.39372100
H	-1.39430500	-1.76611800	1.66840800
H	-1.91140100	0.55665700	1.46278800
H	1.80608300	0.43176900	1.44609700
O	0.57961400	-1.40741000	2.22291300
H	0.23778600	-1.46135400	3.12956500
O	-0.20385900	-3.15397600	0.00451300
H	0.01818100	-3.50989200	-0.87111300
O	1.31948000	-1.86678600	-1.89356400
H	2.22000300	-1.71805400	-2.22162000
O	2.71577700	0.41132700	-1.26285500
H	2.74052500	1.22312900	-1.79239700
C	1.91383900	2.40579700	0.61512800
H	1.65851000	2.89930100	1.56031800
H	3.00516200	2.32419100	0.55507900
O	1.38099100	3.11865300	-0.50037200
H	1.71434600	4.02771900	-0.47184800
O	-0.10218800	1.17833000	1.00524300
O	-4.36255000	0.33301500	-1.25906800
H	-4.30149800	0.81367700	-2.09740300
C	-4.86628200	1.22942600	-0.25740700
H	-5.85750200	1.61290700	-0.52840500

H	-4.95057500	0.65768300	0.66993300
H	-4.18551600	2.07443900	-0.09703800

Scan Point for comp3_3_beta_4.4Å

C	1.22343200	-1.27993800	-0.59712900
C	-0.15079500	-1.72995100	-0.07457900
C	-0.49339200	-1.21080500	1.33370500
C	1.42777800	0.24214200	-0.72419300
C	-0.86353800	0.25095900	1.26656800
C	1.38063100	1.00091800	0.62495400
H	2.00733800	-1.68127200	0.05724400
H	-0.92390800	-1.36877200	-0.76836500
H	0.67301100	0.66179700	-1.39820800
H	-1.38326600	-1.74696100	1.67539200
H	-1.88796500	0.57810100	1.45989900
H	1.82953900	0.43063400	1.43912900
O	0.59369800	-1.39759000	2.22494000
H	0.25354300	-1.44312700	3.13269100
O	-0.20264600	-3.14826900	0.01548800
H	0.00980300	-3.50916400	-0.86043600
O	1.32258500	-1.87520900	-1.89184700
H	2.22155400	-1.72733300	-2.22461500
O	2.73200000	0.39693200	-1.27302200
H	2.76031300	1.20743800	-1.80440100
C	1.94762000	2.40138000	0.60219400
H	1.69918000	2.89852100	1.54733800
H	3.03816700	2.31252900	0.53809700
O	1.41490100	3.11517100	-0.51273100
H	1.75288000	4.02259500	-0.48665000
O	-0.07524000	1.18757900	0.99957100
O	-4.46921500	0.33247400	-1.25382700
H	-4.43882700	0.81725900	-2.09139700
C	-4.95479500	1.21810500	-0.23398700
H	-5.96149400	1.58414300	-0.46964200
H	-4.99639600	0.64351300	0.69460100
H	-4.28377200	2.07454000	-0.09446100

Oxocarbenium Compound 3, Conformer 7

Scan Point for comp3_7_alpha_1.4Å

C	-1.01330300	-1.19244200	0.77043600
C	-1.40905100	-0.80042900	-0.66372500
C	-1.36555000	0.70137000	-1.01139200
C	0.36855700	-0.70494300	1.24267200
C	0.04833300	1.35614000	-0.87705600
C	1.46733500	-0.39410700	0.21272500
H	-1.75494700	-0.78431600	1.46980800
H	-0.74971300	-1.32533400	-1.35896900
H	0.76056100	-1.43545900	1.95045800
H	-1.61797200	0.75634500	-2.07359900
H	0.22398500	1.99888000	-1.74255700
H	2.24430200	0.16916600	0.74662700
O	-2.39324700	1.44129800	-0.36060200
H	-2.20134600	1.52540900	0.58635900
O	-2.71863900	-1.31246500	-0.92612600
H	-3.36466100	-0.73125400	-0.48963400
O	-0.98238200	-2.61757100	0.88380200
H	-1.81093100	-2.95576500	0.50579300
O	0.12848700	0.50955900	2.08423600
H	0.82465400	0.61852300	2.76277200
C	2.10865700	-1.67527700	-0.31318000
H	2.39069500	-2.30574100	0.53856600
H	1.40499700	-2.22704300	-0.94622600
O	3.27086000	-1.29985100	-1.05915200
H	3.63373100	-2.09477500	-1.47680100
O	1.07986300	0.38473400	-0.94707900
C	1.10962300	3.21086400	0.25584000
H	0.87221200	3.88760200	-0.56785000
H	2.11200700	2.79288700	0.13953800
H	1.01541300	3.72762900	1.21069000
O	0.11623000	2.14615500	0.27675000
H	0.12001900	1.36133000	1.43247200

Scan Point for comp3_7_alpha_1.5Å

C	-1.05401100	-1.15434500	0.79891200
C	-1.43593300	-0.77009000	-0.64003700
C	-1.32523700	0.71763400	-1.02578500
C	0.33813200	-0.69296900	1.27072700
C	0.11283300	1.30848600	-0.91193700
C	1.45019600	-0.48150300	0.23034200
H	-1.78561200	-0.72019800	1.49298800
H	-0.80106900	-1.33409500	-1.32755100
H	0.70548500	-1.44143500	1.97559600

H	-1.55430300	0.75243000	-2.09472100
H	0.30684400	1.97822400	-1.74883600
H	2.27046400	0.02180000	0.75705100
O	-2.32288800	1.52812800	-0.42126700
H	-2.17089300	1.60607400	0.53350700
O	-2.76506900	-1.22704700	-0.90325500
H	-3.38869500	-0.61642200	-0.47468600
O	-1.06501200	-2.58040500	0.92255700
H	-1.90945300	-2.89875800	0.56380900
O	0.14583400	0.53835200	2.04244800
H	0.85614600	0.62866300	2.70227600
C	1.99954100	-1.78833000	-0.32782800
H	2.23126900	-2.45505000	0.51158500
H	1.26731600	-2.27935200	-0.97737600
O	3.19018200	-1.47685200	-1.06003200
H	3.50419000	-2.28643000	-1.48888300
O	1.13343800	0.37341600	-0.91670600
C	1.23774900	3.22457000	0.26678400
H	1.01854100	3.89237500	-0.56563500
H	2.21090700	2.74551300	0.15503100
H	1.15709700	3.74904700	1.21788100
O	0.17890800	2.20639000	0.28781400
H	0.17900000	1.58103700	1.18843100

Scan Point for comp3_7_alpha_1.6Å

C	1.42851900	0.66435600	0.79988500
C	1.63378700	0.16605700	-0.63783400
C	0.96021200	-1.16386400	-1.01964600
C	-0.03360600	0.75755400	1.27499700
C	-0.59566300	-1.14180600	-0.95194900
C	-1.13764100	1.00626000	0.23533400
H	1.94476600	-0.01327300	1.49236900
H	1.25948800	0.92865000	-1.32568400
H	-0.08746200	1.58986400	1.98059300
H	1.17205900	-1.29324300	-2.08557400
H	-1.02802600	-1.69722800	-1.78251300
H	-2.08938200	0.87062000	0.76148900
O	1.54991000	-2.29773600	-0.40248800
H	1.38677500	-2.29899400	0.55377400
O	3.03443500	0.08276900	-0.90813200
H	3.39042300	-0.70187800	-0.45829300
O	1.97792200	1.98138800	0.92098100
H	2.88022200	1.95712000	0.56252800

O	-0.32276800	-0.45575300	2.02676900
H	-1.00550500	-0.26433700	2.69161000
C	-1.12942900	2.41528500	-0.34053700
H	-1.03506700	3.12586800	0.48914700
H	-0.28790200	2.55984800	-1.02597800
O	-2.37287500	2.60851800	-1.02423100
H	-2.35591800	3.48014400	-1.44629000
O	-1.21183100	0.07092100	-0.90172200
C	-2.45192100	-2.45799700	0.25879500
H	-2.59030100	-3.07650000	-0.62694300
H	-3.09319100	-1.57594400	0.23783900
H	-2.60857300	-3.04028300	1.16649800
O	-1.04135100	-2.05571600	0.28341700
H	-0.80548200	-1.50063300	1.14441000

Scan Point for comp3_7_alpha_1.7Å

C	1.42791400	-0.56216600	0.84289100
C	1.28713600	-0.99778500	-0.62134600
C	-0.11686000	-1.42423000	-1.08202000
C	0.49308300	0.57505600	1.29445100
C	-1.20932700	-0.33048600	-0.98921000
C	-0.06773700	1.54172100	0.24012700
H	1.22242700	-1.42214300	1.49423100
H	1.60853600	-0.17625800	-1.26627900
H	1.06509600	1.19995100	1.98511200
H	-0.02478200	-1.59138300	-2.16083000
H	-1.93805700	-0.41961900	-1.79147000
H	-0.79168500	2.17668700	0.76237300
O	-0.51903500	-2.67950200	-0.56147400
H	-0.67461000	-2.61803300	0.39413100
O	2.20778100	-2.05592800	-0.88888500
H	1.85404900	-2.87562900	-0.50377000
O	2.76631500	-0.10541300	1.06438300
H	3.36592200	-0.78039700	0.70511500
O	-0.58820200	-0.02829500	2.05303500
H	-0.96931500	0.63551700	2.65387800
C	0.97789000	2.45666500	-0.38006700
H	1.58629400	2.87644900	0.42987000
H	1.63595900	1.91291200	-1.06478800
O	0.28258400	3.49666600	-1.07622900
H	0.93274300	4.03200600	-1.55465700
O	-0.86991200	0.95838300	-0.85637400
C	-3.50515200	-0.09263700	0.29390600

H	-4.03509700	-0.40738600	-0.60456700
H	-3.35205700	0.98794400	0.30591400
H	-4.03651800	-0.42087000	1.18796000
O	-2.21710000	-0.78412300	0.30253600
H	-1.67004500	-0.52086800	1.13944900

Scan Point for comp3_7_alpha_1.8Å

C	1.46946100	-0.47786100	0.84622000
C	1.36314800	-0.89731400	-0.62345200
C	-0.00909600	-1.40544700	-1.09936800
C	0.46418400	0.59750600	1.30124400
C	-1.16706100	-0.38717300	-1.02079800
C	-0.15745400	1.53385000	0.25123600
H	1.30391900	-1.35748300	1.48209400
H	1.63872800	-0.04850100	-1.25301100
H	1.00259400	1.25616100	1.98713100
H	0.10018200	-1.55600300	-2.18022000
H	-1.91386600	-0.53250300	-1.80004900
H	-0.91503600	2.12576000	0.77475100
O	-0.33620000	-2.68628000	-0.59191300
H	-0.49747200	-2.64156500	0.36384700
O	2.34572900	-1.89656300	-0.90158400
H	2.04135600	-2.74013100	-0.52671700
O	2.77799800	0.05386600	1.08509400
H	3.42017100	-0.58989300	0.74263400
O	-0.56776000	-0.07496500	2.06098000
H	-0.98550900	0.56783100	2.65855700
C	0.81857700	2.51092600	-0.38658600
H	1.40235100	2.97428000	0.41848500
H	1.50877600	2.01518000	-1.07495400
O	0.04542500	3.49820900	-1.07694900
H	0.65143200	4.07581900	-1.56275100
O	-0.95311700	0.90413400	-0.83514600
C	-3.51237300	-0.30732000	0.30208800
H	-4.03680500	-0.65445200	-0.58815600
H	-3.38950900	0.77746800	0.28842900
H	-4.04356300	-0.62460000	1.20086800
O	-2.21463100	-0.96873600	0.32247600
H	-1.68362400	-0.68768200	1.14188800

Scan Point for comp3_7_alpha_1.9Å

C	1.46416700	-0.59387800	0.83180000
C	1.29679500	-1.02081600	-0.63095400
C	-0.12273100	-1.40028900	-1.08430100
C	0.53387300	0.53873200	1.30753300
C	-1.16670400	-0.26518600	-1.04331900
C	-0.00591000	1.53809900	0.27329600
H	1.26915800	-1.45687800	1.48124900
H	1.64001500	-0.20939900	-1.27713000
H	1.11532400	1.14689500	2.00649400
H	-0.03681700	-1.58698400	-2.16238200
H	-1.92944400	-0.34030500	-1.81594700
H	-0.71255800	2.18425100	0.80263700
O	-0.57506700	-2.62847700	-0.54665300
H	-0.74911200	-2.53884600	0.40340000
O	2.17872000	-2.10778300	-0.91146900
H	1.81413300	-2.91298600	-0.50652700
O	2.80588600	-0.13605900	1.03335900
H	3.40381700	-0.82046600	0.69079200
O	-0.55047700	-0.07063000	2.04021400
H	-0.88911300	0.56529400	2.69055000
C	1.03704400	2.43554500	-0.37529500
H	1.67134800	2.84105900	0.42244600
H	1.66946500	1.88742200	-1.07984600
O	0.33721000	3.48694900	-1.04795700
H	0.98212000	4.01939200	-1.53678300
O	-0.87145100	0.98516900	-0.80807000
C	-3.59233300	-0.00528200	0.26995100
H	-4.14216500	-0.32532600	-0.61550700
H	-3.36485700	1.06264200	0.21942000
H	-4.17039500	-0.22601500	1.17025100
O	-2.37469400	-0.79210200	0.32530100
H	-1.83713300	-0.54783200	1.13681200

Scan Point for comp3_7_alpha_2.0Å

C	-0.30107500	1.36169700	0.91930400
C	-0.14331600	1.59219300	-0.58702000
C	0.85327100	0.65196600	-1.31402100
C	-0.86943200	-0.02008700	1.32498100
C	0.80041300	-0.84082800	-1.03892700
C	-1.32113900	-1.02586200	0.25034000
H	0.68222700	1.46264600	1.39682000
H	-1.11981700	1.49722500	-1.06388300

H	-1.77063800	0.16806100	1.91764800
H	0.59030400	0.69184800	-2.38196600
H	1.45371900	-1.43600000	-1.67390200
H	-1.56104300	-1.94643400	0.78928200
O	2.18846900	1.11720900	-1.22930100
H	2.58285200	0.76804300	-0.40985600
O	0.25217400	2.94019800	-0.82731300
H	1.21885300	2.99242600	-0.72470500
O	-1.19107400	2.34481300	1.45507800
H	-0.86298900	3.21527600	1.17446700
O	0.12455000	-0.63077900	2.17187400
H	-0.25239200	-1.40746600	2.61631500
C	-2.54533700	-0.68179100	-0.58839300
H	-3.26642100	-0.16257300	0.05489100
H	-2.29698000	-0.03453400	-1.43383800
O	-3.08643600	-1.91850600	-1.06353000
H	-3.82542300	-1.71972400	-1.65777800
O	-0.22859100	-1.51317000	-0.64132100
C	2.90381700	-2.16788700	0.41188800
H	3.58389900	-2.07045600	-0.43487200
H	2.26276800	-3.04585100	0.28909800
H	3.47581000	-2.24749700	1.33976000
O	2.10891700	-0.96050900	0.46888400
H	1.49796700	-0.97544700	1.25862900

Scan Point for comp3_7_alpha_2.1Å

C	-0.30685500	1.35479200	0.91857500
C	-0.17889500	1.59433400	-0.58933600
C	0.81273000	0.66213500	-1.33366300
C	-0.86801300	-0.02766300	1.33064300
C	0.76822300	-0.82903900	-1.07713700
C	-1.31831600	-1.03863100	0.26072900
H	0.68659200	1.45194500	1.37510300
H	-1.16279600	1.49792100	-1.05076700
H	-1.77104900	0.15814400	1.92189000
H	0.53837900	0.70715000	-2.39996600
H	1.44632400	-1.41943100	-1.69055500
H	-1.54325900	-1.96240900	0.79980200
O	2.14765000	1.12766500	-1.25748800
H	2.55247000	0.75586600	-0.45164700
O	0.20824600	2.94419600	-0.83063700
H	1.17490700	3.00240300	-0.73097100
O	-1.18324100	2.33626700	1.47920800

H	-0.85427600	3.20837200	1.20503300
O	0.13078900	-0.62873800	2.17525000
H	-0.24061900	-1.40492400	2.62482900
C	-2.54642800	-0.71348000	-0.57950000
H	-3.26911000	-0.19226400	0.06026600
H	-2.30431300	-0.07382600	-1.43261600
O	-3.07782200	-1.95976500	-1.03906500
H	-3.82137500	-1.77493100	-1.63209500
O	-0.21790700	-1.51744800	-0.63267500
C	2.96938900	-2.12970200	0.40523100
H	3.63424600	-2.03205100	-0.45396000
H	2.32746100	-3.00864400	0.28918200
H	3.56121700	-2.21950900	1.32040900
O	2.17760600	-0.92433600	0.47674800
H	1.57161100	-0.95300900	1.26207000

Scan Point for comp3_7_alpha_2.2Å

C	-0.26026600	1.34911300	0.91873300
C	-0.17666000	1.59405700	-0.59151500
C	0.76116600	0.63326600	-1.36953200
C	-0.86316100	-0.01152700	1.34575600
C	0.69251600	-0.85244100	-1.11644200
C	-1.35116900	-1.01827700	0.28820900
H	0.75305800	1.40178500	1.33674500
H	-1.17725400	1.53484100	-1.02181500
H	-1.75866700	0.20693300	1.93796100
H	0.45241000	0.68448500	-2.42724100
H	1.37031700	-1.45898200	-1.71494100
H	-1.58564200	-1.93631100	0.83278500
O	2.11128900	1.05823000	-1.33580600
H	2.52929200	0.65353900	-0.55072000
O	0.24957700	2.93077300	-0.83864200
H	1.21947900	2.95737500	-0.75804600
O	-1.07444000	2.36076000	1.51740800
H	-0.72323200	3.22122100	1.23426100
O	0.12216400	-0.63437300	2.18734800
H	-0.26564900	-1.40079400	2.63943800
C	-2.57926600	-0.67642200	-0.54395300
H	-3.29671300	-0.16494000	0.10965800
H	-2.34054800	-0.02080100	-1.38568000
O	-3.11455200	-1.91255900	-1.02389300
H	-3.84572900	-1.71476300	-1.62810600
O	-0.26526500	-1.52663200	-0.61375600

C	3.01655900	-2.11892200	0.41030500
H	3.68260000	-2.02040100	-0.44822900
H	2.38503900	-3.00587000	0.29477700
H	3.61000500	-2.20399900	1.32556500
O	2.21322800	-0.92290100	0.47178700
H	1.61690400	-0.95278800	1.25866100

Scan Point for comp3_7_alpha_2.3Å

C	-0.24100000	1.33550700	0.92223100
C	-0.19718300	1.59627300	-0.58721000
C	0.71879600	0.63765600	-1.39208300
C	-0.85172500	-0.02097600	1.35141200
C	0.64391900	-0.84763100	-1.16179500
C	-1.35865400	-1.02018600	0.29632700
H	0.78495800	1.36816500	1.30994900
H	-1.20819900	1.54730800	-0.99373200
H	-1.74210200	0.20400700	1.94935600
H	0.39708300	0.70519000	-2.44585600
H	1.32939200	-1.45155300	-1.75452700
H	-1.58606400	-1.94166600	0.83769900
O	2.07429800	1.04629100	-1.36774300
H	2.49458800	0.62258000	-0.59197600
O	0.23282700	2.93187000	-0.83288100
H	1.20396300	2.95281600	-0.76593200
O	-1.02221400	2.35127000	1.55641600
H	-0.66881900	3.21017600	1.27130700
O	0.13355100	-0.65370700	2.18316000
H	-0.25914900	-1.41353900	2.64180800
C	-2.59581800	-0.67176000	-0.51820100
H	-3.30001000	-0.15617800	0.14653900
H	-2.36569400	-0.01706700	-1.36317300
O	-3.14521900	-1.90427700	-0.99032900
H	-3.89257800	-1.70189300	-1.57294700
O	-0.28294800	-1.52702500	-0.62305500
C	3.08288300	-2.09276100	0.39325800
H	3.73544600	-1.98309000	-0.47445000
H	2.46338500	-2.98893900	0.28090900
H	3.69239200	-2.17795000	1.29851600
O	2.26524100	-0.90924500	0.46839500
H	1.66981800	-0.95651800	1.25118200

Scan Point for comp3_7_alpha_2.4Å

C	-0.22765200	1.32197200	0.92454700
C	-0.22270200	1.59607200	-0.58325600
C	0.67903600	0.64498500	-1.41109000
C	-0.83786100	-0.03360900	1.35674500
C	0.60098200	-0.84053500	-1.20101600
C	-1.36224000	-1.02627900	0.30471800
H	0.80880100	1.34191500	1.28378400
H	-1.24260400	1.54831900	-0.96678800
H	-1.72147600	0.19270100	1.96456000
H	0.35019500	0.72895000	-2.46203200
H	1.29554500	-1.44000900	-1.78882500
H	-1.58110000	-1.95155100	0.84272200
O	2.03812700	1.04219200	-1.38795900
H	2.45813300	0.60295400	-0.61830400
O	0.19988700	2.93368300	-0.82903200
H	1.17162600	2.95845600	-0.77274600
O	-0.98125200	2.33837300	1.58982100
H	-0.62582700	3.19624900	1.30385600
O	0.15372600	-0.67291600	2.17385000
H	-0.23822100	-1.42923900	2.63868900
C	-2.60848000	-0.67390800	-0.49329700
H	-3.30025300	-0.15322500	0.18038300
H	-2.38701600	-0.02226500	-1.34326000
O	-3.17067400	-1.90414700	-0.95527100
H	-3.94409400	-1.69878000	-1.50188300
O	-0.29515100	-1.52760400	-0.63092700
C	3.14275700	-2.06497300	0.36624600
H	3.77794300	-1.94695100	-0.51342600
H	2.52336800	-2.96175400	0.25594500
H	3.77193600	-2.16159500	1.25731000
O	2.32665800	-0.88449900	0.46635000
H	1.72944400	-0.94719000	1.24376100

Scan Point for comp3_7_alpha_2.5Å

C	-0.19932200	1.30840800	0.92813700
C	-0.23131000	1.59897700	-0.57637000
C	0.64267900	0.64676700	-1.43099600
C	-0.82024000	-0.04182500	1.36267400
C	0.54729100	-0.83816600	-1.24018800
C	-1.37611400	-1.02094300	0.31508200
H	0.84671200	1.30762200	1.25858300

H	-1.26044800	1.56456300	-0.93562800
H	-1.69091400	0.19263700	1.98611800
H	0.30236500	0.75084700	-2.47689400
H	1.23912900	-1.43903800	-1.83110500
H	-1.59189900	-1.94911000	0.84914800
O	2.00914500	1.01886300	-1.41730300
H	2.42812800	0.56720600	-0.65228900
O	0.19944900	2.93387300	-0.82085900
H	1.17211300	2.95018400	-0.77994100
O	-0.91690700	2.32885300	1.62600300
H	-0.55134600	3.18397900	1.34475300
O	0.17577100	-0.69921100	2.15846700
H	-0.21868900	-1.45086000	2.62859600
C	-2.63289900	-0.65244800	-0.45818000
H	-3.30929800	-0.13705000	0.23493300
H	-2.42335600	0.00936600	-1.30355800
O	-3.20902600	-1.87394000	-0.92523700
H	-3.99937600	-1.65874900	-1.44319300
O	-0.32701200	-1.52433700	-0.64250300
C	3.18011500	-2.05926400	0.34074400
H	3.81316200	-1.93065400	-0.53924000
H	2.55387000	-2.94936800	0.21490500
H	3.81316500	-2.18046100	1.22645400
O	2.37532900	-0.87477700	0.46478700
H	1.76149000	-0.95474200	1.22608900

Scan Point for comp3_7_alpha_2.6Å

C	-0.18018900	1.29371800	0.93413100
C	-0.24111100	1.59979400	-0.56693800
C	0.60195000	0.64745600	-1.45137600
C	-0.80024800	-0.05555000	1.37240300
C	0.48871000	-0.83782400	-1.28018600
C	-1.38874800	-1.02074900	0.33062500
H	0.87196300	1.28570100	1.24379600
H	-1.27817600	1.58159900	-0.90377900
H	-1.65427600	0.18001600	2.01811100
H	0.24633300	0.77344700	-2.48997900
H	1.17047500	-1.43885300	-1.88396400
H	-1.59952300	-1.95279800	0.85965300
O	1.97529400	0.99354900	-1.45387000
H	2.39672100	0.52933900	-0.69530700
O	0.20054300	2.93191500	-0.80691900
H	1.17377100	2.93776900	-0.78114000

O	-0.87822200	2.31235100	1.65477000
H	-0.51152600	3.16787800	1.37644900
O	0.20909400	-0.72741600	2.13755400
H	-0.17916800	-1.48040600	2.61066800
C	-2.65681700	-0.63628300	-0.41526400
H	-3.32113300	-0.13772000	0.30147700
H	-2.46282200	0.04560700	-1.24819600
O	-3.23860400	-1.84797200	-0.89985400
H	-4.03385600	-1.62286700	-1.40594600
O	-0.36098700	-1.52405100	-0.65293100
C	3.23490600	-2.03230700	0.32643400
H	3.85155400	-1.91078700	-0.56638100
H	2.61099600	-2.92655300	0.21918700
H	3.88484100	-2.14414000	1.20146700
O	2.42791100	-0.85049700	0.45167500
H	1.80286500	-0.93977600	1.20152400

Scan Point for comp3_7_alpha_2.7Å

C	-0.19434300	1.28768200	0.93562000
C	-0.26206100	1.60095900	-0.56408800
C	0.57611400	0.65801200	-1.46157600
C	-0.78641800	-0.07353300	1.37460000
C	0.45910100	-0.82801500	-1.31065100
C	-1.38472200	-1.03625700	0.33805100
H	0.85825700	1.29837400	1.24366400
H	-1.30085200	1.58361100	-0.89593000
H	-1.62897900	0.14547800	2.04082700
H	0.22123400	0.80089700	-2.49844500
H	1.13774900	-1.42173400	-1.92609300
H	-1.57802800	-1.97468300	0.86205900
O	1.95232700	0.99237300	-1.45769300
H	2.37114700	0.50954600	-0.70637400
O	0.17591300	2.93571800	-0.79660700
H	1.14873700	2.94641400	-0.76112600
O	-0.90916700	2.29189300	1.66030400
H	-0.55139600	3.15409400	1.39133400
O	0.24662900	-0.74054500	2.11141500
H	-0.12381800	-1.50248700	2.58470200
C	-2.66661900	-0.65546400	-0.38409300
H	-3.32445700	-0.17622900	0.35165900
H	-2.49444600	0.04372000	-1.20738500
O	-3.24246200	-1.86503000	-0.87985100
H	-4.04774100	-1.64030800	-1.37003300

O	-0.36646700	-1.52409800	-0.66554900
C	3.28478700	-1.99654300	0.31457200
H	3.92233600	-1.85942600	-0.56124900
H	2.64743700	-2.87524900	0.16549900
H	3.91412000	-2.14925100	1.19855600
O	2.49743800	-0.80429500	0.45983600
H	1.83996900	-0.91194400	1.17888300

Scan Point for comp3_7_alpha_2.8Å

C	-0.20588500	1.29562500	0.92760700
C	-0.24882400	1.60883600	-0.57380400
C	0.59413000	0.66672300	-1.46373800
C	-0.78168700	-0.07308400	1.36735500
C	0.44138700	-0.81740100	-1.33863000
C	-1.38821300	-1.03622300	0.33773300
H	0.84081200	1.32339900	1.25468900
H	-1.28186300	1.59399700	-0.92371500
H	-1.61624700	0.13817900	2.04590900
H	0.26383900	0.83208800	-2.50571400
H	1.10800700	-1.41554800	-1.96372700
H	-1.55759800	-1.98180400	0.85712200
O	1.97702300	0.96761500	-1.42649000
H	2.37275200	0.46285200	-0.67359500
O	0.19450800	2.94393700	-0.79484300
H	1.16444600	2.96046900	-0.71674700
O	-0.94956900	2.29113600	1.63561100
H	-0.60130400	3.15807100	1.36955000
O	0.26313400	-0.73721600	2.08999000
H	-0.09929700	-1.50179400	2.56536500
C	-2.69091400	-0.66548400	-0.35068300
H	-3.34409000	-0.22705000	0.41414600
H	-2.55355500	0.06626500	-1.15145600
O	-3.24784400	-1.87151600	-0.87475800
H	-4.06474600	-1.64944000	-1.34658600
O	-0.38480800	-1.50902500	-0.69149200
C	3.26726400	-2.01830100	0.30942900
H	3.93522300	-1.87166600	-0.54193400
H	2.58387300	-2.84779400	0.09556100
H	3.86328500	-2.25907100	1.19706600
O	2.54860100	-0.79018600	0.50498400
H	1.85454700	-0.90324900	1.18844200

Scan Point for comp3_7_alpha_2.9Å

C	-0.20991400	1.30054600	0.92330100
C	-0.24616700	1.61345700	-0.57847700
C	0.59824300	0.67522100	-1.46800900
C	-0.77063400	-0.07461700	1.36272900
C	0.41851300	-0.80719900	-1.37104200
C	-1.38497600	-1.03778800	0.33839700
H	0.83405800	1.34162400	1.25786900
H	-1.27807400	1.59573200	-0.93282700
H	-1.59839500	0.12928000	2.05185000
H	0.28810600	0.86537100	-2.51175100
H	1.06962700	-1.40478100	-2.01317600
H	-1.53698100	-1.98789100	0.85474700
O	1.98643400	0.94603900	-1.40465800
H	2.36548100	0.42717600	-0.64923000
O	0.19393200	2.95041000	-0.79638300
H	1.16139700	2.97561800	-0.69629600
O	-0.97154400	2.28769300	1.62429600
H	-0.63518700	3.15886400	1.35675600
O	0.28465100	-0.73596200	2.07197800
H	-0.07018300	-1.50150600	2.55163400
C	-2.70175700	-0.67357300	-0.32641200
H	-3.34589400	-0.24724300	0.45276100
H	-2.58212300	0.06678300	-1.12234400
O	-3.25652300	-1.87981900	-0.85153400
H	-4.08419900	-1.66148000	-1.30597300
O	-0.39760300	-1.49930600	-0.71335200
C	3.25442500	-2.02838500	0.29613300
H	3.95469300	-1.87322300	-0.52739500
H	2.53402300	-2.80549200	0.01689800
H	3.80929700	-2.35124800	1.18434400
O	2.59761900	-0.77436500	0.54218100
H	1.87222600	-0.89107100	1.19218500

Scan Point for comp3_7_alpha_3.0Å

C	-0.20798500	1.30021100	0.92160700
C	-0.24923000	1.61524000	-0.57937000
C	0.58755200	0.67844600	-1.47559000
C	-0.75798000	-0.07907500	1.36121900
C	0.38757800	-0.80207100	-1.40116300
C	-1.38631700	-1.03881300	0.34237000

H	0.83637700	1.34750900	1.25430900
H	-1.28309600	1.60026400	-0.92902800
H	-1.57517700	0.11923400	2.06448400
H	0.28884600	0.89071200	-2.51800400
H	1.02286400	-1.39867300	-2.06021100
H	-1.52670200	-1.99220900	0.85568600
O	1.98050000	0.92301100	-1.39926300
H	2.35226000	0.39726400	-0.64199200
O	0.19358700	2.95164400	-0.79645700
H	1.16059400	2.97582100	-0.69252100
O	-0.97428800	2.28216500	1.62488200
H	-0.64261400	3.15551400	1.35858600
O	0.30913200	-0.74214700	2.05031900
H	-0.03783900	-1.50836400	2.53476700
C	-2.71422100	-0.67304000	-0.29927000
H	-3.34581500	-0.25082200	0.49224600
H	-2.60624800	0.07150000	-1.09313400
O	-3.27634900	-1.87708700	-0.82120600
H	-4.10958600	-1.65700300	-1.26441800
O	-0.41689100	-1.49433700	-0.73044100
C	3.26327100	-2.02489300	0.28126900
H	3.99001800	-1.86540000	-0.51825700
H	2.51930800	-2.75866500	-0.04885400
H	3.78224500	-2.40767200	1.16731900
O	2.65202100	-0.75569100	0.56610700
H	1.89684900	-0.87550600	1.18106000

Scan Point for comp3_7_alpha_3.1Å

C	-0.18291700	1.29573500	0.92079200
C	-0.24753000	1.61742400	-0.57757000
C	0.56222100	0.67526500	-1.49152900
C	-0.74319500	-0.07887600	1.36336500
C	0.33093900	-0.80106600	-1.43803200
C	-1.39890700	-1.02976600	0.35301900
H	0.86795400	1.32755800	1.23403400
H	-1.28791100	1.61641700	-0.90865800
H	-1.54554800	0.12637800	2.08156000
H	0.26811600	0.91500100	-2.52851200
H	0.93520000	-1.40103200	-2.12266900
H	-1.53400000	-1.98458400	0.86476700
O	1.96270900	0.87888000	-1.41581900
H	2.32895400	0.34563100	-0.65866400
O	0.20850100	2.94901900	-0.79782800

H	1.17682400	2.96174900	-0.70530100
O	-0.92231300	2.28444800	1.64284200
H	-0.58125800	3.15424100	1.37667500
O	0.32776400	-0.75776200	2.03078000
H	-0.02045100	-1.51806900	2.52368000
C	-2.73702200	-0.65296600	-0.26075600
H	-3.35245600	-0.23446300	0.54521600
H	-2.63830800	0.09757300	-1.05018000
O	-3.31285200	-1.85064000	-0.78200100
H	-4.14847600	-1.62361100	-1.21696700
O	-0.45884700	-1.48804900	-0.74546100
C	3.29653600	-2.02041900	0.26732700
H	4.09410800	-1.83402600	-0.45515800
H	2.57027900	-2.71695300	-0.16688900
H	3.72891000	-2.46592200	1.17045300
O	2.68911000	-0.75435200	0.57364700
H	1.90474200	-0.89022800	1.14764700

Scan Point for comp3_7_alpha_3.2Å

C	-0.17204500	1.31275800	0.90071800
C	-0.23879600	1.62108500	-0.60005800
C	0.57198000	0.67331600	-1.50264400
C	-0.73035900	-0.05688700	1.35941900
C	0.30274700	-0.79776300	-1.47233600
C	-1.38735400	-1.02040500	0.36212100
H	0.87968400	1.34720500	1.21078700
H	-1.27931100	1.61892900	-0.93198700
H	-1.53292200	0.15721900	2.07478000
H	0.32960700	0.94415600	-2.54335400
H	0.87451800	-1.40174400	-2.18080000
H	-1.50818300	-1.97360800	0.88039200
O	1.97624100	0.82121100	-1.36706600
H	2.30137000	0.29025800	-0.58336200
O	0.22007200	2.95109700	-0.83023200
H	1.18698100	2.96637500	-0.72485600
O	-0.90881400	2.30918500	1.61542600
H	-0.57078400	3.17600800	1.33581100
O	0.33916900	-0.72632800	2.03842600
H	-0.01045000	-1.47830400	2.54274800
C	-2.73621200	-0.65450800	-0.23512100
H	-3.34512200	-0.24095100	0.57819600
H	-2.65121100	0.09689900	-1.02523800
O	-3.30944400	-1.85635800	-0.74914400

H	-4.15572500	-1.63674900	-1.16689300
O	-0.46737200	-1.47983800	-0.75372900
C	3.21646700	-2.05579900	0.23580400
H	4.03599400	-1.88811900	-0.46641100
H	2.43744800	-2.65251400	-0.25265400
H	3.59707400	-2.59970200	1.10745100
O	2.71615600	-0.76612300	0.62872700
H	1.92441000	-0.87891000	1.19871800

Scan Point for comp3_7_alpha_3.3Å

C	-0.15512200	1.31078800	0.89932100
C	-0.22596400	1.61716400	-0.60159300
C	0.55283100	0.65222300	-1.51490500
C	-0.71702300	-0.05523400	1.36383200
C	0.24803200	-0.81276000	-1.49002200
C	-1.40536000	-1.00891600	0.37794300
H	0.89762200	1.34126700	1.20575000
H	-1.26994300	1.63774300	-0.92262200
H	-1.50183600	0.16404900	2.09707900
H	0.30915300	0.93623700	-2.55127500
H	0.78791600	-1.42411700	-2.21687200
H	-1.53249900	-1.95938600	0.89950400
O	1.96229100	0.76057100	-1.39379100
H	2.28923600	0.24666200	-0.59799100
O	0.25938500	2.93684300	-0.83752900
H	1.22746100	2.93051900	-0.74316400
O	-0.88453300	2.31265200	1.61418400
H	-0.53689200	3.17706000	1.33915700
O	0.36001000	-0.73843700	2.01641200
H	0.01351000	-1.48948700	2.52437600
C	-2.75636000	-0.62240100	-0.20085600
H	-3.35214900	-0.20858300	0.62199700
H	-2.67003900	0.13473300	-0.98547600
O	-3.34805900	-1.81353600	-0.71879600
H	-4.19037800	-1.58026700	-1.13703900
O	-0.51428800	-1.48350600	-0.75335800
C	3.23260900	-2.04353900	0.22871100
H	4.05206300	-1.88919300	-0.47663200
H	2.43535600	-2.61405800	-0.26166000
H	3.60389000	-2.60749000	1.09158600
O	2.76803500	-0.74563100	0.63955200
H	1.97293700	-0.85129800	1.20531100

Scan Point for comp3_7_alpha_3.4Å

C	-0.15702700	1.29173200	0.91086100
C	-0.19864400	1.59914400	-0.59117700
C	0.55919600	0.62266500	-1.50880300
C	-0.70628100	-0.08400500	1.36194600
C	0.21238100	-0.83384800	-1.49186900
C	-1.44677000	-1.00157400	0.37997900
H	0.88626500	1.34077600	1.24547800
H	-1.23872100	1.63800300	-0.92232800
H	-1.45429100	0.11991700	2.13691700
H	0.30460500	0.91106400	-2.54226500
H	0.73709500	-1.45700600	-2.22012500
H	-1.58777400	-1.95605800	0.89098500
O	1.96972900	0.71487300	-1.41246700
H	2.30928900	0.23571800	-0.59991200
O	0.31193700	2.91041800	-0.81969300
H	1.27985900	2.88290800	-0.72840900
O	-0.92573600	2.27925300	1.60482100
H	-0.59372200	3.15159600	1.33630600
O	0.39326600	-0.79471000	1.94292000
H	0.07055800	-1.56938300	2.43101800
C	-2.80164200	-0.57232400	-0.15815700
H	-3.37347300	-0.18753000	0.69532900
H	-2.72305900	0.21834700	-0.91024400
O	-3.42033700	-1.73283600	-0.71264900
H	-4.28370600	-1.47860800	-1.07169400
O	-0.58553500	-1.48280300	-0.77346500
C	3.31144600	-1.98027700	0.23045900
H	4.18334100	-1.81277000	-0.40565200
H	2.54373900	-2.51197100	-0.34323400
H	3.60725200	-2.58800700	1.09266900
O	2.84046900	-0.69104300	0.66051700
H	2.02644400	-0.81130000	1.19586000

Scan Point for comp3_7_alpha_3.5Å

C	-0.13113100	1.22946000	0.94444400
C	-0.19315700	1.58825200	-0.54727900
C	0.50220500	0.62264700	-1.52557100
C	-0.69038000	-0.15427700	1.35797700
C	0.11521700	-0.82347500	-1.53763800

C	-1.50142500	-1.00394900	0.37078500
H	0.91676500	1.25611500	1.26618600
H	-1.23972900	1.67285000	-0.84777700
H	-1.39251100	0.02872900	2.17978000
H	0.20883000	0.94661900	-2.53837700
H	0.61062200	-1.44090300	-2.29123200
H	-1.66101700	-1.97314300	0.84764100
O	1.91677600	0.67871700	-1.49350200
H	2.28294000	0.20883200	-0.68779200
O	0.35239300	2.89044900	-0.74336400
H	1.32114000	2.83033300	-0.68120900
O	-0.88017200	2.20327600	1.67801500
H	-0.54365200	3.08006600	1.43018900
O	0.41774300	-0.92108300	1.84256000
H	0.09638400	-1.70075700	2.32343300
C	-2.85542500	-0.50261700	-0.10369700
H	-3.37617300	-0.11354100	0.78027400
H	-2.76934700	0.30067700	-0.84131800
O	-3.54848700	-1.61938100	-0.66038200
H	-4.41619200	-1.31698200	-0.96838700
O	-0.69001500	-1.46962500	-0.82485400
C	3.58169200	-1.85320700	0.25133600
H	4.46188800	-1.56314900	-0.32664800
H	2.95274800	-2.51435900	-0.35638400
H	3.90328300	-2.38371400	1.15425100
O	2.88167900	-0.64549400	0.59895100
H	2.07911000	-0.86955600	1.11583600

Scan Point for comp3_7_alpha_3.6Å

C	-0.11104100	1.20787200	0.95042300
C	-0.18438100	1.58582500	-0.53669300
C	0.47770200	0.62219300	-1.53750300
C	-0.67286100	-0.17716300	1.35493200
C	0.05342800	-0.81387600	-1.56958200
C	-1.52001200	-0.99899100	0.37431600
H	0.93924700	1.22682400	1.26452000
H	-1.23326400	1.69306900	-0.82237600
H	-1.35016500	-0.00150100	2.19892000
H	0.18714000	0.97291600	-2.54154600
H	0.51787200	-1.42699100	-2.34603200
H	-1.68357100	-1.97312000	0.83916900
O	1.89422000	0.63457100	-1.51794400
H	2.26210300	0.18035700	-0.70414500

O	0.38018700	2.88165500	-0.72272300
H	1.34813500	2.80831000	-0.66343500
O	-0.84995600	2.17797600	1.69999500
H	-0.51336600	3.05584900	1.45602000
O	0.43876400	-0.96596400	1.79248800
H	0.12124900	-1.74686600	2.27366300
C	-2.87648400	-0.47012500	-0.06149900
H	-3.37218900	-0.08946900	0.84022800
H	-2.79323000	0.34433600	-0.78691800
O	-3.59757900	-1.56670500	-0.62270200
H	-4.46446400	-1.24503800	-0.91291000
O	-0.74533400	-1.45762000	-0.84772400
C	3.64126000	-1.82299400	0.24756900
H	4.52061200	-1.52113600	-0.32554500
H	3.02209700	-2.48969100	-0.36421200
H	3.96478200	-2.35170800	1.15092300
O	2.92434400	-0.62493300	0.59424500
H	2.12418500	-0.86443300	1.10681100

Scan Point for comp3_7_alpha_3.7Å

C	-0.09565500	1.17434100	0.95461700
C	-0.16738900	1.56413400	-0.52954200
C	0.44917600	0.58717200	-1.54670900
C	-0.65869000	-0.21189300	1.35015900
C	-0.02219000	-0.83441500	-1.58390700
C	-1.56384600	-0.98989100	0.38788200
H	0.95395000	1.18843700	1.27111700
H	-1.21527500	1.70880600	-0.80286600
H	-1.29178100	-0.04899300	2.23067700
H	0.15053500	0.95375900	-2.54288700
H	0.41005300	-1.45380700	-2.37393700
H	-1.75062800	-1.96349100	0.84576000
O	1.86462200	0.55356300	-1.55694200
H	2.24173700	0.13002800	-0.73013500
O	0.43582100	2.84286200	-0.71136200
H	1.40114900	2.74145100	-0.65016400
O	-0.83366500	2.14118400	1.70990900
H	-0.49164600	3.01988800	1.47724900
O	0.45972200	-1.02930900	1.70948700
H	0.15146100	-1.84530600	2.13504000
C	-2.90869500	-0.40423400	-0.00434400
H	-3.36891400	-0.02142300	0.91526200
H	-2.81102800	0.41955500	-0.71660400

O	-3.68423700	-1.46166800	-0.56890400
H	-4.51241700	-1.08680100	-0.90498900
O	-0.83374300	-1.45891900	-0.85887300
C	3.78913700	-1.71313400	0.26685300
H	4.65090900	-1.34317200	-0.29275800
H	3.24381100	-2.43931300	-0.34719400
H	4.13837000	-2.20136700	1.18333300
O	2.96560800	-0.57723400	0.58333100
H	2.17559700	-0.87456400	1.07987400

Scan Point for comp3_7_alpha_3.8Å

C	-0.08915400	1.15527100	0.95325200
C	-0.16193200	1.55090200	-0.52901000
C	0.43484700	0.56924800	-1.55255900
C	-0.64612000	-0.23432300	1.34111400
C	-0.06863100	-0.84245800	-1.60050700
C	-1.58506400	-0.98677300	0.39113300
H	0.96033700	1.17088900	1.27022200
H	-1.20947300	1.70904400	-0.79647100
H	-1.25046400	-0.08452100	2.24383600
H	0.14318700	0.94986500	-2.54534600
H	0.34003800	-1.46169500	-2.40311100
H	-1.78103000	-1.96168600	0.84253700
O	1.84904600	0.50352700	-1.56695400
H	2.22670800	0.10984600	-0.72738700
O	0.45448500	2.82348300	-0.70939700
H	1.41820200	2.71517100	-0.63706700
O	-0.83105500	2.11534300	1.71330700
H	-0.49131400	2.99667600	1.48770500
O	0.47665800	-1.06700500	1.64676800
H	0.17590500	-1.87423700	2.09360700
C	-2.92356500	-0.36900300	0.02945200
H	-3.35465300	0.02347000	0.95912600
H	-2.82102300	0.45317500	-0.68378500
O	-3.73663100	-1.40640300	-0.51994300
H	-4.55513600	-1.00878600	-0.85343600
O	-0.88598000	-1.45676500	-0.87344200
C	3.86409300	-1.65399300	0.26840200
H	4.70879100	-1.26033800	-0.30100700
H	3.33009300	-2.39236200	-0.34101400
H	4.23746200	-2.13574600	1.17876600
O	3.01583600	-0.53994300	0.59825400
H	2.23664900	-0.85987600	1.09642500

Scan Point for comp3_7_alpha_3.9Å

C	-0.07573100	1.12667500	0.95601500
C	-0.14905300	1.53997000	-0.52088300
C	0.42515000	0.55962000	-1.55760600
C	-0.63272600	-0.26761300	1.32379900
C	-0.11789200	-0.83807000	-1.62691200
C	-1.61034400	-0.98168100	0.38184000
H	0.97397300	1.13681900	1.27209400
H	-1.19588500	1.71471500	-0.78115100
H	-1.20613100	-0.13697800	2.24930800
H	0.14146500	0.96200600	-2.54414700
H	0.26513800	-1.45254400	-2.44571600
H	-1.81763200	-1.96086100	0.81856000
O	1.83706200	0.45841700	-1.57799500
H	2.21486900	0.08499000	-0.73123100
O	0.48248600	2.80632800	-0.69123300
H	1.44440100	2.68847200	-0.61220300
O	-0.81618800	2.07697700	1.72963600
H	-0.47614500	2.96123000	1.51651300
O	0.48837600	-1.12247600	1.56600000
H	0.19534900	-1.91829900	2.03761500
C	-2.94117800	-0.32529500	0.06241700
H	-3.33035100	0.08055000	1.00473900
H	-2.83547500	0.49304400	-0.65483600
O	-3.80467900	-1.33610500	-0.45866500
H	-4.62216800	-0.91220600	-0.76098100
O	-0.94711600	-1.44236300	-0.90510600
C	3.93852500	-1.60163200	0.27890800
H	4.74195700	-1.19569500	-0.33958000
H	3.40904000	-2.38027600	-0.28228000
H	4.36923100	-2.03671200	1.18758100
O	3.06135700	-0.50974300	0.60794300
H	2.29748000	-0.84838100	1.11559100

Scan Point for comp3_7_alpha_4.0Å

C	0.07216200	1.07764600	-0.95872300
C	0.12476700	1.49300500	0.51865100
C	-0.41187100	0.49317000	1.55839300
C	0.60355800	-0.33158500	-1.29664400

C	0.18670700	-0.88288700	1.62143700
C	1.66649600	-0.97154400	-0.39532400
H	-0.96936200	1.10757300	-1.29924100
H	1.16617100	1.69121100	0.78210600
H	1.08573300	-0.25686000	-2.27867500
H	-0.10749900	0.89550600	2.54064700
H	-0.17177800	-1.51417000	2.43895000
H	1.91044400	-1.94850500	-0.81800700
O	-1.81799600	0.36861200	1.62255200
H	-2.22024300	0.04202700	0.76982000
O	-0.53503600	2.74309500	0.69344600
H	-1.49391300	2.60501500	0.61441500
O	0.85387400	2.00168200	-1.72226400
H	0.52378500	2.89598500	-1.53825400
O	-0.52911500	-1.20014200	-1.36869600
H	-0.27397600	-2.04735900	-1.76741600
C	2.96701300	-0.23268300	-0.14736200
H	3.30075400	0.15348100	-1.11885000
H	2.84167100	0.61032300	0.53690200
O	3.90011200	-1.17540500	0.38114800
H	4.72603300	-0.70947000	0.58151500
O	1.06805100	-1.43809800	0.92141100
C	-4.11887500	-1.42399900	-0.37404500
H	-4.91725400	-0.94911300	0.20033100
H	-3.71940000	-2.27125700	0.19528700
H	-4.52601000	-1.78374400	-1.32553700
O	-3.10733100	-0.42727100	-0.60156500
H	-2.35536800	-0.82716500	-1.08054400

Scan Point for comp3_7_alpha_4.1Å

C	0.06163100	1.06612900	-0.94759100
C	0.10805900	1.47739300	0.53128700
C	-0.40705700	0.46612000	1.56932900
C	0.58604400	-0.34521800	-1.28034800
C	0.24257000	-0.88887700	1.64149700
C	1.68287400	-0.96166300	-0.40352400
H	-0.97751300	1.10069600	-1.29458600
H	1.14765600	1.68800200	0.79341600
H	1.03362200	-0.28498500	-2.27955700
H	-0.12548000	0.88328500	2.55177000
H	-0.07812400	-1.52027900	2.47454000
H	1.93173600	-1.93870200	-0.82332800
O	-1.80862800	0.29052900	1.62560200

H	-2.20551100	-0.00367200	0.75989200
O	-0.56710400	2.71824100	0.71314100
H	-1.52354700	2.57164500	0.62393600
O	0.85254200	1.98582600	-1.70662400
H	0.52337000	2.88175000	-1.52939400
O	-0.54358400	-1.22054700	-1.29686000
H	-0.30061500	-2.06429200	-1.71027000
C	2.97568400	-0.19779200	-0.19409900
H	3.27939300	0.18589900	-1.17619600
H	2.85076500	0.64809700	0.48681000
O	3.93814500	-1.11929800	0.31886800
H	4.76553400	-0.64042000	0.47855800
O	1.12920600	-1.42470200	0.93339100
C	-4.16811700	-1.37218800	-0.40093500
H	-4.94548900	-0.88721300	0.19358500
H	-3.78095900	-2.23802500	0.14861700
H	-4.59911500	-1.70670700	-1.35117800
O	-3.13648300	-0.39646700	-0.62776200
H	-2.39861200	-0.80716700	-1.11835800

Scan Point for comp3_7_alpha_4.2Å

C	0.05907200	1.06788400	-0.93291500
C	0.10268600	1.46895000	0.54905400
C	-0.39981600	0.44512900	1.57977800
C	0.57388800	-0.34482400	-1.26935100
C	0.28822200	-0.89302500	1.65505900
C	1.69214500	-0.95534700	-0.41566000
H	-0.97910200	1.10829100	-1.28298900
H	1.14142400	1.68383300	0.81187400
H	0.99678500	-0.29113000	-2.27969900
H	-0.14298100	0.87003600	2.56493000
H	-0.00161200	-1.52381900	2.49981300
H	1.93510800	-1.93322900	-0.83721400
O	-1.79639400	0.22437900	1.62143600
H	-2.18332300	-0.04193700	0.74498400
O	-0.57896400	2.70465600	0.74153400
H	-1.53262100	2.56143300	0.62414300
O	0.85678300	1.98592200	-1.68610600
H	0.52845900	2.88272100	-1.51231900
O	-0.55675000	-1.21854900	-1.25185100
H	-0.32325500	-2.06386200	-1.66779800
C	2.98643700	-0.18650400	-0.23652800
H	3.27290600	0.18630100	-1.22793700

H	2.87149200	0.66649300	0.43720000
O	3.95955800	-1.10046800	0.27018900
H	4.78840900	-0.61791000	0.40984500
O	1.17395900	-1.41518400	0.93623400
C	-4.21455500	-1.34142700	-0.41408900
H	-4.97779400	-0.85301100	0.19582300
H	-3.82445200	-2.21192900	0.12596200
H	-4.66518600	-1.67014000	-1.35735100
O	-3.18068600	-0.37199100	-0.65474800
H	-2.45279000	-0.78728000	-1.15486000

Scan Point for comp3_7_alpha_4.3Å

C	0.05002500	1.07424500	-0.91145000
C	0.09513000	1.45627700	0.57586200
C	-0.38745300	0.41082100	1.59375200
C	0.56241900	-0.33536400	-1.26337800
C	0.33942800	-0.90896300	1.66229200
C	1.70187500	-0.94385100	-0.43585700
H	-0.98863500	1.11806700	-1.26007400
H	1.13330900	1.67811600	0.83598500
H	0.96397500	-0.27642600	-2.28225400
H	-0.15932600	0.83788100	2.58392200
H	0.08241600	-1.54312400	2.51500000
H	1.94464900	-1.91678900	-0.86889600
O	-1.77598100	0.13414900	1.61602800
H	-2.14682300	-0.10204500	0.72692500
O	-0.59766200	2.68236100	0.78984800
H	-1.54789500	2.54126600	0.64603600
O	0.84717100	1.99896800	-1.65650500
H	0.51366800	2.89380500	-1.48332000
O	-0.56438400	-1.21280800	-1.22442600
H	-0.33330000	-2.05754400	-1.64291400
C	2.99236700	-0.16507000	-0.27333700
H	3.26152700	0.21377900	-1.26722100
H	2.87954500	0.68427300	0.40552300
O	3.98056500	-1.07214000	0.21644000
H	4.80771000	-0.58305100	0.34254700
O	1.21734700	-1.41580300	0.92384500
C	-4.25627100	-1.30279700	-0.42338600
H	-4.99831100	-0.80928500	0.20829800
H	-3.86261800	-2.18015200	0.10294800
H	-4.73500900	-1.62275600	-1.35586600
O	-3.21886000	-0.34268000	-0.68460300

H	-2.50556900	-0.76417700	-1.19865000

Scan Point for comp3_7_alpha_4.4Å

C	0.03758700	1.06896700	-0.90095200
C	0.09667400	1.45024100	0.58627300
C	-0.36434200	0.39751200	1.60601700
C	0.54968400	-0.33981600	-1.25515500
C	0.39173700	-0.90792900	1.67687100
C	1.71021200	-0.93745100	-0.44843400
H	-1.00524600	1.10853900	-1.23792500
H	1.13578600	1.68165700	0.83432400
H	0.92998000	-0.28518900	-2.28251300
H	-0.15219500	0.83268800	2.59546800
H	0.16523000	-1.53664600	2.54205500
H	1.95148500	-1.90996200	-0.88338500
O	-1.74741000	0.08676100	1.62198100
H	-2.11001700	-0.13360300	0.72905600
O	-0.60639400	2.66862900	0.81101900
H	-1.55656700	2.51895500	0.67552100
O	0.82398800	1.99454300	-1.65552400
H	0.48701100	2.88854800	-1.48530500
O	-0.57182600	-1.22163000	-1.18654200
H	-0.34227300	-2.07061100	-1.59734900
C	2.99786300	-0.14912900	-0.31123900
H	3.24947900	0.22510100	-1.31143000
H	2.88919500	0.70378200	0.36394500
O	3.99926900	-1.04646100	0.16964100
H	4.82460000	-0.55077800	0.28050700
O	1.26001000	-1.40777400	0.92337900
C	-4.30663500	-1.27450700	-0.42232200
H	-5.03706200	-0.76461900	0.21001500
H	-3.91789400	-2.14927400	0.11198800
H	-4.79857800	-1.60204800	-1.34544000
O	-3.26193900	-0.32884400	-0.70542000
H	-2.55519100	-0.76565100	-1.21415800

Scan Point for comp3_7_beta_1.4Å

C	1.77918300	0.68390000	-0.36296100
C	1.26873300	-0.67672300	-0.88547800
C	0.58741200	-1.59178800	0.14896700

C	0.94170500	1.38637600	0.72888100
C	-0.86833300	-1.21364800	0.52970500
C	-0.59049600	1.29054900	0.68543700
H	2.76967500	0.51874200	0.08228800
H	0.55502800	-0.48266400	-1.69204300
H	1.18254500	2.45262400	0.65941400
H	0.52115900	-2.58342700	-0.31419800
H	-1.20822400	-1.95963500	1.25359700
H	-0.95051000	1.94964500	1.48063000
O	1.33830000	-1.77456800	1.33808800
H	1.42015100	-0.90795400	1.79586200
O	2.34391600	-1.37186300	-1.52817400
H	3.01230500	-1.60111600	-0.86209700
O	1.90453200	1.60473900	-1.45429900
H	2.51812300	1.22899200	-2.10507300
O	1.32668800	0.89617500	2.02718800
H	2.21387800	1.22881600	2.23638100
C	-1.21381800	1.78797400	-0.61428600
H	-0.76825300	2.76446000	-0.84056000
H	-1.02232700	1.12139400	-1.45973900
O	-2.62474500	1.92094400	-0.40107500
H	-3.02186200	2.26940100	-1.21291200
O	-1.10011600	0.00534100	1.15075700
C	-3.15631700	-1.52997300	-0.38422100
H	-3.46889000	-0.75783200	0.31187500
H	-3.27906600	-2.53753800	0.01118100
H	-3.60494300	-1.40149700	-1.36625300
O	-1.68864900	-1.30839700	-0.60082800
H	-1.35661100	-1.90138800	-1.30787700

Scan Point for comp3_7_beta_1.5Å

C	1.77811500	0.68025500	-0.38074200
C	1.25818400	-0.68363700	-0.88400900
C	0.59414700	-1.58827900	0.16877700
C	0.95354200	1.39055700	0.71549200
C	-0.84251700	-1.19821800	0.58502100
C	-0.57832600	1.30190200	0.68412800
H	2.77390300	0.51864600	0.05390500
H	0.52882200	-0.49579500	-1.67745800
H	1.19561700	2.45600800	0.63791300
H	0.51103500	-2.58198400	-0.28567400
H	-1.21237600	-1.94795600	1.28721000
H	-0.93211000	1.96322200	1.47963800

O	1.36761200	-1.77134600	1.34505700
H	1.46064500	-0.90410700	1.79904000
O	2.32020200	-1.38571100	-1.53963900
H	3.00245600	-1.60678400	-0.88500200
O	1.88927000	1.59163200	-1.48077500
H	2.49273600	1.20927300	-2.13714500
O	1.34730200	0.90625700	2.01275100
H	2.23366400	1.24423500	2.21687200
C	-1.21453700	1.78611400	-0.61333200
H	-0.76426300	2.75586800	-0.85847000
H	-1.03814100	1.10502600	-1.45023800
O	-2.62102000	1.93226100	-0.38331400
H	-3.02811800	2.26284100	-1.19772500
O	-1.09398600	0.01699800	1.15824400
C	-3.17175900	-1.53004900	-0.37575500
H	-3.47191500	-0.73755900	0.30347800
H	-3.30522400	-2.52348800	0.05179100
H	-3.64678000	-1.42686800	-1.34907500
O	-1.71826500	-1.32284300	-0.62639700
H	-1.38996200	-1.98044000	-1.27396400

Scan Point for comp3_7_beta_1.6Å

C	1.77328300	0.69008300	-0.39267400
C	1.25544600	-0.67786200	-0.88441600
C	0.61755000	-1.58338600	0.18204100
C	0.95295300	1.39469800	0.70966300
C	-0.80560900	-1.19950100	0.63175300
C	-0.57735200	1.30219700	0.68297900
H	2.77472700	0.53767000	0.03230100
H	0.50683800	-0.49927400	-1.66141500
H	1.18774400	2.46176100	0.63199500
H	0.52679300	-2.57737700	-0.26821500
H	-1.19360000	-1.95392500	1.31729700
H	-0.93297600	1.95638500	1.48295500
O	1.41178100	-1.76560000	1.34597400
H	1.50696300	-0.89922300	1.80083400
O	2.30920800	-1.37348700	-1.55862700
H	3.00782800	-1.58450600	-0.91812700
O	1.86423400	1.59985200	-1.49519000
H	2.46051000	1.22004800	-2.15950500
O	1.35424700	0.91174100	2.00448800
H	2.23573900	1.26172200	2.20963200
C	-1.22517700	1.77908000	-0.61012100

H	-0.76283400	2.73747800	-0.87640400
H	-1.07306000	1.08123800	-1.43782900
O	-2.62452400	1.95260300	-0.35865200
H	-3.04431600	2.25719900	-1.17676400
O	-1.09337900	0.00946700	1.15209500
C	-3.18361700	-1.51357300	-0.36909100
H	-3.44479300	-0.66713700	0.25967100
H	-3.36009600	-2.46767600	0.12819400
H	-3.68051800	-1.45599400	-1.33614100
O	-1.73609100	-1.38608400	-0.65642100
H	-1.44362500	-2.14674200	-1.19862900

Scan Point for comp3_7_beta_1.7Å

C	1.76805500	0.69284200	-0.41816900
C	1.25366800	-0.68665900	-0.87812600
C	0.63821600	-1.57725500	0.21257000
C	0.95778700	1.40524400	0.68563900
C	-0.77270300	-1.19203200	0.68359100
C	-0.57114900	1.31191700	0.67497700
H	2.77767700	0.55735700	-0.00700300
H	0.48875800	-0.52702200	-1.64306200
H	1.18614400	2.47266400	0.59410000
H	0.54591600	-2.57869800	-0.21785100
H	-1.18518000	-1.94492900	1.35498600
H	-0.92024800	1.96158200	1.48093000
O	1.44644900	-1.73959600	1.37133800
H	1.54738600	-0.86545000	1.81016200
O	2.29965700	-1.38667600	-1.55868400
H	3.01177100	-1.58189300	-0.92815200
O	1.83081600	1.58601500	-1.53542100
H	2.41818600	1.20094500	-2.20455800
O	1.37326600	0.93890700	1.98149000
H	2.25344300	1.29790600	2.17686600
C	-1.23923300	1.78165200	-0.60909500
H	-0.76690100	2.72816400	-0.89914200
H	-1.11735100	1.06856200	-1.42872200
O	-2.62862200	1.98317900	-0.32646400
H	-3.06678600	2.26838000	-1.14193200
O	-1.09060500	0.01387300	1.14509900
C	-3.19232200	-1.52646700	-0.36426500
H	-3.44161200	-0.61335700	0.16994500
H	-3.38366200	-2.41496600	0.23917000
H	-3.71087800	-1.57091400	-1.32172900

O	-1.75594900	-1.45130000	-0.67876300
H	-1.49067000	-2.26901000	-1.14552700

Scan Point for comp3_7_beta_1.8Å

C	1.77129000	0.66997400	-0.45107500
C	1.23627300	-0.71432200	-0.86977100
C	0.63014100	-1.57262900	0.25100100
C	0.98723200	1.41188600	0.65154200
C	-0.75772300	-1.15602000	0.74868700
C	-0.54168500	1.34297700	0.66521100
H	2.78729700	0.53550600	-0.05553100
H	0.45839600	-0.56410600	-1.62326400
H	1.22670500	2.47480100	0.53748200
H	0.51044900	-2.58053000	-0.15520500
H	-1.20734800	-1.89848700	1.40651300
H	-0.87071300	2.00117200	1.47219900
O	1.45564500	-1.72624400	1.40011100
H	1.58570100	-0.84409900	1.81505800
O	2.26201600	-1.44145200	-1.55146800
H	2.98459900	-1.62730000	-0.93006200
O	1.81911400	1.53741600	-1.58854500
H	2.38586200	1.12957400	-2.26193600
O	1.41507000	0.96307100	1.94898100
H	2.29878500	1.32101600	2.12994600
C	-1.22901700	1.80140000	-0.61190000
H	-0.75430000	2.74082200	-0.92062400
H	-1.12538600	1.07674600	-1.42383800
O	-2.61110000	2.01523000	-0.30607200
H	-3.06357000	2.28990000	-1.11735900
O	-1.08053700	0.05215200	1.15150400
C	-3.22146100	-1.54008100	-0.35535300
H	-3.46678600	-0.61590800	0.16350000
H	-3.41427600	-2.41257600	0.27175200
H	-3.76314300	-1.60398400	-1.30000500
O	-1.79649500	-1.47198100	-0.68697400
H	-1.53228200	-2.30718800	-1.11896900

Scan Point for comp3_7_beta_1.9Å

C	1.76674300	0.66297700	-0.47946300
C	1.22177800	-0.72667200	-0.86269100

C	0.64343500	-1.56526300	0.28654400
C	0.99874000	1.42351300	0.62090400
C	-0.72468200	-1.13572500	0.81554900
C	-0.52902700	1.36213500	0.65340400
H	2.78844500	0.53484400	-0.09666000
H	0.42280200	-0.58863900	-1.59593800
H	1.23721300	2.48452000	0.48807700
H	0.50779300	-2.57873800	-0.09952400
H	-1.19276800	-1.86829700	1.47045200
H	-0.84745900	2.02306600	1.46202400
O	1.49301300	-1.70408500	1.42091300
H	1.63655100	-0.81492300	1.81592400
O	2.22838200	-1.46538000	-1.55913800
H	2.96829000	-1.64057400	-0.95525700
O	1.79685700	1.50964100	-1.63263300
H	2.34812900	1.08666100	-2.30951300
O	1.44047900	0.99340700	1.91949200
H	2.32313200	1.35967500	2.08887100
C	-1.23817100	1.80483600	-0.61619500
H	-0.75268300	2.72659100	-0.95921000
H	-1.16808900	1.05761700	-1.41135500
O	-2.60706600	2.05448300	-0.28066300
H	-3.07765000	2.30637300	-1.08908500
O	-1.07271300	0.07123700	1.15223700
C	-3.23840800	-1.53519700	-0.36029900
H	-3.44781500	-0.55489900	0.06377800
H	-3.48067400	-2.32889100	0.34997200
H	-3.78758000	-1.66679500	-1.29475900
O	-1.81576200	-1.56236000	-0.68028800
H	-1.58560700	-2.45674600	-0.99366300

Scan Point for comp3_7_beta_2.0Å

C	1.77614800	0.62628500	-0.51005200
C	1.19896300	-0.76081300	-0.85195000
C	0.62512100	-1.56186800	0.32554700
C	1.03691300	1.42517900	0.58267700
C	-0.71602600	-1.09102100	0.87712100
C	-0.49062900	1.39644000	0.63798100
H	2.80008100	0.48777800	-0.13732000
H	0.38875100	-0.62410500	-1.57286400
H	1.29129900	2.47883900	0.42360800
H	0.45566700	-2.57930500	-0.03519200
H	-1.22060300	-1.80794600	1.52174500

H	-0.78522900	2.07234200	1.44292700
O	1.48976100	-1.69479600	1.45042200
H	1.66178700	-0.79932100	1.81978600
O	2.17785300	-1.53516000	-1.54807400
H	2.92393500	-1.71356300	-0.95280500
O	1.80666600	1.44486000	-1.68301100
H	2.34922400	1.00038500	-2.35317400
O	1.48711300	1.01475300	1.88450900
H	2.37633300	1.37235000	2.03738600
C	-1.21822400	1.82364800	-0.62558900
H	-0.72457600	2.72983300	-0.99744300
H	-1.17460200	1.05782300	-1.40488500
O	-2.57544000	2.10169600	-0.26799600
H	-3.06055300	2.33374900	-1.07379800
O	-1.05739500	0.11959500	1.16163600
C	-3.28380400	-1.52739700	-0.34706700
H	-3.48903800	-0.51940200	0.01081900
H	-3.52082500	-2.26618600	0.42285000
H	-3.85725900	-1.72413200	-1.25623800
O	-1.87074100	-1.57556500	-0.68231800
H	-1.64770700	-2.48492400	-0.94875000

Scan Point for comp3_7_beta_2.1Å

C	1.79169100	0.58562300	-0.52934800
C	1.17752400	-0.79143000	-0.84695100
C	0.59784500	-1.56403700	0.34618300
C	1.08186500	1.41483300	0.55992300
C	-0.71271700	-1.04981300	0.92298600
C	-0.44462800	1.42700900	0.62836200
H	2.81487100	0.42688600	-0.16294200
H	0.36216200	-0.64542100	-1.56028500
H	1.36022900	2.46036400	0.38820800
H	0.38912700	-2.57852600	-0.00198000
H	-1.25164200	-1.75229600	1.55548300
H	-0.71724900	2.11351200	1.43180000
O	1.47376200	-1.71106200	1.46201400
H	1.67580200	-0.81646700	1.81883800
O	2.12983500	-1.59876800	-1.54122600
H	2.87798800	-1.78538700	-0.95108400
O	1.83224900	1.38742100	-1.71305100
H	2.36592000	0.92495900	-2.37826200
O	1.53110700	1.00546400	1.86240500
H	2.42772300	1.34731300	2.00812400

C	-1.17991100	1.85331000	-0.63095600
H	-0.67309600	2.74628900	-1.01703200
H	-1.15735100	1.07772100	-1.40164300
O	-2.52693600	2.15835900	-0.26034500
H	-3.01904300	2.38443400	-1.06362000
O	-1.04001100	0.16423000	1.16779100
C	-3.35067600	-1.49877900	-0.32712300
H	-3.54687100	-0.47491700	-0.00945100
H	-3.57399200	-2.19912600	0.48279700
H	-3.95653100	-1.73417900	-1.20660900
O	-1.95040800	-1.56501900	-0.69339400
H	-1.74078900	-2.48045500	-0.94434500

Scan Point for comp3_7_beta_2.2Å

C	1.80530500	0.55489000	-0.54067300
C	1.16045000	-0.81103800	-0.84553300
C	0.57857400	-1.56753000	0.35630600
C	1.11957300	1.40070200	0.55042900
C	-0.70490400	-1.02119100	0.95587300
C	-0.40511100	1.44856900	0.62443200
H	2.82759400	0.37741900	-0.18039200
H	0.33886200	-0.65236900	-1.54926900
H	1.42034200	2.43991700	0.37820200
H	0.33529400	-2.57540700	0.01165900
H	-1.27178900	-1.71304900	1.57572800
H	-0.66204900	2.13750400	1.43072900
O	1.46425600	-1.73792700	1.46198600
H	1.68977400	-0.84838500	1.81694800
O	2.08795400	-1.64064900	-1.54580600
H	2.83862900	-1.83907800	-0.96276900
O	1.85274800	1.34989400	-1.72814500
H	2.37442500	0.87498600	-2.39416900
O	1.56304100	0.97973000	1.85098400
H	2.46507400	1.30685700	1.99720000
C	-1.14099400	1.88447000	-0.63095900
H	-0.61388900	2.76143000	-1.02658400
H	-1.14291600	1.10241700	-1.39574400
O	-2.47606000	2.22567600	-0.25096100
H	-2.96993500	2.45662000	-1.05179400
O	-1.02624800	0.19375100	1.16662500
C	-3.41256800	-1.46501700	-0.30462500
H	-3.57098600	-0.43615700	0.01995100
H	-3.63407200	-2.15635500	0.51431000

H	-4.05983700	-1.68164600	-1.16001400
O	-2.03009100	-1.57096300	-0.71194900
H	-1.85127500	-2.49391900	-0.95736300

Scan Point for comp3_7_beta_2.3Å

C	1.82259300	0.49874700	-0.55868800
C	1.12343800	-0.84478300	-0.84234900
C	0.53655700	-1.57195200	0.37453600
C	1.18091300	1.37667700	0.53352900
C	-0.70667400	-0.97078900	0.99952100
C	-0.33942000	1.48333100	0.61882700
H	2.84146000	0.28598600	-0.20797900
H	0.29413400	-0.66170600	-1.53121200
H	1.51978900	2.40288000	0.35410600
H	0.24076100	-2.56899100	0.03960100
H	-1.30697400	-1.63860200	1.61494000
H	-0.56843400	2.18478400	1.42252900
O	1.43543700	-1.77728500	1.46392400
H	1.69860500	-0.89651500	1.81338100
O	2.00655700	-1.71223100	-1.55274100
H	2.76469000	-1.92711200	-0.98534600
O	1.88450900	1.28190800	-1.75267800
H	2.37850100	0.78263000	-2.42199400
O	1.61645300	0.94286400	1.83212900
H	2.53004000	1.23877700	1.97249800
C	-1.07394100	1.92788500	-0.63392400
H	-0.52527200	2.78701200	-1.03928200
H	-1.10151400	1.13999900	-1.39245800
O	-2.39651700	2.30586300	-0.24706700
H	-2.88436200	2.56088400	-1.04433100
O	-0.99984000	0.25103200	1.17656300
C	-3.49928100	-1.41840600	-0.28181200
H	-3.63958300	-0.38687900	0.04461000
H	-3.71400900	-2.10298500	0.54518700
H	-4.17223100	-1.62888100	-1.11951600
O	-2.12892000	-1.54081100	-0.71578900
H	-1.96213600	-2.46625300	-0.95730400

Scan Point for comp3_7_beta_2.4Å

C	1.84388500	0.40070700	-0.58720200

C	1.05563100	-0.89938100	-0.83342300
C	0.46336500	-1.57514700	0.41063900
C	1.27578500	1.33312900	0.50045100
C	-0.72417900	-0.89305400	1.05745900
C	-0.23399900	1.52797400	0.60786700
H	2.85359300	0.12983200	-0.25016300
H	0.21645000	-0.67410000	-1.49786000
H	1.66842600	2.33526600	0.29564000
H	0.09944300	-2.55734200	0.10001900
H	-1.36550900	-1.51643700	1.67885100
H	-0.41438800	2.25520500	1.40087300
O	1.37404800	-1.81517300	1.48294800
H	1.69480700	-0.94547900	1.81144500
O	1.86008400	-1.82625900	-1.56070200
H	2.62397600	-2.08133900	-1.01813300
O	1.93039200	1.15975200	-1.79463000
H	2.38078100	0.62178000	-2.46471400
O	1.71033600	0.89730000	1.79809000
H	2.64268000	1.14007700	1.91464900
C	-0.96460100	1.97957000	-0.64405200
H	-0.39530500	2.82179800	-1.05649200
H	-1.01425000	1.18900000	-1.39810400
O	-2.27498200	2.39161700	-0.25274900
H	-2.75838100	2.66064000	-1.04812900
O	-0.95536800	0.34239500	1.19887500
C	-3.61489600	-1.33385900	-0.24765600
H	-3.75438800	-0.30371700	0.08479400
H	-3.81167700	-2.01978700	0.58321500
H	-4.30690700	-1.54548700	-1.06999000
O	-2.25378300	-1.44743100	-0.70690500
H	-2.09110600	-2.36716500	-0.96981800

Scan Point for comp3_7_beta_2.5Å

C	-1.84173000	0.36001800	0.63142500
C	-1.02630700	-0.93326300	0.82535500
C	-0.44508700	-1.56885100	-0.44488700
C	-1.32610700	1.31878100	-0.45879600
C	0.70436100	-0.84447900	-1.11160200
C	0.17456300	1.55595800	-0.59852700
H	-2.86006900	0.08155500	0.32822300
H	-0.17800000	-0.70898800	1.47881800
H	-1.74029300	2.30781900	-0.23297500
H	-0.04314300	-2.54384300	-0.15892500

H	1.36032400	-1.44242300	-1.74352900
H	0.31914700	2.29691400	-1.38628700
O	-1.37224700	-1.82031800	-1.50049900
H	-1.72710200	-0.95531300	-1.80570400
O	-1.79817500	-1.89500300	1.54240900
H	-2.55357300	-2.16857200	0.99678700
O	-1.89217000	1.09800600	1.85367700
H	-2.30501700	0.54204900	2.53306900
O	-1.77958900	0.88516400	-1.75033900
H	-2.71859300	1.11083300	-1.84622800
C	0.92756100	2.00353300	0.64084200
H	0.35634300	2.83311500	1.07563500
H	1.00496300	1.20485800	1.38343600
O	2.22279200	2.43672100	0.22357300
H	2.72299500	2.69893200	1.01082100
O	0.91312300	0.39502700	-1.22248400
C	3.68661500	-1.31459300	0.23177100
H	3.82648200	-0.28773000	-0.11160000
H	3.87807100	-2.00704400	-0.59529700
H	4.38671000	-1.52000400	1.04942000
O	2.32915100	-1.42050700	0.69899200
H	2.16445200	-2.33750500	0.96822000

Scan Point for comp3_7_beta_2.6Å

C	-1.84407100	0.33617600	0.65428200
C	-1.01441300	-0.95185400	0.82072800
C	-0.44379300	-1.56748700	-0.46432000
C	-1.35589000	1.30885900	-0.43575800
C	0.68325700	-0.82186400	-1.14341500
C	0.13935600	1.56797500	-0.59094200
H	-2.86548500	0.05211500	0.36724700
H	-0.15850400	-0.72607100	1.46404000
H	-1.78091600	2.29069600	-0.19883500
H	-0.02215300	-2.53835300	-0.19262800
H	1.34676200	-1.40623900	-1.78093700
H	0.26629000	2.31475900	-1.37636700
O	-1.38102400	-1.82479500	-1.50957500
H	-1.75159100	-0.96233900	-1.80328800
O	-1.76566400	-1.92996500	1.53720600
H	-2.52697600	-2.20449900	1.00019000
O	-1.87783200	1.06258400	1.88383000
H	-2.26941900	0.49562200	2.56663800
O	-1.81777900	0.87654300	-1.72457500

H	-2.75832000	1.09859400	-1.81371900
C	0.90488500	2.01373900	0.64081700
H	0.32781800	2.82900900	1.09443000
H	1.00656900	1.20708100	1.37174100
O	2.18612100	2.47193200	0.20773500
H	2.69834300	2.72411100	0.99056000
O	0.88598800	0.41832300	-1.23210300
C	3.74394200	-1.27530700	0.20649800
H	3.83102700	-0.25130600	-0.16287800
H	3.94606700	-1.97598500	-0.61134000
H	4.47496400	-1.43148600	1.00834700
O	2.40475100	-1.42810000	0.70832400
H	2.27939700	-2.34929100	0.98271600

Scan Point for comp3_7_beta_2.7Å

C	-1.85688800	0.32803400	0.65689700
C	-1.02216100	-0.95660500	0.82321500
C	-0.45133500	-1.57225500	-0.46169700
C	-1.37361300	1.29993400	-0.43580100
C	0.66526200	-0.82197600	-1.15079600
C	0.12012900	1.56649700	-0.59099100
H	-2.87773600	0.04009500	0.37177400
H	-0.16536300	-0.72639100	1.46412000
H	-1.80350200	2.28053400	-0.20238800
H	-0.01949500	-2.53822100	-0.18759300
H	1.33285700	-1.40574200	-1.78526600
H	0.24466900	2.31141300	-1.37859600
O	-1.38892400	-1.84238500	-1.50351200
H	-1.76585000	-0.98417800	-1.80105600
O	-1.76738900	-1.93710700	1.54219200
H	-2.52932800	-2.21489200	1.00764000
O	-1.89085600	1.05600700	1.88526200
H	-2.28258100	0.49005200	2.56881600
O	-1.83187000	0.86038800	-1.72329400
H	-2.77308200	1.07850600	-1.81501800
C	0.88718000	2.01513100	0.63844100
H	0.30386800	2.82226400	1.09852300
H	1.00114300	1.20618400	1.36506900
O	2.16101200	2.48859700	0.20048400
H	2.67800200	2.73472500	0.98213200
O	0.87105400	0.41653600	-1.23171700
C	3.80203400	-1.22651900	0.17209900
H	3.82251900	-0.21145900	-0.23053400

H	4.00175600	-1.94105600	-0.63456100
H	4.57819600	-1.32093200	0.94085200
O	2.49632200	-1.42645600	0.73913100
H	2.43548100	-2.33899400	1.05951900

Scan Point for comp3_7_beta_2.8Å

C	-1.85899400	0.30268900	0.68013400
C	-1.01048700	-0.97624700	0.81757600
C	-0.45076500	-1.56978100	-0.48260300
C	-1.40341500	1.29114700	-0.40949000
C	0.64397000	-0.79797900	-1.18164700
C	0.08460700	1.57799000	-0.58213500
H	-2.88177000	0.00829000	0.40915200
H	-0.14679000	-0.74601000	1.44943000
H	-1.84192200	2.26416100	-0.16088800
H	0.00024300	-2.53188600	-0.22502600
H	1.31362100	-1.36750600	-1.82747300
H	0.19056700	2.33163100	-1.36427600
O	-1.39852000	-1.84303200	-1.51423500
H	-1.79133800	-0.98722100	-1.79805600
O	-1.73582700	-1.97379200	1.53336800
H	-2.50438100	-2.25010600	1.00741500
O	-1.87893000	1.01644100	1.91693700
H	-2.24313900	0.43494000	2.60268900
O	-1.87370800	0.85767300	-1.69460300
H	-2.81690400	1.07157600	-1.77535700
C	0.86578200	2.02012900	0.64042800
H	0.28220600	2.81645000	1.11864500
H	0.99777800	1.20317400	1.35501500
O	2.12867300	2.50969600	0.18902800
H	2.65633900	2.74845900	0.96583300
O	0.84034100	0.44192800	-1.24519700
C	3.86183300	-1.18750000	0.14466600
H	3.84749800	-0.16920700	-0.25046700
H	4.05483800	-1.89072700	-0.67373000
H	4.66260200	-1.26968100	0.88941400
O	2.57740500	-1.42087100	0.74548500
H	2.54990300	-2.33335700	1.06984900

Scan Point for comp3_7_beta_2.9Å

C	-1.86325700	0.28008000	0.69826500
C	-1.00391800	-0.99391400	0.81207500
C	-0.45251800	-1.56905600	-0.49997800
C	-1.42972100	1.28248500	-0.38763100
C	0.62690500	-0.78025000	-1.20337800
C	0.05330200	1.58544300	-0.57472900
H	-2.88717800	-0.01943700	0.43783600
H	-0.13523800	-0.76330800	1.43713000
H	-1.87389100	2.24935200	-0.12541700
H	0.01210600	-2.52857200	-0.25594900
H	1.30075800	-1.33775000	-1.85589900
H	0.14409900	2.34512500	-1.35302000
O	-1.40717900	-1.84241800	-1.52480000
H	-1.81254900	-0.98819700	-1.79581800
O	-1.71315900	-2.00535700	1.52412400
H	-2.48734900	-2.27991800	1.00544200
O	-1.87235800	0.98150900	1.94214700
H	-2.21802700	0.38867500	2.62781800
O	-1.91143800	0.85576500	-1.67064400
H	-2.85656300	1.06511000	-1.74009000
C	0.84433800	2.02445900	0.64246900
H	0.26024500	2.81252500	1.13350800
H	0.98970900	1.20210800	1.34833900
O	2.09865300	2.52646900	0.18124900
H	2.63414000	2.76100900	0.95397900
O	0.81446900	0.46080600	-1.25332500
C	3.91718000	-1.14284600	0.11229500
H	3.85864000	-0.12280900	-0.27435300
H	4.09973500	-1.83454500	-0.71845500
H	4.74841300	-1.20654500	0.82491800
O	2.66430900	-1.41834700	0.75922700
H	2.68270200	-2.32865000	1.08988000

Scan Point for comp3_7_beta_3.0Å

C	-1.86153700	0.26486400	0.72033500
C	-0.99956100	-1.00964900	0.80401700
C	-0.46609500	-1.56625500	-0.52325500
C	-1.44633300	1.28205200	-0.35913400
C	0.60296800	-0.76687900	-1.23014500
C	0.03302000	1.59037200	-0.56542600
H	-2.88905800	-0.03227600	0.47219800
H	-0.12201100	-0.78579400	1.41922700
H	-1.88708200	2.24497700	-0.07721700

H	0.00320500	-2.52848300	-0.29831000
H	1.27442300	-1.31539700	-1.89324700
H	0.11116000	2.35745900	-1.33787900
O	-1.43321900	-1.82643700	-1.53950500
H	-1.84454600	-0.96925600	-1.79232200
O	-1.69675000	-2.03173000	1.51246000
H	-2.47937000	-2.29930400	1.00280600
O	-1.85141200	0.95003000	1.97325700
H	-2.18417600	0.34763700	2.65698300
O	-1.94882700	0.87204500	-1.63953400
H	-2.89453700	1.08378200	-1.69131700
C	0.84052900	2.01863800	0.64481700
H	0.26350200	2.80206600	1.15151000
H	0.99499500	1.18915800	1.34042900
O	2.08853000	2.52452100	0.17121300
H	2.64086900	2.73721300	0.93833300
O	0.78940600	0.47421400	-1.26466700
C	3.95578800	-1.11619900	0.07725700
H	3.87229300	-0.08969300	-0.28690000
H	4.10459400	-1.79005200	-0.77479300
H	4.82113500	-1.18725800	0.74735800
O	2.73712200	-1.41498000	0.77618400
H	2.78312700	-2.32773500	1.09706500

Scan Point for comp3_7_beta_3.1Å

C	-1.86060400	0.23751400	0.73961400
C	-0.98548500	-1.02950500	0.79565600
C	-0.46326400	-1.56272100	-0.54555900
C	-1.47040200	1.27252900	-0.33277600
C	0.58820400	-0.74252700	-1.25515900
C	0.00248300	1.60011500	-0.55491900
H	-2.88847900	-0.06613700	0.50125800
H	-0.10192200	-0.80453600	1.40213500
H	-1.91726300	2.22710600	-0.03263000
H	0.01980500	-2.52242600	-0.33898200
H	1.25975100	-1.27579100	-1.93087000
H	0.06240700	2.37621700	-1.32002200
O	-1.43934100	-1.82109700	-1.55346200
H	-1.86302900	-0.96546100	-1.79054300
O	-1.66240500	-2.06797800	1.49956600
H	-2.45096500	-2.33554200	0.99905200
O	-1.83983000	0.90783600	2.00035900
H	-2.16327600	0.29696400	2.68094500

O	-1.98641400	0.87412100	-1.61142400
H	-2.93693600	1.06786100	-1.64311200
C	0.81999200	2.02302400	0.65039200
H	0.23859200	2.78960100	1.17730500
H	0.99681000	1.18448200	1.33005200
O	2.05380600	2.55467700	0.16790400
H	2.60829500	2.77660600	0.93090400
O	0.76360500	0.50000900	-1.27442100
C	3.99355600	-1.07506300	0.04874100
H	3.89785200	-0.02121700	-0.22262600
H	4.08598000	-1.67486100	-0.86452600
H	4.89673100	-1.20528000	0.65708500
O	2.81493200	-1.42595200	0.79047300
H	2.87394100	-2.36071400	1.03668700

Scan Point for comp3_7_beta_3.2Å

C	-1.86825200	0.22580500	0.74256300
C	-0.98632100	-1.03661800	0.79560600
C	-0.46388400	-1.56542200	-0.54732600
C	-1.48545500	1.26346200	-0.32998800
C	0.57988500	-0.73777500	-1.25940700
C	-0.01497600	1.60083500	-0.55202000
H	-2.89499300	-0.08276500	0.50564300
H	-0.10229500	-0.80802900	1.40054300
H	-1.93834700	2.21512800	-0.02968600
H	0.02755800	-2.52126600	-0.34183600
H	1.25298900	-1.26638700	-1.93751800
H	0.04045000	2.37747600	-1.31693200
O	-1.44023300	-1.83165100	-1.55268600
H	-1.86918200	-0.97886200	-1.79023200
O	-1.65611000	-2.07971700	1.49928200
H	-2.44505800	-2.35007700	1.00080500
O	-1.84850300	0.89548500	2.00354700
H	-2.17089600	0.28394500	2.68399600
O	-1.99890000	0.86174900	-1.60855800
H	-2.95083000	1.04860700	-1.64001000
C	0.79964800	2.02754200	0.65372300
H	0.20795000	2.78025800	1.18897300
H	0.99210500	1.18597600	1.32568700
O	2.02301800	2.58296900	0.17161400
H	2.57685700	2.80699900	0.93451900
O	0.75250100	0.50490900	-1.27277600
C	4.01244200	-1.01412100	0.01547200

H	3.81727800	0.02915500	-0.24237000
H	4.10543400	-1.60125200	-0.90596000
H	4.95380400	-1.07259800	0.57542700
O	2.90666800	-1.46308700	0.81423800
H	3.05113600	-2.39381300	1.03992100

Scan Point for comp3_7_beta_3.3Å

C	-1.84145200	0.19734800	0.79090300
C	-0.95305300	-1.06136400	0.77081600
C	-0.47586400	-1.54587900	-0.60458400
C	-1.49989500	1.27039100	-0.26083800
C	0.53449500	-0.69023100	-1.33021400
C	-0.03939800	1.62096700	-0.52438400
H	-2.87550700	-0.10642400	0.58054100
H	-0.04834000	-0.84549800	1.34924300
H	-1.94439800	2.21002200	0.08671200
H	0.03154800	-2.50202500	-0.44314800
H	1.18255000	-1.19454000	-2.05031500
H	-0.01344300	2.42156400	-1.26591300
O	-1.48423400	-1.79484800	-1.58273400
H	-1.92420500	-0.93976900	-1.78681300
O	-1.59068700	-2.12976100	1.46589900
H	-2.39873400	-2.38659400	0.99151300
O	-1.77666500	0.82704700	2.07082800
H	-2.08186600	0.19810100	2.74320300
O	-2.05757800	0.90882900	-1.53232400
H	-3.01445800	1.07022700	-1.51299900
C	0.81852500	2.01116700	0.66326100
H	0.24689700	2.74431000	1.24552100
H	1.03773600	1.14901500	1.30014300
O	2.02252400	2.58458000	0.15417600
H	2.61043900	2.77106400	0.90150600
O	0.70485600	0.55213700	-1.30773100
C	4.01099500	-1.02394400	-0.01800400
H	3.81801700	0.02359300	-0.25996900
H	4.07147900	-1.60232300	-0.94779400
H	4.96755500	-1.09693900	0.51368100
O	2.92410700	-1.47070600	0.80768500
H	3.07002700	-2.40274600	1.02675500

Scan Point for comp3_7_beta_3.5Å

C	-1.80890100	0.11141600	0.85920700
C	-0.88466600	-1.11314800	0.72660400
C	-0.47084500	-1.51565200	-0.69455600
C	-1.55361500	1.24811800	-0.14851800
C	0.46826300	-0.59194900	-1.43095600
C	-0.12028800	1.65774700	-0.46893200
H	-2.84323100	-0.21415500	0.68431200
H	0.04474200	-0.89332000	1.26209500
H	-2.00692300	2.15375900	0.27107300
H	0.07725200	-2.45890000	-0.60697900
H	1.08786900	-1.03888300	-2.21175500
H	-0.15700700	2.49515500	-1.16783300
O	-1.52267200	-1.75634600	-1.62825100
H	-1.99808100	-0.90860400	-1.77158800
O	-1.44643600	-2.23364000	1.40466500
H	-2.27831100	-2.48894700	0.97256200
O	-1.69579500	0.67154700	2.16755500
H	-1.91704600	-0.01394000	2.81747700
O	-2.16405500	0.93346900	-1.40808400
H	-3.12404100	1.05338500	-1.33056700
C	0.79585600	2.01067600	0.68717300
H	0.23828000	2.69027900	1.34340300
H	1.08020800	1.12299400	1.26016300
O	1.94842500	2.65182600	0.14148300
H	2.57129500	2.82334800	0.86371500
O	0.60710600	0.65177500	-1.34937000
C	4.06645000	-0.97586000	-0.08378800
H	3.83807400	0.07288800	-0.28691800
H	4.09266600	-1.52812600	-1.03090300
H	5.05040800	-1.04017900	0.39660200
O	3.03317300	-1.47015000	0.78264000
H	3.21235800	-2.40268600	0.97262500

Scan Point for comp3_7_beta_3.6Å

C	-1.74972700	0.06998600	0.91632600
C	-0.82966600	-1.14312900	0.68202900
C	-0.48209100	-1.47293900	-0.77601100
C	-1.54717800	1.25351800	-0.04831500
C	0.41374100	-0.50782900	-1.51515700
C	-0.13244300	1.68734700	-0.41573900
H	-2.78979500	-0.25272300	0.77526800
H	0.12201900	-0.94752400	1.18609400

H	-1.98472400	2.13613400	0.43205700
H	0.07544700	-2.41458200	-0.76132000
H	0.99460900	-0.91360300	-2.34674600
H	-0.20621000	2.55740400	-1.07003900
O	-1.57954600	-1.67822400	-1.66455300
H	-2.07433900	-0.83183700	-1.73046100
O	-1.35983000	-2.29836000	1.32650100
H	-2.21487000	-2.52614600	0.92557700
O	-1.57742800	0.56966300	2.24256400
H	-1.79965100	-0.13547100	2.87041700
O	-2.21517400	0.99014400	-1.29079500
H	-3.16961800	1.11752100	-1.16801600
C	0.83720700	1.98964200	0.71014500
H	0.31549000	2.65253100	1.41154800
H	1.13711200	1.08146000	1.24157500
O	1.97069300	2.63920500	0.13497000
H	2.62125400	2.79301600	0.83637100
O	0.55458900	0.73045900	-1.37951500
C	3.96026200	-1.00974700	-0.15494300
H	3.70127300	0.03329000	-0.35105700
H	3.93252800	-1.56983500	-1.09764300
H	4.97577200	-1.05183500	0.25738200
O	2.99637800	-1.51500300	0.78169900
H	3.22562500	-2.43196900	0.99201700

Scan Point for comp3_7_beta_3.7Å

C	-1.73913500	0.06162500	0.93896200
C	-0.83613700	-1.15693400	0.66745400
C	-0.52456800	-1.46558300	-0.80335400
C	-1.54431700	1.25981700	-0.00929900
C	0.37202700	-0.49983900	-1.54077000
C	-0.13319100	1.68504100	-0.40020400
H	-2.78473700	-0.24901000	0.81274500
H	0.12781400	-0.97921600	1.15487300
H	-1.96113300	2.13867000	0.49564400
H	0.01558400	-2.41721800	-0.81974200
H	0.93698500	-0.89816800	-2.38685900
H	-0.21243400	2.56330600	-1.04286300
O	-1.64535200	-1.63111900	-1.67033900
H	-2.12820900	-0.77494600	-1.69988700
O	-1.36636700	-2.31672000	1.30330300
H	-2.22807800	-2.53199100	0.90981000
O	-1.53715000	0.53792700	2.26961200

H	-1.76163300	-0.17243400	2.89067100
O	-2.24210100	1.02577800	-1.24153500
H	-3.19177200	1.16633700	-1.09864600
C	0.85887000	1.96798100	0.71131100
H	0.35452800	2.62704300	1.42872800
H	1.16047100	1.05177500	1.22803800
O	1.98697200	2.61549200	0.12358200
H	2.65210500	2.75335800	0.81453800
O	0.52892900	0.73447300	-1.38716100
C	3.99560100	-1.01348300	-0.19645200
H	3.73781600	0.03030500	-0.39066600
H	3.91993900	-1.58091700	-1.13211900
H	5.02761700	-1.06205000	0.17174200
O	3.06880200	-1.50021100	0.78659400
H	3.29036400	-2.42156300	0.98565500

Scan Point for comp3_7_beta_3.8Å

C	-1.71800100	0.07897600	0.95335100
C	-0.83954800	-1.15360400	0.66421700
C	-0.55228400	-1.46093700	-0.81178500
C	-1.51598300	1.27811600	0.00812800
C	0.35184600	-0.50794600	-1.55617300
C	-0.10297000	1.68036400	-0.39947100
H	-2.77028900	-0.21365900	0.84073700
H	0.13357000	-0.99387500	1.13969700
H	-1.91011100	2.16182700	0.52285100
H	-0.03194800	-2.42323200	-0.84025400
H	0.89806500	-0.91066900	-2.41233900
H	-0.17504700	2.56295700	-1.03704200
O	-1.68713200	-1.59834700	-1.66533700
H	-2.15322800	-0.73231600	-1.68147500
O	-1.38179400	-2.30697700	1.30148800
H	-2.25076700	-2.50666400	0.91568200
O	-1.48976500	0.54606100	2.28307700
H	-1.72050300	-0.16159000	2.90493600
O	-2.23392000	1.06237300	-1.21575800
H	-3.17922800	1.21771000	-1.06033300
C	0.90800200	1.94140000	0.70071800
H	0.42200100	2.60133700	1.42988600
H	1.20401200	1.01714200	1.20608200
O	2.03637000	2.57859000	0.10244600
H	2.72213800	2.68084100	0.77928100
O	0.52967500	0.72328200	-1.39954300

C	3.84886100	-1.13893100	-0.30709700
H	3.57779400	-0.13346600	-0.63720400
H	3.59255800	-1.85720400	-1.09542500
H	4.93049300	-1.17337200	-0.12765200
O	3.11300600	-1.39904700	0.89778100
H	3.33942600	-2.28786500	1.20800600

Scan Point for comp3_7_beta_3.9Å

C	-1.71159400	0.05869900	0.96416400
C	-0.81789000	-1.16122700	0.66753000
C	-0.53883300	-1.46399700	-0.81077000
C	-1.53563900	1.26087900	0.01729900
C	0.34201500	-0.49641700	-1.56444300
C	-0.13218900	1.68376800	-0.40265900
H	-2.76045100	-0.24896200	0.85972900
H	0.15686800	-0.98839400	1.13512500
H	-1.93833500	2.13848700	0.53576700
H	-0.00282000	-2.41755100	-0.84406400
H	0.88278600	-0.89036500	-2.42809000
H	-0.22232000	2.56661500	-1.03758300
O	-1.67908800	-1.62085100	-1.65350500
H	-2.16024800	-0.76315100	-1.66490500
O	-1.33801400	-2.32254000	1.30862900
H	-2.20702800	-2.53450300	0.92971300
O	-1.47972400	0.52836700	2.29228900
H	-1.70207600	-0.18050400	2.91579200
O	-2.26156700	1.03418300	-1.19981500
H	-3.20841500	1.16650300	-1.03225700
C	0.88471300	1.95563500	0.68923800
H	0.39828700	2.61261400	1.42086800
H	1.19331800	1.03541200	1.19427700
O	2.00302600	2.60143200	0.08151800
H	2.69561200	2.70364700	0.75138300
O	0.50341400	0.73722300	-1.40977000
C	3.80272500	-1.17409700	-0.36591600
H	3.49445700	-0.20572600	-0.76681800
H	3.45054500	-1.97049400	-1.03303800
H	4.89830100	-1.20372700	-0.32019200
O	3.22243500	-1.29125600	0.94182200
H	3.50780300	-2.13182100	1.32829500

Scan Point for comp3_7_beta_4.0Å

C	-1.72183000	0.07695900	0.95821800
C	-0.82138900	-1.14561700	0.69819800
C	-0.53977600	-1.48762100	-0.77085100
C	-1.54286800	1.25650600	-0.01566100
C	0.34084300	-0.53692000	-1.54598600
C	-0.13742700	1.67084900	-0.43677800
H	-2.76866000	-0.23754400	0.85214600
H	0.15234500	-0.95511700	1.16181900
H	-1.95063600	2.14542800	0.47897800
H	-0.00058500	-2.43997300	-0.77772700
H	0.88188800	-0.95039300	-2.40015800
H	-0.22375100	2.53771200	-1.09386800
O	-1.67704000	-1.67100400	-1.61197600
H	-2.15907000	-0.81488800	-1.65209900
O	-1.33628200	-2.28985000	1.37313200
H	-2.20808200	-2.51226300	1.00692000
O	-1.50273000	0.57783700	2.27695800
H	-1.71717800	-0.12202500	2.91338400
O	-2.26059500	0.99848800	-1.23129000
H	-3.20828200	1.13711000	-1.07398000
C	0.87289900	1.96892100	0.65366300
H	0.38120800	2.64067200	1.36817500
H	1.18155600	1.06095500	1.18009700
O	1.99308900	2.60361900	0.03782700
H	2.68452200	2.71542400	0.70735100
O	0.50282700	0.69978800	-1.41853900
C	3.72745300	-1.26502900	-0.39863200
H	3.42475300	-0.34234400	-0.89893300
H	3.20584400	-2.11386000	-0.85748000
H	4.80852100	-1.39876500	-0.52761000
O	3.38008700	-1.12509000	0.98719800
H	3.65332600	-1.92871600	1.45347500

Scan Point for comp3_7_beta_4.1Å

C	-1.69154700	0.05211600	0.99582600
C	-0.80062800	-1.16439100	0.67594100
C	-0.56332200	-1.46713300	-0.80914900
C	-1.54533800	1.25463100	0.04423200
C	0.29058100	-0.49556300	-1.58769700
C	-0.15410400	1.68118100	-0.41070600
H	-2.74133600	-0.26026500	0.91764000

H	0.18644700	-0.98828300	1.11652100
H	-1.93767700	2.13092500	0.57277900
H	-0.02395900	-2.41819900	-0.85748200
H	0.80604300	-0.88673600	-2.46784500
H	-0.26098600	2.56626600	-1.03987100
O	-1.72607800	-1.63096700	-1.61867500
H	-2.20904400	-0.77437500	-1.62184300
O	-1.29870700	-2.32705800	1.33161600
H	-2.17556600	-2.54334200	0.97396300
O	-1.42888500	0.52262100	2.31771800
H	-1.64149300	-0.18402200	2.94713800
O	-2.30181900	1.02506300	-1.15358700
H	-3.24483500	1.14840300	-0.95920500
C	0.88867500	1.95000800	0.65711700
H	0.41936600	2.60601300	1.40075300
H	1.20888600	1.02926700	1.15359900
O	1.99297600	2.59578000	0.02456000
H	2.70211800	2.69330300	0.67763800
O	0.45475200	0.73806700	-1.43593000
C	3.71528500	-1.25537400	-0.43874900
H	3.41475200	-0.31532800	-0.90713900
H	3.15159300	-2.08144700	-0.88922600
H	4.78565300	-1.41437200	-0.61884200
O	3.43546800	-1.13405600	0.96415800
H	3.70076800	-1.95626700	1.40164100

Scan Point for comp3_7_beta_4.2Å

C	-1.51636200	-0.01859400	1.12431900
C	-0.72984200	-1.20954000	0.54183600
C	-0.69726600	-1.32914500	-0.98834900
C	-1.43555400	1.28927300	0.31531400
C	0.10602100	-0.29820100	-1.74401900
C	-0.09408100	1.72626400	-0.26165600
H	-2.58116000	-0.28683500	1.15059300
H	0.31260200	-1.12003400	0.86551400
H	-1.71432400	2.10328500	0.99429400
H	-0.21806300	-2.28527500	-1.22028300
H	0.49711800	-0.59140100	-2.72091200
H	-0.23695000	2.68569000	-0.76151100
O	-1.95644600	-1.34838900	-1.65795100
H	-2.39140100	-0.47960100	-1.50561100
O	-1.18737700	-2.43248200	1.11294500
H	-2.11019200	-2.58289500	0.85053100

O	-1.06164100	0.27424800	2.44586600
H	-1.17787500	-0.51528600	2.99718900
O	-2.34860100	1.23992100	-0.78978400
H	-3.25140000	1.35929300	-0.45395800
C	1.08384700	1.82571300	0.68841600
H	0.73860500	2.39271900	1.56180800
H	1.41960700	0.83977300	1.02156200
O	2.13077000	2.51513900	0.00644400
H	2.91014600	2.52574700	0.58196800
O	0.34081300	0.90151300	-1.46480900
C	3.42162900	-1.33077900	-0.58981900
H	3.40690500	-0.27994100	-0.88743100
H	2.61517900	-1.86426300	-1.10906800
H	4.38350600	-1.76847400	-0.88395300
O	3.24432800	-1.37080100	0.83290100
H	3.27257700	-2.29564800	1.11811600

Scan Point for comp3_7_beta_4.3Å

C	-1.52327700	-0.02562800	1.13033400
C	-0.73298100	-1.21378400	0.54733200
C	-0.70551600	-1.33608300	-0.98296300
C	-1.45093500	1.28066700	0.31824900
C	0.08652600	-0.30172500	-1.74530800
C	-0.11276800	1.72208600	-0.26321800
H	-2.58675700	-0.29872800	1.16032200
H	0.31008100	-1.11823300	0.86759300
H	-1.73198600	2.09499000	0.99588700
H	-0.22019100	-2.28927200	-1.21464400
H	0.47185600	-0.59418700	-2.72476000
H	-0.26014000	2.68156000	-0.76164900
O	-1.96730500	-1.36629400	-1.64720100
H	-2.40708500	-0.49965300	-1.49707500
O	-1.18275900	-2.43796700	1.12150300
H	-2.10611500	-2.59247700	0.86316400
O	-1.06578000	0.27202200	2.44978200
H	-1.17825900	-0.51629200	3.00363100
O	-2.36606400	1.22426700	-0.78475700
H	-3.26865200	1.34017200	-0.44718200
C	1.06865900	1.82463600	0.68225000
H	0.72464000	2.38880900	1.55792100
H	1.41042500	0.83974800	1.01284500
O	2.10964500	2.51963100	-0.00298100
H	2.88873900	2.54011800	0.57267300

O	0.31836800	0.89925000	-1.46875600
C	3.43546900	-1.30086300	-0.60654200
H	3.39234900	-0.25161500	-0.90703400
H	2.59336400	-1.84153200	-1.05724700
H	4.37317100	-1.73576800	-0.97384700
O	3.37407400	-1.33425800	0.82682300
H	3.44207100	-2.25667500	1.11329600

Scan Point for comp3_7_beta_4.4Å

C	-1.53412800	-0.02545200	1.13451200
C	-0.74753900	-1.21665900	0.55240600
C	-0.72385300	-1.34255500	-0.97764500
C	-1.46053400	1.27865800	0.31900800
C	0.06755900	-0.31116600	-1.74444900
C	-0.12229400	1.71560200	-0.26579200
H	-2.59807500	-0.29622600	1.16753200
H	0.29652700	-1.12254100	0.86991300
H	-1.73884500	2.09531300	0.99493800
H	-0.23991700	-2.29675500	-1.20823800
H	0.44934100	-0.60676200	-2.72434500
H	-0.26805600	2.67470400	-0.76540400
O	-1.98727400	-1.37357900	-1.63875600
H	-2.42542800	-0.50580400	-1.49104400
O	-1.19853800	-2.43850200	1.13043700
H	-2.12199400	-2.59265100	0.87228500
O	-1.07292300	0.27431200	2.45218100
H	-1.19062600	-0.51081200	3.00944800
O	-2.37740300	1.22121400	-0.78250100
H	-3.27919600	1.34092600	-0.44416200
C	1.06142100	1.81663200	0.67707200
H	0.72029300	2.38171200	1.55328200
H	1.40235000	0.83129800	1.00775900
O	2.10198000	2.50958400	-0.01066900
H	2.88257500	2.52869900	0.56300100
O	0.30360600	0.88964400	-1.47090100
C	3.45926500	-1.27304300	-0.61572400
H	3.40312300	-0.22314600	-0.91153800
H	2.58260200	-1.80672700	-1.00477600
H	4.36444300	-1.71422300	-1.05096400
O	3.50240700	-1.30750600	0.81857000
H	3.58664600	-2.23043800	1.09910000

8.2: Geometries for Relaxed PES Scans of Tier 1 and Bare Septanoside Model Systems

Scan Point for comp6_alpha_1.4Å

C	0.03583600	1.58828300	-0.15469500
H	-0.91758000	2.10748800	-0.03034600
H	0.25168400	1.48950100	-1.22152600
H	0.81049400	2.19616000	0.31995000
C	0.00375700	0.24354300	0.54484400
C	2.08347400	-0.45668300	-0.50741200
H	2.88627800	-1.14860600	-0.24976500
H	1.55199900	-0.82674700	-1.38893800
H	2.50540000	0.53259300	-0.70458300
O	1.22182400	-0.42619800	0.65470700
H	-0.36867100	0.33696300	1.56992200
O	-0.84906100	-0.62859400	-0.14223500
H	-0.68617600	-1.55548300	0.13957300
C	-2.31663900	-0.34358900	-0.19606100
H	-2.75669500	-1.24348700	-0.61850900
H	-2.65967200	-0.14985900	0.82001300
H	-2.43773500	0.51048700	-0.85561700

Scan Point for comp6_alpha_1.5Å

C	0.06298500	1.58543800	-0.15885000
H	-0.89182300	2.10026400	-0.03023000
H	0.27115000	1.47183400	-1.22524800
H	0.84017200	2.20468900	0.29855300
C	0.04853400	0.26090200	0.56437700
C	2.09689900	-0.46640500	-0.51060300
H	2.88368000	-1.17820600	-0.25951400
H	1.55861500	-0.81084400	-1.39762800
H	2.53704700	0.51850000	-0.68653500
O	1.22933100	-0.43875900	0.64958000
H	-0.34882500	0.33377500	1.57900600
O	-0.89572700	-0.65226200	-0.15984900
H	-0.76888400	-1.56370500	0.17941900
C	-2.34188300	-0.31298900	-0.18793100
H	-2.83476700	-1.19801000	-0.58483100
H	-2.66669300	-0.08539200	0.82759900
H	-2.44770700	0.53358700	-0.86040500

Scan Point for comp6_alpha_1.6Å

C	0.09535100	1.58519700	-0.16996900
H	-0.86362100	2.09286300	-0.04622400
H	0.30475300	1.45362800	-1.23370000
H	0.86978100	2.21911800	0.27418500
C	0.09372400	0.28265000	0.57930900
C	2.11316600	-0.48532400	-0.50596500
H	2.87909700	-1.21762400	-0.25129900
H	1.57165300	-0.80918100	-1.39806500
H	2.57472900	0.49198800	-0.66559000
O	1.23263200	-0.44889500	0.64700800
H	-0.33363700	0.33742600	1.58101700
O	-0.94425700	-0.66437000	-0.18603300
H	-0.83071500	-1.56449500	0.18217600
C	-2.37225300	-0.29054200	-0.16924600
H	-2.91022300	-1.15813000	-0.54821300
H	-2.66806500	-0.04961700	0.85272700
H	-2.48068400	0.55825700	-0.83958900

Scan Point for comp6_alpha_1.7Å

C	0.19018800	1.59617400	-0.18917900
H	-0.76401100	2.12085400	-0.11451800
H	0.44919700	1.45063600	-1.23962000
H	0.95515500	2.22118500	0.28589100
C	0.13149300	0.30903200	0.57219500
C	2.14189900	-0.53570200	-0.46093800
H	2.86067300	-1.30554800	-0.18256700
H	1.62997300	-0.81595800	-1.38409600
H	2.64758700	0.42600600	-0.57029700
O	1.20186000	-0.48834800	0.64680500
H	-0.35387900	0.35111000	1.54638400
O	-1.01376900	-0.61804700	-0.27568600
H	-0.86355300	-1.54161600	0.00797800
C	-2.43160400	-0.27698800	-0.10254000
H	-3.00068900	-1.06820400	-0.59049700
H	-2.66835400	-0.21695900	0.96127300
H	-2.58868900	0.67455500	-0.60611100

Scan Point for comp6_alpha_1.8Å

C	0.22641500	1.59324500	-0.20290000
H	-0.72964000	2.11467800	-0.13437500
H	0.48622700	1.42543900	-1.24961000
H	0.99214900	2.23109200	0.25661800
C	0.17952400	0.33131000	0.58949300
C	2.15438000	-0.55920200	-0.46140600
H	2.84903600	-1.35117400	-0.18538000
H	1.63299200	-0.81824600	-1.38498500
H	2.68332200	0.39051600	-0.55992900
O	1.20942200	-0.49361100	0.64489900
H	-0.33046300	0.36268800	1.55037800
O	-1.06597900	-0.62675400	-0.28848000
H	-0.92859500	-1.54086800	0.02509000
C	-2.46528000	-0.25544100	-0.09044300
H	-3.07382600	-1.02439300	-0.56844100
H	-2.68888300	-0.18940000	0.97669500
H	-2.61009200	0.70311100	-0.58587400

Scan Point for comp6_alpha_1.9Å

C	0.24805200	1.58701200	-0.21480000
H	-0.71077100	2.10153600	-0.13876300
H	0.49279000	1.39387400	-1.26058000
H	1.01838000	2.24329600	0.21319800
C	0.23323800	0.35473900	0.61338400
C	2.16074300	-0.57674700	-0.47831200
H	2.83714100	-1.38732200	-0.21241900
H	1.61638200	-0.81837300	-1.39283000
H	2.70901400	0.36137900	-0.57759000
O	1.22967900	-0.49076900	0.64166100
H	-0.28688500	0.37812000	1.56839900
O	-1.11397600	-0.65395400	-0.26840500
H	-1.00424900	-1.54361800	0.11420700
C	-2.49613700	-0.22970800	-0.09979200
H	-3.14006500	-1.00237700	-0.52470500
H	-2.72183400	-0.07977500	0.95918900
H	-2.61090700	0.69926400	-0.65703300

Scan Point for comp6_alpha_2.0Å

C	0.27033500	1.57847500	-0.22093100
H	-0.69013900	2.08773500	-0.13537800

H	0.50118600	1.36667800	-1.26618500
H	1.04482600	2.24874200	0.18017200
C	0.28375700	0.36956400	0.63195700
C	2.17840900	-0.58567800	-0.48960100
H	2.84648300	-1.40390900	-0.22742800
H	1.62439500	-0.81728500	-1.40053500
H	2.73249700	0.34914100	-0.58403900
O	1.24930500	-0.49528200	0.63463400
H	-0.24901200	0.37989100	1.57963200
O	-1.16895300	-0.67888800	-0.25707600
H	-1.09215000	-1.54739300	0.17574200
C	-2.52967900	-0.20021300	-0.10443000
H	-3.21247600	-0.95587600	-0.50085600
H	-2.75269500	-0.00160000	0.94785700
H	-2.61265700	0.71434600	-0.69141600

Scan Point for comp6_alpha_2.1Å

C	0.29864700	1.57221000	-0.22890700
H	-0.66518000	2.07435700	-0.14027300
H	0.52272300	1.34235500	-1.27185800
H	1.07234900	2.25771500	0.15028900
C	0.33484400	0.38579400	0.64716900
C	2.19752200	-0.60058600	-0.49794100
H	2.85995700	-1.42185900	-0.23206800
H	1.63620800	-0.83191200	-1.40418800
H	2.75467100	0.33173700	-0.59529000
O	1.26902800	-0.50018400	0.62893000
H	-0.20876000	0.38849800	1.58845000
O	-1.22748600	-0.69562700	-0.24706500
H	-1.17680200	-1.54855000	0.21714500
C	-2.56915400	-0.17436100	-0.10579900
H	-3.28258500	-0.91148700	-0.48523000
H	-2.79005000	0.05590300	0.94118000
H	-2.62602400	0.73139000	-0.71020600

Scan Point for comp6_alpha_2.2Å

C	0.33523900	1.57175100	-0.24280400
H	-0.63159600	2.06856400	-0.15489800
H	0.55508200	1.32034200	-1.28171000
H	1.10742000	2.27199100	0.11452500

C	0.38787800	0.41056200	0.65981900
C	2.20689800	-0.63023300	-0.50571000
H	2.85661000	-1.45952600	-0.23414100
H	1.63144900	-0.86205800	-1.40270300
H	2.77688500	0.29242100	-0.61646500
O	1.28697700	-0.50135300	0.62797100
H	-0.16370600	0.41633900	1.59653000
O	-1.28372200	-0.70589100	-0.23420800
H	-1.24640200	-1.53928700	0.26342600
C	-2.61104000	-0.15492400	-0.10638700
H	-3.34596200	-0.87661500	-0.47672100
H	-2.83358000	0.09847100	0.93544000
H	-2.64608900	0.74437000	-0.72290300

Scan Point for comp6_alpha_2.3Å

C	0.33625800	1.56150000	-0.21780700
H	-0.60774800	2.07969300	-0.04777800
H	0.45159800	1.28419100	-1.26723900
H	1.15431000	2.25290200	0.04294500
C	0.45868600	0.41879300	0.69765300
C	2.19717100	-0.63095300	-0.57671500
H	2.84997200	-1.46951500	-0.34523900
H	1.57114800	-0.84604700	-1.44341100
H	2.76727900	0.28922500	-0.70543000
O	1.33702900	-0.50272000	0.60608400
H	-0.05032200	0.41725100	1.65822900
O	-1.34637500	-0.76400200	-0.09780200
H	-1.41880500	-1.47838600	0.55534300
C	-2.62579100	-0.11082600	-0.20127500
H	-3.39922700	-0.84077500	-0.46223800
H	-2.89434100	0.38584800	0.73753600
H	-2.54704400	0.62830700	-1.00010400

Scan Point for comp6_alpha_2.4Å

C	0.37284400	1.56107500	-0.22739900
H	-0.57034100	2.08002200	-0.05414600
H	0.47922400	1.26773200	-1.27354900
H	1.19294600	2.25791100	0.01385000
C	0.50544700	0.43470100	0.70318800
C	2.21226900	-0.65548000	-0.58052700

H	2.85249900	-1.50239400	-0.34492900
H	1.57660000	-0.86678100	-1.44099100
H	2.79469400	0.25564600	-0.71702200
O	1.35803100	-0.50505200	0.60615100
H	-0.01128800	0.43454900	1.66011200
O	-1.40819400	-0.77530900	-0.09296000
H	-1.48985300	-1.46262500	0.58667000
C	-2.66806400	-0.08902200	-0.19819300
H	-3.46735500	-0.79634900	-0.44546800
H	-2.91819400	0.42961300	0.73424100
H	-2.57260000	0.63792000	-1.00671100

Scan Point for comp6_alpha_2.5Å

C	0.39591700	1.56427100	-0.24243600
H	-0.54277400	2.08430900	-0.04825600
H	0.46724500	1.24057600	-1.28225100
H	1.21876700	2.27425900	-0.05060100
C	0.57315400	0.47431900	0.71979000
C	2.17233300	-0.71033700	-0.62077100
H	2.79594300	-1.57111700	-0.39186800
H	1.47942500	-0.92631600	-1.43438300
H	2.77523000	0.17519700	-0.82190400
O	1.39393000	-0.48830000	0.60791200
H	0.09960300	0.50907800	1.69902000
O	-1.45918000	-0.79413900	0.00520800
H	-1.59758800	-1.37814100	0.76655500
C	-2.67810300	-0.07566900	-0.24899200
H	-3.49635700	-0.77098000	-0.46869400
H	-2.95509600	0.55298200	0.60500900
H	-2.50220600	0.55416400	-1.12312700

Scan Point for comp6_alpha_2.6Å

C	0.42914800	1.56291500	-0.24234600
H	-0.49826300	2.09455000	-0.02652100
H	0.46663700	1.22220900	-1.27855900
H	1.26284700	2.27015800	-0.08875000
C	0.62828800	0.48843500	0.73053200
C	2.16479500	-0.73871500	-0.64396400
H	2.78643600	-1.60196800	-0.41953500
H	1.44625800	-0.95986000	-1.43357900

H	2.76909500	0.13861600	-0.87460300
O	1.42158100	-0.49243500	0.60249000
H	0.17768900	0.53601600	1.72053400
O	-1.52624200	-0.80482800	0.06309700
H	-1.71716400	-1.32250700	0.86008700
C	-2.70027700	-0.05159600	-0.28195700
H	-3.54857300	-0.72037100	-0.46885900
H	-2.96596700	0.65819300	0.50994300
H	-2.47343800	0.49682900	-1.19845000

Scan Point for comp6_alpha_2.7Å

C	0.47818700	1.56185400	-0.24455500
H	-0.44117700	2.10499800	-0.02258600
H	0.50161000	1.21225900	-1.27844400
H	1.32071900	2.26212500	-0.10625500
C	0.67618600	0.49303100	0.73307200
C	2.18624600	-0.76004900	-0.64817700
H	2.79651200	-1.63117300	-0.42321700
H	1.46333600	-0.97264600	-1.43615600
H	2.80100100	0.10968200	-0.87967000
O	1.44697200	-0.50319200	0.59951200
H	0.22673400	0.54500300	1.72375900
O	-1.59984700	-0.80147300	0.07433600
H	-1.80049400	-1.29711100	0.88249700
C	-2.75690800	-0.02996600	-0.28528900
H	-3.62595700	-0.67984800	-0.44155300
H	-2.99600100	0.71452800	0.48321300
H	-2.52554400	0.48028000	-1.22267400

Scan Point for comp6_alpha_2.8Å

C	0.51377500	1.55827000	-0.24876500
H	-0.40528000	2.10033000	-0.02169400
H	0.52853900	1.19941300	-1.27967100
H	1.35430700	2.26407300	-0.12496100
C	0.72465200	0.50031900	0.73655700
C	2.20188100	-0.77974300	-0.65598500
H	2.80679500	-1.65440000	-0.43045000
H	1.46841200	-0.99213700	-1.43416600
H	2.82099700	0.08350800	-0.89949000
O	1.47749700	-0.50752700	0.59802100

H	0.28753700	0.56248500	1.73262100
O	-1.66870600	-0.80281100	0.09337200
H	-1.88505100	-1.27354900	0.91207100
C	-2.80321500	-0.01131100	-0.29219000
H	-3.68823700	-0.64106300	-0.44193900
H	-3.02994800	0.75643700	0.45716900
H	-2.55095000	0.47239400	-1.23834100

Scan Point for comp6_alpha_2.9Å

C	0.54673600	1.55679300	-0.24681900
H	-0.36766400	2.10274400	-0.01000400
H	0.54717400	1.19175800	-1.27571700
H	1.38996900	2.26226600	-0.13848500
C	0.76758700	0.50500500	0.74189900
C	2.20796300	-0.79733100	-0.66833300
H	2.80719500	-1.67697100	-0.44722100
H	1.46225700	-1.00553200	-1.43593400
H	2.83166200	0.05971700	-0.92173500
O	1.50197500	-0.51420000	0.59442500
H	0.34440600	0.57483500	1.74386800
O	-1.73886500	-0.81595900	0.12323000
H	-1.97193100	-1.20618400	0.97880800
C	-2.82853200	0.01152900	-0.31227100
H	-3.74628300	-0.57668700	-0.43268600
H	-3.01734300	0.83026900	0.39237200
H	-2.54683900	0.42908500	-1.28136500

Scan Point for comp6_alpha_3.0Å

C	0.57426200	1.54986200	-0.23424400
H	-0.33408500	2.09787900	0.02005300
H	0.55467600	1.18466600	-1.26312100
H	1.42159500	2.25295500	-0.14276800
C	0.80986800	0.49624900	0.74859500
C	2.23633800	-0.79863700	-0.68314000
H	2.84326300	-1.67470400	-0.46915200
H	1.48478200	-1.00981900	-1.44413100
H	2.85151800	0.06370700	-0.93942200
O	1.53949800	-0.52357500	0.58701500
H	0.39541800	0.55936700	1.75489300
O	-1.82022400	-0.81876100	0.15415100

H	-2.08807400	-1.16805900	1.01698300
C	-2.86834000	0.03145700	-0.33601100
H	-3.80010400	-0.53064800	-0.47372700
H	-3.05381500	0.87157700	0.34396000
H	-2.54213900	0.41818300	-1.30410400

Scan Point for comp6_alpha_3.1Å

C	-0.60306800	1.54409900	0.21914500
H	0.30557700	2.08664400	-0.04593200
H	-0.57793700	1.18615300	1.25052100
H	-1.44825000	2.25006600	0.12854300
C	-0.84943000	0.48459100	-0.75421900
C	-2.26870400	-0.79796000	0.69660500
H	-2.87696000	-1.67530200	0.49205900
H	-1.51388200	-1.00337900	1.45591000
H	-2.88174600	0.06736100	0.94767100
O	-1.57727400	-0.53380000	-0.57920400
H	-0.43828000	0.53679800	-1.76270600
O	1.90394700	-0.81996100	-0.18233200
H	2.21097400	-1.14242800	-1.04234000
C	2.90877800	0.05108900	0.35937400
H	3.85298600	-0.48472200	0.51636000
H	3.08923100	0.91076200	-0.29708700
H	2.53944200	0.40721900	1.32385900

Scan Point for comp6_alpha_3.2Å

C	0.62424500	1.53465100	-0.21941300
H	-0.28842500	2.06897600	0.04936800
H	0.59613400	1.17201900	-1.24913100
H	1.46264700	2.24984900	-0.13699400
C	0.88715600	0.48187100	0.75678000
C	2.30403900	-0.79822300	-0.69922800
H	2.92007900	-1.66996700	-0.49424500
H	1.54559600	-1.01264600	-1.45234500
H	2.90855300	0.07083300	-0.95783900
O	1.61857800	-0.53326100	0.58007100
H	0.48074000	0.53399900	1.76741500
O	-1.97282600	-0.82929600	0.17253500
H	-2.29378800	-1.17852200	1.01679600
C	-2.96084200	0.07227400	-0.34917200

H	-3.91365600	-0.44264700	-0.52331000
H	-3.12916900	0.91790300	0.32856400
H	-2.58231600	0.44721500	-1.30292000

Scan Point for comp6_alpha_3.3Å

C	0.64337700	1.52628800	-0.21869900
H	-0.27198900	2.05418900	0.05417000
H	0.61183600	1.15992300	-1.24700300
H	1.47610900	2.24910600	-0.14358500
C	0.92159000	0.47977200	0.75989300
C	2.33228600	-0.79980100	-0.70316300
H	2.95469500	-1.66719700	-0.49912200
H	1.56873000	-1.02164000	-1.44888600
H	2.92962500	0.07165700	-0.97015300
O	1.65562000	-0.53285300	0.58076100
H	0.52301900	0.53366400	1.77372800
O	-2.04235700	-0.84471700	0.16765600
H	-2.37621700	-1.19357100	1.00699400
C	-2.99857800	0.09565100	-0.34428000
H	-3.97017700	-0.38260400	-0.51922800
H	-3.13419900	0.94207500	0.33979100
H	-2.60958700	0.46350000	-1.29655300

Scan Point for comp6_alpha_3.5Å

C	-0.72583900	1.53128600	0.19956400
H	0.18717300	2.06106900	-0.07854400
H	-0.69693400	1.18158900	1.23342500
H	-1.56109200	2.24939900	0.10798500
C	-0.99388200	0.47092300	-0.76658000
C	-2.36389000	-0.82670100	0.72051900
H	-2.96991600	-1.70814100	0.52780200
H	-1.58979200	-1.02786100	1.46123000
H	-2.97666500	0.03436700	0.98588900
O	-1.70376900	-0.55564800	-0.57140100
H	-0.60558300	0.52394700	-1.78450100
O	2.20088000	-0.84813400	-0.21559100
H	2.62193900	-1.16627700	-1.02746300
C	3.05381900	0.13992400	0.38226200
H	4.03066400	-0.28482100	0.64386900
H	3.20217700	0.99763900	-0.28482700

H	2.55989500	0.47674800	1.29648800

Scan Point for comp6_alpha_3.6Å

C	-0.72021100	1.51974100	0.16833700
H	0.24699600	1.96051500	-0.08514700
H	-0.77180800	1.21733900	1.21484600
H	-1.47804400	2.30512500	-0.00720500
C	-1.02638100	0.45228300	-0.77695200
C	-2.38807900	-0.81564900	0.74665800
H	-3.00498700	-1.69295800	0.57039800
H	-1.60496000	-1.01796900	1.47729100
H	-2.98877400	0.05391900	1.01122900
O	-1.74474200	-0.56339400	-0.55867300
H	-0.65446300	0.49003300	-1.80180700
O	2.29904500	-0.83974800	-0.29513600
H	2.81756900	-1.07805300	-1.07760300
C	3.03089500	0.14288300	0.45315300
H	4.00562200	-0.24586800	0.77242800
H	3.18354200	1.05866100	-0.13078100
H	2.43753600	0.37883700	1.33965100

Scan Point for comp6_alpha_3.7Å

C	-0.86542600	1.56414500	0.20996100
H	0.21445700	1.76918500	0.22045400
H	-1.24846400	1.38654600	1.21274900
H	-1.32244300	2.46771500	-0.22511700
C	-1.09240800	0.48807900	-0.74576900
C	-2.38739500	-0.91929600	0.72212600
H	-2.81005100	-1.90567600	0.54965300
H	-1.62493300	-0.93817300	1.50021300
H	-3.16201700	-0.17836000	0.91735300
O	-1.73803000	-0.58111700	-0.56209200
H	-0.68891600	0.56596100	-1.75680200
O	2.38413500	-0.73173500	-0.40568900
H	2.90058900	-0.81152600	-1.22095700
C	3.12270400	0.08048600	0.51852200
H	4.10371200	-0.35755000	0.73923300
H	3.26292900	1.09842500	0.13384600
H	2.54144400	0.12578500	1.44257800

Scan Point for comp6_alpha_3.8Å

C	-0.90299400	1.56543500	0.27946300
H	0.17853600	1.76614300	0.24951900
H	-1.22878900	1.31514000	1.28698900
H	-1.37249200	2.49906300	-0.06770000
C	-1.17637600	0.55924900	-0.73730100
C	-2.27657100	-1.01862400	0.71498500
H	-2.73283800	-1.97831100	0.48680500
H	-1.43179600	-1.12688400	1.39454400
H	-3.01078200	-0.29995000	1.07748900
O	-1.76274800	-0.54865300	-0.58816700
H	-0.86466800	0.73229100	-1.76880400
O	2.38103100	-0.73616400	-0.41061700
H	2.87950100	-0.83471700	-1.23491300
C	3.13575900	0.10274500	0.47693400
H	4.12050100	-0.32941700	0.69238000
H	3.26750500	1.10900200	0.06043900
H	2.57014400	0.17335200	1.40904100

Scan Point for comp6_alpha_3.9Å

C	-0.90352600	1.55912600	0.27982300
H	0.18293300	1.73332900	0.24747400
H	-1.23050400	1.31007400	1.28724500
H	-1.35015600	2.50615700	-0.06007000
C	-1.20129400	0.56454000	-0.74145400
C	-2.29737400	-1.01323400	0.71363500
H	-2.76208300	-1.96886900	0.48542800
H	-1.44586100	-1.13046500	1.38314900
H	-3.02328100	-0.29219000	1.08800900
O	-1.79554600	-0.53922400	-0.59278200
H	-0.90105200	0.74241300	-1.77555800
O	2.42286900	-0.81480500	-0.32574500
H	2.89403800	-0.99732100	-1.15188900
C	3.16496600	0.16765900	0.41280000
H	4.18113000	-0.18271900	0.63105000
H	3.22226200	1.11807500	-0.13183700
H	2.63735600	0.32520300	1.35638200

Scan Point for comp6_alpha_4.0Å

C	-0.72912200	1.41828700	0.34854500
H	0.36616500	1.37214700	0.23880600
H	-1.02962800	1.14049000	1.35662200
H	-0.98975800	2.46338500	0.12535400
C	-1.28283600	0.59965500	-0.72069200
C	-2.47380700	-0.93719300	0.70039100
H	-3.11630500	-1.77521100	0.44301800
H	-1.59387100	-1.26122700	1.25540900
H	-3.02485200	-0.15160900	1.21608400
O	-2.02681000	-0.41410400	-0.60768500
H	-1.05559500	0.83841700	-1.76120500
O	2.45840500	-0.76502100	-0.34551300
H	2.82448800	-0.93154000	-1.22641000
C	3.37741800	0.06772600	0.37777300
H	4.35912400	-0.41205900	0.47356700
H	3.49891700	1.04389200	-0.10783700
H	2.95864400	0.21546100	1.37607200

Scan Point for comp6_alpha_4.1Å

C	0.71987900	1.38902500	-0.36470700
H	-0.37311000	1.27670900	-0.27623800
H	1.05379800	1.12545100	-1.36618700
H	0.91440000	2.44754000	-0.14006900
C	1.29663600	0.60255500	0.71659200
C	2.54561000	-0.91388000	-0.67879400
H	3.20571200	-1.73323300	-0.40647400
H	1.67951400	-1.26495600	-1.23893800
H	3.08260100	-0.12082900	-1.19793400
O	2.07421500	-0.38745800	0.61953300
H	1.05547400	0.84483400	1.75315700
O	-2.51118000	-0.83718700	0.22909800
H	-2.79113900	-1.08110000	1.12325400
C	-3.44463800	0.12108600	-0.29146600
H	-4.46204800	-0.28765300	-0.32008300
H	-3.44448800	1.04359700	0.30225200
H	-3.12992600	0.35407900	-1.31153900

Scan Point for comp6_alpha_4.2Å

C	0.73191000	1.35528300	-0.42216300
H	-0.35483200	1.17289700	-0.36793000
H	1.11380200	1.08566300	-1.40482500
H	0.85103300	2.42832000	-0.21985100
C	1.31369400	0.62628300	0.69612100
C	2.60968700	-0.91784300	-0.62516500
H	3.26727200	-1.72482400	-0.31254000
H	1.75653400	-1.29056900	-1.19103400
H	3.15459700	-0.13915800	-1.15776600
O	2.11148000	-0.35113900	0.64628700
H	1.05444900	0.90285400	1.71961400
O	-2.56239900	-0.87509500	0.09467800
H	-2.79211500	-1.29183600	0.93804300
C	-3.51710600	0.16310400	-0.17387800
H	-4.53688700	-0.23726300	-0.22720600
H	-3.47886300	0.94936200	0.59001100
H	-3.25674900	0.59347200	-1.14372900

Scan Point for comp6_alpha_4.3Å

C	0.72982900	1.29898600	-0.51042700
H	-0.36176500	1.16303000	-0.44544500
H	1.10686500	0.94737800	-1.46847400
H	0.88959600	2.38016900	-0.38811700
C	1.29337900	0.64275700	0.66054000
C	2.69283100	-0.91094800	-0.53895900
H	3.39278100	-1.65293500	-0.16359600
H	1.87943500	-1.37250100	-1.09771600
H	3.20010200	-0.13265600	-1.10781700
O	2.12756500	-0.30452600	0.68499500
H	0.99067900	0.95975200	1.66018400
O	-2.64456800	-0.91857200	-0.07756300
H	-2.77913400	-1.45304700	0.71851900
C	-3.53358600	0.20771500	-0.02478100
H	-4.58021300	-0.11430900	0.03624300
H	-3.30582000	0.85801300	0.82881400
H	-3.39123100	0.77083700	-0.95028700

Scan Point for comp6_alpha_4.4Å

C	-0.67554700	1.19720900	0.60404000
H	0.40093800	1.05776800	0.41378500

H	-0.97013100	0.70680900	1.52925900
H	-0.81289600	2.28645600	0.66524200
C	-1.36587900	0.74260300	-0.59464800
C	-2.66068300	-0.98964700	0.46903700
H	-3.37837100	-1.68685000	0.04464200
H	-1.79452400	-1.50598200	0.88136900
H	-3.12859000	-0.32117900	1.19105800
O	-2.21592700	-0.18606700	-0.68921300
H	-1.15904000	1.22058800	-1.55404900
O	2.66123400	-0.91109400	0.04379800
H	2.80136800	-1.45739400	-0.74322000
C	3.55673000	0.20977400	-0.01561500
H	4.60212000	-0.11827600	-0.06413100
H	3.33913900	0.85051200	-0.87904800
H	3.40981100	0.78520400	0.90153200

Scan Point for comp6_alpha_4.5Å

C	-0.69234400	1.17784800	0.61463500
H	0.38229400	1.11227000	0.38310900
H	-0.93041000	0.62754400	1.52230700
H	-0.88851400	2.25375500	0.73917700
C	-1.40519200	0.75424100	-0.58241300
C	-2.68230200	-1.00711000	0.45649300
H	-3.40015600	-1.69850000	0.02297000
H	-1.80822300	-1.52740500	0.84646600
H	-3.14635900	-0.35971400	1.19990700
O	-2.25736900	-0.17139800	-0.68646100
H	-1.21991900	1.26149100	-1.53113100
O	2.72755500	-0.91490100	0.03753300
H	2.86910100	-1.44949000	-0.75723900
C	3.59959600	0.22422200	-0.01929800
H	4.65127300	-0.08182300	-0.07577600
H	3.36446900	0.86624100	-0.87721200
H	3.44640400	0.79081900	0.90234100

Scan Point for comp6_alpha_4.6Å

C	-0.72120800	1.16078000	0.62024500
H	0.35202400	1.07124500	0.38802700
H	-0.96980300	0.61330600	1.52683800
H	-0.89333100	2.24026500	0.74689200

C	-1.44237800	0.75371100	-0.57761200
C	-2.72811700	-1.00821200	0.44983500
H	-3.44668200	-1.69542000	0.01088700
H	-1.85511500	-1.53228800	0.83711400
H	-3.19193200	-0.36512000	1.19715900
O	-2.30137600	-0.16494500	-0.68694100
H	-1.25642900	1.26785000	-1.52247000
O	2.80178900	-0.91040800	0.03697800
H	2.95122600	-1.44834900	-0.75408200
C	3.66668200	0.23400800	-0.02123000
H	4.72100400	-0.06507200	-0.06434600
H	3.43588700	0.86668600	-0.88719800
H	3.49998100	0.80800100	0.89345400

Scan Point for comp9_alpha_1.4Å

C	-2.37942900	-0.75548700	-0.25362200
C	-1.40751500	-1.80381200	0.31226100
C	0.00398900	-1.72322000	-0.29285400
C	-2.05895500	0.70819400	0.08421000
C	0.88781600	-0.66560700	0.36993700
C	-0.63957900	1.16616500	-0.25661700
H	-2.41234600	-0.87230100	-1.34600600
H	-1.35148200	-1.72979100	1.40644500
H	-2.21790500	0.89497500	1.15503400
H	0.52341600	-2.68152600	-0.18026200
H	1.29864800	-1.03997700	1.31211400
H	-0.36147600	0.86188400	-1.27273700
C	-0.45267200	2.66951800	-0.11327900
H	0.57943200	2.95820600	-0.33687500
H	-1.11371000	3.19605100	-0.80932000
O	0.29902500	0.55055000	0.69021600
H	-0.69470900	2.99691900	0.90452800
H	-2.76264400	1.35419500	-0.45584600
H	-3.39014700	-0.97883700	0.11009400
H	-1.80595500	-2.79967900	0.08933600
H	-0.06971400	-1.52014400	-1.36929000
O	1.96824700	-0.40963500	-0.48279200
H	2.14922300	-1.10470900	-1.15076200
C	3.22263400	0.15455100	0.09461300
H	3.66060200	-0.60240000	0.74440100
H	3.85118700	0.38899800	-0.76122500
H	2.92166400	1.04900900	0.63309600

Scan Point for comp9_alpha_1.5Å

C	-2.40779900	-0.70607900	-0.25033300
C	-1.46146600	-1.78605000	0.29803700
C	-0.04273800	-1.72346800	-0.29799800
C	-2.04574200	0.74444800	0.10124200
C	0.83968900	-0.69339800	0.39402700
C	-0.62343300	1.17189600	-0.26316100
H	-2.45031700	-0.80848000	-1.34370700
H	-1.41040500	-1.73608700	1.39386000
H	-2.18105400	0.92330900	1.17653500
H	0.45765400	-2.69210900	-0.19127000
H	1.27030400	-1.07320600	1.32311500
H	-0.36342200	0.85522400	-1.27941600
C	-0.39654900	2.66925800	-0.12455800
H	0.63915400	2.93191900	-0.36235700
H	-1.05303300	3.20927800	-0.81431200
O	0.31874100	0.53854000	0.67627900
H	-0.61850200	3.00457500	0.89508000
H	-2.74135700	1.41465100	-0.41906700
H	-3.42164100	-0.90619000	0.11779300
H	-1.87860100	-2.76861000	0.05208700
H	-0.10128100	-1.50384100	-1.37094200
O	2.01777200	-0.46623500	-0.50626000
H	2.26387800	-1.26166300	-1.02409100
C	3.21871100	0.15048600	0.10877600
H	3.64629600	-0.55720600	0.81898200
H	3.89267900	0.36563000	-0.71794900
H	2.87350000	1.06180300	0.58932000

Scan Point for comp9_alpha_1.6Å

C	-2.41349100	-0.72137200	-0.26090200
C	-1.46576000	-1.79997300	0.28664500
C	-0.03715000	-1.71532300	-0.28745700
C	-2.06111500	0.72826200	0.10466100
C	0.80868100	-0.67970200	0.42701900
C	-0.64580800	1.17138800	-0.26436200
H	-2.44717100	-0.81480100	-1.35529900
H	-1.43185000	-1.76534700	1.38364500
H	-2.19415900	0.89704200	1.18172300
H	0.47534500	-2.67655900	-0.17632100

H	1.27981600	-1.04580400	1.34020700
H	-0.38069200	0.85326100	-1.27821300
C	-0.42845500	2.66909200	-0.12525200
H	0.60669100	2.93748000	-0.35869200
H	-1.08474100	3.20201700	-0.82052400
O	0.30946800	0.54697100	0.67585200
H	-0.65864100	3.00492200	0.89221700
H	-2.76271400	1.39830000	-0.40744100
H	-3.42876800	-0.92952300	0.09841700
H	-1.86720500	-2.78351500	0.01983500
H	-0.08228900	-1.48903500	-1.35918000
O	2.07118700	-0.45077900	-0.52884400
H	2.31939600	-1.27141900	-1.00144300
C	3.25562800	0.15228300	0.11001100
H	3.67646600	-0.55526900	0.82518000
H	3.95178500	0.37874400	-0.69617100
H	2.90830600	1.06204200	0.59382000

Scan Point for comp9_alpha_1.7Å

C	-2.41898800	-0.73635300	-0.27394800
C	-1.47099200	-1.81312100	0.27532400
C	-0.03212800	-1.70736200	-0.27471700
C	-2.07675900	0.71223200	0.10565500
C	0.77665500	-0.66711400	0.46208200
C	-0.66825500	1.17168900	-0.26623500
H	-2.44188400	-0.82123600	-1.36920500
H	-1.45545800	-1.79250600	1.37299100
H	-2.20874600	0.87094100	1.18423200
H	0.49186300	-2.66113400	-0.15787200
H	1.28479300	-1.01706600	1.36053500
H	-0.39648500	0.85284500	-1.27755300
C	-0.46125900	2.66964000	-0.12467300
H	0.57328700	2.94473100	-0.35245900
H	-1.11697200	3.19585600	-0.82541300
O	0.29960800	0.55546800	0.67499700
H	-0.70091000	3.00441700	0.89076600
H	-2.78370000	1.38194900	-0.39907700
H	-3.43622200	-0.95222100	0.07478700
H	-1.85598400	-2.79756400	-0.01129900
H	-0.06247900	-1.47456300	-1.34517000
O	2.12723400	-0.44424800	-0.54601900
H	2.38105000	-1.28621600	-0.97248500
C	3.29372000	0.15980700	0.10639000

H	3.71118100	-0.53743100	0.83452800
H	4.01014500	0.39120000	-0.68175600
H	2.93982300	1.07173400	0.58335300

Scan Point for comp9_alpha_1.8Å

C	-2.43785600	-0.69621900	-0.29972800
C	-1.52555600	-1.79734300	0.25905000
C	-0.07060600	-1.71004900	-0.25491000
C	-2.06706200	0.74015200	0.09809800
C	0.72641500	-0.68790100	0.50809700
C	-0.65213100	1.18128600	-0.27042900
H	-2.44362300	-0.77165400	-1.39578000
H	-1.53673300	-1.79050000	1.35683600
H	-2.19752200	0.88977000	1.17806200
H	0.43762300	-2.67068400	-0.12909700
H	1.24546900	-1.03456300	1.40086100
H	-0.37743300	0.85835900	-1.27924000
C	-0.42178900	2.67379400	-0.11777500
H	0.61824300	2.93459100	-0.33628700
H	-1.06404300	3.21290800	-0.82098200
O	0.31119500	0.54766500	0.67348300
H	-0.66522300	3.00609200	0.89745200
H	-2.75899600	1.43003700	-0.39989200
H	-3.46571400	-0.88973700	0.02995300
H	-1.91839400	-2.77168200	-0.05030500
H	-0.06989600	-1.46953200	-1.32354000
O	2.18723000	-0.54645900	-0.53402300
H	2.49117500	-1.44492200	-0.76383600
C	3.29416600	0.19303300	0.06680100
H	3.63073700	-0.30952500	0.97604900
H	4.09309100	0.23880400	-0.67488900
H	2.92036000	1.19208600	0.28373100

Scan Point for comp9_alpha_1.9Å

C	-2.44239400	-0.71339800	-0.31363900
C	-1.52839000	-1.81006400	0.25024200
C	-0.06410300	-1.70476000	-0.24092000
C	-2.08570500	0.72390200	0.09446200
C	0.69601700	-0.67624800	0.53967800
C	-0.67619100	1.18124600	-0.27136200

H	-2.43680000	-0.78344500	-1.40991600
H	-1.55623100	-1.81204600	1.34763600
H	-2.21995900	0.86700600	1.17471900
H	0.45484600	-2.65797200	-0.10744700
H	1.25317200	-1.00660300	1.41475000
H	-0.39093900	0.85703000	-1.27646600
C	-0.45592900	2.67408400	-0.11636700
H	0.58363600	2.94137300	-0.32874500
H	-1.09689100	3.20704400	-0.82534300
O	0.29510100	0.55401200	0.67729500
H	-0.70912600	3.00564000	0.89654200
H	-2.78181600	1.41077400	-0.40156900
H	-3.47182100	-0.91561200	0.00545700
H	-1.90460400	-2.78633300	-0.07305400
H	-0.04999900	-1.45961600	-1.30828500
O	2.24327400	-0.53082600	-0.55341300
H	2.54451000	-1.43189300	-0.76902900
C	3.33847000	0.19756200	0.06684500
H	3.67949800	-0.32047200	0.96657100
H	4.14725300	0.27739300	-0.66261600
H	2.95762200	1.18829400	0.31209200

Scan Point for comp9_alpha_2.0Å

C	-2.44841200	-0.72883700	-0.32663500
C	-1.53324500	-1.82126800	0.24259100
C	-0.06043600	-1.70050800	-0.22719900
C	-2.10490400	0.70919100	0.09047300
C	0.66652300	-0.66682000	0.56792900
C	-0.70028500	1.18098500	-0.27225500
H	-2.43220800	-0.79424800	-1.42296600
H	-1.57644500	-1.83102300	1.33928500
H	-2.24314300	0.84675900	1.17083100
H	0.46723500	-2.64726100	-0.08646900
H	1.25915200	-0.98105300	1.42498500
H	-0.40513800	0.85569200	-1.27387700
C	-0.48889600	2.67399700	-0.11522100
H	0.55053500	2.94667900	-0.32077000
H	-1.12748100	3.20140300	-0.83043300
O	0.27814300	0.55917400	0.68091000
H	-0.75208100	3.00529400	0.89506900
H	-2.80452300	1.39315500	-0.40442000
H	-3.47920300	-0.93901400	-0.01748200
H	-1.89398400	-2.79917500	-0.09287900

H	-0.03408500	-1.45110600	-1.29337300
O	2.30135400	-0.51264000	-0.57380500
H	2.60082700	-1.41277600	-0.78978100
C	3.38645200	0.19971300	0.07087100
H	3.72961000	-0.33935600	0.95817000
H	4.20467400	0.31472600	-0.64459900
H	2.99949700	1.18031400	0.34854000

Scan Point for comp9_alpha_2.1Å

C	-2.45741900	-0.73866500	-0.34038800
C	-1.54549000	-1.82968800	0.23522200
C	-0.06448300	-1.69798600	-0.21166700
C	-2.12226700	0.69849500	0.08618900
C	0.63641800	-0.66112900	0.59379600
C	-0.72161600	1.18187800	-0.27410500
H	-2.42963600	-0.79957000	-1.43665100
H	-1.60491400	-1.84738800	1.33082800
H	-2.26314400	0.82997500	1.16687600
H	0.46841600	-2.64009900	-0.06321800
H	1.25809800	-0.96097900	1.43495000
H	-0.41868600	0.85661500	-1.27326800
C	-0.51743900	2.67468700	-0.11303900
H	0.52218400	2.95190200	-0.31107300
H	-1.15308100	3.19878400	-0.83326500
O	0.26453600	0.56371000	0.68141000
H	-0.79017200	3.00409900	0.89521600
H	-2.82404000	1.38182100	-0.40635500
H	-3.49052200	-0.95323700	-0.04242300
H	-1.89297300	-2.80788600	-0.11293200
H	-0.02476700	-1.44556400	-1.27690400
O	2.36486900	-0.50660800	-0.58882000
H	2.67237900	-1.40324500	-0.80440000
C	3.43518300	0.20500300	0.07337900
H	3.77802600	-0.33992400	0.95797200
H	4.26376100	0.34462500	-0.62688300
H	3.03650800	1.17768800	0.36448600

Scan Point for comp9_alpha_2.2Å

C	-2.46644500	-0.74556100	-0.35712800
C	-1.56093100	-1.83617900	0.22787400

C	-0.07125000	-1.69691500	-0.19313600
C	-2.13854200	0.69028100	0.07892600
C	0.60637800	-0.65672300	0.62029800
C	-0.74015100	1.18304100	-0.27533400
H	-2.42472800	-0.80282500	-1.45304800
H	-1.63844700	-1.86033600	1.32197800
H	-2.28429900	0.81594400	1.15958700
H	0.46430400	-2.63547600	-0.03476700
H	1.25339900	-0.94297500	1.44685500
H	-0.42777800	0.85799100	-1.27164600
C	-0.54240500	2.67558500	-0.10963400
H	0.49784500	2.95651300	-0.29863500
H	-1.17382500	3.19745600	-0.83510600
O	0.25031800	0.56776300	0.68407500
H	-0.82537700	3.00270400	0.89644600
H	-2.84049500	1.37378700	-0.41293100
H	-3.50269000	-0.96275900	-0.07259400
H	-1.89615400	-2.81424800	-0.13212600
H	-0.01578000	-1.44350200	-1.25764300
O	2.42911900	-0.50642000	-0.60241400
H	2.74377800	-1.40205800	-0.80768300
C	3.48301000	0.21180900	0.07239800
H	3.82481400	-0.33075800	0.95944400
H	4.32134900	0.36932400	-0.61350800
H	3.07060100	1.17844700	0.36649600

Scan Point for comp9_alpha_2.3Å

C	-2.47413300	-0.75600200	-0.37496900
C	-1.57361300	-1.84476900	0.22021600
C	-0.07556600	-1.69680800	-0.17141100
C	-2.15777900	0.67914900	0.07087100
C	0.57992500	-0.64945300	0.64573600
C	-0.76236800	1.18374100	-0.27602200
H	-2.41667700	-0.80915400	-1.47032700
H	-1.67053100	-1.87559800	1.31242600
H	-2.30972800	0.79864800	1.15133500
H	0.46270400	-2.63114100	0.00034700
H	1.25294600	-0.91950100	1.45705500
H	-0.44015000	0.85946300	-1.26948300
C	-0.57330800	2.67638100	-0.10623900
H	0.46746200	2.96212900	-0.28501100
H	-1.20018200	3.19541600	-0.83764800
O	0.23301400	0.57384200	0.68772100

H	-0.86780000	3.00104900	0.89727700
H	-2.86113000	1.36109200	-0.42112800
H	-3.51337700	-0.97831700	-0.10573100
H	-1.89502200	-2.82290600	-0.15188200
H	-0.00148000	-1.44496400	-1.23571500
O	2.49571700	-0.50111200	-0.61827900
H	2.81206800	-1.39840000	-0.80949600
C	3.53451600	0.21970500	0.07204800
H	3.86651300	-0.32081500	0.96456100
H	4.38570000	0.38583400	-0.59679800
H	3.11279700	1.18365000	0.36331500

Scan Point for comp9_alpha_2.4Å

C	-2.49036600	-0.74668800	-0.39154600
C	-1.60468100	-1.84238800	0.21197900
C	-0.09844400	-1.70102900	-0.15354400
C	-2.17036500	0.68456600	0.06355500
C	0.54879600	-0.65502200	0.66722900
C	-0.77235200	1.18544000	-0.27596100
H	-2.41975500	-0.79635500	-1.48623100
H	-1.71872900	-1.87842500	1.30221200
H	-2.32704600	0.79983000	1.14376000
H	0.43261600	-2.63729700	0.02878700
H	1.23965700	-0.91967700	1.46565700
H	-0.44450300	0.85824200	-1.26658500
C	-0.57669000	2.67642300	-0.10298800
H	0.46668600	2.95694900	-0.27437800
H	-1.19573800	3.19875200	-0.83868400
O	0.22061300	0.57031800	0.69208300
H	-0.87698200	3.00168600	0.89854200
H	-2.86781700	1.37236100	-0.42863300
H	-3.53399600	-0.96366900	-0.13560400
H	-1.92297700	-2.81729200	-0.17080800
H	-0.00460500	-1.45012700	-1.21707300
O	2.56185100	-0.50802700	-0.63123200
H	2.89271900	-1.39841600	-0.82703600
C	3.58356900	0.21874900	0.07487400
H	3.90806200	-0.31980300	0.97180100
H	4.44562600	0.39607700	-0.57779300
H	3.15027200	1.17852500	0.36366900

Scan Point for comp9_alpha_2.5Å

C	-2.50761000	-0.72726900	-0.41504400
C	-1.64512000	-1.83441500	0.20014800
C	-0.12927100	-1.70630000	-0.13240900
C	-2.17874000	0.69847900	0.05039900
C	0.51227700	-0.66603200	0.69625900
C	-0.77318000	1.18749600	-0.27322600
H	-2.41917100	-0.77412200	-1.50849800
H	-1.78187400	-1.87559600	1.28743300
H	-2.34581800	0.81098700	1.12931900
H	0.38926700	-2.64729600	0.06068000
H	1.21037600	-0.93216100	1.48846000
H	-0.43500300	0.85481800	-1.25846400
C	-0.56464000	2.67602800	-0.09760000
H	0.48352400	2.94619300	-0.25568400
H	-1.16876600	3.20374500	-0.84181800
O	0.20712300	0.56274100	0.70597500
H	-0.87506400	3.00474600	0.89966400
H	-2.86355500	1.39570600	-0.44626800
H	-3.55760700	-0.93327700	-0.17699700
H	-1.96307300	-2.80428000	-0.19524900
H	-0.01078600	-1.45537100	-1.19404500
O	2.62135300	-0.52342800	-0.63845700
H	2.96544600	-1.40657300	-0.84201400
C	3.63469900	0.21342700	0.06720100
H	3.96259800	-0.31945200	0.96661800
H	4.49840100	0.39890100	-0.58170700
H	3.19280200	1.17004000	0.35404800

Scan Point for comp9_alpha_2.6Å

C	-2.52359300	-0.71361100	-0.43736500
C	-1.68033700	-1.82884900	0.18910000
C	-0.15684400	-1.70989000	-0.11370600
C	-2.19018400	0.70796100	0.03707800
C	0.47735800	-0.67392400	0.72288100
C	-0.77826100	1.18836500	-0.27027600
H	-2.41773900	-0.75838300	-1.52932800
H	-1.83775500	-1.87367600	1.27329500
H	-2.36875900	0.81859200	1.11433100
H	0.35244700	-2.65405100	0.08789400
H	1.17793000	-0.94075100	1.51327800
H	-0.42948000	0.85119700	-1.25021300

C	-0.56111400	2.67524400	-0.09310200
H	0.49110800	2.93744800	-0.23685700
H	-1.15064700	3.20601500	-0.84679300
O	0.18970600	0.55719800	0.72006400
H	-0.88334500	3.00768700	0.89911500
H	-2.86391900	1.41190600	-0.46518300
H	-3.57876100	-0.91173000	-0.21651300
H	-1.99587800	-2.79504700	-0.21686100
H	-0.01723700	-1.45785900	-1.17297700
O	2.68460600	-0.53467500	-0.64411000
H	3.03938200	-1.41204700	-0.85271100
C	3.69111800	0.21117800	0.06039000
H	4.02145000	-0.31629500	0.96243700
H	4.55599800	0.40278600	-0.58560500
H	3.24186000	1.16518300	0.34505800

Scan Point for comp9_alpha_2.7Å

C	-2.54004600	-0.69765100	-0.45536300
C	-1.71580900	-1.82130600	0.18075300
C	-0.18618300	-1.71487000	-0.09856500
C	-2.19950500	0.71986500	0.02572200
C	0.44563100	-0.68407200	0.74381400
C	-0.78123100	1.18909200	-0.26807000
H	-2.41976100	-0.74165500	-1.54586500
H	-1.88937800	-1.86711600	1.26230900
H	-2.38797000	0.83048200	1.10125200
H	0.31222600	-2.66326600	0.10974500
H	1.14772200	-0.95338400	1.53276300
H	-0.42514700	0.84718700	-1.24363600
C	-0.55219700	2.67380200	-0.08951200
H	0.50441300	2.92550100	-0.21903200
H	-1.12571400	3.20881000	-0.85254100
O	0.17538700	0.54956500	0.73118000
H	-0.88510500	3.01109100	0.89749000
H	-2.86176100	1.43073900	-0.48208600
H	-3.59979400	-0.88634000	-0.24891800
H	-2.03247300	-2.78392300	-0.23257000
H	-0.02909900	-1.46253200	-1.15580200
O	2.74858900	-0.54495500	-0.65869500
H	3.11752700	-1.41583300	-0.86889100
C	3.73627100	0.20776300	0.06386400
H	4.05728600	-0.31964300	0.96964800
H	4.61059200	0.41137700	-0.56586500

H	3.27304300	1.15588500	0.34626600

Scan Point for comp9_alpha_2.8Å

C	-2.55771500	-0.68629100	-0.46951700
C	-1.74780100	-1.81637900	0.17318000
C	-0.21373300	-1.71943200	-0.08678700
C	-2.21242300	0.72798100	0.01737800
C	0.41589500	-0.69170200	0.75919700
C	-0.78975500	1.18922600	-0.26677400
H	-2.42657900	-0.72906500	-1.55881600
H	-1.93394200	-1.86347500	1.25249400
H	-2.40790700	0.83798200	1.09168100
H	0.27609800	-2.67077000	0.12798600
H	1.11990500	-0.96245400	1.54652000
H	-0.42884200	0.84370600	-1.23924500
C	-0.55181700	2.67227300	-0.08729300
H	0.50781500	2.91602100	-0.20687300
H	-1.11391900	3.21025800	-0.85670200
O	0.15887200	0.54370000	0.73849200
H	-0.89183700	3.01321400	0.89598400
H	-2.86646000	1.44398000	-0.49386300
H	-3.62065600	-0.86839200	-0.27411300
H	-2.06482600	-2.77609800	-0.24641100
H	-0.04186800	-1.46803800	-1.14247800
O	2.81835200	-0.54891200	-0.67182100
H	3.19935600	-1.41330300	-0.88647700
C	3.78895500	0.20531200	0.07148800
H	4.09690600	-0.32497700	0.98038500
H	4.67390400	0.41811500	-0.54031700
H	3.31541800	1.14907000	0.35164600

Scan Point for comp9_alpha_2.9Å

C	-2.57903900	-0.67580500	-0.47400000
C	-1.77895500	-1.81207800	0.16976100
C	-0.24268200	-1.72488300	-0.08176200
C	-2.22576800	0.73518900	0.01637700
C	0.39159300	-0.69944600	0.76231300
C	-0.80102900	1.18913100	-0.26846000
H	-2.44478000	-0.71752800	-1.56295200
H	-1.97004800	-1.86018300	1.24809200

H	-2.42016200	0.84406800	1.09098400
H	0.23986400	-2.67897300	0.13694500
H	1.10190300	-0.97142900	1.54408500
H	-0.44216300	0.84084400	-1.24071100
C	-0.55386400	2.67046500	-0.08850100
H	0.50718000	2.90764000	-0.20857900
H	-1.11301200	3.21189400	-0.85764400
O	0.14695200	0.53766300	0.73561500
H	-0.89149500	3.01322400	0.89495600
H	-2.87576000	1.45617300	-0.49301800
H	-3.64370600	-0.85130600	-0.28212100
H	-2.09938500	-2.76899900	-0.25350000
H	-0.06356500	-1.47595900	-1.13740100
O	2.89765500	-0.55207000	-0.68956100
H	3.30475600	-1.40006000	-0.92050700
C	3.83327600	0.20460800	0.09418300
H	4.13013300	-0.33954500	0.99878300
H	4.72897500	0.45061800	-0.48917500
H	3.33322500	1.13169000	0.38387100

Scan Point for comp9_alpha_3.0Å

C	-2.59827400	-0.70126200	-0.45571100
C	-1.77756700	-1.82832100	0.17756600
C	-0.24514900	-1.72309600	-0.08943700
C	-2.25398400	0.71326800	0.03087800
C	0.38783800	-0.68634800	0.74077400
C	-0.84118300	1.18667900	-0.27957600
H	-2.47854600	-0.74131100	-1.54635500
H	-1.95554800	-1.87974100	1.25793600
H	-2.42970100	0.81745800	1.10916400
H	0.25100200	-2.67038300	0.12832100
H	1.11627100	-0.94575900	1.51045300
H	-0.49476100	0.84292700	-1.25798700
C	-0.61074000	2.67087700	-0.10245700
H	0.44372100	2.92355200	-0.24624100
H	-1.19516000	3.20530500	-0.85753200
O	0.13426000	0.54826900	0.70772100
H	-0.93124700	3.00692200	0.88900600
H	-2.92258100	1.42677900	-0.46473400
H	-3.65818900	-0.88865200	-0.24930500
H	-2.09052200	-2.78881000	-0.24314500
H	-0.07866300	-1.47634700	-1.14805800
O	3.01110900	-0.54820600	-0.70814500

H	3.49182800	-1.34458600	-0.97800100
C	3.86399000	0.23063700	0.14463000
H	4.15336100	-0.33004600	1.04171900
H	4.76828200	0.55205800	-0.38639400
H	3.29790900	1.11552700	0.44454500

Scan Point for comp9_alpha_3.1Å

C	-2.60306700	-0.70795100	-0.46852700
C	-1.78666500	-1.83210500	0.17501200
C	-0.25156900	-1.72429300	-0.07485100
C	-2.26678400	0.70764400	0.02007100
C	0.37254300	-0.68308700	0.75591000
C	-0.85315500	1.18475400	-0.27998800
H	-2.47160200	-0.74895000	-1.55780100
H	-1.97583800	-1.88193800	1.25353300
H	-2.45150900	0.81215100	1.09679900
H	0.24404100	-2.66981300	0.15150400
H	1.10169500	-0.93693800	1.52723700
H	-0.49790900	0.83967200	-1.25474900
C	-0.62807600	2.66981300	-0.10391500
H	0.42712300	2.92483500	-0.23778800
H	-1.20613800	3.20089100	-0.86623000
O	0.11825800	0.55081400	0.71540700
H	-0.95931100	3.00746700	0.88344400
H	-2.93306500	1.41920000	-0.48145400
H	-3.66467000	-0.89754900	-0.27316400
H	-2.09262600	-2.79400200	-0.24758100
H	-0.07287700	-1.48051100	-1.13257300
O	3.08242300	-0.54120900	-0.74289600
H	3.59582100	-1.31789300	-1.00986800
C	3.87464300	0.23507900	0.16852400
H	4.12734600	-0.33867800	1.06845100
H	4.79933800	0.58221900	-0.30837400
H	3.27751400	1.10387000	0.45510900

Scan Point for comp9_alpha_3.2Å

C	-2.61977900	-0.69376800	-0.47119400
C	-1.81417000	-1.82535000	0.17278000
C	-0.27756800	-1.73098000	-0.07369900
C	-2.27219800	0.71831900	0.01948100

C	0.35600300	-0.69470900	0.75556000
C	-0.85473800	1.18407900	-0.28002600
H	-2.48673500	-0.73470100	-1.56028900
H	-2.00566700	-1.87449600	1.25088200
H	-2.45670200	0.82330800	1.09619500
H	0.20910600	-2.68084900	0.15371400
H	1.08796900	-0.95358200	1.52288900
H	-0.50221600	0.83617200	-1.25477000
C	-0.61685400	2.66699700	-0.10312600
H	0.44065900	2.91275100	-0.23599700
H	-1.18948200	3.20323600	-0.86594200
O	0.11318300	0.54123000	0.71417300
H	-0.94611600	3.00728400	0.88398500
H	-2.93215100	1.43600800	-0.48170700
H	-3.68325500	-0.87457600	-0.27784300
H	-2.12738400	-2.78420900	-0.25134500
H	-0.09495400	-1.48908800	-1.13150600
O	3.15319200	-0.51646300	-0.78844800
H	3.67423200	-1.29237100	-1.04257200
C	3.88276900	0.21266100	0.21028700
H	4.05221400	-0.39666900	1.10620900
H	4.84930000	0.55735900	-0.17720900
H	3.27938900	1.08278600	0.47911400

Scan Point for comp9_alpha_3.3Å

C	-2.63484000	-0.69418700	-0.48580600
C	-1.83610900	-1.82559200	0.16698500
C	-0.29712000	-1.73213400	-0.06449600
C	-2.29142400	0.71815800	0.00706300
C	0.32877900	-0.69544700	0.77005400
C	-0.87087500	1.18300700	-0.27892700
H	-2.49114600	-0.73610300	-1.57351000
H	-2.03819200	-1.87374100	1.24319800
H	-2.48642200	0.82414200	1.08182900
H	0.18685800	-2.68203200	0.16848600
H	1.05306900	-0.95400400	1.54473800
H	-0.50898400	0.83410600	-1.24987600
C	-0.63404500	2.66596800	-0.10097000
H	0.42482900	2.91113000	-0.22371300
H	-1.19894700	3.20181600	-0.86979900
O	0.08694400	0.54056600	0.72525300
H	-0.97278100	3.00724700	0.88258700
H	-2.94609700	1.43572400	-0.50117600

H	-3.70024500	-0.87434200	-0.30273600
H	-2.14559800	-2.78466400	-0.25938700
H	-0.10402500	-1.49123100	-1.12066600
O	3.22887400	-0.51390300	-0.79407300
H	3.75172100	-1.29054800	-1.04217000
C	3.94868600	0.21502200	0.21187200
H	4.10818700	-0.39403700	1.10979900
H	4.91954500	0.55860400	-0.16566700
H	3.34337100	1.08585400	0.47397500

Scan Point for comp9_alpha_3.5Å

C	-2.66526200	-0.69495600	-0.51417900
C	-1.88011200	-1.82601100	0.15549000
C	-0.33691300	-1.73433600	-0.04691700
C	-2.32992200	0.71788400	-0.01718500
C	0.27403100	-0.69684400	0.79766100
C	-0.90376100	1.18097200	-0.27695300
H	-2.50100900	-0.73879400	-1.59890100
H	-2.10261100	-1.87220400	1.22776200
H	-2.54516000	0.82581200	1.05352400
H	0.14167100	-2.68428900	0.19675200
H	0.98327100	-0.95478200	1.58635900
H	-0.52385400	0.83014500	-1.24030300
C	-0.66895500	2.66400800	-0.09695200
H	0.39229400	2.90800600	-0.19999200
H	-1.21867600	3.19910400	-0.87723300
O	0.03425600	0.53931400	0.74625700
H	-1.02596200	3.00721200	0.87945400
H	-2.97417300	1.43520900	-0.53891500
H	-3.73412400	-0.87383900	-0.35105000
H	-2.18236400	-2.78550300	-0.27511300
H	-0.12359600	-1.49535000	-1.09963600
O	3.38089900	-0.50994400	-0.80310100
H	3.90770300	-1.28740800	-1.04002000
C	4.08222400	0.22012700	0.21500600
H	4.22425700	-0.38751500	1.11682600
H	5.06032100	0.56228500	-0.14474600
H	3.47279100	1.09189200	0.46416400

Scan Point for comp9_alpha_3.6Å

C	2.70887700	-0.64109400	0.47642400
C	1.93577400	-1.80298200	-0.15333500
C	0.39720900	-1.75098100	0.09491700
C	2.31699400	0.75554800	-0.02560800
C	-0.26837200	-0.74011600	-0.73917000
C	0.88807600	1.18248300	0.27880100
H	2.58168500	-0.67551900	1.56641300
H	2.12639100	-1.85853300	-1.23120900
H	2.49249300	0.85665700	-1.10420800
H	-0.06235700	-2.71614200	-0.12400600
H	-0.99867500	-1.02712100	-1.49855100
H	0.55017100	0.83039600	1.25732800
C	0.60459200	2.65623100	0.09360400
H	-0.45920200	2.87030400	0.23069900
H	1.16454400	3.21405100	0.85034600
O	-0.06704500	0.50307300	-0.70527100
H	0.91868400	3.00018800	-0.89713800
H	2.95822900	1.49668100	0.46556900
H	3.77646300	-0.79132700	0.27985200
H	2.27729800	-2.74754600	0.28069300
H	0.21060100	-1.50506100	1.15157600
O	-3.47054000	-0.41933700	0.87427600
H	-4.03709100	-1.14473200	1.17583700
C	-4.03308200	0.12364900	-0.32995100
H	-4.07741400	-0.63046400	-1.12516100
H	-5.04017800	0.52148900	-0.15507400
H	-3.38136700	0.94036100	-0.64909500

Scan Point for comp9_alpha_3.7Å

C	2.71446700	-0.67288500	0.47884300
C	1.92359500	-1.82073500	-0.15435100
C	0.38560200	-1.74535200	0.09155000
C	2.34515800	0.73063600	-0.02073500
C	-0.26313600	-0.72197800	-0.74042800
C	0.92324900	1.17943600	0.28375900
H	2.58570500	-0.70767900	1.56863500
H	2.11443100	-1.87669600	-1.23216900
H	2.52263100	0.83059500	-1.09910900
H	-0.08822400	-2.70282100	-0.13083800
H	-0.99816100	-0.99501700	-1.50048400
H	0.57987600	0.83085100	1.26157800
C	0.66354800	2.65781300	0.10088900
H	-0.39663300	2.88913000	0.23819100

H	1.23243700	3.20538600	0.85844400
O	-0.04231400	0.51773900	-0.70227500
H	0.98320100	2.99810900	-0.88935200
H	2.99781600	1.46080200	0.47188500
H	3.77971900	-0.83985900	0.28303200
H	2.24954300	-2.77163600	0.27784400
H	0.19985100	-1.49970200	1.14851200
O	-3.57327700	-0.41156900	0.88332300
H	-4.18615100	-1.10748700	1.16199600
C	-4.05263800	0.14708400	-0.34953500
H	-4.08845100	-0.60891900	-1.14334100
H	-5.04984900	0.58691700	-0.22583800
H	-3.35208200	0.93454300	-0.63732700

Scan Point for comp9_alpha_3.8Å

C	2.73491700	-0.66640100	0.47522200
C	1.94675500	-1.81728400	-0.15590000
C	0.40947700	-1.74959900	0.09647900
C	2.35722700	0.73592000	-0.02157500
C	-0.24828000	-0.72808600	-0.73059400
C	0.93462200	1.17806500	0.28945200
H	2.61079600	-0.70273500	1.56549300
H	2.13340400	-1.87120900	-1.23454600
H	2.52977400	0.83772800	-1.10057700
H	-0.06079200	-2.70897100	-0.12520400
H	-0.98700900	-1.00329200	-1.48635100
H	0.59720600	0.82718000	1.26853100
C	0.66712100	2.65534900	0.10889100
H	-0.39343200	2.88156400	0.25166400
H	1.23721100	3.20507500	0.86396900
O	-0.03273300	0.51255900	-0.69229900
H	0.98031500	2.99773400	-0.88268200
H	3.00859800	1.46856600	0.46907200
H	3.80010300	-0.82825600	0.27485800
H	2.27902900	-2.76709600	0.27383800
H	0.22734500	-1.50648600	1.15474100
O	-3.68082400	-0.44775000	0.87532600
H	-4.36879400	-1.08572000	1.11430400
C	-4.05023100	0.17464900	-0.36467200
H	-4.11416200	-0.56004200	-1.17665000
H	-5.00960400	0.69891900	-0.27654800
H	-3.27118100	0.90288600	-0.60194700

Scan Point for comp9_alpha_3.9Å

C	2.73753500	-0.64838900	0.50438700
C	1.97415300	-1.80704700	-0.14272700
C	0.43180300	-1.75572100	0.08001200
C	2.35526000	0.74997800	0.00043900
C	-0.22194600	-0.74047500	-0.75805000
C	0.92255300	1.17782800	0.28396700
H	2.59174400	-0.68640700	1.59195600
H	2.18217100	-1.85762900	-1.21763200
H	2.54784000	0.85402300	-1.07495600
H	-0.02422100	-2.71980500	-0.15059900
H	-0.94649800	-1.02241800	-1.52508100
H	0.56952500	0.82351100	1.25630100
C	0.64388200	2.65243000	0.09822000
H	-0.42174800	2.86765400	0.21829000
H	1.19202000	3.20742000	0.86562200
O	-0.01997900	0.50233100	-0.71552000
H	0.97439700	2.99884400	-0.88630500
H	2.98938200	1.48911100	0.50370700
H	3.80817100	-0.79902800	0.32550800
H	2.30807900	-2.75369100	0.29267400
H	0.22770700	-1.51492300	1.13493400
O	-3.73952400	-0.44142000	0.89940800
H	-4.44759200	-1.06461100	1.11785200
C	-4.03833400	0.15777200	-0.37077000
H	-4.08046800	-0.59494800	-1.16749400
H	-4.98962200	0.70293300	-0.33968000
H	-3.23429200	0.86440500	-0.58906200

Scan Point for comp9_alpha_4.0Å

C	2.75165500	-0.66580500	0.49198000
C	1.97010600	-1.81861900	-0.14382900
C	0.43065400	-1.75266700	0.09622600
C	2.37588900	0.73534600	-0.00937300
C	-0.22149600	-0.73346800	-0.73798100
C	0.95018200	1.17552000	0.28987700
H	2.61891900	-0.70097700	1.58129000
H	2.16530800	-1.87367600	-1.22090200
H	2.55691500	0.83639000	-1.08705000
H	-0.03645400	-2.71310000	-0.12745600

H	-0.95341800	-1.01076600	-1.49958700
H	0.60530800	0.82462300	1.26635700
C	0.68174400	2.65223100	0.10614700
H	-0.38051100	2.87662600	0.23881400
H	1.24367000	3.20326500	0.86638800
O	-0.00812800	0.50753200	-0.69936300
H	1.00349300	2.99490300	-0.88258400
H	3.02216100	1.46951500	0.48569700
H	3.81861600	-0.82644400	0.30028100
H	2.30013600	-2.76739100	0.28990500
H	0.24000000	-1.50777200	1.15263000
O	-3.85707500	-0.42129700	0.90062900
H	-4.60056600	-1.01936700	1.06502300
C	-4.02497600	0.16461000	-0.39922000
H	-4.01884000	-0.59980000	-1.18580700
H	-4.95995500	0.73494900	-0.46100600
H	-3.18571000	0.84625200	-0.55508800

Scan Point for comp9_alpha_4.1Å

C	2.75057400	-0.67396300	0.51281500
C	1.97409900	-1.82262600	-0.13645700
C	0.43170600	-1.75231800	0.08252600
C	2.38649800	0.72928000	0.00915000
C	-0.20585900	-0.72950900	-0.75857400
C	0.95828600	1.17359500	0.28936200
H	2.60230600	-0.71095100	1.60008300
H	2.18371100	-1.87530400	-1.21095600
H	2.58292600	0.83178100	-1.06567600
H	-0.03515300	-2.71094800	-0.14920200
H	-0.92876000	-1.00268700	-1.53023500
H	0.59888700	0.82203200	1.26030200
C	0.69765100	2.65157600	0.10459500
H	-0.36575500	2.87946600	0.22119200
H	1.24967100	3.19917500	0.87452000
O	0.01115300	0.51070600	-0.71427600
H	1.03557900	2.99517600	-0.87839900
H	3.02811200	1.46047500	0.51455300
H	3.81958600	-0.83793100	0.33588900
H	2.29510100	-2.77358500	0.29926400
H	0.22707200	-1.50869800	1.13667800
O	-3.94145000	-0.42740900	0.90396900
H	-4.71562500	-0.99832700	1.01471600
C	-4.00912000	0.17851300	-0.39554000

H	-3.98587600	-0.57717400	-1.19022000
H	-4.91608800	0.78556700	-0.50510000
H	-3.13634000	0.82827700	-0.49221500

Scan Point for comp9_alpha_4.2Å

C	2.75014700	-0.67336900	0.53765600
C	1.98557000	-1.82195800	-0.12563000
C	0.43979900	-1.75410300	0.06860200
C	2.39291700	0.72983400	0.02932800
C	-0.18620300	-0.73130700	-0.78123000
C	0.95984700	1.17253900	0.28626800
H	2.58402300	-0.71157900	1.62232100
H	2.21231600	-1.87226700	-1.19676600
H	2.60702800	0.83337000	-1.04199000
H	-0.02183700	-2.71321900	-0.17135900
H	-0.89785700	-1.00432800	-1.56335500
H	0.58505200	0.82029200	1.25112000
C	0.70127200	2.65040100	0.09756500
H	-0.36410800	2.87765600	0.19584400
H	1.23983700	3.19813100	0.87687300
O	0.02914400	0.50909600	-0.73264800
H	1.05563300	2.99447700	-0.87945000
H	3.02519400	1.46140400	0.54577800
H	3.82208600	-0.83618600	0.37821000
H	2.30082600	-2.77326500	0.31351200
H	0.21791400	-1.51193900	1.11966400
O	-4.01733300	-0.42150200	0.91181800
H	-4.81739600	-0.96169200	0.98711000
C	-3.99584100	0.17490900	-0.39357800
H	-3.97163700	-0.58829000	-1.18100200
H	-4.86694300	0.82305400	-0.54966900
H	-3.08967200	0.78194900	-0.45407900

Scan Point for comp9_alpha_4.3Å

C	2.76813800	-0.67909800	0.53003100
C	1.99438900	-1.82713800	-0.12350500
C	0.45044300	-1.75349300	0.08324300
C	2.41088100	0.72392900	0.02117500
C	-0.17860900	-0.73104000	-0.76464400
C	0.98143100	1.17152200	0.28934100

H	2.61121000	-0.71397600	1.61617100
H	2.21216700	-1.88167100	-1.19629000
H	2.61600100	0.82418700	-1.05222000
H	-0.01629400	-2.71175100	-0.15025700
H	-0.89619500	-1.00406400	-1.54129900
H	0.61380100	0.82231500	1.25806000
C	0.72546900	2.64970400	0.09961600
H	-0.33845400	2.88011800	0.20612100
H	1.27177400	3.19761400	0.87338900
O	0.04071400	0.50880200	-0.72062700
H	1.07283000	2.99070300	-0.88099300
H	3.04988700	1.45481200	0.53030800
H	3.83816700	-0.84563000	0.36185800
H	2.31004000	-2.77811600	0.31606800
H	0.23796400	-1.50747400	1.13531400
O	-4.12876100	-0.40249000	0.90217200
H	-4.95520000	-0.90589700	0.93578000
C	-3.99774500	0.16999300	-0.40796600
H	-3.95273700	-0.60714600	-1.18071100
H	-4.83047600	0.84841800	-0.63096900
H	-3.06649400	0.74078700	-0.41644200

Scan Point for comp9_alpha_4.4Å

C	2.78556400	-0.69888800	0.51418700
C	1.99290600	-1.83927800	-0.13034500
C	0.45249400	-1.75107800	0.09579700
C	2.43491400	0.70789500	0.01123100
C	-0.17711800	-0.72131800	-0.74345600
C	1.01320100	1.16846700	0.29844200
H	2.64238500	-0.73327400	1.60229500
H	2.19640000	-1.89540700	-1.20570400
H	2.62664400	0.80706400	-1.06473900
H	-0.02613600	-2.70453900	-0.13333900
H	-0.90564900	-0.98689200	-1.51265300
H	0.65528200	0.82158100	1.27167900
C	0.76825300	2.64904500	0.11333400
H	-0.29183500	2.88927600	0.23561000
H	1.33072900	3.19113100	0.87939300
O	0.05394000	0.51638500	-0.70008500
H	1.10457200	2.98755800	-0.87201300
H	3.08775500	1.43208100	0.51251100
H	3.85168300	-0.87517600	0.33216800
H	2.30492100	-2.79356600	0.30472500

H	0.25521300	-1.50469500	1.15058700
O	-4.27110100	-0.45137100	0.84600200
H	-5.16227200	-0.82628900	0.78727900
C	-3.98085400	0.22634800	-0.38580200
H	-3.99196000	-0.46804100	-1.23488000
H	-4.69551500	1.03686500	-0.57456500
H	-2.98109100	0.65504400	-0.28602300

Scan Point for comp9_alpha_4.5Å

C	2.80685000	-0.71324000	0.50961900
C	2.00412400	-1.84781600	-0.13199600
C	0.46531900	-1.74903800	0.09919700
C	2.46410700	0.69563100	0.00692100
C	-0.16203800	-0.71348900	-0.73399000
C	1.04805100	1.16796800	0.30153800
H	2.66714200	-0.74642400	1.59814200
H	2.20360500	-1.90521000	-1.20817100
H	2.65046900	0.79176600	-1.07027200
H	-0.02087500	-2.69872400	-0.12985500
H	-0.89973400	-0.97260200	-1.49659500
H	0.69274100	0.82546700	1.27729400
C	0.81455500	2.65032600	0.11578300
H	-0.24257500	2.89993400	0.24451000
H	1.38672100	3.18898800	0.87723700
O	0.07719700	0.52258600	-0.69046000
H	1.14745300	2.98423000	-0.87225900
H	3.12512800	1.41558300	0.50342900
H	3.87118300	-0.89700000	0.32403800
H	2.31096300	-2.80423300	0.30201600
H	0.27281800	-1.50333200	1.15519700
O	-4.36972700	-0.44049000	0.83787000
H	-5.26184800	-0.80988300	0.76531600
C	-4.05576700	0.23252700	-0.39076400
H	-4.06045400	-0.46338900	-1.23872200
H	-4.76060000	1.04891100	-0.59056000
H	-3.05309300	0.65195100	-0.27788600

Scan Point for comp9_beta_1.4Å

C	-1.70363000	1.51353300	-0.48097400
C	-0.36227700	2.15691400	-0.11320600
C	0.41484500	1.44346500	1.00563200

C	-1.62549100	0.02466300	-0.84306200
C	1.02727800	0.07193200	0.71058700
C	-1.25918900	-0.89770600	0.32755200
H	-2.40116700	1.62882400	0.36034300
H	0.26488200	2.25208400	-1.01075700
H	-0.91978000	-0.14584100	-1.66893600
H	1.25419500	2.07385500	1.31861200
H	-1.69470900	-0.50389400	1.25469600
C	-1.73570100	-2.32857500	0.11923100
H	-1.40234600	-2.97371700	0.93848700
H	-2.82957000	-2.35268900	0.08998800
O	0.18215100	-1.02922600	0.55464400
H	-1.35509400	-2.73582300	-0.82473800
H	-2.60956400	-0.29362300	-1.20731500
H	-2.14002300	2.06520200	-1.32258700
H	-0.53969700	3.18418800	0.22579900
H	-0.21994500	1.30904400	1.88900400
H	1.71978900	-0.18103500	1.51696400
O	1.86057200	0.16793700	-0.41030700
H	1.38406800	0.35239500	-1.24812000
C	2.88354000	-0.89710300	-0.63109300
H	2.37041400	-1.84657900	-0.76955400
H	3.42652700	-0.58295100	-1.51963200
H	3.51398600	-0.88186800	0.25504000

Scan Point for comp9_beta_1.5Å

C	-1.69152000	1.51287900	-0.50214400
C	-0.35263300	2.15398500	-0.12204600
C	0.40543000	1.45373500	1.01827400
C	-1.61561200	0.02158700	-0.85423000
C	0.99430800	0.07216000	0.76220200
C	-1.27224100	-0.89532900	0.32519000
H	-2.39980200	1.63687100	0.32884400
H	0.28930000	2.23344700	-1.00985800
H	-0.90209600	-0.15788300	-1.67132200
H	1.24786000	2.07977000	1.33010600
H	-1.72847700	-0.50251700	1.24214100
C	-1.72731700	-2.33111400	0.10937800
H	-1.41120700	-2.96984600	0.94023500
H	-2.81963800	-2.36472600	0.05052300
O	0.16903200	-1.01444000	0.59719900
H	-1.31751000	-2.73783400	-0.82237600
H	-2.59677900	-0.29558200	-1.22686200

H	-2.11373500	2.06048800	-1.35349200
H	-0.53079400	3.18610000	0.20128000
H	-0.24185800	1.34240600	1.89693600
H	1.72232800	-0.17908200	1.53544200
O	1.88868700	0.17833600	-0.43730300
H	1.38173300	0.31875000	-1.26377000
C	2.87304200	-0.91438100	-0.63821900
H	2.33944400	-1.85699700	-0.74887100
H	3.42300300	-0.64543400	-1.53802800
H	3.51572300	-0.90022600	0.23947600

Scan Point for comp9_beta_1.6Å

C	-1.67431600	1.51569000	-0.52430100
C	-0.33731000	2.15307300	-0.13280000
C	0.40016700	1.46557700	1.02865100
C	-1.60219000	0.02184300	-0.86589800
C	0.95840500	0.07102300	0.81565000
C	-1.29043500	-0.89167200	0.32234500
H	-2.39298800	1.64955400	0.29611400
H	0.31916800	2.21435600	-1.01064100
H	-0.87920000	-0.16858700	-1.67188700
H	1.24998500	2.08313800	1.33565200
H	-1.77242100	-0.50073000	1.22623400
C	-1.72304600	-2.33167700	0.09496000
H	-1.43161800	-2.96524300	0.93852200
H	-2.81216400	-2.37399700	-0.00282600
O	0.14734700	-0.99853000	0.64891300
H	-1.27702100	-2.73659800	-0.82060300
H	-2.57972600	-0.29180800	-1.25064100
H	-2.08174300	2.05891500	-1.38549000
H	-0.51350500	3.19048300	0.17390800
H	-0.25826100	1.38361300	1.90358700
H	1.72094600	-0.18070700	1.55327400
O	1.91489800	0.17913600	-0.46240800
H	1.38900700	0.29054800	-1.27946900
C	2.86409900	-0.93588500	-0.64517100
H	2.31219600	-1.87131400	-0.73414300
H	3.42285300	-0.70814600	-1.55185200
H	3.51428200	-0.92615500	0.22760500

Scan Point for comp9_beta_1.7Å

C	-1.68435700	1.48893300	-0.54523500
C	-0.36039500	2.15275500	-0.15645400
C	0.37565700	1.50192400	1.02585700
C	-1.58520900	-0.00646600	-0.87255400
C	0.92064900	0.10138100	0.86987700
C	-1.29224900	-0.91031900	0.32521300
H	-2.40967100	1.61929400	0.26986900
H	0.30442200	2.20043200	-1.02822900
H	-0.84799200	-0.19517800	-1.66551100
H	1.22716000	2.12545700	1.31407900
H	-1.81969000	-0.53762500	1.21062900
C	-1.65655500	-2.36527600	0.07979800
H	-1.38327500	-2.98688400	0.93802000
H	-2.73684100	-2.44946600	-0.07265600
O	0.13777400	-0.96662900	0.72085400
H	-1.14909000	-2.75100400	-0.81140000
H	-2.55182600	-0.33688200	-1.27060800
H	-2.09630900	2.01527500	-1.41459100
H	-0.55266000	3.19413900	0.12581600
H	-0.28475800	1.44976100	1.90324600
H	1.72214500	-0.13164200	1.57019100
O	1.93277400	0.19991300	-0.49243500
H	1.39304000	0.28135800	-1.30258400
C	2.85115400	-0.93386000	-0.64939300
H	2.28465800	-1.86471800	-0.69799300
H	3.40739700	-0.75979500	-1.57045900
H	3.51673000	-0.91322800	0.21217100

Scan Point for comp9_beta_1.8Å

C	1.68796200	-1.47336200	-0.56745800
C	0.37454500	-2.15035400	-0.16742400
C	-0.35033400	-1.51965500	1.03208000
C	1.57021600	0.02239800	-0.88629200
C	-0.88153600	-0.11620500	0.91881500
C	1.30098000	0.91961400	0.32023200
H	2.42518400	-1.60162500	0.23721500
H	-0.30397700	-2.18773300	-1.02857100
H	0.81490200	0.20980400	-1.66186200
H	-1.20282900	-2.14340700	1.31531300
H	1.85268800	0.55280300	1.19269900
C	1.62875700	2.38163700	0.07070700
H	1.36504600	2.99485600	0.93777500

H	2.70308700	2.48688600	-0.10801700
O	-0.12286800	0.94742600	0.75996700
H	1.09217100	2.75959200	-0.80645100
H	2.52535500	0.36316500	-1.30287600
H	2.09289800	-1.99099300	-1.44517000
H	0.57649500	-3.19384600	0.09938100
H	0.31808200	-1.48707200	1.90606100
H	-1.71088900	0.11079900	1.58688100
O	-1.96391200	-0.21386300	-0.51608000
H	-1.41765900	-0.26752700	-1.32240400
C	-2.86241400	0.93048700	-0.64301800
H	-2.28894700	1.85948100	-0.65616200
H	-3.41938200	0.80397900	-1.57245900
H	-3.53703900	0.89497600	0.21169300

Scan Point for comp9_beta_1.9Å

C	1.68163100	-1.46899900	-0.59375100
C	0.37706100	-2.14722900	-0.16924700
C	-0.32840100	-1.52440800	1.04631600
C	1.55492500	0.02715000	-0.90583600
C	-0.84338800	-0.11851200	0.96611800
C	1.31661700	0.91858200	0.31029900
H	2.43670100	-1.59925400	0.19376300
H	-0.31954500	-2.17803500	-1.01564200
H	0.78000800	0.21741800	-1.66064900
H	-1.18210700	-2.14402900	1.33365500
H	1.88089700	0.54609200	1.17190800
C	1.63370300	2.38281500	0.06568600
H	1.38416900	2.98853000	0.94205400
H	2.70459300	2.49109100	-0.13068600
O	-0.10301700	0.93749400	0.78067200
H	1.08137100	2.76559800	-0.79931800
H	2.49887000	0.37149700	-1.34436600
H	2.06666900	-1.98405400	-1.48176000
H	0.58336300	-3.19183100	0.08922800
H	0.35259200	-1.50683900	1.91262500
H	-1.69331100	0.11241800	1.60536300
O	-2.00535900	-0.22044300	-0.53369300
H	-1.45437300	-0.25563300	-1.33586400
C	-2.88309400	0.93525900	-0.63412700
H	-2.30025100	1.85963500	-0.62070900
H	-3.44548800	0.85109700	-1.56615900
H	-3.56146000	0.89194400	0.21797700

Scan Point for comp9_beta_2.0Å

C	1.66868500	-1.47084300	-0.62201000
C	0.37147800	-2.14417000	-0.16989800
C	-0.30645400	-1.52482500	1.06374100
C	1.53941000	0.02644300	-0.92555900
C	-0.80327500	-0.11651000	1.01181800
C	1.33702900	0.91351600	0.29879300
H	2.44272600	-1.60766500	0.14557700
H	-0.34547800	-2.16676800	-0.99882800
H	0.74445800	0.22295700	-1.65734300
H	-1.16081000	-2.13794700	1.36177500
H	1.91108300	0.53291700	1.15009900
C	1.65195400	2.37799600	0.05863600
H	1.41882200	2.97798200	0.94330200
H	2.71999400	2.48355600	-0.15385800
O	-0.07854500	0.93138300	0.79595700
H	1.08731100	2.76798200	-0.79492600
H	2.47217000	0.37026200	-1.38789800
H	2.02859100	-1.98420200	-1.52132700
H	0.57801600	-3.19051500	0.08077800
H	0.39168900	-1.52126700	1.91804100
H	-1.67038700	0.12106800	1.62418600
O	-2.05208800	-0.22230200	-0.54679500
H	-1.50706700	-0.25119400	-1.35190700
C	-2.90722600	0.94599600	-0.62220700
H	-2.31196900	1.86318300	-0.59018400
H	-3.47927400	0.90051500	-1.55207500
H	-3.58441600	0.90086300	0.23140500

Scan Point for comp9_beta_2.1Å

C	1.66622200	-1.46222000	-0.65059100
C	0.38019100	-2.14047600	-0.17465900
C	-0.27138300	-1.53120000	1.07908800
C	1.52708100	0.03624000	-0.94378500
C	-0.76206600	-0.12462300	1.05449900
C	1.35182800	0.91689500	0.28813200
H	2.45754400	-1.60199900	0.09855500
H	-0.35644900	-2.15576300	-0.98578300
H	0.71313000	0.23501600	-1.65357000

H	-1.11903800	-2.14577100	1.39191500
H	1.93955700	0.53387800	1.12879200
C	1.65138100	2.38451800	0.05192800
H	1.42935400	2.97705200	0.94439100
H	2.71517100	2.49772100	-0.17709400
O	-0.05883300	0.92185700	0.81174600
H	1.07044300	2.77593400	-0.78981100
H	2.44753000	0.38525500	-1.42652400
H	2.00660700	-1.97006500	-1.56045900
H	0.59317400	-3.18801900	0.06488300
H	0.44716200	-1.53555800	1.91769700
H	-1.64546100	0.11154400	1.64319800
O	-2.10047100	-0.23236500	-0.56014200
H	-1.55870700	-0.24604100	-1.36677700
C	-2.94128000	0.94302500	-0.60573000
H	-2.33927100	1.85555200	-0.54840300
H	-3.51890900	0.93668600	-1.53420600
H	-3.61924800	0.88567700	0.24707700

Scan Point for comp9_beta_2.2Å

C	1.67093200	-1.44878100	-0.67669200
C	0.39449700	-2.13339800	-0.18472100
C	-0.23322000	-1.54214200	1.09070800
C	1.52321400	0.05086000	-0.95906100
C	-0.72112400	-0.13855900	1.09538500
C	1.36546700	0.92426600	0.27924400
H	2.47513700	-1.59166000	0.05793200
H	-0.35932300	-2.13580000	-0.97970200
H	0.69644600	0.25162500	-1.65325500
H	-1.07358100	-2.16117900	1.41367200
H	1.96863600	0.54331800	1.10964400
C	1.64101000	2.39634400	0.04507300
H	1.42937800	2.98180000	0.94458300
H	2.69878600	2.52306500	-0.20380600
O	-0.03987600	0.90920400	0.82869000
H	1.03941500	2.78417000	-0.78363100
H	2.43450400	0.40624300	-1.45433000
H	1.99662900	-1.95020300	-1.59535800
H	0.61176200	-3.18373500	0.03755700
H	0.50394900	-1.55649100	1.91400400
H	-1.61717400	0.09316100	1.66646800
O	-2.14937100	-0.24347600	-0.57467500
H	-1.59371100	-0.22655000	-1.37076100

C	-2.98697100	0.93158600	-0.58732000
H	-2.38639700	1.84290700	-0.49534500
H	-3.56446300	0.96333800	-1.51618500
H	-3.66885700	0.84911700	0.26069300

Scan Point for comp9_beta_2.3Å

C	-1.64247100	1.48298600	-0.69267700
C	-0.35281100	2.12380500	-0.17697700
C	0.22683500	1.51837900	1.11564900
C	-1.53750200	-0.01930300	-0.97848300
C	0.67806200	0.10617500	1.12423300
C	-1.41657000	-0.89831500	0.25908800
H	-2.45408600	1.65024500	0.02837000
H	0.41795600	2.09337000	-0.95465000
H	-0.70824700	-0.24149500	-1.66276000
H	1.07329400	2.11604800	1.46147800
H	-2.01026700	-0.50009200	1.08809600
C	-1.72880800	-2.36241500	0.02603000
H	-1.53823600	-2.95062100	0.92842000
H	-2.78834300	-2.46026500	-0.22829300
O	-0.00952200	-0.91996200	0.81591200
H	-1.13352100	-2.76802000	-0.79854700
H	-2.45329600	-0.34740800	-1.48414400
H	-1.93490000	1.99758800	-1.61515700
H	-0.53687000	3.18221600	0.03611400
H	-0.53270900	1.55047200	1.91840200
H	1.57806400	-0.15370300	1.67674300
O	2.23196100	0.22117300	-0.56756200
H	1.72573200	0.23741400	-1.39502200
C	3.05567300	-0.96054000	-0.56470700
H	2.44594800	-1.86915500	-0.61888000
H	3.75324900	-0.93679000	-1.40838800
H	3.62226800	-0.95412100	0.36848000

Scan Point for comp9_beta_2.4Å

C	-1.62376300	1.48813300	-0.72492500
C	-0.33843700	2.11472300	-0.18256900
C	0.19241200	1.51779000	1.13652500
C	-1.53347400	-0.01703700	-0.99999900
C	0.63136700	0.10443400	1.16405800

C	-1.44516900	-0.88996100	0.24392800
H	-2.44909000	1.67087400	-0.02353100
H	0.45443800	2.05965600	-0.93586800
H	-0.69604600	-0.25410700	-1.66882500
H	1.03140700	2.11148400	1.50618700
H	-2.04890800	-0.48244300	1.06087200
C	-1.75977600	-2.35371800	0.01497500
H	-1.59188800	-2.93585500	0.92570100
H	-2.81423700	-2.44703500	-0.26118500
O	-0.04456500	-0.91579700	0.82657100
H	-1.14961300	-2.76840900	-0.79397800
H	-2.44509900	-0.33664800	-1.51855500
H	-1.88758600	2.00104400	-1.65685100
H	-0.51061900	3.17857200	0.01191200
H	-0.59577700	1.56274700	1.91076200
H	1.53537600	-0.16122700	1.70788100
O	2.29627300	0.21706200	-0.56087800
H	1.80462500	0.24281300	-1.39618300
C	3.10702500	-0.97180300	-0.55014500
H	2.48947000	-1.87467900	-0.61688800
H	3.82105000	-0.95597100	-1.38081400
H	3.65772300	-0.97631600	0.39273400

Scan Point for comp9_beta_2.5Å

C	-1.61391600	1.49523000	-0.74568500
C	-0.32963500	2.10381400	-0.18127800
C	0.15577100	1.51020200	1.15921800
C	-1.54168700	-0.01184500	-1.01582000
C	0.59080900	0.09753500	1.18883800
C	-1.47517000	-0.88326000	0.22996200
H	-2.44836200	1.69260200	-0.05927900
H	0.48117100	2.02193000	-0.91258200
H	-0.70199100	-0.26185200	-1.67690500
H	0.98377700	2.10167500	1.55585600
H	-2.08159000	-0.46972100	1.04164200
C	-1.79514000	-2.34544100	0.00120400
H	-1.64161800	-2.92598400	0.91542200
H	-2.84681300	-2.43263900	-0.28733700
O	-0.07573900	-0.91613600	0.82366400
H	-1.17810800	-2.76555600	-0.79964500
H	-2.45323000	-0.32065900	-1.54106400
H	-1.85310100	2.00914300	-1.68367400
H	-0.48516800	3.17266100	-0.00169100

H	-0.65995700	1.55819700	1.90390800
H	1.50386000	-0.17458500	1.71501300
O	2.36241200	0.21440100	-0.57120800
H	1.87985200	0.21565100	-1.41176400
C	3.17866500	-0.96827900	-0.51951100
H	2.56722600	-1.87721000	-0.56196600
H	3.90006400	-0.97620100	-1.34439700
H	3.72242100	-0.94131600	0.42724600

Scan Point for comp9_beta_2.6Å

C	-1.59794700	1.52698700	-0.74389100
C	-0.29576500	2.08843500	-0.17233600
C	0.14858000	1.48418000	1.17963800
C	-1.57428900	0.02006900	-1.02317200
C	0.55167700	0.06384300	1.19955600
C	-1.52795900	-0.86264900	0.21476300
H	-2.42710100	1.74896300	-0.05864900
H	0.51963400	1.96414800	-0.89252200
H	-0.74559200	-0.25065700	-1.68981500
H	0.98223100	2.05448200	1.59462000
H	-2.12349200	-0.44373200	1.03158000
C	-1.87684400	-2.31589300	-0.02628400
H	-1.73305900	-2.90770100	0.88221700
H	-2.93070300	-2.37894600	-0.31317300
O	-0.12591800	-0.92906200	0.80562800
H	-1.27014800	-2.74057600	-0.83252500
H	-2.49746200	-0.25725600	-1.54563600
H	-1.81686100	2.05307200	-1.68008300
H	-0.40828700	3.16393800	-0.00152600
H	-0.68246700	1.54914200	1.90541400
H	1.46783200	-0.23494000	1.70606200
O	2.44386600	0.19335500	-0.57888400
H	1.98256900	0.17293900	-1.43075900
C	3.27843000	-0.97315200	-0.48575900
H	2.68340900	-1.89380900	-0.51251200
H	4.01271700	-0.99177400	-1.29940800
H	3.80790300	-0.91255000	0.46767400

Scan Point for comp9_beta_2.7Å

C	-1.59159600	1.53085000	-0.76332700

C	-0.29261800	2.07853500	-0.17142700
C	0.11253900	1.47999300	1.19691500
C	-1.58313600	0.02272900	-1.03739700
C	0.51090100	0.05954600	1.22072000
C	-1.55716000	-0.85822200	0.20198600
H	-2.42914800	1.76654400	-0.09307700
H	0.53633300	1.93398900	-0.87210700
H	-0.75254800	-0.25937300	-1.69682900
H	0.93757200	2.04772000	1.63196800
H	-2.15891300	-0.43542500	1.01206700
C	-1.90796000	-2.31042900	-0.04066900
H	-1.78108100	-2.90043900	0.87146700
H	-2.95745400	-2.36935000	-0.34401000
O	-0.15878900	-0.92886600	0.80691600
H	-1.29070100	-2.73946300	-0.83649600
H	-2.50529500	-0.24527800	-1.56650600
H	-1.78769900	2.05541300	-1.70541000
H	-0.39202200	3.15702700	-0.01226600
H	-0.73879300	1.55097400	1.89777300
H	1.43020300	-0.24330900	1.72022300
O	2.51581200	0.19305300	-0.58275100
H	2.07320100	0.16312900	-1.44391000
C	3.34955100	-0.97061500	-0.45943700
H	2.75529400	-1.89225600	-0.47488000
H	4.09331800	-1.00511600	-1.26416900
H	3.86842600	-0.89259700	0.49867000

Scan Point for comp9_beta_2.8Å

C	-1.55387300	1.53351400	-0.81207000
C	-0.28194700	2.06921200	-0.15211400
C	0.04033500	1.46333100	1.23904300
C	-1.55899400	0.02199300	-1.07055600
C	0.46776700	0.05212500	1.24448900
C	-1.57622200	-0.84325100	0.18056500
H	-2.42283200	1.78989200	-0.19129500
H	0.58272200	1.91790200	-0.80615600
H	-0.71524900	-0.27963800	-1.70403300
H	0.82493200	2.03896000	1.73375900
H	-2.17650300	-0.39201900	0.97577800
C	-1.95913600	-2.28946100	-0.04361400
H	-1.86178400	-2.86684300	0.88021700
H	-3.00520100	-2.32622200	-0.36209400
O	-0.18234400	-0.93326700	0.79623500

H	-1.34140700	-2.74722600	-0.82280100
H	-2.47033800	-0.23827600	-1.62161800
H	-1.68884100	2.05124600	-1.76864900
H	-0.38053400	3.14802900	0.00432700
H	-0.86061800	1.50718500	1.87578500
H	1.39867100	-0.24618700	1.72595900
O	2.58659400	0.19728100	-0.58020400
H	2.15152500	0.16017300	-1.44470300
C	3.40097900	-0.97615000	-0.43067700
H	2.79344100	-1.88945100	-0.43350400
H	4.14993500	-1.03777800	-1.22924000
H	3.91463700	-0.88973700	0.52962800

Scan Point for comp9_beta_2.9Å

C	-1.50220000	1.62514700	-0.76023800
C	-0.18602600	2.03358000	-0.09411600
C	0.09347700	1.35589100	1.27488300
C	-1.63338100	0.12812100	-1.06738900
C	0.43270200	-0.07597400	1.20912300
C	-1.68590900	-0.77521000	0.15619900
H	-2.34294800	1.93075700	-0.12320100
H	0.65971700	1.83543300	-0.76046700
H	-0.83189500	-0.21687600	-1.73290100
H	0.91333900	1.85985900	1.78962200
H	-2.22436000	-0.30468900	0.98408600
C	-2.18839300	-2.17822400	-0.10267900
H	-2.11088200	-2.79486400	0.79728000
H	-3.24316000	-2.12243000	-0.38841300
O	-0.28454400	-0.99301800	0.72182500
H	-1.63222500	-2.65475200	-0.91626000
H	-2.57599000	-0.04077700	-1.60093000
H	-1.60037800	2.18391200	-1.69800200
H	-0.19676600	3.11058200	0.09994600
H	-0.80432700	1.43428700	1.91126200
H	1.35843900	-0.45361300	1.64238900
O	2.72325000	0.15269900	-0.55470600
H	2.32117600	0.13277500	-1.43547900
C	3.57107200	-0.99830300	-0.41690600
H	2.99253400	-1.92930400	-0.45795600
H	4.34016100	-1.01625300	-1.19837100
H	4.05986000	-0.92166500	0.55718200

Scan Point for comp9_beta_3.0Å

C	1.58598700	-1.49264400	-0.87690700
C	0.34983000	-2.05597000	-0.17319500
C	0.09843700	-1.48684200	1.25070200
C	1.56691900	0.02374700	-1.10502700
C	-0.37131900	-0.09139700	1.28424100
C	1.61051500	0.86802600	0.15942700
H	2.48268900	-1.75396500	-0.29931200
H	-0.54721300	-1.89473700	-0.78020800
H	0.70150000	0.32723100	-1.70757600
H	-0.63964000	-2.09146100	1.78075400
H	2.24436500	0.41716300	0.92892200
C	1.95074100	2.32630500	-0.05225500
H	1.86709000	2.88663500	0.88334200
H	2.98550700	2.39420100	-0.40125700
O	0.23015000	0.91414400	0.81694700
H	1.29857100	2.78023300	-0.80518900
H	2.45894800	0.30466200	-1.67724600
H	1.68398100	-1.98884900	-1.84930500
H	0.46285700	-3.13739900	-0.04848500
H	1.03961000	-1.51718000	1.82515700
H	-1.30949900	0.17208100	1.77377200
O	-2.75402400	-0.22917000	-0.53337700
H	-2.36301200	-0.22052900	-1.41916900
C	-3.58416500	0.93461400	-0.39435100
H	-2.99246000	1.85690100	-0.44548700
H	-4.36056000	0.95968900	-1.16842600
H	-4.06341400	0.87050700	0.58533800

Scan Point for comp9_beta_3.1Å

C	1.60519700	-1.48359500	-0.88982700
C	0.38183800	-2.05418000	-0.16935000
C	0.14857200	-1.48525700	1.25883200
C	1.57770700	0.03326400	-1.11526400
C	-0.33544700	-0.09502900	1.28976100
C	1.63092800	0.87619100	0.14988200
H	2.51086700	-1.74258000	-0.32544000
H	-0.52498100	-1.89986200	-0.76371300
H	0.70402600	0.33408900	-1.70723800
H	-0.57573100	-2.09532300	1.80133500
H	2.27305300	0.42733700	0.91378900

C	1.96171900	2.33640800	-0.06258800
H	1.88274800	2.89495800	0.87449200
H	2.99327000	2.41022500	-0.41984600
O	0.25376900	0.91402600	0.81583600
H	1.30096200	2.78784900	-0.80949000
H	2.46214800	0.31847500	-1.69700200
H	1.69132600	-1.97763900	-1.86445700
H	0.50359300	-3.13466700	-0.04494800
H	1.09966800	-1.50560500	1.81638400
H	-1.27935800	0.16015200	1.77352300
O	-2.83011400	-0.23610700	-0.54510600
H	-2.49624600	-0.22245000	-1.45390300
C	-3.67637000	0.90930100	-0.35801500
H	-3.11264000	1.84427500	-0.46413200
H	-4.50884200	0.90681300	-1.07201200
H	-4.07796500	0.84800200	0.65623900

Scan Point for comp9_beta_3.2Å

C	1.61084300	-1.47576600	-0.91022400
C	0.40104000	-2.05182800	-0.17145000
C	0.19089700	-1.48923200	1.26280800
C	1.57649300	0.04193800	-1.12890900
C	-0.29528800	-0.10013300	1.30767300
C	1.64954700	0.87979100	0.13861400
H	2.52648300	-1.73517600	-0.36236200
H	-0.51604400	-1.89697500	-0.74970600
H	0.69226500	0.34338200	-1.70468800
H	-0.52289500	-2.10300100	1.81498000
H	2.30543500	0.42913900	0.88965800
C	1.97375900	2.34155000	-0.07339400
H	1.90957200	2.89607600	0.86719900
H	2.99895100	2.41898400	-0.44778100
O	0.28380800	0.91206700	0.82801400
H	1.29952000	2.79468800	-0.80710200
H	2.45032800	0.33136100	-1.72443100
H	1.68139900	-1.96564400	-1.88820200
H	0.52706300	-3.13255900	-0.05358600
H	1.15134700	-1.50990300	1.80407000
H	-1.23135700	0.15112700	1.80842300
O	-2.90187400	-0.24289100	-0.54309200
H	-2.58351500	-0.22463400	-1.45735600
C	-3.74660800	0.90028800	-0.33651100
H	-3.18617900	1.83664000	-0.44782900

H	-4.59099700	0.89971100	-1.03637500
H	-4.13095200	0.83372700	0.68407600

Scan Point for comp9_beta_3.3Å

C	1.68290400	-1.43544200	-0.89287800
C	0.48512000	-2.06035500	-0.17469200
C	0.23368800	-1.50898300	1.25815700
C	1.59056300	0.07944900	-1.11561300
C	-0.31540500	-0.14400200	1.28777300
C	1.60299200	0.92276300	0.15003600
H	2.59847400	-1.65615600	-0.32816000
H	-0.42901200	-1.93955100	-0.76571500
H	0.70682800	0.34378300	-1.71004500
H	-0.46016200	-2.15261900	1.80145100
H	2.26552700	0.50560000	0.91459700
C	1.86060100	2.39809600	-0.06016900
H	1.75463800	2.95016100	0.87807400
H	2.88696500	2.52400900	-0.41778200
O	0.22267400	0.89211900	0.81287300
H	1.17767200	2.81767600	-0.80573200
H	2.46416600	0.40328400	-1.69368300
H	1.79121500	-1.92282200	-1.86857100
H	0.65126500	-3.13550100	-0.05629700
H	1.18762800	-1.48816000	1.80983800
H	-1.27776200	0.06278800	1.75992800
O	-2.99469500	-0.33617800	-0.62911900
H	-2.68324000	-0.26511100	-1.54321200
C	-3.64251300	0.89558400	-0.27575900
H	-2.93820200	1.73627800	-0.29669500
H	-4.48108100	1.10987600	-0.94932900
H	-4.02645300	0.77626900	0.74017600

Scan Point for comp9_beta_3.5Å

C	1.69206600	-1.42389800	-0.93226500
C	0.51972400	-2.05591800	-0.17913700
C	0.31446000	-1.51425300	1.26476100
C	1.58952800	0.09219100	-1.14203600
C	-0.23582400	-0.15057900	1.32139500
C	1.64210300	0.92742000	0.12797500
H	2.62616200	-1.64626700	-0.39937200

H	-0.41359800	-1.93328100	-0.73902100
H	0.68613500	0.35845600	-1.70529200
H	-0.36000600	-2.16278300	1.82635400
H	2.33029100	0.50674100	0.86757900
C	1.88986700	2.40461500	-0.08103600
H	1.81389200	2.95042300	0.86378700
H	2.90365200	2.53495900	-0.47150000
O	0.28443900	0.88967700	0.83579800
H	1.18188100	2.82755100	-0.80092500
H	2.44298400	0.42155900	-1.74650600
H	1.76917300	-1.90480500	-1.91414700
H	0.69173900	-3.13145100	-0.07322600
H	1.28598200	-1.49506100	1.78498700
H	-1.18241400	0.05124100	1.82647900
O	-3.14192000	-0.34649300	-0.61928100
H	-2.86106100	-0.26909000	-1.54274600
C	-3.77973800	0.88180000	-0.23677000
H	-3.07790200	1.72393300	-0.27562300
H	-4.64053100	1.09879600	-0.88083800
H	-4.12964700	0.75533400	0.79055100

Scan Point for comp9_beta_3.6Å

C	1.59944200	-1.47000400	-0.94287300
C	0.42783000	-2.05263500	-0.14870600
C	0.29341500	-1.49509000	1.29939800
C	1.55338700	0.04863400	-1.15610800
C	-0.22414400	-0.11933800	1.34547800
C	1.66217100	0.88725100	0.10885000
H	2.54036700	-1.73024700	-0.44052300
H	-0.51806100	-1.89629400	-0.67925600
H	0.65093600	0.34848400	-1.70365200
H	-0.37698100	-2.11979300	1.89183500
H	2.35005700	0.44757300	0.83712000
C	1.95758500	2.35331700	-0.11484000
H	1.91296300	2.90879400	0.82632300
H	2.97023900	2.44548500	-0.51894000
O	0.31506400	0.89977500	0.83683400
H	1.25546300	2.79472200	-0.82926500
H	2.40725500	0.34172300	-1.77815100
H	1.62371200	-1.95611800	-1.92494300
H	0.56109500	-3.13346500	-0.04141700
H	1.28435800	-1.49503900	1.78043300
H	-1.16644700	0.11157000	1.84751400

O	-3.18501900	-0.30909600	-0.69344500
H	-2.92606500	-0.18310000	-1.61780800
C	-3.64982400	0.94707700	-0.17708300
H	-2.85551700	1.70343200	-0.18619900
H	-4.50811500	1.31980500	-0.74921700
H	-3.96478700	0.77176300	0.85434000

Scan Point for comp9_beta_3.7Å

C	-1.57161600	1.55746400	-0.87575400
C	-0.34177100	2.02903800	-0.09555400
C	-0.21809600	1.41676500	1.33146200
C	-1.63613200	0.04741100	-1.14217800
C	0.21528000	0.01175600	1.31564100
C	-1.75910900	-0.82987400	0.09540800
H	-2.47822400	1.86366700	-0.33742400
H	0.57767800	1.82025100	-0.65414100
H	-0.77403300	-0.29037700	-1.73114800
H	0.50119900	1.97687200	1.93110500
H	-2.39666000	-0.37770200	0.86092500
C	-2.15230200	-2.26477500	-0.17393300
H	-2.12617600	-2.85808500	0.74450800
H	-3.17690300	-2.27588700	-0.55790500
O	-0.39583300	-0.95218000	0.78166500
H	-1.49528700	-2.72252200	-0.92014800
H	-2.52786700	-0.16551000	-1.74315600
H	-1.58786700	2.07905500	-1.83962900
H	-0.39202500	3.11281200	0.04686800
H	-1.19896400	1.46199500	1.83069900
H	1.15339500	-0.29440500	1.78398300
O	3.27653300	0.23812100	-0.75014700
H	3.08471900	0.04443600	-1.67934500
C	3.79546700	-0.95215200	-0.13774500
H	3.05608000	-1.76227400	-0.14839700
H	4.70868400	-1.29219800	-0.64109900
H	4.03632100	-0.70144600	0.89807400

Scan Point for comp9_beta_3.8Å

C	1.58045600	-1.48802200	-0.95086000
C	0.41216900	-2.04542900	-0.13341900
C	0.31893700	-1.48438900	1.31706700

C	1.56037300	0.03103600	-1.16654100
C	-0.17578800	-0.10062300	1.36723300
C	1.70514600	0.86997300	0.09501400
H	2.52512200	-1.76626000	-0.46548300
H	-0.54023300	-1.86814500	-0.64585200
H	0.65516200	0.34717000	-1.70002200
H	-0.34902500	-2.09668300	1.92500800
H	2.39720300	0.42008500	0.81280600
C	2.02261600	2.32985300	-0.13716900
H	2.00552700	2.88832700	0.80312900
H	3.02954300	2.40261000	-0.55921000
O	0.37073800	0.90751000	0.84505500
H	1.31610600	2.78228400	-0.84021900
H	2.40985700	0.30688200	-1.80228400
H	1.57641900	-1.97626500	-1.93214800
H	0.52362000	-3.12892600	-0.02825700
H	1.31983500	-1.49910200	1.77667400
H	-1.10661100	0.14715300	1.88264000
O	-3.20514900	-0.12827000	-0.92671600
H	-3.11188900	0.32105600	-1.77951900
C	-3.78476600	0.79270900	0.01020000
H	-3.13550400	1.66193400	0.17088000
H	-4.76960900	1.13759900	-0.32806500
H	-3.90509400	0.25570100	0.95406000

Scan Point for comp9_beta_3.9Å

C	1.70044400	-1.50463200	-0.89131200
C	0.48135600	-2.03584800	-0.13286500
C	0.32295000	-1.44922100	1.30257400
C	1.71091000	0.01078600	-1.13429700
C	-0.17491100	-0.06629700	1.29041100
C	1.78342400	0.87389300	0.11682500
H	2.61157600	-1.78452700	-0.34630000
H	-0.44002900	-1.85427000	-0.69802000
H	0.84411400	0.32410300	-1.72984400
H	-0.37475900	-2.04766700	1.89043700
H	2.42676400	0.43524700	0.88533400
C	2.12061100	2.32770800	-0.12490700
H	2.05350300	2.90428100	0.80207900
H	3.14957500	2.38823700	-0.49212800
O	0.40353600	0.93032000	0.78055400
H	1.45640000	2.76905800	-0.87471900
H	2.60155000	0.26611900	-1.72032300

H	1.74816400	-2.00976200	-1.86287800
H	0.57220000	-3.11884300	-0.00551200
H	1.30239300	-1.45693300	1.80519300
H	-1.14243700	0.18889300	1.72910900
O	-3.36531600	-0.05647500	-0.95262600
H	-3.26855500	0.50671600	-1.73422600
C	-4.10415700	0.67079400	0.04044300
H	-3.57085600	1.57666800	0.35380000
H	-5.09871600	0.94994300	-0.32848400
H	-4.22041100	0.00887000	0.90183200

Scan Point for comp9_beta_4.0Å

C	1.80298900	-1.47156400	-0.89138500
C	0.57410200	-2.04171300	-0.17917200
C	0.35148700	-1.47584900	1.25622500
C	1.78168700	0.04606800	-1.11722300
C	-0.17315600	-0.10255900	1.24579500
C	1.80106100	0.89312900	0.14637700
H	2.70324500	-1.73399800	-0.32005000
H	-0.33172300	-1.87741600	-0.77349800
H	0.92261200	0.34578900	-1.73065300
H	-0.35465100	-2.09604400	1.81051000
H	2.42869500	0.45439100	0.92774500
C	2.11695400	2.35684400	-0.06233700
H	2.00916800	2.91615500	0.87143800
H	3.15540900	2.44351500	-0.39594400
O	0.40058300	0.91272900	0.76876400
H	1.46755400	2.79767500	-0.82529700
H	2.68032900	0.33019900	-1.67733600
H	1.89509700	-1.96419400	-1.86611000
H	0.68828900	-3.12339900	-0.05970200
H	1.31195900	-1.47115800	1.79429400
H	-1.15967500	0.12714400	1.65566200
O	-3.46088300	0.11297400	-1.02233000
H	-3.51802300	0.82087400	-1.68058400
C	-4.25918000	0.48418000	0.11108500
H	-3.88429100	1.40093700	0.58259400
H	-5.30933500	0.62911300	-0.17065600
H	-4.19792500	-0.33641300	0.82993200

Scan Point for comp9_beta_4.1Å

C	1.81919200	-1.47879700	-0.88843400
C	0.58623400	-2.03840200	-0.17465500
C	0.36769800	-1.46586200	1.25899000
C	1.80865500	0.03831000	-1.11914300
C	-0.15169400	-0.09076400	1.23983500
C	1.83028900	0.88988800	0.14148000
H	2.71736300	-1.74581800	-0.31599200
H	-0.31847000	-1.87010200	-0.76963400
H	0.95309300	0.34161100	-1.73572000
H	-0.34102700	-2.08029800	1.81636900
H	2.45354500	0.45071300	0.92601800
C	2.15533400	2.35082800	-0.07207700
H	2.04849700	2.91444200	0.85920100
H	3.19519700	2.42978200	-0.40322200
O	0.42792900	0.91963400	0.75949900
H	1.51075900	2.79257900	-0.83857200
H	2.71045700	0.31455200	-1.67809000
H	1.90808700	-1.97504400	-1.86163800
H	0.69306600	-3.12041800	-0.05147200
H	1.32868800	-1.46318400	1.79589300
H	-1.14031200	0.14442400	1.64186100
O	-3.56184300	0.11328100	-1.02715400
H	-3.62508800	0.83131900	-1.67365700
C	-4.32564700	0.47829400	0.13176800
H	-3.93438700	1.39034400	0.59913100
H	-5.38312500	0.62867400	-0.11812100
H	-4.24538900	-0.34785600	0.84230100

Scan Point for comp9_beta_4.2Å

C	-1.83193300	-1.44621600	0.92480300
C	-0.61359600	-2.04228600	0.21596500
C	-0.39178600	-1.50268500	-1.22930600
C	-1.79311200	0.07472900	1.12432100
C	0.14588500	-0.13459000	-1.24681000
C	-1.81166100	0.89992100	-0.15362500
H	-2.73825500	-1.70854300	0.36311800
H	0.29708500	-1.87949300	0.80322800
H	-0.92725000	0.37600500	1.72731400
H	0.30514400	-2.13945800	-1.77641400
H	-2.44827900	0.45404800	-0.92369400
C	-2.11125500	2.37031800	0.03127500
H	-2.00389400	2.91216200	-0.91280700

H	-3.14655700	2.47374100	0.36992200
O	-0.41491600	0.89461600	-0.78473200
H	-1.45236200	2.81755800	0.78228000
H	-2.68544100	0.37768600	1.68472600
H	-1.92399200	-1.92094900	1.90835400
H	-0.74137400	-3.12430300	0.11462700
H	-1.35467300	-1.49743300	-1.76305300
H	1.13100600	0.07828900	-1.66879600
O	3.61899700	0.22284000	1.08765600
H	3.77239000	1.02688200	1.60519900
C	4.24973100	0.38069900	-0.19190700
H	3.81928900	1.22162300	-0.74919300
H	5.33044500	0.53684400	-0.08714200
H	4.08042700	-0.54365300	-0.74936800

Scan Point for comp9_beta_4.3Å

C	-1.85599800	-1.43489400	0.95139000
C	-0.63505100	-2.03707500	0.25221400
C	-0.41493000	-1.51841600	-1.20122500
C	-1.82490200	0.08952600	1.12512000
C	0.11947200	-0.14938700	-1.23718700
C	-1.84503500	0.89345200	-0.16642500
H	-2.76127000	-1.71148500	0.39491600
H	0.27463700	-1.86202900	0.83753400
H	-0.96137800	0.40516500	1.72411000
H	0.28408000	-2.16130300	-1.73842000
H	-2.47710700	0.43194700	-0.93086200
C	-2.15332300	2.36486400	-0.00607400
H	-2.04598500	2.89249700	-0.95819800
H	-3.19042100	2.46762400	0.32729200
O	-0.44634700	0.88482400	-0.79284900
H	-1.49964000	2.82747700	0.74010700
H	-2.71954300	0.39731400	1.67913100
H	-1.94516400	-1.89319100	1.94296100
H	-0.75857100	-3.12099000	0.16735400
H	-1.37783500	-1.52388100	-1.73471500
H	1.10658700	0.06012800	-1.65649100
O	3.70655400	0.38528600	1.07300300
H	4.02235700	1.19785600	1.49424600
C	4.34971500	0.25895400	-0.20383600
H	4.08153500	1.08795800	-0.87049800
H	5.44085400	0.22147600	-0.09874500
H	4.00552400	-0.67958600	-0.64480800

Scan Point for comp9_beta_4.4Å

C	-1.92240000	-1.39840700	0.96500000
C	-0.70031400	-2.03595700	0.29978200
C	-0.44264600	-1.54767200	-1.15804500
C	-1.86370200	0.12786500	1.11414600
C	0.11824900	-0.18989000	-1.20864300
C	-1.84220600	0.91025200	-0.19084800
H	-2.82233300	-1.66646100	0.39572000
H	0.20117100	-1.86734200	0.89948300
H	-1.00539200	0.43578500	1.72462700
H	0.25406900	-2.21300900	-1.67029400
H	-2.46993700	0.44909900	-0.95896500
C	-2.12308300	2.39002700	-0.05848400
H	-1.99354000	2.90105800	-1.01686100
H	-3.16222600	2.51838900	0.25934600
O	-0.43399500	0.86265200	-0.79137400
H	-1.47042600	2.85142400	0.68938800
H	-2.76228100	0.46333100	1.64503700
H	-2.03954200	-1.83830900	1.96192100
H	-0.84304500	-3.11867200	0.23169300
H	-1.39506100	-1.54512800	-1.71008700
H	1.11585700	-0.00665000	-1.61514900
O	3.82243000	0.53029000	1.05418200
H	4.23259100	1.37287400	1.29831400
C	4.36807500	0.10680100	-0.20398700
H	4.14073500	0.82529000	-1.00112000
H	5.45460300	-0.03044000	-0.14270800
H	3.90545000	-0.85287700	-0.44633600

Scan Point for comp9_beta_4.5Å

C	-1.92826300	-1.39438500	0.97931200
C	-0.71259300	-2.03358200	0.30407100
C	-0.46867500	-1.54930000	-1.15741200
C	-1.86895600	0.13240700	1.12242000
C	0.09098600	-0.19136900	-1.21774700
C	-1.86102700	0.91049400	-0.18519300
H	-2.83379000	-1.66506600	0.42030100
H	0.19451700	-1.86340100	0.89477000
H	-1.00468500	0.44294000	1.72309200

H	0.22349600	-2.21594800	-1.67410600
H	-2.49564900	0.44639500	-0.94583600
C	-2.14170200	2.39047000	-0.05479300
H	-2.02058100	2.89875100	-1.01572700
H	-3.17813900	2.51913800	0.27165000
O	-0.45826300	0.86214400	-0.79894500
H	-1.48289900	2.85437900	0.68610000
H	-2.76231500	0.46919400	1.66126600
H	-2.03493100	-1.83067300	1.97899900
H	-0.85589000	-3.11648600	0.24030300
H	-1.42613000	-1.54876500	-1.70063000
H	1.08457100	-0.00873700	-1.63456100
O	3.90723800	0.53786700	1.05259000
H	4.34726800	1.37021100	1.27982400
C	4.40408400	0.09468700	-0.21894000
H	4.16985300	0.81438200	-1.01303000
H	5.48846300	-0.06807500	-0.18944000
H	3.91191600	-0.85485300	-0.44244900

Scan Point for comp9_beta_4.6Å

C	-1.96216300	-1.37986000	0.98466100
C	-0.74341600	-2.03064000	0.32603600
C	-0.48207500	-1.55830400	-1.13632600
C	-1.89443700	0.14739400	1.11860500
C	0.08582100	-0.20404600	-1.20142800
C	-1.86789200	0.91676700	-0.19409300
H	-2.86359900	-1.64847100	0.41804200
H	0.15866300	-1.86087100	0.92457300
H	-1.03431100	0.45609800	1.72616400
H	0.21130600	-2.23251800	-1.64145700
H	-2.49807800	0.45170600	-0.95773400
C	-2.14081000	2.39919400	-0.07550100
H	-2.00884100	2.90106900	-1.03836300
H	-3.17923600	2.53587200	0.24122700
O	-0.46025200	0.85556800	-0.79410900
H	-1.48570400	2.86385200	0.66820600
H	-2.79098000	0.49379000	1.64582300
H	-2.08177400	-1.80920600	1.98586200
H	-0.89202600	-3.11317800	0.26873900
H	-1.43399700	-1.55631100	-1.68933300
H	1.08329400	-0.03005800	-1.61232400
O	4.02362900	0.63455800	1.02352100
H	4.53736200	1.45045700	1.11122200

C	4.39383300	-0.00305100	-0.20793300
H	4.15894900	0.63055300	-1.07208700
H	5.46240000	-0.25030700	-0.22328000
H	3.81640000	-0.92821000	-0.27469600

8.3: Geometries for Relaxed PES Scans of Single Hydroxyl variations (2-OH through 7-OH and 2-deoxy through 7-deoxy structures)

Scan Point for comp9-c2oh_alpha_1.4Å

C	1.65625400	-1.40016800	-0.60416600
C	0.18792200	-1.64560200	-0.25611400
C	1.90720900	1.11257700	0.03544000
C	-0.78881500	-0.54965400	-0.77375400
C	0.41606600	1.35020400	0.27310000
H	2.29422300	-0.59932100	1.29482900
H	1.70856700	-1.15716700	-1.67397600
H	2.14267000	1.45596800	-0.98117400
H	-0.14394400	-2.58109100	-0.71542600
H	0.09138600	0.87652400	1.20659600
C	0.04891100	2.82645100	0.29350600
H	-1.02944800	2.96211000	0.42316300
H	0.55877300	3.32599900	1.12362700
O	-0.34614400	0.76235800	-0.83935800
H	0.35330700	3.31444200	-0.63948900
H	2.46590600	1.75847600	0.72433800
H	3.44505700	-0.38589200	-0.01091900
H	2.17735000	-2.35603400	-0.47707100
O	-0.03970600	-1.73819400	1.17479400
H	-0.09639700	-2.67027900	1.43444900
H	-1.12391800	-0.79235900	-1.78363200
O	-1.89679100	-0.69108400	0.07027600
H	-1.55567800	-1.03539900	0.95773700
C	-3.01291800	0.27582700	0.07385200
H	-3.76493200	-0.16981400	0.72140800
H	-2.65579800	1.23157200	0.45105300
H	-3.35923000	0.34186300	-0.95580100

Scan Point for comp9-c2oh_alpha_1.5Å

C	1.63986900	-1.43983400	-0.60772000

C	0.17294000	-1.63352200	-0.21059200
C	1.93568700	1.08099100	-0.01999500
C	-0.76232500	-0.53837300	-0.77221600
C	0.46019700	1.33742300	0.28505900
H	2.36615900	-0.61357500	1.24713500
H	1.67198500	-1.23092500	-1.68560500
H	2.12481100	1.40818800	-1.05136900
H	-0.19440300	-2.57496200	-0.63000000
H	0.16351500	0.86115300	1.22509300
C	0.10787400	2.81571900	0.32262800
H	-0.96242300	2.95988600	0.50077600
H	0.65764100	3.30628700	1.13212400
O	-0.35801200	0.76441500	-0.80257500
H	0.37616400	3.30436200	-0.62086400
H	2.53008100	1.73242800	0.63258300
H	3.46063600	-0.42918700	-0.11048900
H	2.14042100	-2.40415200	-0.46298600
O	-0.02090300	-1.66401000	1.22162400
H	-0.03345800	-2.58510000	1.52161000
H	-1.10504000	-0.79070900	-1.77578200
O	-1.99097600	-0.70638500	0.07169700
H	-1.67687500	-0.95252300	0.98442500
C	-3.06527500	0.30071000	0.01694900
H	-3.85344700	-0.09025700	0.65784900
H	-2.68693800	1.25799500	0.36992000
H	-3.38495600	0.34552100	-1.02243500

Scan Point for comp9-c2oh_alpha_1.6Å

C	1.63296400	-1.46860400	-0.60106900
C	0.16260000	-1.62595200	-0.19113900
C	1.95718400	1.05630900	-0.04458400
C	-0.73208100	-0.52455700	-0.78569500
C	0.49227700	1.33134900	0.29112300
H	2.39547600	-0.62810300	1.23263600
H	1.66483300	-1.28179500	-1.68310400
H	2.12768700	1.37221700	-1.08255900
H	-0.22637700	-2.56540800	-0.59535000
H	0.20339500	0.85368600	1.23169400
C	0.15305500	2.81140800	0.33176400
H	-0.91395700	2.96474400	0.52091800
H	0.71521700	3.29399400	1.13738700
O	-0.35547600	0.76602600	-0.78596600
H	0.41721500	3.29936500	-0.61305500

H	2.56937300	1.70950900	0.58927500
H	3.46910600	-0.46622200	-0.14445300
H	2.11613100	-2.43898500	-0.43897200
O	-0.02545700	-1.62439000	1.23823600
H	-0.00575400	-2.53830900	1.55878600
H	-1.09589500	-0.77893600	-1.78041500
O	-2.06828400	-0.71699700	0.07310100
H	-1.76355400	-0.91363800	0.99393500
C	-3.09682700	0.32705000	-0.00453600
H	-3.91665600	-0.02243700	0.62191900
H	-2.69387900	1.27433100	0.35013300
H	-3.39853900	0.38152100	-1.04910500

Scan Point for comp9-c2oh_alpha_1.7Å

C	1.61057600	-1.51118500	-0.59505700
C	0.13626700	-1.61819200	-0.17250500
C	1.98946400	1.01339900	-0.07210100
C	-0.70781200	-0.50290600	-0.79533700
C	0.54035900	1.32412200	0.29711600
H	2.41670200	-0.66412500	1.21729300
H	1.64288000	-1.34693700	-1.68068400
H	2.14297900	1.31460100	-1.11693100
H	-0.28395300	-2.55148800	-0.56049000
H	0.25730400	0.84982000	1.23982400
C	0.23098100	2.80946100	0.33694600
H	-0.82948400	2.98523400	0.54191500
H	0.81499400	3.27998900	1.13400800
O	-0.34624000	0.77277300	-0.76514100
H	0.49223800	3.29040400	-0.61207800
H	2.62728000	1.66228500	0.54029200
H	3.47155700	-0.53774700	-0.17812800
H	2.06660900	-2.49169100	-0.41618500
O	-0.04932500	-1.57649800	1.25208400
H	0.10422800	-2.46223400	1.61372800
H	-1.09755200	-0.75259400	-1.78078500
O	-2.15274200	-0.71034000	0.07595500
H	-1.86721100	-0.87890500	1.00305500
C	-3.13714500	0.36466700	-0.02472500
H	-3.98143300	0.06563000	0.59702800
H	-2.70645900	1.30492000	0.31891200
H	-3.42910600	0.41907900	-1.07250800

Scan Point for comp9-c2oh_alpha_1.8Å

C	1.66687400	-1.48626100	-0.55756700
C	0.17781700	-1.62005200	-0.19236200
C	1.96613900	1.05008500	-0.04008900
C	-0.65010500	-0.51960500	-0.85432900
C	0.50318300	1.33512300	0.28985600
H	2.38232900	-0.60750500	1.27847600
H	1.74009200	-1.33158500	-1.64252300
H	2.14144500	1.34432300	-1.08342200
H	-0.21135900	-2.55946400	-0.59765200
H	0.20001700	0.85760400	1.22379200
C	0.15561000	2.81152300	0.30438200
H	-0.91551700	2.96124100	0.47058300
H	0.69882600	3.30195400	1.11804600
O	-0.34490400	0.75389900	-0.79633300
H	0.43929300	3.29090500	-0.63880100
H	2.57218400	1.71936400	0.58236700
H	3.48678600	-0.46600600	-0.07659500
H	2.13328900	-2.45617200	-0.34989700
O	-0.06226600	-1.58156800	1.22262100
H	0.14236600	-2.45166100	1.59759200
H	-1.04505900	-0.77783700	-1.83475800
O	-2.19864500	-0.78386200	0.02441400
H	-1.88574500	-1.02247300	0.92629300
C	-3.09629000	0.36116300	0.05472700
H	-3.93201500	0.09419100	0.70364600
H	-2.57774200	1.24418700	0.43076800
H	-3.44117000	0.51639500	-0.96712500

Scan Point for comp9-c2oh_alpha_1.9Å

C	1.64782000	-1.52567900	-0.55072400
C	0.15344100	-1.61430900	-0.18185500
C	2.00058700	1.00913800	-0.05679300
C	-0.62510800	-0.49933400	-0.86684800
C	0.55042400	1.32922800	0.29462300
H	2.39570700	-0.64508100	1.27183100
H	1.72617300	-1.39000800	-1.63785200
H	2.16768800	1.29195200	-1.10449100
H	-0.26289200	-2.54579400	-0.57816400
H	0.24554600	0.85435700	1.22861600
C	0.23084300	2.81061900	0.30905500

H	-0.83440400	2.98064000	0.49156700
H	0.79515700	3.29000700	1.11480600
O	-0.32726800	0.76138600	-0.78486400
H	0.51089700	3.28329100	-0.63839900
H	2.62773000	1.67135300	0.55197300
H	3.49072800	-0.53672300	-0.09392000
H	2.08668400	-2.50479300	-0.32732000
O	-0.08469000	-1.54824200	1.22956100
H	0.14734000	-2.40355800	1.62286700
H	-1.05103900	-0.74964300	-1.83594300
O	-2.27702300	-0.76532000	0.03339000
H	-1.96981700	-0.97730600	0.94003300
C	-3.14317900	0.39776300	0.03677300
H	-3.98758500	0.18226000	0.69499300
H	-2.60376500	1.28158900	0.38374100
H	-3.48941800	0.53615800	-0.98757400

Scan Point for comp9-c2oh_alpha_2.0Å

C	1.62466500	-1.56826400	-0.54211700
C	0.12425700	-1.60819800	-0.18000100
C	2.03798800	0.96057100	-0.06264000
C	-0.60003400	-0.47430400	-0.88321700
C	0.60142100	1.32431500	0.29963600
H	2.39278300	-0.69468600	1.27592500
H	1.71521600	-1.44772500	-1.63007000
H	2.20503700	1.23216400	-1.11323100
H	-0.31915000	-2.52759100	-0.57498300
H	0.28494500	0.85860900	1.23398100
C	0.32113200	2.81273600	0.30519700
H	-0.73931800	3.01254800	0.48446300
H	0.89647300	3.27853300	1.11106400
O	-0.30239800	0.77366400	-0.77629500
H	0.61741100	3.27346900	-0.64307100
H	2.68592000	1.61107600	0.53674400
H	3.49017700	-0.62079300	-0.09049200
H	2.03057000	-2.55797000	-0.30396100
O	-0.11832900	-1.52320500	1.22735700
H	0.12707700	-2.36941900	1.63263900
H	-1.05645800	-0.71020000	-1.84185000
O	-2.35670500	-0.73865000	0.03560100
H	-2.05366500	-0.94260100	0.94264200
C	-3.19091700	0.44221300	0.03354200
H	-4.05155400	0.25804200	0.68164000

H	-2.63473100	1.31465000	0.38598800
H	-3.52341600	0.59435000	-0.99383400

Scan Point for comp9-c2oh_alpha_2.1Å

C	1.60617100	-1.60426800	-0.53552000
C	0.10190500	-1.60194300	-0.17764600
C	2.07322900	0.91885200	-0.06831500
C	-0.57446100	-0.45349400	-0.89578600
C	0.65007400	1.31980800	0.30454300
H	2.39457200	-0.73737200	1.27752800
H	1.70553700	-1.49793900	-1.62412800
H	2.23880000	1.18139200	-1.12137100
H	-0.36498000	-2.51048600	-0.57055100
H	0.32405500	0.86251500	1.23938600
C	0.40161700	2.81301800	0.30249900
H	-0.65394200	3.03646200	0.48228900
H	0.98793000	3.26810900	1.10656500
O	-0.27583400	0.78356600	-0.76811500
H	0.70763100	3.26334900	-0.64755100
H	2.73990300	1.55799000	0.52253600
H	3.49109200	-0.69322600	-0.09109500
H	1.98349100	-2.60216300	-0.28488100
O	-0.14271900	-1.49864700	1.22609500
H	0.12110900	-2.33353200	1.64364200
H	-1.06059400	-0.67528900	-1.84322200
O	-2.43570100	-0.71481200	0.04096300
H	-2.13662300	-0.90572300	0.94974900
C	-3.24836900	0.47728400	0.02619000
H	-4.11564400	0.32459700	0.67492200
H	-2.67779700	1.34611000	0.36730100
H	-3.57828800	0.62604100	-1.00288500

Scan Point for comp9-c2oh_alpha_2.2Å

C	1.59910000	-1.63141800	-0.52266100
C	0.08977200	-1.59627300	-0.18095700
C	2.10156800	0.88728300	-0.06483100
C	-0.54502300	-0.43940200	-0.91632000
C	0.68667500	1.31669800	0.30526200
H	2.38718100	-0.76677400	1.29195200
H	1.71386700	-1.53822900	-1.61086100

H	2.27362000	1.14106200	-1.11891800
H	-0.39140800	-2.49712400	-0.57416200
H	0.34664500	0.86659200	1.23829000
C	0.46126500	2.81270900	0.29421500
H	-0.59196800	3.05304300	0.46567800
H	1.04867300	3.26048600	1.10160300
O	-0.24974700	0.78979500	-0.77096000
H	0.78188300	3.25479600	-0.65478300
H	2.77760900	1.51883100	0.52345500
H	3.49403600	-0.74699500	-0.06891400
H	1.95207400	-2.63456500	-0.25778200
O	-0.16779600	-1.47549400	1.21783100
H	0.10794400	-2.29979200	1.64899500
H	-1.05400300	-0.65059900	-1.85440500
O	-2.50975500	-0.70165200	0.03817100
H	-2.20228900	-0.89351800	0.94246000
C	-3.29568600	0.50533000	0.03508900
H	-4.16128000	0.37879200	0.69281500
H	-2.70272100	1.36337200	0.36790700
H	-3.63427100	0.66421400	-0.99004700

Scan Point for comp9-c2oh_alpha_2.3Å

C	1.59375400	-1.65597900	-0.50964100
C	0.08033400	-1.59079600	-0.18486600
C	2.12784500	0.85826500	-0.06010200
C	-0.51629100	-0.42756200	-0.93619300
C	0.72031100	1.31354800	0.30533400
H	2.37933100	-0.79291000	1.30710200
H	1.72314700	-1.57506400	-1.59711000
H	2.30713400	1.10370100	-1.11488900
H	-0.41338200	-2.48466800	-0.57836500
H	0.36653300	0.87006600	1.23620300
C	0.51644400	2.81178400	0.28632800
H	-0.53381400	3.06811300	0.45263400
H	1.10685200	3.25290800	1.09522200
O	-0.22421800	0.79541200	-0.77564600
H	0.84809900	3.24586900	-0.66248100
H	2.81155500	1.48276500	0.52674100
H	3.49684200	-0.79579900	-0.04516500
H	1.92444600	-2.66322300	-0.23181900
O	-0.19160300	-1.45221500	1.20854200
H	0.08883200	-2.26776600	1.65355200
H	-1.04186700	-0.62956000	-1.86752900

O	-2.58322500	-0.69158000	0.03750000
H	-2.25268000	-0.87630000	0.93409500
C	-3.34056000	0.53118700	0.04312700
H	-4.18308200	0.44483000	0.73728800
H	-2.71499000	1.38291800	0.33195800
H	-3.71685400	0.67935800	-0.97080000

Scan Point for comp9-c2oh_alpha_2.4Å

C	1.60990700	-1.66384300	-0.48887700
C	0.08926700	-1.59099800	-0.19597300
C	2.14072400	0.85221800	-0.04109300
C	-0.48111500	-0.42955100	-0.96648800
C	0.72992700	1.31446000	0.30085600
H	2.36153100	-0.79277600	1.33855500
H	1.76268100	-1.59140400	-1.57390100
H	2.33866500	1.09256200	-1.09363000
H	-0.39998000	-2.48502000	-0.59458700
H	0.35809700	0.87453800	1.22622200
C	0.52703000	2.81205400	0.26993200
H	-0.52580000	3.06926700	0.41746500
H	1.10344200	3.25631600	1.08718100
O	-0.20284000	0.79113900	-0.79431400
H	0.87484300	3.24189000	-0.67492700
H	2.81596700	1.47759200	0.55458500
H	3.50506300	-0.80495300	0.00823300
H	1.93021300	-2.67050500	-0.19720400
O	-0.21339000	-1.43911800	1.18923200
H	0.06639200	-2.24639500	1.64983400
H	-1.01175300	-0.62968400	-1.89588000
O	-2.64908800	-0.70106800	0.02657300
H	-2.27565100	-0.89383900	0.90408200
C	-3.35998500	0.54672700	0.07183100
H	-4.15698500	0.50351000	0.82215400
H	-2.68605100	1.37893300	0.30514500
H	-3.79928500	0.70087400	-0.91593800

Scan Point for comp9-c2oh_alpha_2.5Å

C	1.61662400	-1.68017800	-0.46340900
C	0.08923700	-1.58952200	-0.21132300
C	2.15666000	0.83399900	-0.01703800

C	-0.44803900	-0.42601900	-1.00017000
C	0.74510500	1.31356000	0.29525100
H	2.33045500	-0.80436000	1.37706800
H	1.79869600	-1.61749200	-1.54445100
H	2.37861400	1.06585700	-1.06664500
H	-0.39884700	-2.48078000	-0.61748800
H	0.34909600	0.88231100	1.21460000
C	0.55656100	2.81211600	0.24821500
H	-0.49640500	3.08017700	0.37365000
H	1.12135900	3.25715500	1.07312500
O	-0.17670500	0.79118000	-0.81539000
H	0.92613300	3.23155300	-0.69300000
H	2.82508600	1.45732800	0.58838600
H	3.50576200	-0.83365400	0.07465400
H	1.91816600	-2.68805100	-0.15640400
O	-0.25057100	-1.42282200	1.16341800
H	0.02257400	-2.22232700	1.64131700
H	-0.97958900	-0.62061500	-1.93086900
O	-2.71956900	-0.70170100	0.00688000
H	-2.30308700	-0.92509000	0.85728300
C	-3.36733100	0.57502200	0.11336400
H	-4.13698700	0.55289000	0.89322200
H	-2.64699200	1.37019200	0.33774400
H	-3.83778500	0.77635200	-0.85151800

Scan Point for comp9-c2oh_alpha_2.6Å

C	-1.58929400	-1.71890000	0.44820300
C	-0.06108100	-1.57838200	0.22382500
C	-2.19735700	0.77735800	-0.00387600
C	0.42325600	-0.40100300	1.02421300
C	-0.79836300	1.30523800	-0.29316800
H	-2.29440000	-0.86199800	-1.40443300
H	-1.79181100	-1.66200700	1.52594600
H	-2.44353900	0.99850300	1.04257300
H	0.44804100	-2.45511100	0.63571300
H	-0.37203200	0.89102200	-1.20681200
C	-0.66114000	2.80850800	-0.23385200
H	0.38375900	3.11404200	-0.33840100
H	-1.22607900	3.23825400	-1.06675900
O	0.12744500	0.80663300	0.82993100
H	-1.06224300	3.20936800	0.70247200
H	-2.87531800	1.38154100	-0.61798800
H	-3.49286500	-0.93024000	-0.12447800

H	-1.85220600	-2.73576300	0.13565300
O	0.29948900	-1.39230100	-1.14269700
H	0.04626400	-2.19111900	-1.63254900
H	0.96161600	-0.57785800	1.95514000
O	2.80060000	-0.66423100	0.00492700
H	2.35638900	-0.90219900	-0.82694700
C	3.42607700	0.61891000	-0.14015400
H	4.19484900	0.59111100	-0.92131600
H	2.69242800	1.39602100	-0.38414400
H	3.89622500	0.85676000	0.81664700

Scan Point for comp9-c2oh_alpha_2.7Å

C	-1.56636900	-1.75113800	0.43516100
C	-0.03873500	-1.56696400	0.23653100
C	-2.23710700	0.72715400	-0.02497300
C	0.39536500	-0.37728800	1.04597100
C	-0.85063000	1.29801400	-0.29164900
H	-2.25940400	-0.91129300	-1.42969000
H	-1.78791100	-1.69938200	1.50945000
H	-2.50638800	0.93846800	1.01773500
H	0.48849600	-2.42908500	0.65639700
H	-0.39659500	0.89902200	-1.19866200
C	-0.75596100	2.80404400	-0.22379900
H	0.28215000	3.13765800	-0.30764100
H	-1.31650400	3.22098600	-1.06615800
O	0.07444200	0.82087600	0.84490200
H	-1.18608600	3.18958200	0.70594700
H	-2.92290400	1.31250200	-0.64858400
H	-3.48006600	-1.01672800	-0.17339600
H	-1.79436900	-2.77510600	0.11857300
O	0.34068300	-1.36642200	-1.12256800
H	0.10801200	-2.16641700	-1.62098600
H	0.93729200	-0.53754000	1.97843900
O	2.87763800	-0.62855300	0.01389400
H	2.40475600	-0.87036100	-0.80060000
C	3.49861400	0.65250500	-0.16177200
H	4.25646000	0.61590000	-0.95359200
H	2.76067100	1.42562900	-0.40609200
H	3.98343000	0.90726200	0.78350100

Scan Point for comp9-c2oh_alpha_2.8Å

C	-1.53023900	-1.78989700	0.41846300
C	-0.00622800	-1.55211800	0.25420400
C	-2.27838600	0.66391600	-0.04693800
C	0.36871900	-0.34713900	1.07001700
C	-0.91113500	1.28796300	-0.29096600
H	-2.21024400	-0.96712500	-1.45887000
H	-1.77626800	-1.74959600	1.48780500
H	-2.57072200	0.85941200	0.99255900
H	0.54119300	-2.39510100	0.68684100
H	-0.42854300	0.91059700	-1.19239900
C	-0.87117800	2.79587600	-0.21347000
H	0.15599700	3.16563700	-0.27616100
H	-1.42991300	3.19657500	-1.06494200
O	0.01744100	0.83886100	0.85762500
H	-1.33325000	3.16042700	0.70924900
H	-2.97610800	1.22709000	-0.67775100
H	-3.45430000	-1.12201000	-0.23089600
H	-1.71439200	-2.82036800	0.09440500
O	0.39814500	-1.33718100	-1.09590600
H	0.19983100	-2.14245200	-1.60112200
H	0.91131900	-0.48514900	2.00620800
O	2.95533300	-0.58558500	0.02475600
H	2.43881800	-0.83042600	-0.76206100
C	3.55805100	0.69820300	-0.18767200
H	4.28802000	0.66061000	-1.00560100
H	2.80506900	1.46267400	-0.41338800
H	4.07466700	0.96917200	0.73619400

Scan Point for comp9-c2oh_alpha_2.9Å

C	-1.51913500	-1.81989200	0.36697100
C	0.00396600	-1.54467500	0.28669800
C	-2.29561400	0.62473100	-0.09426600
C	0.32035300	-0.33812700	1.12639600
C	-0.93500300	1.28159000	-0.27904800
H	-2.12828100	-0.98025500	-1.52717000
H	-1.82039600	-1.80713200	1.42265600
H	-2.62961600	0.79705900	0.93673700
H	0.54816100	-2.38052100	0.73650800
H	-0.40835900	0.92333600	-1.16337000
C	-0.93026000	2.78874600	-0.18524400
H	0.09056500	3.18018500	-0.20252600
H	-1.46222100	3.18589500	-1.05536900

O	-0.04032400	0.84121200	0.90228300
H	-1.43779400	3.13377200	0.72089900
H	-2.98181400	1.18336800	-0.74147600
H	-3.42459700	-1.18118500	-0.36131000
H	-1.66064500	-2.84782500	0.01456000
O	0.47475400	-1.30224400	-1.03885400
H	0.36809000	-2.11958000	-1.55222700
H	0.83877100	-0.46822300	2.07788700
O	3.00913800	-0.55270900	0.06131900
H	2.38985100	-0.81665800	-0.64287000
C	3.56947300	0.72652700	-0.26387600
H	4.12407400	0.68695300	-1.20947000
H	2.79322900	1.49855500	-0.33403400
H	4.25953200	0.99048600	0.54123300

Scan Point for comp9-c2oh_alpha_3.0Å

C	-1.53876500	-1.82351500	0.33406000
C	-0.01369100	-1.54817700	0.31065000
C	-2.29696400	0.62477400	-0.13396500
C	0.27579900	-0.34639200	1.16654800
C	-0.93201000	1.28342400	-0.27098000
H	-2.08245800	-0.96896900	-1.57350700
H	-1.87735600	-1.81941400	1.37842500
H	-2.66244500	0.78849200	0.88775100
H	0.51410700	-2.38724100	0.77376200
H	-0.37703100	0.93211600	-1.14064400
C	-0.93077900	2.78940400	-0.16401100
H	0.08990500	3.18121700	-0.14579700
H	-1.43543800	3.19408600	-1.04683700
O	-0.07306000	0.83408000	0.93511700
H	-1.46628700	3.12650300	0.72894000
H	-2.96257000	1.18932000	-0.79738700
H	-3.41754300	-1.17767900	-0.45393000
H	-1.66733100	-2.84858400	-0.03136300
O	0.50644100	-1.29522500	-0.99498500
H	0.42280400	-2.10959300	-1.51748200
H	0.77116300	-0.47985100	2.13034900
O	3.05982200	-0.55135700	0.06782000
H	2.39045400	-0.82380300	-0.58638300
C	3.58007200	0.73169200	-0.30473600
H	4.08721700	0.68762200	-1.27653900
H	2.78806500	1.48976400	-0.34601600
H	4.30539600	1.02053900	0.45994300

Scan Point for comp9-c2oh_alpha_3.1Å

C	-1.54594700	-1.83182700	0.30154300
C	-0.02285100	-1.54968400	0.33277400
C	-2.29953500	0.61672500	-0.17019100
C	0.23359200	-0.35172500	1.20407300
C	-0.93471500	1.28274800	-0.26253100
H	-2.03179600	-0.96376300	-1.61589900
H	-1.91980100	-1.83910000	1.33370300
H	-2.69570900	0.76947700	0.84170300
H	0.49283600	-2.38966300	0.80771800
H	-0.35228300	0.93935300	-1.11731100
C	-0.94331100	2.78769100	-0.14553500
H	0.07456000	3.18404200	-0.09471200
H	-1.42355200	3.19595400	-1.04029100
O	-0.10864300	0.82868800	0.96628000
H	-1.50605600	3.11689400	0.73351800
H	-2.94820000	1.18413500	-0.84782400
H	-3.40088300	-1.18784900	-0.54156100
H	-1.65696400	-2.85420000	-0.07695000
O	0.54217700	-1.28327500	-0.95183500
H	0.47426300	-2.09092800	-1.48711200
H	0.70507900	-0.48704300	2.17999300
O	3.11276700	-0.54566100	0.07149000
H	2.39390000	-0.82516600	-0.52570800
C	3.58065700	0.74504700	-0.34123500
H	3.98645600	0.71432000	-1.36021000
H	2.78119900	1.49548500	-0.29758800
H	4.37688800	1.03743400	0.34793600

Scan Point for comp9-c2oh_alpha_3.2Å

C	-1.54837700	-1.83970700	0.28586300
C	-0.02789800	-1.54803700	0.34646800
C	-2.30827300	0.60624500	-0.19191800
C	0.20315600	-0.35135400	1.22562000
C	-0.94607800	1.28039900	-0.25986200
H	-2.00588400	-0.96855100	-1.63727400
H	-1.94067400	-1.85284200	1.31116200
H	-2.72315500	0.75383200	0.81321700
H	0.48399100	-2.38626800	0.82858400

H	-0.34699800	0.94156600	-1.10490400
C	-0.96418200	2.78487800	-0.13979100
H	0.05077400	3.18620700	-0.07183900
H	-1.43187900	3.19256900	-1.04144900
O	-0.13827000	0.82778100	0.98263200
H	-1.54258200	3.10963200	0.73071300
H	-2.94852700	1.17163200	-0.87918700
H	-3.39195300	-1.20401100	-0.58756200
H	-1.64618700	-2.86142700	-0.09789000
O	0.56136000	-1.27162700	-0.92501000
H	0.50418500	-2.07522000	-1.46759600
H	0.65954100	-0.48542400	2.20912500
O	3.17373400	-0.54890600	0.05231900
H	2.42259600	-0.82019800	-0.50789900
C	3.59416600	0.76293700	-0.34432900
H	3.94848700	0.77175300	-1.38282800
H	2.78322200	1.49445600	-0.23669100
H	4.41901500	1.05214500	0.31191900

Scan Point for comp9-c2oh_alpha_3.3Å

C	-1.57269100	-1.83594300	0.25619600
C	-0.05341000	-1.55465000	0.37230900
C	-2.29819300	0.61760300	-0.23475700
C	0.15831500	-0.36319500	1.26384000
C	-0.93073100	1.28422100	-0.25131100
H	-1.95329800	-0.95119400	-1.67734400
H	-2.00080200	-1.85035600	1.26726100
H	-2.74875000	0.76261500	0.75530200
H	0.43624700	-2.39873300	0.86697700
H	-0.30481900	0.94738600	-1.07743200
C	-0.94431300	2.78792700	-0.12145800
H	0.06994400	3.18280600	-0.01543000
H	-1.37734400	3.20488900	-1.03612500
O	-0.16584800	0.81918000	1.01495400
H	-1.55087800	3.11041200	0.73051200
H	-2.90988700	1.19085700	-0.94127400
H	-3.37881000	-1.18271400	-0.68048800
H	-1.66369200	-2.85514200	-0.13562300
O	0.58058400	-1.27555600	-0.87701500
H	0.54373300	-2.07908500	-1.42139900
H	0.58606400	-0.50380900	2.25940500
O	3.21349500	-0.55953200	0.03204200
H	2.41829500	-0.82267500	-0.46899200

C	3.59007200	0.76465100	-0.36609100
H	3.83392600	0.80622400	-1.43526900
H	2.79394100	1.48913300	-0.15208600
H	4.47861700	1.03896700	0.20839900

Scan Point for comp9-c2oh_alpha_3.4Å

C	-1.58567700	-1.83817200	0.22361600
C	-0.07150600	-1.55713300	0.39555800
C	-2.29339200	0.61812600	-0.27984400
C	0.10700400	-0.37110300	1.30129500
C	-0.92713600	1.28547400	-0.24249500
H	-1.89516800	-0.94246600	-1.71761400
H	-2.04970900	-1.85681600	1.21868400
H	-2.77966800	0.75733300	0.69408700
H	0.40117400	-2.40406400	0.90176700
H	-0.27059300	0.95384100	-1.04656100
C	-0.94571500	2.78830000	-0.10279400
H	0.06416800	3.18197800	0.04254700
H	-1.34514600	3.21202000	-1.02954200
O	-0.20832000	0.81254100	1.04822300
H	-1.58273500	3.10485000	0.72892600
H	-2.87957900	1.19500200	-1.00477100
H	-3.35628900	-1.17970300	-0.77496000
H	-1.66248100	-2.85538900	-0.17613800
O	0.60476600	-1.26997300	-0.82922900
H	0.57847800	-2.06736200	-1.38321700
H	0.49995100	-0.51730700	2.31033700
O	3.25569500	-0.55507900	0.03169000
H	2.43350900	-0.82116400	-0.42233600
C	3.60831200	0.76616400	-0.39639700
H	3.80860800	0.79702400	-1.47512100
H	2.81727700	1.48869300	-0.15826100
H	4.51785000	1.05200500	0.13831600

Scan Point for comp9-c2oh_alpha_3.5Å

C	-1.58505800	-1.84628700	0.18912300
C	-0.07980700	-1.55733500	0.41680300
C	-2.29083300	0.60881800	-0.32572400
C	0.05345300	-0.37736100	1.33711200
C	-0.93165500	1.28432500	-0.23418300

H	-1.83131800	-0.94052300	-1.75685200
H	-2.08476500	-1.87396200	1.16629300
H	-2.81195400	0.73913000	0.63130800
H	0.38029400	-2.40467700	0.93392200
H	-0.24285100	0.96141600	-1.01437300
C	-0.96423800	2.78586000	-0.08358800
H	0.03751500	3.18389300	0.10086000
H	-1.33307800	3.21472200	-1.02056300
O	-0.25973500	0.80596400	1.08044000
H	-1.63258100	3.09150500	0.72736500
H	-2.85465100	1.18592700	-1.06796600
H	-3.32304400	-1.19327400	-0.86796000
H	-1.64097500	-2.86142600	-0.21937800
O	0.63722800	-1.25729000	-0.78112100
H	0.62153000	-2.04563200	-1.34831200
H	0.40656200	-0.52874300	2.36006500
O	3.30121700	-0.53852600	0.04248700
H	2.45966700	-0.81738400	-0.36624400
C	3.62370200	0.77501700	-0.43096400
H	3.79647700	0.77946700	-1.51494700
H	2.82832300	1.49246500	-0.19191400
H	4.54217400	1.08729600	0.07287000

Scan Point for comp9-c2oh_alpha_3.6Å

C	-1.48403200	-1.91768900	0.14208400
C	-0.02087100	-1.51301000	0.45303500
C	-2.35204600	0.48078500	-0.40329100
C	-0.03523000	-0.33342500	1.38254000
C	-1.05622100	1.26028700	-0.23451400
H	-1.69741600	-1.01845500	-1.81061900
H	-2.03254000	-1.99766900	1.08964000
H	-2.93213300	0.56481600	0.52455400
H	0.47520000	-2.32464300	0.99406300
H	-0.30061500	0.99850100	-0.97505700
C	-1.21282000	2.75373900	-0.07871500
H	-0.25660800	3.22382000	0.16797400
H	-1.55685100	3.16245400	-1.03393000
O	-0.42615900	0.82371400	1.11411600
H	-1.94949800	2.99961900	0.69239900
H	-2.91805500	1.01634800	-1.17441800
H	-3.20968300	-1.39301400	-1.00291900
H	-1.43570500	-2.92941100	-0.27607900
O	0.73301500	-1.15315200	-0.70444300

H	0.77083800	-1.92577100	-1.29204800
H	0.26815700	-0.46564000	2.42393100
O	3.35368800	-0.37264200	0.16858200
H	2.50413300	-0.63534500	-0.23529100
C	3.86103200	0.77382000	-0.52524600
H	4.08608800	0.54124600	-1.57427200
H	3.15164400	1.61053200	-0.48969800
H	4.78545600	1.07520800	-0.02565900

Scan Point for comp9-c2oh_alpha_3.7Å

C	-1.43900300	-1.94290900	0.12781800
C	0.00330900	-1.49280500	0.47393600
C	-2.36670300	0.42792200	-0.43599100
C	-0.07215500	-0.31720500	1.40475600
C	-1.10013500	1.24713500	-0.23501100
H	-1.63376700	-1.04883800	-1.82931800
H	-2.00771600	-2.04049300	1.06173800
H	-2.97151000	0.49138400	0.47758000
H	0.51169300	-2.28976800	1.02543200
H	-0.31877300	1.01087200	-0.95714100
C	-1.30857700	2.73440000	-0.08251400
H	-0.37519100	3.23512300	0.18991800
H	-1.64028400	3.13297100	-1.04637600
O	-0.49064500	0.82837600	1.12817000
H	-2.07296100	2.95597900	0.66878400
H	-2.93046500	0.94755000	-1.21953000
H	-3.15224500	-1.46999100	-1.05740500
H	-1.34899200	-2.95231700	-0.28911400
O	0.77146400	-1.10801800	-0.66558000
H	0.82472100	-1.87022800	-1.26581000
H	0.20674900	-0.44321800	2.45374900
O	3.41186200	-0.34787300	0.15949200
H	2.53942600	-0.59055400	-0.20726700
C	3.89922700	0.81018900	-0.52889900
H	4.07474600	0.60145600	-1.59234300
H	3.20184100	1.65312700	-0.44092100
H	4.84847700	1.09046500	-0.06475600

Scan Point for comp9-c2oh_alpha_3.8Å

C	-1.43578100	-1.94595200	0.12090200

C	0.00107300	-1.49295800	0.48715000
C	-2.35999000	0.42384200	-0.45300100
C	-0.09208500	-0.32029100	1.41930300
C	-1.09809500	1.24516100	-0.23283900
H	-1.60375900	-1.04947400	-1.83771100
H	-2.01750800	-2.04526200	1.04655600
H	-2.97812900	0.48444800	0.45179400
H	0.50430300	-2.28987800	1.04345400
H	-0.30605100	1.01118300	-0.94393700
C	-1.31155000	2.73179800	-0.08174200
H	-0.38299300	3.23436100	0.20344000
H	-1.63138600	3.13033700	-1.04963600
O	-0.50815500	0.82525500	1.13855800
H	-2.08641300	2.95125200	0.65938100
H	-2.91365900	0.94331500	-1.24379200
H	-3.13244600	-1.47482800	-1.08872400
H	-1.33789400	-2.95474400	-0.29574000
O	0.78272000	-1.10296800	-0.64097200
H	0.83206000	-1.85766500	-1.25116900
H	0.16956700	-0.44848400	2.47251400
O	3.46759100	-0.39111800	0.09126300
H	2.56321600	-0.61154200	-0.20602700
C	3.85612600	0.85642200	-0.49609100
H	3.86376500	0.80030300	-1.59240700
H	3.19015300	1.67213700	-0.18608700
H	4.86856500	1.07919300	-0.14914500

Scan Point for comp9-c2oh_alpha_3.9Å

C	-1.42325400	-1.95405900	0.11112300
C	0.00321700	-1.48721400	0.50303100
C	-2.36083300	0.40632700	-0.47862200
C	-0.12250800	-0.31867100	1.43574800
C	-1.11223300	1.24002900	-0.23194100
H	-1.56142600	-1.05725600	-1.84980100
H	-2.02081600	-2.05794200	1.02610600
H	-2.99806400	0.45864000	0.41337300
H	0.50437400	-2.28028200	1.06672300
H	-0.30412100	1.01590600	-0.92800200
C	-1.34441900	2.72394100	-0.08235700
H	-0.42682900	3.23612500	0.22053800
H	-1.65103300	3.12060400	-1.05529300
O	-0.54563400	0.82303500	1.14956800
H	-2.13516300	2.93379300	0.64467700

H	-2.90382400	0.92123000	-1.27970000
H	-3.10012300	-1.49975400	-1.13220200
H	-1.30835100	-2.96201700	-0.30325000
O	0.80076100	-1.08628600	-0.60955900
H	0.85083900	-1.83108300	-1.23202000
H	0.11810900	-0.44730800	2.49396700
O	3.52345100	-0.39954900	0.05356000
H	2.60261900	-0.61285500	-0.19398700
C	3.85668000	0.88789700	-0.47983300
H	3.80963700	0.89293700	-1.57658700
H	3.19175900	1.66898200	-0.08920600
H	4.88124900	1.11312800	-0.17217800

Scan Point for comp9-c2oh_alpha_4.0Å

C	-1.40820800	-1.96309600	0.06208700
C	-0.00372200	-1.49443100	0.52626100
C	-2.33302500	0.40015000	-0.53782400
C	-0.18286700	-0.34256700	1.47083100
C	-1.10496300	1.23748600	-0.21602100
H	-1.45731300	-1.03758200	-1.88971700
H	-2.04605800	-2.08227100	0.94746100
H	-3.01597200	0.43497200	0.32060300
H	0.47616800	-2.29355200	1.09970900
H	-0.26285900	1.03076100	-0.87635700
C	-1.35488900	2.71707500	-0.05282600
H	-0.45430900	3.23140700	0.29414200
H	-1.62583500	3.12637000	-1.03108300
O	-0.60131500	0.80063300	1.18401500
H	-2.17582600	2.90953100	0.64500200
H	-2.83808700	0.92367800	-1.35797000
H	-3.02582100	-1.50039600	-1.25484500
H	-1.26890400	-2.96458700	-0.36039500
O	0.84222600	-1.06961500	-0.54071900
H	0.92288900	-1.80018400	-1.17699700
H	0.00920600	-0.48764100	2.53693900
O	3.56685700	-0.36813400	0.07838300
H	2.64050200	-0.62615200	-0.09444600
C	3.79533000	0.90938600	-0.52815500
H	3.62671300	0.87610500	-1.61225500
H	3.15088300	1.68276300	-0.09036000
H	4.83893300	1.17756200	-0.34338300

Scan Point for comp9-c2oh_alpha_4.1Å

C	-1.33958800	-1.99332700	0.05203100
C	0.03176900	-1.46197500	0.54739600
C	-2.35184000	0.32786700	-0.57288600
C	-0.22267300	-0.32249600	1.48928400
C	-1.16923400	1.21729000	-0.22035700
H	-1.38617900	-1.07262400	-1.90211700
H	-1.99146000	-2.14019200	0.92296800
H	-3.05831300	0.33521200	0.26693000
H	0.53487300	-2.24057200	1.12945300
H	-0.30252300	1.04640300	-0.85860900
C	-1.48688900	2.68482900	-0.06393700
H	-0.61795500	3.23649100	0.30552500
H	-1.75068200	3.08326400	-1.04859000
O	-0.68280800	0.80204300	1.19236400
H	-2.33239000	2.84057400	0.61334700
H	-2.85614300	0.82881700	-1.40735900
H	-2.94630400	-1.60217400	-1.30032900
H	-1.14645800	-2.98761300	-0.36612800
O	0.88055700	-0.99392800	-0.49847700
H	0.96950200	-1.69825500	-1.16228600
H	-0.05179900	-0.46184500	2.55976000
O	3.62826300	-0.32896600	0.08206900
H	2.69379000	-0.57331000	-0.06416500
C	3.85762400	0.94487300	-0.53187900
H	3.66366400	0.91202300	-1.61177500
H	3.23312100	1.72659300	-0.08035600
H	4.90847600	1.20047500	-0.37197300

Scan Point for comp9-c2oh_alpha_4.2Å

C	-1.24573600	-2.02609300	0.04869600
C	0.08072900	-1.41498500	0.57230700
C	-2.37568800	0.23326800	-0.60289300
C	-0.25805100	-0.29058700	1.50578700
C	-1.25240200	1.18879200	-0.22829000
H	-1.30628200	-1.11235000	-1.90889000
H	-1.90722700	-2.21161300	0.90475600
H	-3.09858700	0.20292100	0.22216100
H	0.61519400	-2.16291600	1.16674800
H	-0.36347000	1.06460400	-0.84628400
C	-1.65502900	2.63654500	-0.08612400

H	-0.82807900	3.23667400	0.30369700
H	-1.91430000	3.01722200	-1.07898900
O	-0.77416000	0.80589200	1.19585700
H	-2.52536100	2.74724200	0.56813500
H	-2.88967700	0.70451600	-1.44867700
H	-2.84544100	-1.72912600	-1.33590200
H	-0.98511000	-3.00726300	-0.36378900
O	0.92399000	-0.89987900	-0.45550100
H	1.00185200	-1.56749000	-1.15734900
H	-0.10120600	-0.41785000	2.57991700
O	3.69443100	-0.28255000	0.08528700
H	2.75404300	-0.51471600	-0.04055100
C	3.92623800	0.98817000	-0.53429100
H	3.71453500	0.95571100	-1.61088000
H	3.31707600	1.77662200	-0.07372200
H	4.98211400	1.23329100	-0.39202700

Scan Point for comp9-c2oh_alpha_4.3Å

C	-1.21071500	-2.03607000	0.02185300
C	0.08408300	-1.40264400	0.59443500
C	-2.36920600	0.20596600	-0.64341000
C	-0.31223400	-0.29621000	1.52650500
C	-1.27751500	1.17979700	-0.22548500
H	-1.23393800	-1.10439900	-1.92874500
H	-1.89461100	-2.24897200	0.85321900
H	-3.11563100	0.15287000	0.15930600
H	0.61373200	-2.14482500	1.20035500
H	-0.36688000	1.07825900	-0.81541100
C	-1.71366000	2.61777200	-0.08539600
H	-0.91372000	3.23056000	0.33957200
H	-1.94404500	3.00246100	-1.08382500
O	-0.83958600	0.79314900	1.21010800
H	-2.60939500	2.70514800	0.53742800
H	-2.86743500	0.67472300	-1.49994400
H	-2.77525800	-1.75950200	-1.40654500
H	-0.91436400	-3.00584700	-0.39366700
O	0.94972900	-0.86456900	-0.40224100
H	1.03471500	-1.51462200	-1.11967200
H	-0.19280200	-0.43348000	2.60417500
O	3.73914500	-0.26135500	0.08597900
H	2.79310000	-0.48722000	-0.00106300
C	3.95218800	1.00942000	-0.54013400
H	3.66863400	0.98780600	-1.60021500

H	3.38938500	1.80549500	-0.03552700
H	5.01951000	1.23492700	-0.46819000

Scan Point for comp9-c2oh_alpha_4.4Å

C	-1.04098800	-2.06719500	0.01549700
C	0.16333800	-1.30530400	0.62956900
C	-2.40586100	0.04592000	-0.68797300
C	-0.37630800	-0.24465100	1.54409400
C	-1.42960800	1.12437000	-0.24284000
H	-1.11318700	-1.14554500	-1.94008000
H	-1.72053700	-2.35250300	0.82862200
H	-3.16746900	-0.08106300	0.09201300
H	0.74257700	-1.99099700	1.25639600
H	-0.49629600	1.11078900	-0.80565500
C	-2.00570800	2.51446200	-0.12362400
H	-1.28043400	3.20175800	0.32102900
H	-2.24134900	2.87298400	-1.13050800
O	-1.00040000	0.78574700	1.20674000
H	-2.92411500	2.51856500	0.47154300
H	-2.92219500	0.46034000	-1.56161500
H	-2.58907000	-1.95264000	-1.45058100
H	-0.63293200	-2.99890400	-0.39217400
O	1.00871100	-0.68424100	-0.33568800
H	1.09204900	-1.27461200	-1.10238900
H	-0.27902800	-0.36817800	2.62562400
O	3.80887700	-0.13621000	0.19040800
H	2.85919900	-0.33365000	0.07819000
C	4.12434800	1.01294800	-0.60524900
H	3.92323200	0.83177600	-1.66903600
H	3.55872700	1.89532000	-0.27911300
H	5.19141300	1.21451200	-0.47926200

Scan Point for comp9-c2oh_beta_1.4Å

C	0.45242300	-1.85490200	-0.81965600
C	-0.37075900	-1.54129600	0.43038500
C	1.58260600	0.46231700	-1.00232200
C	-1.02296800	-0.13531100	0.51911900
C	1.19920200	1.07509600	0.34772000
H	2.46145400	-1.33569900	-0.20450000
H	-0.19019000	-1.72288100	-1.70053000
H	0.85724300	0.77554200	-1.76744100

H	-1.22125200	-2.23408700	0.45157000
H	1.73201500	0.55057100	1.14844600
C	1.50872200	2.56366800	0.42549200
H	1.16670900	2.98137500	1.37789900
H	2.58971000	2.71974100	0.35437600
O	-0.23323800	0.99514500	0.67678700
H	1.02379700	3.11090100	-0.39116500
H	2.54150000	0.91208500	-1.28640700
H	2.20995900	-1.37312600	-1.94098700
H	0.68156600	-2.92614700	-0.77940000
H	-1.71144100	-0.15037000	1.36842400
O	-1.86815800	0.01466400	-0.58685000
H	-1.40009800	0.12474000	-1.44333600
C	-3.02223000	0.96460900	-0.49479900
H	-2.62716700	1.96807200	-0.34851800
H	-3.54899000	0.85368700	-1.43962900
H	-3.61523000	0.61405400	0.34665100
O	0.43994600	-1.73914100	1.58850300
H	-0.13044800	-1.86977000	2.36145700

Scan Point for comp9-c2oh_beta_1.5Å

C	0.50837500	-1.83019100	-0.84087600
C	-0.31328400	-1.56558600	0.42120100
C	1.55877000	0.52660600	-1.00596300
C	-0.98557500	-0.18003300	0.56277700
C	1.17394300	1.11565000	0.35258900
H	2.50179900	-1.24758600	-0.23007600
H	-0.14675400	-1.70737900	-1.71301800
H	0.81877000	0.82474400	-1.76259300
H	-1.14636000	-2.27852500	0.43525700
H	1.74556200	0.61535100	1.14150100
C	1.40199900	2.61783400	0.43033300
H	1.06153100	3.01308900	1.39261400
H	2.47066500	2.83317800	0.33298400
O	-0.24842200	0.95786500	0.72357400
H	0.86803500	3.13949900	-0.37225100
H	2.49979100	1.01147300	-1.29207000
H	2.24211000	-1.27677300	-1.96544000
H	0.77517400	-2.89320800	-0.81634800
H	-1.71024300	-0.22037100	1.37902000
O	-1.89427400	-0.03446700	-0.62173600
H	-1.40598900	0.17178200	-1.44657700
C	-3.05305000	0.88812600	-0.47867100

H	-2.68036400	1.89154600	-0.27854400
H	-3.58603300	0.82547400	-1.42517200
H	-3.64517100	0.48936200	0.34197400
O	0.51342000	-1.76643500	1.56972000
H	-0.04675500	-1.93702500	2.34238400

Scan Point for comp9-c2oh_beta_1.6Å

C	0.78115200	-1.72480000	-0.87613700
C	-0.05397600	-1.62782200	0.40127600
C	1.42217400	0.77443600	-1.00861000
C	-0.90942400	-0.36199900	0.61329800
C	0.98678900	1.28179400	0.36488500
H	2.65883300	-0.82982000	-0.27349200
H	0.10134800	-1.68879900	-1.73676600
H	0.62252600	0.95463400	-1.74093100
H	-0.77102300	-2.45675300	0.40111500
H	1.66485900	0.89352900	1.13169900
C	0.92939600	2.79893700	0.44845900
H	0.56304000	3.12017700	1.42847800
H	1.93355900	3.21104800	0.30884000
O	-0.36864600	0.85425300	0.79557000
H	0.27363600	3.21330300	-0.32559300
H	2.26094600	1.41309600	-1.31000300
H	2.38356900	-0.87315100	-2.00627800
H	1.21709900	-2.73046200	-0.88104800
H	-1.65019200	-0.53117600	1.39664500
O	-1.90823400	-0.32863600	-0.63620900
H	-1.44377100	-0.08278000	-1.46117300
C	-3.09850900	0.53364800	-0.47564400
H	-2.77977400	1.56134500	-0.30493900
H	-3.66366300	0.43117000	-1.40070600
H	-3.65015700	0.12907600	0.37068700
O	0.81255300	-1.73441800	1.53497400
H	0.29618400	-2.00133900	2.31119400

Scan Point for comp9-c2oh_beta_1.7Å

C	0.74938000	-1.72255000	-0.88907300
C	-0.04621200	-1.62676800	0.41313600
C	1.40052000	0.77298200	-1.03119500
C	-0.87176600	-0.35338600	0.66777700

C	1.00961900	1.28128300	0.35370100
H	2.64727900	-0.84036000	-0.33281600
H	0.04547300	-1.67753400	-1.72900300
H	0.58243200	0.96118500	-1.74015000
H	-0.77280700	-2.44632500	0.43104000
H	1.70126700	0.88639300	1.10423100
C	0.95314500	2.79691000	0.44513000
H	0.61467700	3.11415200	1.43628400
H	1.95382700	3.20767600	0.27981900
O	-0.33804900	0.84916800	0.82175800
H	0.27724800	3.21458100	-0.30930200
H	2.23429300	1.40808100	-1.35337700
H	2.32649000	-0.87616600	-2.05793700
H	1.17876300	-2.73082300	-0.90980200
H	-1.63866700	-0.50992600	1.42697900
O	-1.95105400	-0.32764900	-0.64541500
H	-1.48829100	-0.05618000	-1.46138300
C	-3.11878500	0.54350100	-0.44935800
H	-2.78907100	1.56191100	-0.24133200
H	-3.69888500	0.49238000	-1.37044500
H	-3.67727400	0.12204100	0.38473100
O	0.85347700	-1.74755400	1.52076600
H	0.36427100	-2.04391800	2.30372000

Scan Point for comp9-c2oh_beta_1.8Å

C	0.69853800	-1.72541400	-0.90281500
C	-0.05794600	-1.62564600	0.42134900
C	1.39165100	0.75786400	-1.05093300
C	-0.83647800	-0.33750800	0.71957700
C	1.04910400	1.26951200	0.34377200
H	2.62522000	-0.88068400	-0.38797200
H	-0.02684400	-1.66049600	-1.72227100
H	0.55998600	0.96465700	-1.73798300
H	-0.80413300	-2.42633200	0.45327700
H	1.74921200	0.86005700	1.07805000
C	1.01095000	2.78424700	0.44247200
H	0.70476700	3.10214700	1.44364100
H	2.01205400	3.18177400	0.25027000
O	-0.29523700	0.84748300	0.84669500
H	0.32033900	3.21214500	-0.29237100
H	2.22856300	1.37909400	-1.39159700
H	2.26271900	-0.90324900	-2.10507600
H	1.10801600	-2.74148300	-0.94079100

H	-1.62794700	-0.47184000	1.45638600
O	-1.99784800	-0.30094400	-0.65515300
H	-1.53245300	-0.00791800	-1.46037400
C	-3.13737800	0.58563000	-0.42186500
H	-2.78864300	1.59319200	-0.18773600
H	-3.73980300	0.58287600	-1.33109300
H	-3.69735500	0.15733400	0.40839000
O	0.86717600	-1.77578000	1.50583500
H	0.39448800	-2.09126800	2.29150800

Scan Point for comp9-c2oh_beta_1.9Å

C	0.45896800	-1.78159000	-0.90492000
C	-0.25073200	-1.58848600	0.43249900
C	1.47599600	0.58460000	-1.07039400
C	-0.82511000	-0.20831600	0.75929100
C	1.23935100	1.13775900	0.32903300
H	2.49374400	-1.20373200	-0.42843000
H	-0.27085700	-1.60819800	-1.70387200
H	0.66333400	0.89880500	-1.73911700
H	-1.10402500	-2.27269400	0.47257300
H	1.89048900	0.63844700	1.05234200
C	1.39105800	2.64475500	0.42998500
H	1.14541500	2.99289300	1.43772500
H	2.42976400	2.91579100	0.21870800
O	-0.14167400	0.88832300	0.86301300
H	0.74363100	3.15591300	-0.29057700
H	2.37866400	1.09123100	-1.43231600
H	2.09637000	-1.17595600	-2.13795700
H	0.72515200	-2.84364900	-0.95585500
H	-1.65172400	-0.21907600	1.46867100
O	-2.03073300	-0.01502900	-0.69642700
H	-1.53267500	0.37547200	-1.43775800
C	-3.15528200	0.85393200	-0.37897900
H	-2.79956500	1.82496400	-0.02578400
H	-3.75500900	0.97116500	-1.28350700
H	-3.73490300	0.34731700	0.39234100
O	0.65669600	-1.87626800	1.50645800
H	0.15215500	-2.14761200	2.28922200

Scan Point for comp9-c2oh_beta_2.0Å

C	0.43190200	-1.76900900	-0.91885500
C	-0.23320700	-1.59040400	0.44281300
C	1.45163300	0.59290300	-1.09362300
C	-0.78109500	-0.21327400	0.81224200
C	1.26312400	1.13730700	0.31527800
H	2.48171700	-1.20400200	-0.49390100
H	-0.32200600	-1.58072600	-1.69119500
H	0.61606300	0.91257000	-1.73050400
H	-1.08950000	-2.26865300	0.50321600
H	1.92965800	0.63049000	1.01866800
C	1.41433000	2.64289000	0.42477600
H	1.19564900	2.98245900	1.44149000
H	2.44723200	2.91531500	0.18836600
O	-0.10760400	0.87990200	0.88656000
H	0.74856200	3.15916200	-0.27494700
H	2.34202200	1.10152100	-1.48191200
H	2.03682000	-1.16040400	-2.19161100
H	0.68987300	-2.83188700	-0.99080100
H	-1.61827200	-0.21273100	1.50848900
O	-2.08276100	-0.01206600	-0.69281100
H	-1.59156300	0.39169300	-1.43030400
C	-3.19386000	0.85557000	-0.34693900
H	-2.83101200	1.82324800	0.01076700
H	-3.81804500	0.98927500	-1.23352900
H	-3.76108400	0.34686800	0.43290100
O	0.70674900	-1.89429300	1.48552600
H	0.22805900	-2.19662400	2.27330200

Scan Point for comp9-c2oh_beta_2.1Å

C	-0.54119100	-1.73149800	0.93452600
C	0.10083700	-1.61690400	-0.44538600
C	-1.37806600	0.69875900	1.11413300
C	0.72779000	-0.28882900	-0.85622200
C	-1.19265100	1.21313400	-0.30610200
H	-2.55553100	-1.02061500	0.55850500
H	0.24402200	-1.59095500	1.68535500
H	-0.49918900	0.95803700	1.71916700
H	0.90624800	-2.35355100	-0.51721300
H	-1.90506000	0.74252600	-0.98908500
C	-1.23779800	2.72279100	-0.43522400
H	-1.02489600	3.03307500	-1.46229600
H	-2.24253900	3.06902900	-0.17526400
O	0.14793600	0.84910400	-0.90539800

H	-0.51975100	3.19984200	0.23987700
H	-2.21449800	1.27767600	1.52310000
H	-2.06187800	-0.99891300	2.24334700
H	-0.87205600	-2.77265200	1.02390800
H	1.57420100	-0.34341100	-1.53870300
O	2.15236400	-0.16790200	0.68194800
H	1.69041100	0.21383900	1.44774900
C	3.24147500	0.71416000	0.32044900
H	2.86166700	1.68651000	-0.00826100
H	3.89784200	0.84243300	1.18537900
H	3.78935200	0.22887700	-0.48815400
O	-0.88268500	-1.86504900	-1.46382200
H	-0.44473000	-2.21579300	-2.25536600

Scan Point for comp9-c2oh_beta_2.2Å

C	-0.55513600	-1.71737600	0.94238800
C	0.04358800	-1.62365000	-0.45806800
C	-1.33875400	0.73124100	1.13627100
C	0.68061300	-0.31143300	-0.89514700
C	-1.18660300	1.23379000	-0.29112800
H	-2.56683400	-0.96772100	0.63154900
H	0.25836200	-1.58947800	1.66466100
H	-0.43583800	0.97923300	1.71016200
H	0.83112900	-2.37666600	-0.55236500
H	-1.92007900	0.76852800	-0.95507700
C	-1.20494700	2.74216800	-0.43247900
H	-1.01609900	3.04008000	-1.46780600
H	-2.19497700	3.10948600	-0.14627800
O	0.13727300	0.83818400	-0.91728600
H	-0.45914400	3.21026900	0.21826800
H	-2.15101700	1.32828800	1.56721100
H	-2.01442600	-0.94709600	2.29797900
H	-0.90442000	-2.75092200	1.04832500
H	1.53630200	-0.37566200	-1.56524700
O	2.21889200	-0.22065700	0.67503000
H	1.76788200	0.15988900	1.44671800
C	3.28251400	0.67402400	0.28291700
H	2.88139500	1.63763800	-0.04829900
H	3.96132600	0.82595700	1.12733200
H	3.82039000	0.19203300	-0.53493200
O	-0.97608700	-1.85284200	-1.44568900
H	-0.56943200	-2.21644100	-2.24822600

Scan Point for comp9-c2oh_beta_2.3Å

C	-0.68086900	-1.66805700	0.95908600
C	-0.12474100	-1.63896800	-0.46162400
C	-1.23588800	0.84248400	1.15402400
C	0.60818500	-0.39309200	-0.93349600
C	-1.08645500	1.32202900	-0.28130900
H	-2.62456700	-0.74353100	0.69901700
H	0.16632100	-1.60774000	1.65062900
H	-0.29465200	1.00911300	1.69476800
H	0.58706300	-2.46090700	-0.57739700
H	-1.87688200	0.91924500	-0.92013800
C	-0.96725000	2.82398200	-0.43629100
H	-0.78907300	3.09707400	-1.48018700
H	-1.90738400	3.28397100	-0.11766900
O	0.17958700	0.79946900	-0.94049600
H	-0.15727700	3.22220800	0.18356300
H	-1.97564300	1.51372700	1.60612300
H	-2.02497200	-0.76150400	2.34943600
H	-1.11684500	-2.66555300	1.08697700
H	1.45955500	-0.53352300	-1.59739000
O	2.26364100	-0.40264000	0.66318000
H	1.82949200	-0.00491200	1.43517100
C	3.33469200	0.46854200	0.24698100
H	2.94693600	1.43644300	-0.08907200
H	4.03386300	0.62003600	1.07545800
H	3.85115300	-0.02886200	-0.57589400
O	-1.19336100	-1.77518300	-1.41455600
H	-0.85200900	-2.19246500	-2.22144700

Scan Point for comp9-c2oh_beta_2.4Å

C	-0.66851100	-1.66102300	0.96873700
C	-0.14780000	-1.63969300	-0.46554100
C	-1.23158800	0.84448300	1.16793400
C	0.56682000	-0.39421300	-0.96277300
C	-1.11143000	1.32313100	-0.26992000
H	-2.62196600	-0.74854500	0.73906300
H	0.19581900	-1.58424000	1.63727000
H	-0.27949300	1.01284800	1.68892600
H	0.56449200	-2.45914000	-0.59387700
H	-1.91028300	0.91704800	-0.89588600

C	-0.99353000	2.82398000	-0.43125300
H	-0.82984600	3.09391000	-1.47830500
H	-1.92965100	3.28433100	-0.10147200
O	0.14636800	0.79728400	-0.95078300
H	-0.17563500	3.22398700	0.17678200
H	-1.96335400	1.51529300	1.63341600
H	-1.99461800	-0.75974300	2.37941800
H	-1.09104400	-2.66164700	1.11573500
H	1.42144100	-0.53107000	-1.62344000
O	2.33963500	-0.40135900	0.65496500
H	1.90997900	0.00611400	1.42359700
C	3.39904100	0.46952200	0.21416400
H	3.00221100	1.42991800	-0.13382400
H	4.11005800	0.64150200	1.02916300
H	3.90916800	-0.03611100	-0.60793800
O	-1.23707300	-1.78362900	-1.39403900
H	-0.91742500	-2.22814700	-2.19524100

Scan Point for comp9-c2oh_beta_2.5Å

C	-0.63281000	-1.66790700	0.96191900
C	-0.17623000	-1.63564500	-0.49483300
C	-1.21362600	0.83351400	1.19420600
C	0.53244300	-0.38745100	-0.99243500
C	-1.13722800	1.31352800	-0.24595100
H	-2.60261100	-0.77403400	0.81909400
H	0.25906100	-1.58730800	1.59260900
H	-0.25105200	1.01651500	1.68985000
H	0.52150900	-2.45978500	-0.66548400
H	-1.94115000	0.89424300	-0.85606400
C	-1.04291900	2.81495800	-0.41193100
H	-0.90142300	3.08522600	-1.46213700
H	-1.98039500	3.26169300	-0.06745000
O	0.11918300	0.80280400	-0.94915200
H	-0.22113200	3.22806300	0.18177600
H	-1.94246100	1.49406300	1.67852700
H	-1.90561500	-0.78289300	2.43049100
H	-1.04162900	-2.67223800	1.12166300
H	1.39779800	-0.51125300	-1.64213500
O	2.42691300	-0.41630500	0.63856200
H	2.00850800	-0.02542900	1.42103900
C	3.44036000	0.49037900	0.16729100
H	2.99909100	1.43266000	-0.17768300
H	4.16733300	0.69849600	0.95989700

H	3.94884200	-0.00048300	-0.66497900
O	-1.30757600	-1.75725900	-1.37327900
H	-1.02812600	-2.18489800	-2.19823000

Scan Point for comp9-c2oh_beta_2.6Å

C	-0.52520600	-1.68896000	0.94650800
C	-0.12446400	-1.62398300	-0.52647400
C	-1.28247500	0.76594100	1.21029900
C	0.52113000	-0.33738300	-1.00818600
C	-1.23586300	1.25982500	-0.22580500
H	-2.55655900	-0.93990000	0.85770100
H	0.37944000	-1.54128400	1.54613400
H	-0.34077800	1.02348300	1.71202000
H	0.60050400	-2.41553800	-0.73366500
H	-2.00977900	0.79879200	-0.84413500
C	-1.22704800	2.76504500	-0.38035100
H	-1.09644500	3.05081300	-1.42788300
H	-2.19065500	3.15430500	-0.03811000
O	0.05647300	0.82933500	-0.92823300
H	-0.43387500	3.22092600	0.22078600
H	-2.06336200	1.36550500	1.69280200
H	-1.82132900	-0.90197600	2.45061300
H	-0.85501100	-2.71968000	1.11996000
H	1.40496200	-0.40065600	-1.64207200
O	2.54541500	-0.33961700	0.62345900
H	2.14962600	0.01424600	1.43409900
C	3.50032500	0.61687900	0.13219400
H	3.00858600	1.54656500	-0.17766300
H	4.25180200	0.84225200	0.89713400
H	3.99511300	0.16390400	-0.72962200
O	-1.28041600	-1.78074600	-1.36398300
H	-1.01224300	-2.17075700	-2.21093500

Scan Point for comp9-c2oh_beta_2.7Å

C	-0.60893900	-1.66849300	0.94273800
C	-0.31291000	-1.62719200	-0.55759700
C	-1.12730800	0.84688700	1.24924200
C	0.44114200	-0.40707400	-1.05358600
C	-1.13763500	1.32235700	-0.19497600
H	-2.56592800	-0.74380400	1.01426600

H	0.34812000	-1.61185800	1.47266600
H	-0.13464900	1.02843600	1.68097100
H	0.30704000	-2.48845800	-0.82166900
H	-1.97239200	0.90284500	-0.76057900
C	-1.03895500	2.82093000	-0.37485000
H	-0.95180600	3.08460400	-1.43264000
H	-1.95394300	3.27664000	0.01566000
O	0.08885000	0.79501000	-0.95206900
H	-0.18435000	3.23090300	0.17278400
H	-1.82100300	1.51220600	1.77656500
H	-1.70268300	-0.76948100	2.54196600
H	-1.02061200	-2.66519200	1.13804000
H	1.31914100	-0.54364500	-1.68489700
O	2.58045900	-0.49634100	0.59120900
H	2.18746900	-0.11343500	1.38988000
C	3.53872100	0.43714200	0.06661100
H	3.05388900	1.36561100	-0.25818800
H	4.30481100	0.67231000	0.81435400
H	4.01636000	-0.04032200	-0.79181500
O	-1.53539500	-1.64949900	-1.30710800
H	-1.36360200	-2.01952800	-2.18785600

Scan Point for comp9-c2oh_beta_2.8Å

C	-0.50140000	-1.69117700	0.92172800
C	-0.26383500	-1.61717200	-0.58962300
C	-1.17886600	0.78299100	1.27215400
C	0.42691400	-0.35582500	-1.07010300
C	-1.23829300	1.26684900	-0.16770100
H	-2.51173700	-0.89996700	1.06050900
H	0.46772800	-1.57375000	1.41902000
H	-0.19689400	1.03275500	1.69357200
H	0.38255800	-2.44631000	-0.89021900
H	-2.04783600	0.79699700	-0.72983300
C	-1.23648200	2.76900400	-0.34016900
H	-1.17977600	3.04196900	-1.39777600
H	-2.17402800	3.16358900	0.06326900
O	0.01911400	0.82394900	-0.93553500
H	-0.40313600	3.23072100	0.19886600
H	-1.91236500	1.39340600	1.81179100
H	-1.60363700	-0.88038600	2.56240500
H	-0.83889200	-2.71444100	1.12135100
H	1.32061400	-0.43410000	-1.68964400
O	2.71831900	-0.44276100	0.53672800

H	2.40501000	-0.18930100	1.41767700
C	3.58176800	0.59548200	0.04725400
H	3.03946800	1.54075900	-0.07592500
H	4.42939100	0.75320500	0.72450600
H	3.96035700	0.26854600	-0.92381600
O	-1.51102800	-1.67948200	-1.29259100
H	-1.35609600	-2.01880200	-2.18867200

Scan Point for comp9-c2oh_beta_2.9Å

C	-0.31838900	-1.70789600	0.89638500
C	-0.09332700	-1.58029700	-0.61458800
C	-1.31706800	0.65077300	1.28466400
C	0.43490300	-0.23056000	-1.05937300
C	-1.43666000	1.13911500	-0.14989500
H	-2.41550300	-1.18960100	1.04648000
H	0.62723400	-1.47129600	1.39708300
H	-0.37794100	1.02328700	1.71315500
H	0.65631200	-2.31243400	-0.92646000
H	-2.16562900	0.56393500	-0.72408200
C	-1.64718000	2.62731700	-0.30970600
H	-1.62735700	2.91502100	-1.36468300
H	-2.63232400	2.88008100	0.09405800
O	-0.11899500	0.88409700	-0.90309400
H	-0.88953700	3.19834700	0.23624400
H	-2.12641800	1.15025200	1.82987700
H	-1.51508000	-1.07472800	2.54886000
H	-0.51909900	-2.76950000	1.07939200
H	1.35091000	-0.17596900	-1.64892600
O	2.85126000	-0.22014300	0.54409500
H	2.54747800	0.04159800	1.42575000
C	3.69636900	0.82043200	0.02868900
H	3.14281800	1.75884500	-0.09739400
H	4.55403900	0.99440400	0.68933900
H	4.06165100	0.48567700	-0.94494400
O	-1.31997400	-1.79495500	-1.32086500
H	-1.12028600	-2.09564200	-2.22185200

Scan Point for comp9-c2oh_beta_3.0Å

C	-0.29416900	-1.70633900	0.88404200
C	-0.09569000	-1.56833700	-0.63088100

C	-1.34217500	0.62867500	1.29306400
C	0.41154600	-0.20704400	-1.06251500
C	-1.48364700	1.11905800	-0.13886900
H	-2.40020400	-1.23708200	1.06584300
H	0.65305700	-1.44980200	1.37190600
H	-0.40868400	1.02242900	1.71503700
H	0.65985100	-2.28728100	-0.95926800
H	-2.20132700	0.52900500	-0.71164300
C	-1.72776000	2.60253100	-0.29189300
H	-1.72024200	2.89471600	-1.34576200
H	-2.71613500	2.83128600	0.11821800
O	-0.16052200	0.89610800	-0.89587900
H	-0.98020800	3.18802300	0.25254000
H	-2.15886800	1.10722300	1.84598700
H	-1.48059600	-1.10392200	2.55504000
H	-0.46803700	-2.77271700	1.06639300
H	1.33681100	-0.12867700	-1.63570900
O	2.93716000	-0.18895100	0.55641800
H	2.65380600	0.09877100	1.43657100
C	3.77893700	0.83050400	-0.00369700
H	3.23253000	1.77235900	-0.13539900
H	4.65691400	1.00869000	0.62870200
H	4.11342800	0.47098100	-0.97969100
O	-1.33053000	-1.79735200	-1.31591500
H	-1.14274300	-2.07449900	-2.22699800

Scan Point for comp9-c2oh_beta_3.1Å

C	-0.54476200	-1.69917300	0.89440600
C	-0.36854800	-1.60903800	-0.62753200
C	-1.20243100	0.77830300	1.29121700
C	0.36380100	-0.35924400	-1.06772900
C	-1.27688800	1.27193000	-0.14483100
H	-2.54459400	-0.90072100	1.10741900
H	0.44437700	-1.58952900	1.35440100
H	-0.21549400	1.02677000	1.70141400
H	0.24105300	-2.45079700	-0.96840200
H	-2.08647700	0.80372800	-0.70726900
C	-1.26804700	2.77385500	-0.31091700
H	-1.21482800	3.05143300	-1.36749000
H	-2.20225200	3.17043600	0.09846600
O	-0.01146300	0.82540800	-0.90698700
H	-0.43056000	3.22913200	0.22709300
H	-1.93012400	1.38402400	1.84382200

H	-1.58661200	-0.89674600	2.57823700
H	-0.87886600	-2.72254200	1.09804100
H	1.29686300	-0.44503500	-1.62820400
O	2.95945900	-0.43195500	0.62557400
H	2.79542100	-0.08906500	1.51634800
C	3.75377800	0.52693800	-0.08913600
H	3.22340900	1.48022400	-0.20317700
H	4.71031300	0.70479700	0.41722200
H	3.95221300	0.10707800	-1.07797200
O	-1.64114100	-1.62148900	-1.27773400
H	-1.52620800	-1.91861100	-2.19483500

Scan Point for comp9-c2oh_beta_3.2Å

C	-0.58347000	-1.70622300	0.87239900
C	-0.47809400	-1.60145500	-0.65780700
C	-1.13371300	0.79497500	1.31029500
C	0.31495900	-0.38737900	-1.08735100
C	-1.23746700	1.29588900	-0.12194200
H	-2.53968500	-0.83686800	1.18521100
H	0.42917800	-1.64016900	1.28751400
H	-0.12542800	1.00972400	1.68632900
H	0.06389900	-2.46977700	-1.04389400
H	-2.07346600	0.85142600	-0.66388300
C	-1.18939700	2.79695000	-0.28575400
H	-1.15206600	3.07520100	-1.34288600
H	-2.10311600	3.21841400	0.14464600
O	-0.00024400	0.81163100	-0.90851900
H	-0.32791100	3.22772700	0.23424000
H	-1.82165800	1.42168500	1.88970800
H	-1.51244000	-0.87348200	2.60759900
H	-0.94901400	-2.71737900	1.08200500
H	1.24938700	-0.51378800	-1.63840700
O	3.02883000	-0.51113600	0.60368100
H	2.87478600	-0.16816100	1.49616600
C	3.78394200	0.46375900	-0.13172600
H	3.23087600	1.40562800	-0.23174900
H	4.74984100	0.66241000	0.34848300
H	3.96436600	0.04771500	-1.12563000
O	-1.78109900	-1.52761700	-1.23383900
H	-1.72750300	-1.76178200	-2.17409600

Scan Point for comp9-c2oh_beta_3.3Å

C	-0.58432100	-1.70606400	0.87161200
C	-0.50380100	-1.60146400	-0.66011400
C	-1.13092100	0.79445200	1.31784600
C	0.28059100	-0.38641400	-1.10259100
C	-1.25840400	1.29493000	-0.11262600
H	-2.53644800	-0.83937400	1.21577800
H	0.43479100	-1.63848700	1.27033100
H	-0.11701600	1.01068600	1.67755300
H	0.03305200	-2.46913400	-1.05474900
H	-2.10240100	0.84920700	-0.64095700
C	-1.21505400	2.79602700	-0.27743300
H	-1.19504900	3.07413800	-1.33506800
H	-2.12234900	3.21629500	0.16747800
O	-0.03333200	0.81220400	-0.91892400
H	-0.34595300	3.22809200	0.22862900
H	-1.81031100	1.42033800	1.90814000
H	-1.48633700	-0.87425100	2.62140800
H	-0.94501500	-2.71768300	1.08728500
H	1.20621800	-0.51167700	-1.66855300
O	3.10725800	-0.50985300	0.59585500
H	2.96721400	-0.16689800	1.49064600
C	3.84918300	0.46583100	-0.15182200
H	3.29338900	1.40697900	-0.24312200
H	4.82243100	0.66582300	0.31272700
H	4.01409500	0.04980200	-1.14842200
O	-1.81602600	-1.52948800	-1.21507300
H	-1.77728600	-1.76391400	-2.15599400

Scan Point for comp9-c2oh_beta_3.5Å

C	-0.58946700	-1.70553800	0.86954900
C	-0.55482500	-1.60150300	-0.66394400
C	-1.12825100	0.79395000	1.33080400
C	0.21328400	-0.38489600	-1.13008300
C	-1.29940000	1.29343500	-0.09545600
H	-2.53246200	-0.84311600	1.27131800
H	0.44091100	-1.63545400	1.23772100
H	-0.10458200	1.01266200	1.66008100
H	-0.02798400	-2.46814700	-1.07402700
H	-2.15773100	0.84553700	-0.59824400
C	-1.26440500	2.79454600	-0.26211500
H	-1.27652300	3.07218400	-1.31999800

H	-2.15901600	3.21296900	0.20942700
O	-0.09776500	0.81309700	-0.93765800
H	-0.38161300	3.22883200	0.21767200
H	-1.79120000	1.41857900	1.94079700
H	-1.44088800	-0.87491800	2.64507900
H	-0.94127000	-2.71786800	1.09629200
H	1.12194600	-0.50833700	-1.72328800
O	3.26381200	-0.50811600	0.58137700
H	3.14967700	-0.16503600	1.47979400
C	3.98092600	0.46888000	-0.18847300
H	3.42050800	1.40871700	-0.26359400
H	4.96711200	0.67131400	0.24681900
H	4.11705500	0.05273200	-1.18936400
O	-1.88315600	-1.53276800	-1.17961800
H	-1.87191500	-1.76755600	-2.12118000

Scan Point for comp9-c2oh_beta_3.6Å

C	-0.64569500	-1.70931900	0.86017400
C	-0.58972200	-1.59743800	-0.67413100
C	-1.15228700	0.79848600	1.32464100
C	0.23592500	-0.40453800	-1.09453400
C	-1.26731700	1.30642500	-0.10449200
H	-2.58047400	-0.81695800	1.22949300
H	0.38049800	-1.65504400	1.24423100
H	-0.13665400	1.00091500	1.68777600
H	-0.08385200	-2.47645000	-1.08402600
H	-2.11529400	0.87656600	-0.63898500
C	-1.19415900	2.80660500	-0.26359500
H	-1.16036300	3.08848000	-1.31984400
H	-2.09730800	3.24173200	0.17557400
O	-0.04201300	0.80075100	-0.90092600
H	-0.32164400	3.22037000	0.25174200
H	-1.82551700	1.43069300	1.91527500
H	-1.51623200	-0.87165600	2.62352800
H	-1.01527300	-2.71708000	1.07824800
H	1.17659200	-0.55552400	-1.63019800
O	3.35617700	-0.50425700	0.69824800
H	3.27838900	-0.03885400	1.54394100
C	3.90440100	0.40308900	-0.27050000
H	3.23656400	1.25576900	-0.44362700
H	4.88713100	0.77446900	0.04473400
H	4.02165500	-0.15547200	-1.20215500
O	-1.90613500	-1.48224100	-1.20664700

H	-1.88679000	-1.71438300	-2.14856600

Scan Point for comp9-c2oh_beta_3.7Å

C	-0.78435300	-1.67155200	0.86797000
C	-0.83452100	-1.57420800	-0.66775000
C	-0.92547500	0.88232400	1.34163000
C	0.10387900	-0.50072500	-1.16471700
C	-1.07771200	1.39906100	-0.08103400
H	-2.55340300	-0.53448700	1.36980900
H	0.26737200	-1.74879800	1.17092700
H	0.13030200	0.95452800	1.63193800
H	-0.47970300	-2.51291800	-1.10312900
H	-2.01414100	1.08824800	-0.54577200
C	-0.81421400	2.87510900	-0.26250900
H	-0.82172600	3.14833600	-1.32145200
H	-1.61485400	3.42885800	0.23772700
O	0.00399600	0.73085300	-0.96262200
H	0.14211200	3.16751700	0.18220000
H	-1.46968500	1.59674700	1.97043800
H	-1.40346500	-0.72530000	2.68139500
H	-1.26222700	-2.62235100	1.12774300
H	0.97538900	-0.77437600	-1.76554600
O	3.31049800	-0.72071100	0.66809800
H	3.25012600	-0.24132400	1.50726100
C	3.81947700	0.17586200	-0.33121000
H	3.13837300	1.01904400	-0.49857400
H	4.80732300	0.56210800	-0.05201800
H	3.91400500	-0.39683100	-1.25687400
O	-2.16213900	-1.29215400	-1.10027900
H	-2.24454200	-1.52751700	-2.03806000

Scan Point for comp9-c2oh_beta_3.8Å

C	-0.76313300	-1.68058300	0.86352200
C	-0.83114100	-1.57941500	-0.67159500
C	-0.94734500	0.86937200	1.34612400
C	0.08586800	-0.48926800	-1.17170500
C	-1.12073600	1.38663000	-0.07390900
H	-2.54758000	-0.57871100	1.38813800
H	0.29286300	-1.73934100	1.15564700
H	0.10927800	0.96116200	1.62767500

H	-0.46553500	-2.51073300	-1.11393300
H	-2.05509300	1.06053900	-0.53221300
C	-0.88485700	2.86749900	-0.25390800
H	-0.90606100	3.14293400	-1.31212600
H	-1.69096000	3.40606500	0.25408700
O	-0.03357200	0.73979700	-0.96510200
H	0.06984400	3.17593100	0.18342100
H	-1.49989400	1.57172400	1.98122300
H	-1.37941800	-0.75063100	2.68616700
H	-1.22071200	-2.64074300	1.12533300
H	0.96025300	-0.74590100	-1.77599300
O	3.40154400	-0.67864900	0.67502400
H	3.36725400	-0.18586500	1.50774100
C	3.87428700	0.20282200	-0.35465700
H	3.19009400	1.04651900	-0.50630700
H	4.87381200	0.58874700	-0.12017800
H	3.93016900	-0.38159500	-1.27620400
O	-2.16748600	-1.31751300	-1.08886600
H	-2.25500000	-1.54594000	-2.02794000

Scan Point for comp9-c2oh_beta_3.9Å

C	-0.77950600	-1.67947400	0.86808400
C	-0.85149200	-1.58110000	-0.66699200
C	-0.95368900	0.87154300	1.34677100
C	0.06746600	-0.49496600	-1.17195700
C	-1.12891800	1.38726100	-0.07359100
H	-2.55917500	-0.57072700	1.39466900
H	0.27715400	-1.74045600	1.15758900
H	0.10412200	0.95942100	1.62516200
H	-0.49008800	-2.51447100	-1.10847900
H	-2.06576500	1.06404600	-0.52888300
C	-0.88768500	2.86690400	-0.25649600
H	-0.91065400	3.14086000	-1.31505900
H	-1.69030800	3.40934700	0.25288800
O	-0.04678100	0.73482600	-0.96701100
H	0.06943900	3.17212800	0.17778300
H	-1.50166400	1.57711000	1.98227100
H	-1.38879400	-0.74456500	2.69050800
H	-1.23892600	-2.63788700	1.13302400
H	0.93887500	-0.75602200	-1.77859900
O	3.48073700	-0.64657500	0.70862100
H	3.55260800	-0.12533700	1.52154100
C	3.89103400	0.17458700	-0.39500300

H	3.21820300	1.03017300	-0.53024100
H	4.91554600	0.54182500	-0.25903100
H	3.85840400	-0.45076400	-1.29037000
O	-2.18806900	-1.31578600	-1.08145800
H	-2.27840600	-1.54521800	-2.02005600

Scan Point for comp9-c2oh_beta_4.0Å

C	-0.83282600	-1.66420600	0.88489500
C	-0.91287500	-1.57684600	-0.64990000
C	-0.91003000	0.89490700	1.34343300
C	0.03354800	-0.52465800	-1.17623400
C	-1.08633100	1.40447500	-0.07907900
H	-2.56654200	-0.48697800	1.41805900
H	0.22336100	-1.76157600	1.16643300
H	0.15410400	0.94543600	1.60666800
H	-0.58460500	-2.52540600	-1.08480700
H	-2.03920700	1.10730600	-0.51874900
C	-0.80009700	2.87388900	-0.27833100
H	-0.82619300	3.13904800	-1.33904200
H	-1.57914500	3.44609200	0.23507400
O	-0.03809500	0.70988000	-0.98079700
H	0.17130700	3.15181700	0.14234700
H	-1.42277600	1.62512000	1.98051000
H	-1.39132400	-0.69361400	2.70495300
H	-1.32439200	-2.60321800	1.16136600
H	0.88667500	-0.81919700	-1.79354900
O	3.53034300	-0.62547800	0.76341300
H	3.60994800	-0.00092700	1.49915200
C	3.86540900	0.06137000	-0.45176300
H	3.16549300	0.88101600	-0.65537800
H	4.88591300	0.46174100	-0.41361500
H	3.80659500	-0.67127700	-1.26021900
O	-2.24359400	-1.27368600	-1.05839600
H	-2.34870500	-1.51309000	-1.99301100

Scan Point for comp9-c2oh_beta_4.1Å

C	-0.83955700	-1.67065100	0.88690100
C	-0.90131200	-1.58567400	-0.64935300
C	-0.97531700	0.88739600	1.34053600
C	0.03609800	-0.51802700	-1.15947600

C	-1.13751500	1.39206100	-0.08536000
H	-2.60380000	-0.52839400	1.39395300
H	0.21424500	-1.74666700	1.18331200
H	0.08271900	0.96122800	1.62217700
H	-0.55107500	-2.52849000	-1.07962300
H	-2.07717300	1.07766300	-0.54106600
C	-0.87412900	2.86621300	-0.28138000
H	-0.88971000	3.13064400	-1.34247300
H	-1.67032500	3.42480800	0.22058000
O	-0.06121900	0.71530200	-0.96757800
H	0.08600000	3.16134300	0.15326000
H	-1.51432500	1.60743700	1.96742000
H	-1.44282800	-0.70889900	2.69733700
H	-1.31607800	-2.61898800	1.15784300
H	0.90770000	-0.79850100	-1.75729800
O	3.65084200	-0.58369600	0.77425100
H	3.74681100	0.04728200	1.50249400
C	3.95450500	0.09332500	-0.45449800
H	3.25137800	0.91334200	-0.64508900
H	4.97675200	0.49095500	-0.44746500
H	3.87129300	-0.64469700	-1.25597400
O	-2.23150500	-1.30522200	-1.07409800
H	-2.31992600	-1.54381300	-2.01055300

Scan Point for comp9-c2oh_beta_4.2Å

C	-0.83824800	-1.66309100	0.90500500
C	-0.91034800	-1.59303800	-0.63120200
C	-0.96916300	0.89852800	1.33700100
C	0.02100000	-0.52952300	-1.16127300
C	-1.14159000	1.39066400	-0.09187400
H	-2.59853100	-0.51535300	1.41432200
H	0.21773600	-1.73585500	1.19454100
H	0.09093000	0.97376200	1.61036100
H	-0.56262300	-2.54001400	-1.05431400
H	-2.08544400	1.07372800	-0.53718600
C	-0.87811800	2.86276000	-0.30292400
H	-0.90222400	3.11799900	-1.36612200
H	-1.66949600	3.42661200	0.20076900
O	-0.07425300	0.70531300	-0.97843700
H	0.08601000	3.16050900	0.12098200
H	-1.50286900	1.62473800	1.96133800
H	-1.42845300	-0.68526200	2.71101500
H	-1.31244600	-2.60892400	1.18846300

H	0.88320000	-0.81427600	-1.77049600
O	3.72639000	-0.50301100	0.81593800
H	3.94679200	0.18662900	1.45883800
C	3.91308500	0.02931600	-0.50396900
H	3.22720000	0.86246900	-0.70041000
H	4.94455400	0.37094800	-0.65375200
H	3.70542300	-0.78101900	-1.20675100
O	-2.24348800	-1.31726800	-1.05044400
H	-2.33669000	-1.56110600	-1.98515000

Scan Point for comp9-c2oh_beta_4.3Å

C	-0.88138100	-1.65868900	0.90792400
C	-0.95955800	-1.58806700	-0.62774200
C	-0.95792200	0.90533800	1.33890500
C	-0.01261900	-0.54181900	-1.16471100
C	-1.13253700	1.39991000	-0.08897000
H	-2.61507900	-0.47506100	1.42694300
H	0.17442600	-1.75350300	1.19191000
H	0.10586800	0.95853200	1.60301200
H	-0.63107200	-2.54149300	-1.05172800
H	-2.08551800	1.09943500	-0.52622500
C	-0.84397800	2.86679600	-0.30328900
H	-0.86984700	3.12136000	-1.36659100
H	-1.62192300	3.44533800	0.20464300
O	-0.08459300	0.69474500	-0.98295400
H	0.12797000	3.14733100	0.11443700
H	-1.47121200	1.64249800	1.96752300
H	-1.44096300	-0.66827300	2.71688200
H	-1.37356100	-2.59445200	1.19413300
H	0.84052700	-0.84308800	-1.77868600
O	3.80778300	-0.53139400	0.80871500
H	4.00763900	0.16678600	1.44905200
C	3.95938600	0.00703600	-0.51337300
H	3.23727200	0.81047100	-0.70397000
H	4.97419600	0.39151300	-0.67274400
H	3.77929400	-0.81195100	-1.21376800
O	-2.28956800	-1.28885500	-1.04124600
H	-2.39260400	-1.53566500	-1.97417000

Scan Point for comp9-c2oh_beta_4.4Å

C	-0.90856700	-1.65740800	0.90881800
C	-0.99697200	-1.58466200	-0.62623000
C	-0.95091200	0.90744600	1.34085100
C	-0.04091400	-0.54962300	-1.16883400
C	-1.13170100	1.40382100	-0.08566000
H	-2.62360500	-0.45309300	1.44223300
H	0.14795800	-1.76600600	1.18509000
H	0.11573500	0.94764100	1.59566000
H	-0.68332800	-2.54168000	-1.05337700
H	-2.09089100	1.11237900	-0.51529900
C	-0.83044700	2.86765900	-0.30292100
H	-0.85992100	3.12148200	-1.36630800
H	-1.60002000	3.45400200	0.20881500
O	-0.09732400	0.68768900	-0.98666900
H	0.14643400	3.13943600	0.10901900
H	-1.44981700	1.65058600	1.97399000
H	-1.44132100	-0.66077600	2.72251600
H	-1.41049300	-2.58705200	1.19799700
H	0.80554300	-0.86116000	-1.78704200
O	3.89188900	-0.54174000	0.80423000
H	4.02496700	0.18056300	1.43505400
C	3.99735700	-0.00893900	-0.52460100
H	3.21466400	0.73416600	-0.72105900
H	4.97933400	0.44973700	-0.69338100
H	3.87615700	-0.84724000	-1.21479000
O	-2.32629200	-1.26887400	-1.02957100
H	-2.44008500	-1.51459800	-1.96153000

Scan Point for comp9-c2oh_beta_4.5Å

C	-0.91018500	-1.67195700	0.89767000
C	-0.97156200	-1.58858200	-0.63848200
C	-1.01766400	0.88780700	1.34904500
C	-0.02517600	-0.53044000	-1.15204500
C	-1.17710900	1.39274800	-0.07711300
H	-2.66159000	-0.50985100	1.40428100
H	0.14293300	-1.75923700	1.19368400
H	0.04162900	0.95013800	1.62881000
H	-0.63044000	-2.53537200	-1.06733300
H	-2.12091500	1.08737700	-0.53045900
C	-0.89865900	2.86380400	-0.27536000
H	-0.91338000	3.12715300	-1.33672200
H	-1.68794800	3.43132300	0.22749300
O	-0.10976400	0.70393800	-0.96093200

H	0.06539700	3.14912800	0.15712200
H	-1.54762700	1.61423200	1.97627300
H	-1.50225600	-0.70222400	2.70750200
H	-1.39668600	-2.61480200	1.17001600
H	0.84142800	-0.81997900	-1.75273800
O	4.05106400	-0.59230800	0.75332600
H	4.26374600	0.04453900	1.45101800
C	3.99434400	0.10978700	-0.49747800
H	3.19566700	0.86164300	-0.49786400
H	4.94934900	0.60019200	-0.72262900
H	3.78890400	-0.63236600	-1.27255000
O	-2.29913700	-1.29641600	-1.06377400
H	-2.39060100	-1.53860000	-1.99904500

Scan Point for comp9-c2oh_beta_4.6Å

C	-0.94471200	-1.65572800	0.92161500
C	-1.01132100	-1.59127000	-0.61484900
C	-0.99922200	0.91113200	1.34080600
C	-0.05019200	-0.55659000	-1.14869700
C	-1.15912300	1.40086800	-0.09048000
H	-2.67028200	-0.45255000	1.42220900
H	0.10807200	-1.75997100	1.21360400
H	0.06309000	0.95545900	1.61243800
H	-0.68880900	-2.54960200	-1.03232800
H	-2.11180800	1.10717300	-0.53293900
C	-0.85479100	2.86385500	-0.30940500
H	-0.87108600	3.11402500	-1.37391200
H	-1.63024900	3.45218600	0.19100200
O	-0.11145800	0.68144300	-0.97329700
H	0.11702700	3.13654700	0.11375600
H	-1.51003300	1.65587000	1.96248200
H	-1.50810600	-0.65169600	2.72197200
H	-1.44820000	-2.58525000	1.20849000
H	0.80527100	-0.86934900	-1.75365800
O	4.12097700	-0.52963400	0.79053300
H	4.35584300	0.19300000	1.39084400
C	3.98255800	0.00531400	-0.53461600
H	3.16257300	0.73192600	-0.58833800
H	4.91010000	0.48552600	-0.86942900
H	3.76253800	-0.83584900	-1.19619200
O	-2.33524200	-1.28127100	-1.03944400
H	-2.43468300	-1.53513000	-1.97081800

Scan Point for comp9-c3oh_alpha_1.4Å

C	1.81853300	-0.70825600	-0.29757000
C	0.55957700	-1.31554900	0.33251100
C	1.13621000	1.78863000	-0.11542900
C	-0.73141700	-0.86459000	-0.35058500
C	-0.31864900	1.49787800	0.25736300
H	2.24261000	0.61176200	1.33341700
H	1.70443600	-0.67243500	-1.39047400
H	1.16712400	2.00166600	-1.19200300
H	0.60050200	-2.40466300	0.23665700
H	-0.39194200	1.11622300	1.28338200
C	-1.21748500	2.71589000	0.10629800
H	-2.25604300	2.46905100	0.34810900
H	-0.88692700	3.50881900	0.78476400
O	-0.85514900	0.48525500	-0.66230500
H	-1.17982600	3.10227100	-0.91861600
H	1.44036100	2.70883700	0.39717000
H	-0.87560100	-1.39936200	-1.29190000
O	-1.79376100	-1.29327800	0.45418200
H	-1.79774900	-0.90353100	1.35583000
C	-3.17038900	-1.33705700	-0.12265900
H	-3.79797400	-1.71407800	0.68138100
H	-3.44688500	-0.33164000	-0.43337600
H	-3.11199000	-2.03706000	-0.95306200
H	0.52805300	-1.08242400	1.40408000
H	3.12971600	0.98271500	-0.14574900
O	2.88492900	-1.62548200	0.02516400
H	3.70995400	-1.27863400	-0.34776700

Scan Point for comp9-c3oh_alpha_1.5Å

C	1.82981300	-0.72082500	-0.29922800
C	0.55237400	-1.31989800	0.30419700
C	1.15736100	1.77737300	-0.11282100
C	-0.71276200	-0.83844000	-0.39169700
C	-0.30007200	1.50296200	0.25883000
H	2.23539800	0.58765600	1.34595500
H	1.73836700	-0.67883700	-1.39410600
H	1.19388300	1.98746200	-1.18968200
H	0.57907600	-2.40770300	0.19437100
H	-0.38050700	1.11405900	1.28070500

C	-1.18883600	2.72713700	0.10786700
H	-2.23064900	2.48673600	0.34149800
H	-0.85620900	3.51189700	0.79457100
O	-0.85030200	0.49578800	-0.66695800
H	-1.14040400	3.12023400	-0.91387200
H	1.46602200	2.69663600	0.39855000
H	-0.90708900	-1.37964500	-1.31876300
O	-1.84187400	-1.30793800	0.47702500
H	-1.83922100	-0.86626700	1.35289000
C	-3.20332900	-1.30871800	-0.11297100
H	-3.86141000	-1.65824300	0.67990800
H	-3.45032600	-0.29945100	-0.43822000
H	-3.16388800	-2.01593700	-0.93887200
H	0.50952300	-1.09729400	1.37705400
H	3.14726200	0.96235100	-0.11751900
O	2.87953000	-1.64929400	0.04171600
H	3.71509800	-1.31143800	-0.31569100

Scan Point for comp9-c3oh_alpha_1.6Å

C	1.83841500	-0.73691300	-0.30001400
C	0.54051300	-1.32422800	0.27465900
C	1.18360900	1.76485600	-0.10650300
C	-0.69547000	-0.80911400	-0.43563300
C	-0.27802100	1.50985400	0.25929300
H	2.22831100	0.55683800	1.36084500
H	1.77041100	-0.68769300	-1.39626800
H	1.22892200	1.97472600	-1.18297100
H	0.55026200	-2.41030400	0.15010000
H	-0.37046300	1.11144000	1.27581400
C	-1.15393300	2.74198500	0.10832000
H	-2.19979500	2.50956800	0.33117900
H	-0.81944800	3.51674700	0.80522300
O	-0.84018400	0.51029600	-0.67600900
H	-1.09170600	3.14319200	-0.90934500
H	1.49807300	2.68095400	0.40676900
H	-0.94227800	-1.35415400	-1.34654100
O	-1.89178700	-1.31383600	0.49929000
H	-1.88194600	-0.82594000	1.34881200
C	-3.23920900	-1.28257800	-0.10009900
H	-3.92473600	-1.59793500	0.68481300
H	-3.45964300	-0.27368200	-0.44790800
H	-3.21833100	-2.00268200	-0.91606000

H	0.48494600	-1.11202900	1.34857600
H	3.16665600	0.93373600	-0.08552600
O	2.86745600	-1.68046000	0.05828500
H	3.71345000	-1.35769300	-0.28835200

Scan Point for comp9-c3oh_alpha_1.7Å

C	-1.84163900	-0.76421600	0.30061900
C	-0.52007900	-1.32700200	-0.24828800
C	-1.22130800	1.74556500	0.10452600
C	0.68266100	-0.77158300	0.47621300
C	0.24459300	1.52266800	-0.26359400
H	-2.23114200	0.51756600	-1.37009100
H	-1.79551000	-0.71189900	1.39777700
H	-1.27097100	1.95013200	1.18175600
H	-0.50408900	-2.41096700	-0.11030700
H	0.34903700	1.11699200	-1.27544500
C	1.09744600	2.76963000	-0.11217500
H	2.14835900	2.55460700	-0.32807500
H	0.75247800	3.53383800	-0.81542100
O	0.83079300	0.53488500	0.67748300
H	1.02104700	3.17464300	0.90289300
H	-1.55111700	2.65829600	-0.40479200
H	0.97997300	-1.31391800	1.37253500
O	1.95086000	-1.31572300	-0.51655300
H	1.93591100	-0.80123000	-1.34858200
C	3.28407800	-1.24937400	0.09234700
H	3.99551400	-1.54267600	-0.67916500
H	3.47974600	-0.23701700	0.44805600
H	3.27940800	-1.96995600	0.90868700
H	-0.45478100	-1.12324200	-1.32287400
H	-3.19162000	0.88560800	0.06426800
O	-2.84239600	-1.72912100	-0.07614200
H	-3.69951000	-1.43058700	0.26485100

Scan Point for comp9-c3oh_alpha_2.0Å

C	-1.89334000	-0.77146000	0.29371900
C	-0.52712200	-1.33184100	-0.15958500
C	-1.25864900	1.73236200	0.08202800

C	0.59456300	-0.72222200	0.61842200
C	0.21090400	1.52566000	-0.27225200
H	-2.20327600	0.48221800	-1.41526700
H	-1.91775500	-0.70385000	1.39022200
H	-1.32771600	1.93762200	1.15768600
H	-0.49952100	-2.40844200	0.01985600
H	0.33337700	1.08511300	-1.26582500
C	1.05982100	2.77289000	-0.13078700
H	2.11464900	2.55373500	-0.32016600
H	0.72733800	3.51358900	-0.86431100
O	0.80794500	0.54803100	0.70036000
H	0.95881500	3.20659700	0.86966800
H	-1.58145700	2.64420000	-0.43282200
H	0.98322200	-1.25645300	1.48207900
O	2.09100400	-1.47715700	-0.47278700
H	1.97127900	-1.13146100	-1.37485500
C	3.40031000	-1.08428000	0.00804200
H	4.15533400	-1.47966900	-0.67596700
H	3.47915500	0.00429200	0.07063200
H	3.52177500	-1.53247300	0.99483300
H	-0.40393600	-1.15504100	-1.23343000
H	-3.22681700	0.87424800	-0.03129900
O	-2.85300700	-1.75154700	-0.13454600
H	-3.72794200	-1.48272900	0.18585600

Scan Point for comp9-c3oh_alpha_2.5Å

C	-1.87781400	-0.96921900	0.28989900
C	-0.40883100	-1.34934700	-0.03453500
C	-1.54098800	1.58443000	0.06014800
C	0.55873500	-0.55277100	0.75197500
C	-0.05699000	1.58827100	-0.28395300
H	-2.23384400	0.20947600	-1.46469900
H	-1.99984200	-0.89387200	1.37871000
H	-1.65336900	1.76822700	1.13583800
H	-0.24575200	-2.40080700	0.20700100
H	0.14243100	1.13531500	-1.25923000
C	0.62113400	2.93423000	-0.15548200
H	1.69752500	2.84929500	-0.32985100
H	0.20490500	3.60722100	-0.91122700
O	0.68518100	0.70514100	0.70998000
H	0.44932500	3.37252900	0.83286300
H	-1.97274900	2.45184200	-0.45123500

H	1.14295700	-1.01237900	1.54669100
O	2.54724200	-1.38836500	-0.51199600
H	2.40586800	-1.07397900	-1.41837700
C	3.75287800	-0.79177000	-0.00391800
H	4.61157900	-1.06721300	-0.62661200
H	3.66968300	0.30036600	0.03646300
H	3.90319200	-1.18219200	1.00467900
H	-0.23165900	-1.20005300	-1.10707500
H	-3.37887100	0.48949000	-0.15008700
O	-2.64790000	-2.07639900	-0.19502300
H	-3.57084000	-1.94697700	0.07336400

Scan Point for comp9-c3oh_alpha_3.0Å

C	-1.89679600	-1.08894200	0.28859000
C	-0.39322800	-1.36863800	0.01630100
C	-1.73548700	1.47684400	0.04869900
C	0.50867200	-0.48441100	0.77667500
C	-0.25818500	1.60007900	-0.29451000
H	-2.28623400	0.05088800	-1.48570900
H	-2.05293200	-1.01463200	1.37271300
H	-1.86547700	1.64576700	1.12472000
H	-0.16128300	-2.39812700	0.29345200
H	-0.02119500	1.16016100	-1.26730500
C	0.31410400	2.99282300	-0.15949800
H	1.39484600	2.99084300	-0.32647200
H	-0.14796600	3.63073700	-0.91903700
O	0.56645500	0.77058800	0.69325200
H	0.10016900	3.41518500	0.82725200
H	-2.23048500	2.31141100	-0.45985400
H	1.18892600	-0.89297800	1.52468700
O	3.03396700	-1.25064200	-0.65013100
H	2.97139700	-0.81497300	-1.51286400
C	4.05171800	-0.59159700	0.11952600
H	5.01927000	-0.62493900	-0.39534600
H	3.78697800	0.45309900	0.32331200
H	4.13592300	-1.13076200	1.06605500
H	-0.19364600	-1.23695200	-1.05761900
H	-3.48451400	0.25286100	-0.20409800
O	-2.56803700	-2.25282700	-0.20724000
H	-3.50248300	-2.19876200	0.04772000

Scan Point for comp9-c3oh_alpha_3.3Å

C	-1.89266800	-1.15512500	0.28850200
C	-0.37425300	-1.36850700	0.04323400
C	-1.84032200	1.41374400	0.04014000
C	0.48623900	-0.43497000	0.78947100
C	-0.37084700	1.60383300	-0.30433000
H	-2.31781600	-0.03905200	-1.49351000
H	-2.06760400	-1.08713300	1.37013300
H	-1.97762000	1.57681500	1.11620100
H	-0.10012000	-2.38194800	0.34010100
H	-0.11358000	1.16679600	-1.27349100
C	0.13781900	3.02156500	-0.17702500
H	1.21886400	3.06597600	-0.33569100
H	-0.34591400	3.63227600	-0.94534100
O	0.49413600	0.81892800	0.68695900
H	-0.10286300	3.44104800	0.80474400
H	-2.37236200	2.22558600	-0.46773700
H	1.20217900	-0.80433900	1.52583400
O	3.32328500	-1.20729500	-0.70875700
H	3.30137800	-0.74662800	-1.56028500
C	4.16359800	-0.46418800	0.18747300
H	5.18343900	-0.37559100	-0.20646100
H	3.76213300	0.53932300	0.37387900
H	4.19654900	-1.01785200	1.12875800
H	-0.16187700	-1.24619900	-1.03061500
H	-3.53365200	0.11373600	-0.22115700
O	-2.50040900	-2.35020600	-0.21528700
H	-3.43753300	-2.34547600	0.03478900

Scan Point for comp9-c3oh_alpha_3.5Å

C	-1.90431600	-1.18951900	0.28355200
C	-0.37732900	-1.36800800	0.06498600
C	-1.90936800	1.37801500	0.01675400
C	0.44797700	-0.40874400	0.81830100
C	-0.43932600	1.60098100	-0.30482400
H	-2.32629400	-0.09674500	-1.51358700
H	-2.09885400	-1.11806800	1.36160500
H	-2.06846300	1.54540500	1.08914500
H	-0.08399900	-2.37242000	0.37394100

H	-0.15550100	1.16338800	-1.26628900
C	0.03301200	3.03142900	-0.17977700
H	1.11518000	3.10074800	-0.32089800
H	-0.45233700	3.62482600	-0.96054100
O	0.42755400	0.84421700	0.70649700
H	-0.23401000	3.45195700	0.79471000
H	-2.45215200	2.17317400	-0.50593300
H	1.16015400	-0.75552100	1.56915400
O	3.50197800	-1.16672900	-0.71419300
H	3.48369000	-0.71343800	-1.56975800
C	4.30891000	-0.39670200	0.18996100
H	5.33283900	-0.28646700	-0.18757400
H	3.88031200	0.59819600	0.36155000
H	4.33927600	-0.94222300	1.13607600
H	-0.15008100	-1.24825800	-1.00610100
H	-3.56649500	0.03580100	-0.26265900
O	-2.47473600	-2.40245300	-0.22121700
H	-3.41568600	-2.41867000	0.01353800

Scan Point for comp9-c3oh_alpha_3.6Å

C	2.00868800	-1.11189200	-0.27873900
C	0.50295800	-1.39605000	-0.02618400
C	1.83833400	1.45189700	-0.04378700
C	-0.40446400	-0.50729900	-0.77116500
C	0.36318600	1.57891900	0.30470900
H	2.38076800	0.03084100	1.49779200
H	2.17531500	-1.03857300	-1.36122100
H	1.96558500	1.61370300	-1.12122500
H	0.27629500	-2.42288400	-0.31727700
H	0.12898200	1.14059600	1.27899800
C	-0.20945000	2.97084700	0.16632900
H	-1.28964700	2.96936100	0.33648900
H	0.25491500	3.61091200	0.92264500
O	-0.47266400	0.74488000	-0.67411200
H	0.00209100	3.38992500	-0.82231000
H	2.33464900	2.29000400	0.45763100
H	-1.10954400	-0.91513300	-1.49818900
O	-3.59953400	-1.21704800	0.72808000
H	-3.75154900	-0.82299800	1.59936700
C	-4.31208200	-0.44471200	-0.25026700
H	-5.38507700	-0.41042400	-0.02579800
H	-3.92275500	0.57900000	-0.31186600

H	-4.17020100	-0.93906600	-1.21430100
H	0.28989100	-1.27805300	1.04834700
H	3.58869400	0.23305800	0.22514200
O	2.67528200	-2.27459700	0.22532600
H	3.61123300	-2.22305200	-0.02457100

Scan Point for comp9-c3oh_alpha_3.8Å

C	1.98493100	-1.16154900	-0.27918700
C	0.46709500	-1.38913000	-0.04363600
C	1.90789800	1.40608600	-0.02997200
C	-0.40118200	-0.46064500	-0.78576600
C	0.43692600	1.58520400	0.31337000
H	2.39079400	-0.04268000	1.50560000
H	2.16486900	-1.09141900	-1.35978600
H	2.04526500	1.56920600	-1.10600700
H	0.20408900	-2.40382300	-0.34623000
H	0.18226800	1.14633200	1.28237300
C	-0.08308600	2.99862900	0.18486800
H	-1.16434700	3.03464100	0.34408300
H	0.39620900	3.61348400	0.95267700
O	-0.42363900	0.79217800	-0.67714200
H	0.15398000	3.41944200	-0.79719200
H	2.43273900	2.22263200	0.47784500
H	-1.11946200	-0.83522400	-1.51783100
O	-3.79899500	-1.22387400	0.73485300
H	-3.88003600	-0.78752300	1.59538500
C	-4.32095700	-0.34266400	-0.27126200
H	-5.37520900	-0.10506300	-0.08386300
H	-3.74540800	0.58958800	-0.32553400
H	-4.24177600	-0.86682800	-1.22669700
H	0.24776700	-1.27319400	1.03016000
H	3.61156700	0.12144900	0.23941800
O	2.59991700	-2.35162500	0.22734800
H	3.53756300	-2.34103200	-0.02062100

Scan Point for comp9-c3oh_alpha_4.0Å

C	2.00325400	-1.17259000	-0.27165200
C	0.48423200	-1.39436700	-0.03803100

C	1.93465200	1.39582100	-0.02876300
C	-0.37985400	-0.46454400	-0.78318000
C	0.46395600	1.58049700	0.31279700
H	2.41114500	-0.05075700	1.51086000
H	2.18485900	-1.10564500	-1.35219900
H	2.07362500	1.55585200	-1.10506200
H	0.21827200	-2.40878200	-0.33900500
H	0.20688900	1.14399600	1.28224800
C	-0.05145700	2.99526800	0.18114900
H	-1.13284900	3.03482200	0.33858900
H	0.42852000	3.60996900	0.94864800
O	-0.39822300	0.78848400	-0.67718700
H	0.18851700	3.41360200	-0.80126800
H	2.46166200	2.21191300	0.47753900
H	-1.09919500	-0.83843000	-1.51456200
O	-3.98408800	-1.13061100	0.81862400
H	-4.24845000	-0.61730100	1.59574600
C	-4.31089200	-0.37508500	-0.35718800
H	-5.38028000	-0.13364800	-0.39022000
H	-3.73041600	0.55417700	-0.41126800
H	-4.06549100	-1.00152500	-1.21809800
H	0.26325500	-1.27549700	1.03517800
H	3.63375000	0.10601500	0.24544800
O	2.61344400	-2.36358700	0.23843900
H	3.55145900	-2.35659400	-0.00829400

Scan Point for comp9-c3oh_alpha_4.4Å

C	2.10275500	-1.12493100	-0.24195700
C	0.59848300	-1.41913700	0.01015100
C	1.90822900	1.44004800	-0.04618200
C	-0.31336800	-0.55079900	-0.75306300
C	0.43061600	1.55725600	0.29545200
H	2.45894100	0.04761900	1.51827000
H	2.27165300	-1.06589800	-1.32495000
H	2.03797000	1.58758800	-1.12534500
H	0.38263500	-2.45267700	-0.26508200
H	0.19723400	1.12887600	1.27435500
C	-0.15555000	2.94123800	0.13749900
H	-1.23607100	2.93122900	0.30535600
H	0.30061900	3.59566800	0.88646100
O	-0.39335600	0.70183900	-0.67538100
H	0.05424400	3.34952000	-0.85600000

H	2.39422100	2.29028000	0.44486800
H	-1.01129700	-0.97683500	-1.47661900
O	-4.36886000	-0.97272600	0.90069200
H	-4.74856900	-0.24652100	1.41644500
C	-4.23282900	-0.53800700	-0.46075300
H	-5.20056600	-0.23953500	-0.88203900
H	-3.53082200	0.30046900	-0.54421700
H	-3.84901600	-1.38798000	-1.02969500
H	0.38055000	-1.28496200	1.08194200
H	3.66890600	0.24136100	0.24615400
O	2.77844000	-2.27402600	0.28054800
H	3.71421800	-2.21840900	0.03068000

Scan Point for comp9-c3oh_beta_1.4Å

C	1.50975600	-0.95463900	-0.25343600
C	0.44445600	-1.17005600	0.83917200
C	1.27861500	1.62028400	-0.48378500
C	-0.93011000	-0.55759200	0.56191800
C	-0.02276400	1.71071400	0.31564400
H	2.59734500	0.52393900	0.84367800
H	1.06437700	-1.09194400	-1.24970600
H	1.01490500	1.62670800	-1.54960100
H	0.28590400	-2.24224600	1.00314100
H	0.16577800	1.56771200	1.38655400
C	-0.75482300	3.02788000	0.10544900
H	-1.69662300	3.04098500	0.66334000
H	-0.13630800	3.86018100	0.45668400
O	-0.93678000	0.66007700	-0.13681100
H	-0.97412900	3.18686300	-0.95667500
H	1.85523100	2.53399700	-0.29680100
H	-1.50258400	-0.48140100	1.49292200
O	-1.67924000	-1.43745900	-0.22842300
H	-1.27473100	-1.61669100	-1.10659400
C	-3.15172000	-1.20509900	-0.36195300
H	-3.30648000	-0.27986300	-0.91252300
H	-3.52045500	-2.07877800	-0.89423100
H	-3.52685700	-1.15996700	0.65766200
H	0.80618200	-0.75959700	1.78744500
O	2.56614100	-1.92067000	-0.08217700
H	2.20454700	-2.80951800	-0.21922700
H	3.02497000	0.42577300	-0.86438800

Scan Point for comp9-c3oh_beta_1.5Å

C	1.50692000	-0.97475900	-0.24401100
C	0.45633100	-1.13779300	0.87106700
C	1.22492600	1.57117600	-0.58856300
C	-0.91776900	-0.53609000	0.62505500
C	0.00649100	1.73162000	0.32201700
H	2.62119700	0.56962900	0.73071700
H	1.05399100	-1.17434200	-1.22564900
H	0.86622200	1.49239900	-1.62322000
H	0.29418300	-2.20153100	1.07817500
H	0.28947000	1.62269700	1.37536000
C	-0.70552300	3.06115600	0.12501200
H	-1.59186100	3.12623200	0.76377900
H	-0.03263100	3.88398800	0.38619900
O	-0.99954400	0.70410200	0.01142600
H	-1.01529300	3.18802200	-0.91859500
H	1.80761600	2.49781100	-0.52799000
H	-1.53095000	-0.58675500	1.53038800
O	-1.66998700	-1.45859300	-0.28771800
H	-1.25831800	-1.50318000	-1.17685900
C	-3.13636300	-1.24263200	-0.41259500
H	-3.31384400	-0.27088500	-0.86986200
H	-3.49125000	-2.06376900	-1.03211800
H	-3.52770500	-1.30659200	0.60031000
H	0.83596500	-0.69638000	1.79975000
O	2.57119000	-1.92164400	-0.02804100
H	2.22042800	-2.81911100	-0.13322200
H	2.97528300	0.38737400	-0.98850300

Scan Point for comp9-c3oh_beta_1.6Å

C	1.83985400	-0.25889500	-0.22870400
C	1.00590800	-0.76660700	0.96462200
C	0.12319600	1.53097900	-0.89818500
C	-0.49808800	-0.90203700	0.81596700
C	-0.78320600	1.52282400	0.33496000
H	1.95474400	1.83640200	0.20409100
H	1.64968500	-0.89486800	-1.10450200
H	-0.29792000	0.86668200	-1.66526300
H	1.37462300	-1.75886500	1.24381800
H	-0.22180500	1.86901500	1.21060600

C	-2.03665100	2.36542000	0.16859100
H	-2.68336000	2.27666000	1.04704800
H	-1.75515900	3.41707200	0.05733200
O	-1.29245100	0.18204000	0.69260800
H	-2.60356300	2.06197300	-0.71869400
H	0.08605200	2.54401400	-1.31308600
H	-0.92001000	-1.55936200	1.57666400
O	-0.73795800	-1.86360100	-0.44016100
H	-0.38876800	-1.48121600	-1.26929400
C	-2.13537200	-2.29042200	-0.64767900
H	-2.75222900	-1.42083100	-0.87136200
H	-2.11144400	-2.99604600	-1.47687600
H	-2.43984300	-2.77965300	0.27582000
H	1.16208000	-0.11077900	1.83056400
O	3.23418800	-0.36430800	0.10881700
H	3.47550400	-1.30081400	0.17817500
H	2.19844900	1.42132000	-1.49339900

Scan Point for comp9-c3oh_beta_1.7Å

C	1.84454500	-0.24075900	-0.23327900
C	1.03533800	-0.75017400	0.97619500
C	0.09505500	1.51890800	-0.90079500
C	-0.46689100	-0.87570000	0.87052200
C	-0.80480300	1.52698900	0.33461600
H	1.92938200	1.85896000	0.18694600
H	1.64939300	-0.88726500	-1.09948700
H	-0.32422700	0.84071900	-1.65606500
H	1.40803500	-1.74246700	1.24824800
H	-0.25340400	1.91723100	1.19730200
C	-2.08871000	2.31569900	0.14266200
H	-2.72883000	2.23844400	1.02680200
H	-1.84550700	3.37136300	-0.01154900
O	-1.26787600	0.17917600	0.75071200
H	-2.64561500	1.95670500	-0.72980700
H	0.04151400	2.52552300	-1.32930000
H	-0.88985000	-1.57461000	1.59089200
O	-0.71917300	-1.89409900	-0.46709400
H	-0.39459300	-1.48546100	-1.29282200
C	-2.11756300	-2.29926600	-0.65317800
H	-2.73617800	-1.42120200	-0.84098500
H	-2.13179900	-2.98584200	-1.49956600
H	-2.41284800	-2.80868800	0.26299300

H	1.21220700	-0.09262200	1.83838700
O	3.24402500	-0.32324400	0.08636600
H	3.50051900	-1.25550200	0.15689200
H	2.16564100	1.43699100	-1.50983000

Scan Point for comp9-c3oh_beta_2.0Å

C	1.79124700	-0.33375100	-0.20895100
C	0.97564800	-0.73072700	1.03926600
C	0.18640000	1.54256700	-0.93100800
C	-0.51621700	-0.70826700	0.98287200
C	-0.71257300	1.66178400	0.29431100
H	2.04889400	1.76626100	0.14100300
H	1.51179000	-0.99435400	-1.03710800
H	-0.28643300	0.89100200	-1.67686600
H	1.26000300	-1.74365400	1.33690900
H	-0.14892900	2.04558200	1.15082300
C	-1.96351400	2.48785100	0.06633700
H	-2.60380400	2.47976500	0.95340100
H	-1.67552500	3.52351400	-0.13711200
O	-1.24061700	0.33909000	0.77081700
H	-2.53431100	2.11151300	-0.78919400
H	0.21451900	2.54336000	-1.37569300
H	-1.04336000	-1.44580400	1.58305900
O	-0.82107300	-1.89944800	-0.59451500
H	-0.77065700	-1.33256700	-1.38378400
C	-2.13393700	-2.51433700	-0.55509800
H	-2.91277300	-1.75720200	-0.42528600
H	-2.29139700	-3.06114600	-1.48794400
H	-2.13199700	-3.21042900	0.28442200
H	1.23693000	-0.05908000	1.87263600
O	3.18413500	-0.52576700	0.08433200
H	3.36285600	-1.47524300	0.16472300
H	2.23634900	1.26855400	-1.54104200

Scan Point for comp9-c3oh_beta_2.5Å

C	1.28629600	-1.24288600	-0.18472700
C	0.55020400	-1.01810900	1.16606800
C	0.98539800	1.16922800	-1.01769700

C	-0.65643200	-0.16578000	1.17789000
C	0.41964500	1.84253000	0.22455400
H	2.73653100	0.33349600	-0.06295900
H	0.56476900	-1.64346100	-0.90430700
H	0.15953900	0.86788100	-1.67438800
H	0.26367500	-1.98610800	1.58270000
H	1.15138800	1.86560000	1.03799000
C	-0.17983200	3.21181500	-0.01340400
H	-0.65235900	3.59442600	0.89578600
H	0.62153900	3.89989700	-0.29827200
O	-0.73312100	1.04305500	0.80935000
H	-0.91997700	3.18481800	-0.81978300
H	1.53667100	1.95060300	-1.55190900
H	-1.55478900	-0.50763700	1.68728900
O	-1.93813500	-1.32775500	-0.62684000
H	-1.63743900	-0.86651200	-1.42503600
C	-3.34918500	-1.09431800	-0.47264700
H	-3.56179200	-0.02902400	-0.32468700
H	-3.89702800	-1.45576600	-1.34998500
H	-3.67332400	-1.65455500	0.40689700
H	1.25210200	-0.54174400	1.87200700
O	2.32485600	-2.20406200	0.02904000
H	1.92752800	-3.07850400	0.16123400
H	2.43440300	-0.27362100	-1.69224500

Scan Point for comp9-c3oh_beta_3.0Å

C	0.75610700	-1.62091200	-0.16827200
C	0.29472600	-1.10248900	1.23406200
C	1.43471400	0.69983200	-1.06172500
C	-0.51808100	0.12332000	1.22200400
C	1.20957500	1.54525400	0.18358700
H	2.73264600	-0.79067100	-0.17946500
H	-0.12304800	-1.67597900	-0.81989100
H	0.54860900	0.76911200	-1.70471100
H	-0.28850300	-1.88016400	1.73074700
H	1.89895600	1.28146600	0.99096100
C	1.18057100	3.03796900	-0.05588600
H	0.90897900	3.57527300	0.85717900
H	2.18085100	3.36160800	-0.35901600
O	-0.16823700	1.24890000	0.77406400
H	0.47395900	3.29643800	-0.85099600
H	2.25095100	1.18690200	-1.60620700

H	-1.51615100	0.13361900	1.65887000
O	-2.73138200	-0.59677500	-0.67081400
H	-2.40847200	-0.35259000	-1.55042900
C	-3.79126400	0.30464800	-0.31457500
H	-3.42613800	1.33516400	-0.22535500
H	-4.60115800	0.27300400	-1.05322400
H	-4.18158800	-0.02259300	0.65193700
H	1.19259900	-0.89674600	1.83891500
O	1.30637700	-2.92599800	0.00221700
H	0.59050400	-3.55469800	0.18317800
H	2.09981100	-1.21919200	-1.76998400

Scan Point for comp9-c3oh_beta_3.3Å

C	0.78096900	-1.62827000	-0.16352200
C	0.35052200	-1.09479400	1.24653400
C	1.49718000	0.67735200	-1.07074700
C	-0.46011100	0.13014000	1.21526900
C	1.27956300	1.53033300	0.17098200
H	2.77218900	-0.83600700	-0.19155000
H	-0.10690500	-1.66399900	-0.80514500
H	0.61440200	0.75996500	-1.71674400
H	-0.22934700	-1.86381400	1.76013100
H	1.96218900	1.26279200	0.98266500
C	1.26492200	3.02198600	-0.07432800
H	0.99591400	3.56555400	0.83577000
H	2.26925500	3.33474000	-0.37550200
O	-0.10675400	1.24740500	0.75209400
H	0.56337400	3.28372300	-0.87277500
H	2.32352700	1.14982600	-1.61284400
H	-1.47209500	0.14201700	1.62164700
O	-3.00664100	-0.58977600	-0.75625500
H	-2.78597900	-0.31051400	-1.65669400
C	-3.91042300	0.37274300	-0.19199600
H	-3.44557300	1.36334700	-0.11662400
H	-4.82890700	0.45111800	-0.78626700
H	-4.16910200	0.02156600	0.80975500
H	1.26116100	-0.88762200	1.83011300
O	1.30469900	-2.94328900	0.00337100
H	0.57790100	-3.55717200	0.19179700
H	2.12008900	-1.25618000	-1.77660700

Scan Point for comp9-c3oh_beta_3.5Å

C	0.76070300	-1.64239000	-0.16106700
C	0.39130000	-1.09429800	1.26065600
C	1.51247000	0.64022700	-1.09716400
C	-0.38458200	0.15331400	1.25234500
C	1.35971200	1.50123300	0.14871600
H	2.77175000	-0.90729500	-0.25558400
H	-0.14809000	-1.65396300	-0.77365500
H	0.61186300	0.74686500	-1.71441700
H	-0.19343800	-1.84551100	1.79468600
H	2.06034400	1.21557200	0.93860600
C	1.37989600	2.99227900	-0.09989000
H	1.15601800	3.54486100	0.81698800
H	2.38255400	3.27557100	-0.43402700
O	-0.01458700	1.25920400	0.77506600
H	0.66074000	3.27269600	-0.87603200
H	2.33388800	1.08793900	-1.66706800
H	-1.38209000	0.19490900	1.69127900
O	-3.17210600	-0.53606800	-0.74877100
H	-2.97244000	-0.26484700	-1.65654300
C	-4.02913700	0.45318000	-0.15838000
H	-3.53366800	1.43002600	-0.10048900
H	-4.96355300	0.55714800	-0.72317400
H	-4.26560600	0.11127600	0.85203700
H	1.32582500	-0.91230900	1.81412400
O	1.25194200	-2.97150900	-0.00753600
H	0.51442800	-3.56410700	0.20577000
H	2.05694400	-1.31154900	-1.81758600

Scan Point for comp9-c3oh_beta_3.6Å

C	-0.41403700	1.69819800	-0.17552700
C	-0.21733000	1.10940600	1.26515100
C	-1.59059600	-0.39284900	-1.12370200
C	0.29467600	-0.26699700	1.28761400
C	-1.64862200	-1.25231400	0.12988200
H	-2.52762800	1.38737200	-0.32511700
H	0.49792900	1.51006200	-0.75368100
H	-0.71615300	-0.68730500	-1.71697200
H	0.48372800	1.73597700	1.81922300

H	-2.30034200	-0.82176500	0.89613200
C	-1.95854000	-2.71270800	-0.10846000
H	-1.88009100	-3.28473200	0.82029200
H	-2.98622300	-2.79336600	-0.47528700
O	-0.27008300	-1.28089100	0.79726100
H	-1.28608300	-3.14325800	-0.85714200
H	-2.47250600	-0.66783900	-1.71280000
H	1.25349600	-0.50092900	1.75387900
O	3.49570800	0.22056700	-0.28581400
H	3.64145800	0.65969300	-1.13663700
C	3.66740700	-1.19259400	-0.47120500
H	2.92435700	-1.59722700	-1.16920600
H	4.67313200	-1.42571600	-0.84123800
H	3.53414800	-1.66521900	0.50467900
H	-1.19197400	1.12396100	1.77620800
O	-0.62456500	3.10218600	-0.05216600
H	0.21624900	3.53502300	0.16202900
H	-1.70259600	1.62097500	-1.86814600

Scan Point for comp9-c3oh_beta_3.8Å

C	-0.15310100	1.67973500	-0.12581400
C	-0.11553600	1.04954700	1.31107200
C	-1.61254000	-0.17957800	-1.15690000
C	0.16873500	-0.39133300	1.32552800
C	-1.85838300	-1.03219600	0.07932300
H	-2.28252200	1.72092800	-0.36542400
H	0.73812000	1.34861800	-0.67102100
H	-0.77389400	-0.60612700	-1.72066800
H	0.65384600	1.54792100	1.90341200
H	-2.45907700	-0.51028500	0.82962300
C	-2.39632500	-2.41822800	-0.19565400
H	-2.44946300	-3.00709300	0.72434400
H	-3.40912100	-2.32303700	-0.59873700
O	-0.53057400	-1.29447800	0.79427600
H	-1.77687100	-2.94509500	-0.92823900
H	-2.50243100	-0.30208200	-1.78379000
H	1.06069800	-0.78222900	1.81905600
O	3.50731300	-0.08191800	-0.46281000
H	3.42533500	0.12768100	-1.40457000
C	3.65260300	-1.50368300	-0.32492900
H	2.75384900	-2.03198500	-0.66592700
H	4.52171700	-1.87118400	-0.88362700

H	3.80590000	-1.70792100	0.73743400
H	-1.09547700	1.21571300	1.78423900
O	-0.13112700	3.09695400	0.01446300
H	0.76031600	3.37822500	0.27277800
H	-1.36546800	1.83466800	-1.86953600

Scan Point for comp9-c3oh_beta_4.0Å

C	0.08947700	1.63557100	-0.11490000
C	-0.00563300	1.02319800	1.32664100
C	-1.57661900	-0.02009700	-1.18066200
C	0.06425400	-0.44332900	1.36468500
C	-1.99222400	-0.80716100	0.05306300
H	-2.00447400	1.96409200	-0.42899300
H	0.94590000	1.18200400	-0.62739700
H	-0.78215900	-0.56831200	-1.70181900
H	0.81039300	1.41155100	1.93842000
H	-2.53996700	-0.19107900	0.77243600
C	-2.71172900	-2.10614700	-0.22768400
H	-2.88340700	-2.66610100	0.69596300
H	-3.68387200	-1.87362500	-0.67275800
O	-0.74276100	-1.24438000	0.82283000
H	-2.14758300	-2.72871700	-0.92923900
H	-2.44703100	-0.02859000	-1.84580000
H	0.87464600	-0.95138000	1.89079400
O	3.66101900	-0.41706800	-0.38534200
H	3.79310000	-0.14353400	-1.30480600
C	3.25861500	-1.79550300	-0.37512000
H	2.28641200	-1.93173300	-0.86426200
H	4.00268100	-2.43056200	-0.87094400
H	3.18063000	-2.09896300	0.67146300
H	-0.96385600	1.33422100	1.76923700
O	0.29633500	3.03894000	0.01572500
H	1.20632100	3.20232700	0.30805600
H	-1.03094200	1.93158700	-1.90102000

Scan Point for comp9-c3oh_beta_4.4Å

C	0.24288300	1.55746500	-0.09422000
C	-0.05630000	1.04199800	1.35870800

C	-1.49495300	0.02407100	-1.23721200
C	-0.13182100	-0.42057700	1.46614500
C	-2.09108500	-0.64853000	-0.00917300
H	-1.75984200	2.08577200	-0.63563600
H	1.09314700	0.99318900	-0.49380400
H	-0.72958300	-0.63459900	-1.66526500
H	0.72909200	1.38731000	2.03313400
H	-2.62927600	0.05770100	0.62956500
C	-2.92037100	-1.88062300	-0.29254200
H	-3.22545100	-2.36955400	0.63686000
H	-3.82321600	-1.57370300	-0.82919600
O	-0.96309100	-1.16793300	0.88542000
H	-2.37102600	-2.59460300	-0.91448100
H	-2.30610100	0.07431400	-1.97212700
H	0.57708700	-0.97460100	2.08452400
O	3.87731900	-0.68141400	-0.32794400
H	4.18902300	-0.51183700	-1.22888700
C	3.06673100	-1.86635300	-0.34286900
H	2.16214200	-1.72758300	-0.94669600
H	3.62638700	-2.72668200	-0.72967800
H	2.78121200	-2.07170300	0.69146800
H	-1.01885000	1.46657000	1.68156400
O	0.57999400	2.93905800	-0.01082100
H	1.47505800	3.02990600	0.35057600
H	-0.66245800	1.85432700	-1.99844900

Scan Plot for comp9-c4oh_alpha_1.4Å

C	1.32272500	-1.53297600	-0.23996500
C	-0.08933900	-1.65456700	0.35271700
C	1.56801900	1.03662400	-0.07411700
C	-1.11987500	-0.77563700	-0.35634800
C	0.09724500	1.28232200	0.27067600
H	2.12595400	-0.42391600	1.40895000
H	1.27899500	-1.47969900	-1.33527400
H	1.69753300	1.18915100	-1.15349000
H	-0.44717500	-2.68443900	0.26481200
H	-0.12712700	0.95618400	1.29362400
C	-0.30023900	2.74243000	0.11097300
H	-1.36302400	2.88373200	0.33064200
H	0.27841600	3.36475600	0.80099400
O	-0.74535600	0.52979200	-0.66310800
H	-0.10481500	3.08807400	-0.91033300
H	2.17261700	1.79624500	0.43766500

H	1.87831400	-2.44201900	0.01360900
H	-1.42463200	-1.22422100	-1.30434900
O	-2.28462800	-0.79112500	0.42025300
H	-2.15293300	-0.49317500	1.34587400
C	-3.54799700	-0.23685500	-0.14941100
H	-4.30809400	-0.44987600	0.59830100
H	-3.41317700	0.82899100	-0.31962100
H	-3.71705500	-0.79138000	-1.06963400
H	-0.07101700	-1.41668700	1.42444600
O	3.46107300	-0.49383300	-0.17674500
H	3.99996100	0.23244600	0.17232900

Scan Plot for comp9-c4oh_alpha_1.5Å

C	1.33104200	-1.54283000	-0.22805700
C	-0.08936400	-1.64469200	0.35254900
C	1.57779500	1.02756000	-0.08542900
C	-1.08815200	-0.76194800	-0.38172400
C	0.11372100	1.28558000	0.27591900
H	2.13687400	-0.41951000	1.40988000
H	1.29866900	-1.50689000	-1.32452800
H	1.69596500	1.16832800	-1.16758700
H	-0.45747900	-2.67070200	0.26756300
H	-0.10655100	0.95863600	1.29848900
C	-0.27883300	2.74601300	0.11571000
H	-1.33963900	2.89216900	0.34109400
H	0.30643200	3.36480800	0.80311600
O	-0.74749500	0.53767400	-0.65245100
H	-0.08624800	3.09014700	-0.90649300
H	2.19005800	1.79080600	0.41130500
H	1.87597100	-2.45222700	0.04588300
H	-1.42312100	-1.20898900	-1.31890600
O	-2.34379100	-0.80558200	0.43770800
H	-2.20322400	-0.45104200	1.34032200
C	-3.57384100	-0.23084100	-0.16101200
H	-4.36010600	-0.40857200	0.56984200
H	-3.41654200	0.82986300	-0.34785500
H	-3.74544900	-0.79219600	-1.07692000
H	-0.07939600	-1.39664300	1.42152700
O	3.46919100	-0.50486500	-0.17768200
H	4.01177600	0.21837700	0.17199700

Scan Plot for comp9-c4oh_alpha_1.6Å

C	1.34479100	-1.54849900	-0.22189100
C	-0.08488000	-1.64125400	0.34197000
C	1.58522700	1.02339600	-0.09112900
C	-1.05507100	-0.75361300	-0.41272300
C	0.12496600	1.28736700	0.27808300
H	2.14050000	-0.41470000	1.41408400
H	1.32688800	-1.52415300	-1.31898300
H	1.69888600	1.15716800	-1.17452000
H	-0.45912400	-2.66417900	0.25289900
H	-0.09527900	0.95692200	1.29866400
C	-0.26937800	2.74612200	0.11678800
H	-1.33063300	2.89085300	0.34042200
H	0.31385600	3.36330000	0.80720100
O	-0.74463500	0.53877400	-0.65045700
H	-0.07393400	3.09170500	-0.90421100
H	2.19930000	1.79004700	0.39778700
H	1.88211900	-2.45693900	0.06924600
H	-1.42596800	-1.19585000	-1.33756100
O	-2.39965300	-0.82538000	0.45153900
H	-2.25138100	-0.45084500	1.34342800
C	-3.59833100	-0.21787300	-0.15769100
H	-4.40668000	-0.37253400	0.55542800
H	-3.41705300	0.84047700	-0.34100300
H	-3.77729500	-0.76671600	-1.08031800
H	-0.08611600	-1.38829300	1.40915000
O	3.47925400	-0.50583200	-0.16799100
H	4.02148100	0.21501600	0.18716800

Scan Plot for comp9-c4oh_alpha_1.7Å

C	1.35450100	-1.55630200	-0.21590400
C	-0.08596600	-1.63557300	0.32708900
C	1.59740100	1.01605000	-0.09705800
C	-1.02416900	-0.73960200	-0.44626000
C	0.14150300	1.29140000	0.27863600
H	2.14064300	-0.41444200	1.41947500
H	1.35369200	-1.54377400	-1.31326500
H	1.70821000	1.14209200	-1.18152400
H	-0.46945900	-2.65395700	0.23094300
H	-0.08124800	0.95658000	1.29657100
C	-0.24932300	2.74999700	0.11767100
H	-1.31054900	2.89685000	0.33953600

H	0.33387200	3.36257100	0.81207900
O	-0.73848800	0.54529300	-0.65090800
H	-0.04937000	3.09752100	-0.90160300
H	2.21542600	1.78401100	0.38448300
H	1.87958100	-2.46557700	0.09394900
H	-1.43361500	-1.17224200	-1.35824600
O	-2.45663900	-0.83935900	0.46372800
H	-2.30236000	-0.45597900	1.34949700
C	-3.63095300	-0.20705400	-0.14907800
H	-4.45577300	-0.33960800	0.55092400
H	-3.43096500	0.84900900	-0.33217600
H	-3.81908100	-0.74600000	-1.07630100
H	-0.10094600	-1.37998000	1.39291500
O	3.48863900	-0.51669600	-0.15438100
H	4.03271300	0.19897100	0.20834800

Scan Plot for comp9-c4oh_alpha_2.0Å

C	1.38969800	-1.57081300	-0.22576100
C	-0.08576800	-1.62914900	0.23723600
C	1.63608800	0.99813500	-0.09950400
C	-0.93837900	-0.70385700	-0.56789900
C	0.18424900	1.30021700	0.26441500
H	2.10163000	-0.42975400	1.44432200
H	1.45209700	-1.56773600	-1.32094300
H	1.76321500	1.11342700	-1.18298600
H	-0.48525500	-2.63565900	0.10198400
H	-0.06604600	0.94705000	1.26865300
C	-0.19626900	2.75854500	0.10196100
H	-1.26154500	2.90866900	0.29952800
H	0.37246800	3.35793000	0.81919100
O	-0.71013200	0.56329300	-0.68410600
H	0.03418100	3.11386500	-0.90772100
H	2.25348600	1.76512400	0.38351200
H	1.87657600	-2.48648300	0.12400300
H	-1.47794600	-1.09768100	-1.42625500
O	-2.61034400	-0.86624900	0.51753200
H	-2.41474400	-0.46089800	1.38125900
C	-3.74161000	-0.18293400	-0.07809400
H	-4.57767300	-0.21409100	0.62485500
H	-3.48632800	0.85363800	-0.31498800
H	-3.99896700	-0.72966700	-0.98580400
H	-0.14891700	-1.38361400	1.30306800
O	3.52082900	-0.54163900	-0.06518700

H	4.06070500	0.13890000	0.36518500

Scan Plot for comp9-c4oh_alpha_2.5Å

C	-1.41056400	-1.61694900	0.23619800
C	0.10157700	-1.59199400	-0.12014400
C	-1.75676900	0.93461200	0.09367900
C	0.83202300	-0.60505900	0.70161400
C	-0.32563500	1.32697300	-0.25735600
H	-2.08107500	-0.50749100	-1.47335200
H	-1.54937500	-1.62835500	1.32344500
H	-1.90387100	1.03246000	1.17612900
H	0.55007600	-2.56903300	0.06310600
H	-0.02939400	0.96982900	-1.24726600
C	-0.02216100	2.80083200	-0.09461600
H	1.03837100	3.00178500	-0.27086300
H	-0.60408600	3.36167500	-0.83196800
O	0.62306000	0.64457300	0.70636700
H	-0.29535700	3.15178300	0.90566700
H	-2.40628700	1.67385400	-0.38996900
H	-1.81127000	-2.55683600	-0.15487800
H	1.50894900	-0.92271600	1.49252400
O	2.95770900	-0.84373100	-0.59240900
H	2.76666300	-0.40860300	-1.43782600
C	4.04702600	-0.15093900	0.04122600
H	4.92864900	-0.14073600	-0.60955900
H	3.77009600	0.87944900	0.29326100
H	4.28662600	-0.69677900	0.95608900
H	0.22129200	-1.35179300	-1.18361300
O	-3.56939900	-0.68348500	-0.03834500
H	-4.12149300	-0.05884800	-0.53349300

Scan Plot for comp9-c4oh_alpha_3.0Å

C	-1.48444400	-1.63450000	0.23694600
C	0.04438400	-1.59406300	-0.04890000
C	-1.84087100	0.91367700	0.07822000
C	0.73367100	-0.58724300	0.77542500
C	-0.41064300	1.32377500	-0.25033700
H	-2.10790300	-0.53232700	-1.49622800
H	-1.66884900	-1.65081800	1.31693400
H	-2.00856200	1.00979500	1.15775200

H	0.49497800	-2.56355800	0.16640600
H	-0.08726400	0.95679100	-1.22787700
C	-0.12338200	2.80097100	-0.09703800
H	0.93924200	3.00870500	-0.25115100
H	-0.69138900	3.34521800	-0.85744500
O	0.53942300	0.65831600	0.73479700
H	-0.42457400	3.16365400	0.89074300
H	-2.48859000	1.64703900	-0.41669400
H	-1.85333700	-2.57836700	-0.17457600
H	1.44744300	-0.87941000	1.54643300
O	3.33384400	-0.82974000	-0.70115700
H	3.19058000	-0.34447300	-1.52703000
C	4.28932300	-0.10725200	0.09081600
H	5.24351300	-0.00147600	-0.43926400
H	3.91388800	0.88714400	0.36111500
H	4.45228600	-0.68721200	1.00219600
H	0.21050200	-1.36093700	-1.11014600
O	-3.63736700	-0.71710700	-0.10591900
H	-4.17971400	-0.10432900	-0.62603500

Scan Plot for comp9-c4oh_alpha_3.3Å

C	-1.53177300	-1.63592000	0.24144600
C	0.00509700	-1.60571400	0.00135300
C	-1.87006300	0.91286400	0.05813300
C	0.67980800	-0.59217900	0.82808700
C	-0.43240100	1.31684300	-0.24290500
H	-2.10706900	-0.54115400	-1.51407400
H	-1.74648500	-1.64515000	1.31584900
H	-2.06043500	1.01538100	1.13331900
H	0.44355700	-2.57501900	0.24099700
H	-0.08913700	0.94171000	-1.21045800
C	-0.14200300	2.79358100	-0.09306200
H	0.92461600	2.99559800	-0.22546200
H	-0.69072300	3.33446600	-0.86988900
O	0.49835800	0.65343800	0.76518300
H	-0.46300100	3.16497000	0.88515000
H	-2.50410500	1.64625700	-0.45413100
H	-1.89270900	-2.58039500	-0.17554500
H	1.38909400	-0.87708800	1.60727700
O	3.54107500	-0.82066400	-0.80008500
H	3.45548200	-0.29116400	-1.60624500
C	4.35033400	-0.09272600	0.13610500
H	5.34836100	0.10637000	-0.27270000

H	3.88023400	0.85682500	0.41916000
H	4.45222500	-0.71871500	1.02566300
H	0.20533100	-1.38526000	-1.05776200
O	-3.66924300	-0.71054500	-0.15823100
H	-4.19704100	-0.09717400	-0.69226500

Scan Plot for comp9-c4oh_alpha_3.5Å

C	-1.55441700	-1.64110800	0.24464800
C	-0.01435000	-1.60475800	0.02855400
C	-1.90369900	0.90438500	0.04480100
C	0.64535700	-0.58210600	0.85601000
C	-0.46480900	1.31554500	-0.23926700
H	-2.11005100	-0.55758200	-1.52447500
H	-1.78513200	-1.64607900	1.31575300
H	-2.10882800	1.00983600	1.11698300
H	0.42479800	-2.57031900	0.28174300
H	-0.10691800	0.93813900	-1.20062000
C	-0.18496400	2.79455300	-0.09197300
H	0.88205400	3.00239500	-0.21153700
H	-0.72684500	3.32885400	-0.87810500
O	0.45827500	0.66197000	0.78292300
H	-0.52065500	3.16822500	0.88042100
H	-2.53504800	1.63224500	-0.47857400
H	-1.90404300	-2.58952400	-0.17301200
H	1.35155900	-0.85776300	1.64156000
O	3.69581000	-0.80198800	-0.84586800
H	3.62027900	-0.23617600	-1.62797100
C	4.43185200	-0.08844900	0.15939900
H	5.43072000	0.18707900	-0.20012100
H	3.90208900	0.81781400	0.47713200
H	4.53772800	-0.75905800	1.01534000
H	0.20218700	-1.39122800	-1.02908800
O	-3.69061400	-0.72994500	-0.19038900
H	-4.21430700	-0.12123700	-0.73370200

Scan Plot for comp9-c4oh_alpha_3.6Å

C	1.52905900	-1.66191400	-0.23011500
C	-0.00335200	-1.58174500	0.02668000
C	1.94940800	0.87440300	-0.07165900
C	-0.66036500	-0.54852900	-0.78878700

C	0.53269100	1.32550200	0.25662700
H	2.16425400	-0.57390700	1.50856800
H	1.72842100	-1.68639100	-1.30720000
H	2.11993600	0.96106900	-1.15152700
H	-0.47378300	-2.53755600	-0.20701800
H	0.19806100	0.96350800	1.23214900
C	0.28718100	2.81029600	0.10691600
H	-0.76878500	3.04832000	0.26303300
H	0.87143400	3.33562600	0.86832300
O	-0.44013300	0.69058500	-0.72991400
H	0.59790200	3.16701900	-0.88008700
H	2.61713900	1.59172500	0.42016500
H	1.86388000	-2.61461900	0.18979100
H	-1.39963400	-0.81101400	-1.54807400
O	-3.84643800	-0.71736600	0.87866300
H	-3.91160400	-0.09738800	1.61975300
C	-4.47148500	-0.12192800	-0.26877700
H	-5.52341000	0.11581100	-0.06879700
H	-3.94969800	0.79054900	-0.58198000
H	-4.42421800	-0.85693000	-1.07581600
H	-0.18800000	-1.35475400	1.08783100
O	3.70145100	-0.80177500	0.13334100
H	4.25468600	-0.20349100	0.65904700

Scan Plot for comp9-c4oh_alpha_3.8Å

C	1.54839300	-1.66191200	-0.22890800
C	0.00902900	-1.58451600	-0.01533600
C	1.96263700	0.87429500	-0.04815300
C	-0.62329500	-0.54968600	-0.84784800
C	0.53621500	1.32152600	0.24143800
H	2.13677200	-0.58069000	1.53092500
H	1.77773200	-1.68156000	-1.30014400
H	2.16441800	0.96660500	-1.12215500
H	-0.45300600	-2.54035400	-0.26494100
H	0.17441700	0.95346300	1.20484000
C	0.29218000	2.80658300	0.09249800
H	-0.76884400	3.04134800	0.21588100
H	0.85028300	3.32877100	0.87541500
O	-0.40658900	0.68940800	-0.77684400
H	0.63315300	3.17019600	-0.88190200
H	2.61462500	1.59018700	0.46636800
H	1.87236700	-2.61594500	0.19639600
H	-1.33675100	-0.80969500	-1.63222500

O	-3.96284700	-0.65722200	0.96205600
H	-4.15992500	-0.00564600	1.65067700
C	-4.46262000	-0.16235700	-0.28941700
H	-5.54045100	0.03439500	-0.23915400
H	-3.94374800	0.75482600	-0.59396200
H	-4.28260200	-0.94014700	-1.03538100
H	-0.20666600	-1.35984100	1.04056400
O	3.70883800	-0.80289200	0.19436400
H	4.24915200	-0.20630600	0.73505300

Scan Plot for comp9-c4oh_alpha_4.0Å

C	1.57993300	-1.65928900	-0.21836700
C	0.03529300	-1.59541800	-0.04202300
C	1.96925400	0.88098500	-0.03017200
C	-0.58492200	-0.56712100	-0.89146100
C	0.53203100	1.31522900	0.22464100
H	2.12216400	-0.57184000	1.55316900
H	1.83477200	-1.67804200	-1.28382100
H	2.19657700	0.97543100	-1.09884500
H	-0.41187900	-2.55566800	-0.30147100
H	0.15010900	0.94399200	1.17911500
C	0.27838400	2.79796500	0.06903700
H	-0.78757300	3.02310300	0.16447900
H	0.81146800	3.32521400	0.86588500
O	-0.38030900	0.67387400	-0.81646300
H	0.64110000	3.16469900	-0.89629400
H	2.60188900	1.60262500	0.50018900
H	1.90204200	-2.60994800	0.21581100
H	-1.27652400	-0.83365300	-1.69312600
O	-4.09330600	-0.58981300	1.02965400
H	-4.35889700	0.12344100	1.62813000
C	-4.44708100	-0.21191500	-0.30905900
H	-5.52312800	-0.01840700	-0.39745200
H	-3.89483700	0.67879500	-0.63312700
H	-4.18696700	-1.05098700	-0.95873500
H	-0.20776000	-1.37150100	1.00809500
O	3.72247600	-0.78314200	0.24809100
H	4.24846300	-0.17854300	0.79371000

Scan Plot for comp9-c4oh_alpha_4.4Å

C	1.61843200	-1.65431300	-0.16188000
C	0.06973700	-1.61317000	-0.01005800
C	1.95799300	0.89821000	-0.01949800
C	-0.54528600	-0.61955100	-0.90340100
C	0.50691100	1.31022600	0.19190500
H	2.11368800	-0.52064800	1.59460900
H	1.89049400	-1.69153300	-1.22256900
H	2.20865200	0.97807000	-1.08412900
H	-0.35741300	-2.58749900	-0.24995900
H	0.10792800	0.95718700	1.14635600
C	0.23225500	2.78394900	-0.00866700
H	-0.83908600	2.99349800	0.05647400
H	0.73872200	3.34073000	0.78543300
O	-0.36549600	0.62661200	-0.85570600
H	0.61102900	3.13085700	-0.97518800
H	2.56402000	1.64158700	0.51183000
H	1.95041500	-2.58924200	0.29826100
H	-1.19928800	-0.92165500	-1.72350500
O	-4.46892700	-0.31745600	1.06478000
H	-5.04551700	0.45164600	1.18108600
C	-4.14767600	-0.43628300	-0.32902300
H	-5.05092900	-0.57335400	-0.93610700
H	-3.60232400	0.44424100	-0.68936900
H	-3.51607900	-1.32150600	-0.43482700
H	-0.19076000	-1.36279200	1.02930100
O	3.73591700	-0.72785400	0.31540200
H	4.24389800	-0.09878500	0.85006100

Scan Point for comp9-c4oh_beta_1.4Å

C	0.98835000	-1.62896000	0.36497700
C	-0.18566700	-1.25338900	1.28287500
C	1.26912000	0.74981500	-0.56877800
C	-1.29456900	-0.37310200	0.70456100
C	0.34484000	1.50171900	0.39695400
H	2.45536700	-0.17667200	0.96449900
H	0.62831700	-2.06208800	-0.57834200
H	0.71401900	0.47684300	-1.47669100
H	-0.68244100	-2.17254600	1.60928100
H	0.74638100	1.44254100	1.41621500
C	0.16959400	2.96531300	0.01789700
H	-0.54029300	3.45593000	0.69144900
H	1.13020900	3.48370600	0.09698900
O	-1.01777800	0.97059500	0.43803300

H	-0.19537400	3.06504900	-1.01060500
H	2.06289200	1.44257900	-0.87334700
H	1.55448700	-2.42409200	0.86167200
H	-2.15074700	-0.38787400	1.38345800
O	-1.78995800	-0.98056800	-0.45542800
H	-1.12841800	-1.07980400	-1.17321800
C	-3.09790800	-0.52481800	-1.01156300
H	-2.99501400	0.50890100	-1.33514500
H	-3.30100600	-1.20357500	-1.83659300
H	-3.81356600	-0.64383100	-0.20115900
H	0.17163700	-0.75398300	2.18984000
O	2.92034200	-1.02939800	-0.86900500
H	3.61946200	-0.37197300	-1.00540000

Scan Point for comp9-c4oh_beta_1.5Å

C	1.01814500	-1.61611700	0.36727200
C	-0.15291600	-1.26586400	1.29873500
C	1.24175900	0.76335000	-0.57574300
C	-1.26632200	-0.37989400	0.75719000
C	0.32828500	1.50986000	0.40158200
H	2.46386000	-0.13347800	0.94744400
H	0.65392300	-2.05560500	-0.57098300
H	0.67521000	0.47516800	-1.47145600
H	-0.63892900	-2.19389900	1.61467000
H	0.75354800	1.47184300	1.41160000
C	0.10374200	2.96148400	0.00622000
H	-0.60065200	3.44360500	0.69140000
H	1.05240600	3.50486700	0.05309900
O	-1.02577900	0.94783000	0.49687100
H	-0.29010000	3.03510600	-1.01370100
H	2.01732900	1.46787600	-0.89924700
H	1.60482500	-2.39967100	0.85833700
H	-2.14825200	-0.43973700	1.39733900
O	-1.78645900	-1.03546600	-0.48767300
H	-1.11501400	-1.08885100	-1.19912900
C	-3.07060300	-0.53456900	-1.03739200
H	-2.94596900	0.50281400	-1.34313600
H	-3.29600100	-1.18801400	-1.87782800
H	-3.79876000	-0.64674300	-0.23679700
H	0.20827600	-0.77731400	2.21145200
O	2.92396700	-0.98319300	-0.88873300
H	3.61177700	-0.31509800	-1.03071900

Scan Point for comp9-c4oh_beta_1.6Å

C	1.05355500	-1.60450800	0.35802900
C	-0.11581600	-1.29013300	1.30394200
C	1.21368500	0.78069500	-0.57775600
C	-1.23529400	-0.39590300	0.80798700
C	0.30771600	1.51859300	0.40965000
H	2.46666500	-0.08920600	0.93656700
H	0.68704400	-2.04366700	-0.57902900
H	0.64166500	0.48045000	-1.46557900
H	-0.59076700	-2.22976300	1.60024900
H	0.75749300	1.50738600	1.40899600
C	0.02500400	2.95401600	-0.00447400
H	-0.67381000	3.42680200	0.69256300
H	0.95724100	3.52668700	0.00462300
O	-1.03134500	0.91831900	0.56429400
H	-0.39976900	2.99537900	-1.01363400
H	1.96980400	1.50028700	-0.91377600
H	1.66160900	-2.37839600	0.83817600
H	-2.14053600	-0.50463800	1.40596800
O	-1.78206000	-1.08671200	-0.52761400
H	-1.10746400	-1.09314000	-1.23577900
C	-3.04863400	-0.54293500	-1.05412500
H	-2.92047900	0.51292900	-1.29065100
H	-3.28048300	-1.13087600	-1.94091800
H	-3.79047900	-0.69936100	-0.27328200
H	0.24814400	-0.82014400	2.22680000
O	2.93627300	-0.92153800	-0.90526900
H	3.60932000	-0.23818000	-1.04581100

Scan Point for comp9-c4oh_beta_1.7Å

C	1.06868500	-1.59847600	0.36073400
C	-0.09364600	-1.29517300	1.31856600
C	1.19922300	0.78452800	-0.58471500
C	-1.20969900	-0.38771300	0.85869800
C	0.30787100	1.52747200	0.40935200
H	2.47449700	-0.06877300	0.92062600
H	0.69456800	-2.04332500	-0.56981500
H	0.61735500	0.47680500	-1.46316700
H	-0.56831400	-2.23683400	1.60719800
H	0.77366500	1.53299700	1.40085200

C	-0.00739400	2.95123200	-0.01817800
H	-0.69612900	3.42367700	0.68881800
H	0.91644100	3.53689700	-0.03958100
O	-1.02320100	0.90820600	0.60835500
H	-0.45595500	2.97141500	-1.01740900
H	1.94575000	1.50713300	-0.93531100
H	1.68809900	-2.36533200	0.83756200
H	-2.13597000	-0.52187000	1.41610400
O	-1.79316500	-1.12288900	-0.55872300
H	-1.11932300	-1.09513300	-1.26483800
C	-3.04402700	-0.54512200	-1.06396900
H	-2.90275600	0.51464000	-1.27922600
H	-3.30331900	-1.10151900	-1.96456700
H	-3.78893100	-0.70045600	-0.28511600
H	0.28003700	-0.83742300	2.24523100
O	2.93184200	-0.90389500	-0.92307200
H	3.60022300	-0.21728000	-1.06996600

Scan Point for comp9-c4oh_beta_2.0Å

C	0.91644000	-1.65221200	0.40373900
C	-0.17052200	-1.20611500	1.39338700
C	1.27989900	0.67214300	-0.62107700
C	-1.16022900	-0.16535200	0.98424100
C	0.50915500	1.55086100	0.35744300
H	2.48821400	-0.26341800	0.89146500
H	0.44889500	-2.05679100	-0.50046900
H	0.64347900	0.40093300	-1.47292100
H	-0.75134300	-2.07668900	1.70602800
H	0.99704100	1.56141600	1.33733600
C	0.28550400	2.96745200	-0.13740700
H	-0.33048700	3.53219100	0.56851600
H	1.25236700	3.47115800	-0.22762300
O	-0.87206400	1.04774700	0.64213600
H	-0.20227400	2.97001300	-1.11782500
H	2.08931600	1.29813200	-1.01548500
H	1.46174000	-2.47545900	0.87626600
H	-2.15528900	-0.22867600	1.41820400
O	-1.91865700	-1.01783600	-0.65833500
H	-1.31868200	-0.79983200	-1.39280500
C	-3.23620400	-0.49913000	-0.97382500
H	-3.22286100	0.59446500	-1.00246400
H	-3.54736500	-0.89952800	-1.94158200
H	-3.91059200	-0.85251700	-0.19314500

H	0.28888000	-0.79185900	2.30617000
O	2.81325900	-1.19955200	-0.93220300
H	3.54246000	-0.58929900	-1.12016400

Scan Point for comp9-c4oh_beta_2.5Å

C	0.64243900	-1.67985200	0.52771800
C	-0.21087800	-0.95573700	1.58814900
C	1.39734300	0.43738500	-0.71061100
C	-1.00561200	0.21695200	1.16559500
C	0.88086800	1.50975900	0.23784600
H	2.50982800	-0.63832000	0.78409400
H	-0.00280900	-2.00177200	-0.29577500
H	0.66230800	0.25175800	-1.50324300
H	-0.90726600	-1.66171800	2.04396700
H	1.40222700	1.48354300	1.19929900
C	0.87445100	2.91005300	-0.33906300
H	0.41667700	3.61614500	0.35947900
H	1.90836900	3.22206800	-0.51335300
O	-0.56734500	1.26911500	0.61212200
H	0.33460200	2.94258600	-1.29085500
H	2.28658800	0.86332200	-1.19019800
H	1.03898200	-2.58040000	1.00622200
H	-2.04389000	0.31146600	1.47648600
O	-2.27014000	-0.88305100	-0.68938800
H	-1.72245400	-0.70012300	-1.46831600
C	-3.54842700	-0.24968500	-0.87256200
H	-3.44722800	0.83977100	-0.94056800
H	-4.03934300	-0.62542300	-1.77722200
H	-4.15973800	-0.50335100	-0.00378800
H	0.43770800	-0.57422600	2.39733900
O	2.46187300	-1.73815200	-0.97567400
H	3.29040100	-1.32294400	-1.25965200

Scan Point for comp9-c4oh_beta_3.0Å

C	0.50505100	-1.66764800	0.58879800
C	-0.14479500	-0.78451600	1.68370800
C	1.54128800	0.26482600	-0.75416600
C	-0.81869200	0.43285500	1.19839300
C	1.18432200	1.43076200	0.15641200
H	2.52031000	-0.93499200	0.74215600

H	-0.23324000	-1.88611800	-0.18950500
H	0.78453100	0.16389100	-1.54156900
H	-0.88313200	-1.36402400	2.23982800
H	1.70610300	1.37868800	1.11656800
C	1.33068100	2.79607500	-0.47882500
H	0.97495100	3.57969900	0.19591500
H	2.39096700	2.97326500	-0.68217400
O	-0.28881900	1.37075500	0.54226800
H	0.77972600	2.85357400	-1.42288900
H	2.48114200	0.54538300	-1.24445800
H	0.76883600	-2.61364100	1.07052300
H	-1.86795700	0.62127700	1.42719100
O	-2.74295100	-0.75443500	-0.77330000
H	-2.34731500	-0.55541400	-1.63436100
C	-3.95255500	0.00805900	-0.64047900
H	-3.74969400	1.08602100	-0.64945600
H	-4.66087200	-0.23148600	-1.44265300
H	-4.39861900	-0.26564000	0.31852600
H	0.62735500	-0.45002500	2.39716200
O	2.22701000	-2.05872500	-0.97874700
H	3.10316600	-1.79655900	-1.30033400

Scan Point for comp9-c4oh_beta_3.3Å

C	0.28082400	-1.60913000	0.63331400
C	-0.22267500	-0.56633300	1.66769900
C	1.69237600	0.04490100	-0.74358400
C	-0.68592100	0.69608000	1.06781800
C	1.49384400	1.29737900	0.09999400
H	2.38821100	-1.24072300	0.83805800
H	-0.46142300	-1.72927200	-0.16290800
H	0.96835800	0.03676000	-1.56714100
H	-1.05169200	-0.98025300	2.24272700
H	1.94368400	1.20481400	1.09284400
C	1.90909800	2.58655800	-0.57312700
H	1.65512100	3.45031900	0.04764800
H	2.99432200	2.57178000	-0.71088500
O	0.01038300	1.49553900	0.38616500
H	1.43426800	2.69311500	-1.55345300
H	2.68996000	0.13727400	-1.18917500
H	0.35399000	-2.56195200	1.16524300
H	-1.71606800	1.03469200	1.19051400
O	-3.11197700	-0.55259500	-0.78827000
H	-2.90529800	-0.43862200	-1.72741400

C	-4.26232300	0.24769200	-0.47654400
H	-4.07070400	1.31226800	-0.65840400
H	-5.13508300	-0.06549900	-1.06262800
H	-4.47862300	0.09865300	0.58399400
H	0.59258100	-0.32048100	2.36658900
O	1.95576600	-2.37170200	-0.84713800
H	2.87584600	-2.28426000	-1.13971200

Scan Point for comp9-c4oh_beta_3.5Å

C	0.29020500	-1.59521200	0.66208800
C	-0.15985500	-0.53172400	1.70003100
C	1.70276900	0.01233400	-0.76777000
C	-0.60901000	0.73629300	1.10124600
C	1.55722000	1.27650100	0.06916200
H	2.41057600	-1.27591400	0.80639700
H	-0.47614300	-1.70425000	-0.11261500
H	0.95661100	0.01451400	-1.57136100
H	-0.98254200	-0.92057000	2.30106600
H	2.03167700	1.18175600	1.05027800
C	1.98453200	2.54939900	-0.62698600
H	1.76826500	3.42439900	-0.00766800
H	3.06493100	2.50730200	-0.79394500
O	0.08729200	1.51282200	0.39358800
H	1.48579000	2.65883500	-1.59504900
H	2.68977500	0.07681600	-1.24098500
H	0.35506300	-2.54491800	1.20062900
H	-1.62706300	1.10068500	1.24865300
O	-3.26593000	-0.54231300	-0.78447500
H	-3.08261000	-0.44157700	-1.72995900
C	-4.38750900	0.28853800	-0.44876100
H	-4.17533900	1.34647100	-0.64594900
H	-5.28353400	-0.00844100	-1.00755000
H	-4.57775800	0.15422300	0.61872100
H	0.67979900	-0.29964300	2.37431500
O	1.90558200	-2.41070800	-0.85593700
H	2.81921800	-2.34800300	-1.17394900

Scan Point for comp9-c4oh_beta_3.6Å

C	0.39593500	-1.61110600	0.69533400
C	-0.00503000	-0.57520800	1.78319200

C	1.64178900	0.06192500	-0.81393200
C	-0.55546600	0.66936000	1.22333400
C	1.50486000	1.31184000	0.04484700
H	2.50954000	-1.22279100	0.68305700
H	-0.42418600	-1.73410600	-0.02032400
H	0.84121500	0.04415900	-1.56325800
H	-0.75861600	-1.00053900	2.44686800
H	2.05015900	1.23045900	0.98929600
C	1.82455500	2.60675700	-0.66790100
H	1.60760500	3.46758900	-0.02938900
H	2.89268200	2.61688300	-0.90452900
O	0.05065500	1.47785500	0.47066900
H	1.25860100	2.69468800	-1.60056400
H	2.58940900	0.17012900	-1.35499700
H	0.53125200	-2.56546100	1.21197000
H	-1.58302000	0.97619600	1.42957200
O	-3.27235700	-0.57212200	-0.78593800
H	-3.07723900	-0.45264900	-1.72679800
C	-4.41375300	0.23266200	-0.45309000
H	-4.21883400	1.29657700	-0.63559400
H	-5.29846900	-0.07525000	-1.02376900
H	-4.61020300	0.08381300	0.61144600
H	0.87917400	-0.31333800	2.38553300
O	1.91471200	-2.35066400	-0.95476900
H	2.79479100	-2.24910100	-1.34849600

Scan Point for comp9-c4oh_beta_3.8Å

C	0.38121500	-1.59379300	0.72080900
C	0.01183200	-0.53239100	1.79581900
C	1.65941300	0.02723200	-0.81935300
C	-0.51892200	0.70998200	1.21319800
C	1.55036400	1.29234600	0.02155600
H	2.50322700	-1.25585400	0.69271400
H	-0.44552500	-1.70728600	0.01106800
H	0.85782700	0.01608000	-1.56768800
H	-0.74519100	-0.93071200	2.47226300
H	2.09509600	1.21265300	0.96629900
C	1.89638300	2.57113700	-0.70800800
H	1.69545700	3.44386400	-0.08039400
H	2.96479100	2.55759100	-0.94314300
O	0.10008600	1.49340900	0.44479600
H	1.33312300	2.65833700	-1.64233300
H	2.60877800	0.10586800	-1.36223300

H	0.49648200	-2.54386000	1.25001300
H	-1.54312600	1.03477000	1.40938500
O	-3.41674800	-0.60084000	-0.86629800
H	-3.35059900	-0.48165900	-1.82488400
C	-4.41560200	0.30023400	-0.36490200
H	-4.13422100	1.34619900	-0.53859000
H	-5.39234700	0.10961600	-0.82612500
H	-4.49253800	0.12512300	0.71088100
H	0.90630400	-0.27904900	2.38600600
O	1.87268700	-2.39349700	-0.92502900
H	2.75511300	-2.32403500	-1.32033600

Scan Point for comp9-c4oh_beta_4.0Å

C	0.53203100	-1.63212900	0.64869300
C	0.04336700	-0.62180800	1.72509100
C	1.75546500	0.10790200	-0.80460000
C	-0.54213700	0.59649500	1.14416100
C	1.53580900	1.34076300	0.06228000
H	2.62656600	-1.15341200	0.70993600
H	-0.25480000	-1.79086600	-0.09695800
H	0.98229500	0.06428200	-1.58117200
H	-0.71566200	-1.08556600	2.35601500
H	2.04531700	1.26725400	1.02715700
C	1.83214300	2.65746500	-0.61962400
H	1.56309700	3.49980800	0.02375000
H	2.90653700	2.70932700	-0.81977100
O	0.05840900	1.43976500	0.42618900
H	1.29481900	2.74036700	-1.56947300
H	2.71520100	0.26174400	-1.31208600
H	0.69291200	-2.58160500	1.16691100
H	-1.59471300	0.84648600	1.29622600
O	-3.77922900	-0.77251700	-0.76554800
H	-3.74403200	-0.78310200	-1.73316400
C	-4.56123900	0.35876200	-0.35377600
H	-4.10183000	1.30093100	-0.67704200
H	-5.58302200	0.30206100	-0.74856800
H	-4.60329100	0.33856800	0.73789800
H	0.89056200	-0.32308200	2.36172000
O	2.13469500	-2.28960400	-0.95609400
H	3.01824300	-2.14192900	-1.32700900

Scan Point for comp9-c4oh_beta_4.4Å

C	1.01526300	-1.74280100	0.22554200
C	-0.02690100	-1.03008900	1.13440200
C	2.20528000	0.40649400	-0.55048300
C	-0.66182200	0.12043600	0.47420200
C	1.41435200	1.42118500	0.26427500
H	2.78264800	-0.87354400	1.08251100
H	0.58157000	-1.92748500	-0.76356100
H	1.77812700	0.33231800	-1.55787200
H	-0.81610000	-1.72702400	1.41843700
H	1.57580300	1.30584100	1.33934900
C	1.59103000	2.85900200	-0.16893900
H	0.92463400	3.52012100	0.39215100
H	2.62310400	3.15788700	0.03714600
O	-0.07733300	1.16418700	0.07917900
H	1.40069700	2.97559100	-1.24036900
H	3.21361100	0.82409700	-0.65585200
H	1.21546700	-2.71403100	0.68654300
H	-1.73306100	0.12960400	0.25861500
O	-4.78728900	-0.84418800	-0.71321500
H	-5.07050900	-0.68974500	-1.62620500
C	-5.16356600	0.29395300	0.07658200
H	-4.66327800	1.20564400	-0.27241100
H	-6.24908700	0.45055200	0.05981100
H	-4.85254700	0.08712400	1.10343100
H	0.46816200	-0.67221100	2.05008000
O	3.17725000	-1.81804800	-0.72327700
H	4.08059800	-1.46652900	-0.70214000

Scan Point for comp9-c5oh_alpha_1.4Å

C	0.69473100	2.16009700	0.30338500
C	-0.63604600	1.77624100	-0.36339300
C	1.83851300	-0.18856600	0.26787800
C	-1.32149600	0.60467500	0.33455600
C	0.56030500	-0.92452300	-0.17359500
H	1.97323100	1.33718700	-1.22849100
H	0.58510000	2.14777000	1.39546000
H	1.90054600	-0.28273600	1.36197000
H	-1.34024500	2.61341500	-0.33269900
H	0.32389300	-0.68153000	-1.21641700
C	0.63186300	-2.43478700	-0.00508500
H	-0.32983600	-2.88475500	-0.27060400

H	1.39902600	-2.85824400	-0.65782000
O	-0.51751400	-0.47283000	0.70140600
H	2.80485000	1.71803900	0.27933100
H	0.92093600	3.19564800	0.02813900
H	-1.80288900	0.93066900	1.25917600
O	-2.38378100	0.18621000	-0.47565200
H	-2.13699700	-0.00157100	-1.40617100
C	-3.34929200	-0.82493600	0.04614800
H	-4.13709100	-0.86811800	-0.70239200
H	-2.82830000	-1.77226700	0.16430700
H	-3.70946000	-0.42247000	0.99027100
O	2.95163300	-0.88208300	-0.32858500
H	3.76305900	-0.40247400	-0.10216400
H	-0.46664000	1.53663500	-1.42161200
H	0.86971600	-2.70237100	1.03050300

Scan Point for comp9-c5oh_alpha_1.5Å

C	0.72789600	2.16427400	0.29273900
C	-0.61551100	1.78241300	-0.35312100
C	1.84121500	-0.19784500	0.26527900
C	-1.28205500	0.62236000	0.36770200
C	0.55921400	-0.92603100	-0.17850700
H	1.98439600	1.31509500	-1.24345800
H	0.63206600	2.16751700	1.38620400
H	1.89698700	-0.28471800	1.36026800
H	-1.31609200	2.62161900	-0.31438000
H	0.31899300	-0.67970700	-1.21920700
C	0.61637800	-2.43574200	-0.00713100
H	-0.35073000	-2.87653700	-0.26783100
H	1.37621100	-2.86597000	-0.66376800
O	-0.51966500	-0.46846500	0.69915800
H	2.83159500	1.69631200	0.25600400
H	0.95789100	3.19411800	0.00029300
H	-1.79135600	0.93831700	1.27948100
O	-2.43955300	0.20642400	-0.49090000
H	-2.17046300	-0.01554800	-1.40658200
C	-3.36795800	-0.81686700	0.04916700
H	-4.16807400	-0.89354500	-0.68436000
H	-2.83089200	-1.75503500	0.17439200
H	-3.73066000	-0.41745700	0.99407100
O	2.94865900	-0.90693800	-0.32142500
H	3.76475600	-0.43950900	-0.08635700
H	-0.46215900	1.53570900	-1.41149000

H	0.85730300	-2.70420100	1.02737000

Scan Point for comp9-c5oh_alpha_1.6Å

C	0.75943800	2.16775700	0.28012500
C	-0.59691600	1.78467600	-0.34185700
C	1.84659800	-0.20563400	0.26154500
C	-1.24260600	0.63691400	0.40494800
C	0.55993100	-0.92747600	-0.17981500
H	1.99305400	1.29365300	-1.26078900
H	0.67911200	2.18762400	1.37462600
H	1.89986800	-0.28436500	1.35721200
H	-1.29515400	2.62489100	-0.29664100
H	0.31007100	-0.67602500	-1.21642800
C	0.60392000	-2.43647600	-0.00784800
H	-0.36935800	-2.86808100	-0.26042300
H	1.35370200	-2.87168500	-0.67255800
O	-0.51656200	-0.46260700	0.70520600
H	2.85713200	1.67778200	0.22873600
H	0.98982000	3.19184400	-0.03113400
H	-1.78187900	0.94174200	1.30206400
O	-2.49182600	0.22189300	-0.50456100
H	-2.20380400	-0.02750300	-1.40598100
C	-3.39686000	-0.80497700	0.04523600
H	-4.20408100	-0.90874600	-0.67827800
H	-2.85143900	-1.73802700	0.18017500
H	-3.76453300	-0.40698300	0.98929800
O	2.94700400	-0.92938100	-0.31827600
H	3.76783500	-0.47385600	-0.07634100
H	-0.46087600	1.52758900	-1.39947800
H	0.85265500	-2.70757600	1.02390800

Scan Point for comp9-c5oh_alpha_1.7Å

C	0.78340000	2.17202000	0.26454300
C	-0.58458900	1.78122200	-0.33183700
C	1.85425100	-0.20783200	0.26010400
C	-1.20357200	0.64451100	0.44159300
C	0.56829300	-0.92894000	-0.18543400
H	2.00100100	1.27621900	-1.27710400
H	0.71807100	2.21107200	1.35943000
H	1.90014100	-0.27709900	1.35670800

H	-1.28380500	2.61968200	-0.27974200
H	0.31202600	-0.66963100	-1.21775600
C	0.60538500	-2.43740300	-0.01703200
H	-0.37080400	-2.86355200	-0.26729200
H	1.35016200	-2.87210600	-0.68753000
O	-0.51165500	-0.46454000	0.70383600
H	2.87676500	1.66885100	0.20378800
H	1.00904100	3.19020800	-0.06829200
H	-1.76547900	0.93459400	1.32852000
O	-2.55434800	0.23962100	-0.50786300
H	-2.26426400	-0.01392300	-1.40603200
C	-3.42981700	-0.79999300	0.04431800
H	-4.25074100	-0.92190100	-0.66213400
H	-2.87237200	-1.72848800	0.16921100
H	-3.79257500	-0.41859100	0.99761000
O	2.95327600	-0.94186200	-0.30695400
H	3.77549000	-0.49285900	-0.05756100
H	-0.46688400	1.51291600	-1.38833800
H	0.85835800	-2.71308500	1.01228000

Scan Point for comp9-c5oh_alpha_2.0Å

C	0.85639400	2.18043800	0.23591200
C	-0.55301800	1.78311400	-0.26910800
C	1.88615300	-0.21138100	0.24046400
C	-1.09705900	0.66329400	0.55226300
C	0.59637100	-0.93909900	-0.18475500
H	1.98624100	1.23009800	-1.34197300
H	0.85503200	2.25685600	1.33017900
H	1.93849700	-0.25122200	1.33811600
H	-1.24843500	2.61968000	-0.17664700
H	0.31170300	-0.67673500	-1.20743000
C	0.62255000	-2.44317500	0.00072600
H	-0.36377000	-2.86290200	-0.21752300
H	1.34327700	-2.88716100	-0.68929700
O	-0.48669800	-0.46582800	0.72042600
H	2.93454700	1.64482700	0.08877300
H	1.06080900	3.18498700	-0.14716400
H	-1.74758700	0.89303100	1.39289400
O	-2.72566800	0.27289900	-0.54100000
H	-2.41279000	0.00010700	-1.42137600
C	-3.55430800	-0.77917600	0.01280700
H	-4.38965800	-0.95954700	-0.66824600
H	-2.97506100	-1.69566600	0.15190900

H	-3.92735400	-0.41467100	0.97045800
O	2.97033700	-0.97081600	-0.31583700
H	3.80005200	-0.53089200	-0.07487400
H	-0.49974900	1.50036700	-1.32636800
H	0.90537100	-2.71051100	1.02395300

Scan Point for comp9-c5oh_alpha_2.5Å

C	0.97138700	2.18727700	0.20402300
C	-0.47189500	1.78142800	-0.21770200
C	1.96328500	-0.21683700	0.22974700
C	-0.95236500	0.67838900	0.63409700
C	0.67604700	-0.95054200	-0.19531700
H	2.04094700	1.18814000	-1.38820500
H	1.02002700	2.30545600	1.29272600
H	2.00720600	-0.23162400	1.32838500
H	-1.16114900	2.61840200	-0.09815800
H	0.37570600	-0.67958500	-1.21078800
C	0.68786600	-2.45171200	-0.00674100
H	-0.30639700	-2.85914600	-0.21150500
H	1.39208800	-2.89903400	-0.71146200
O	-0.42570300	-0.47365600	0.71119200
H	3.03226400	1.62060400	0.00866300
H	1.15188000	3.17510800	-0.22975500
H	-1.70545300	0.84531200	1.40173300
O	-3.05152000	0.23926500	-0.65070400
H	-2.75266700	-0.20306500	-1.46019200
C	-3.88006800	-0.67371400	0.09038200
H	-4.75092800	-0.97388900	-0.50312900
H	-3.31907500	-1.56621400	0.39093100
H	-4.22147000	-0.14276900	0.98147100
O	3.04105600	-0.99715200	-0.30371200
H	3.87418400	-0.55982600	-0.06927600
H	-0.47023700	1.47500600	-1.27059500
H	0.98610400	-2.72321300	1.01047100

Scan Point for comp9-c5oh_alpha_3.0Å

C	1.16221400	2.17904900	0.17120000
C	-0.33343700	1.85141800	-0.11505300
C	2.02372600	-0.27021100	0.18101900
C	-0.82072500	0.76641300	0.74835800

C	0.68412000	-0.95744200	-0.14901700
H	2.04380100	1.08980800	-1.47797600
H	1.30576100	2.31474800	1.24886800
H	2.13675500	-0.25832600	1.27455900
H	-0.96230900	2.72497800	0.06214500
H	0.33744100	-0.69940400	-1.15322800
C	0.64081700	-2.45106900	0.08483200
H	-0.38008800	-2.81917800	-0.05121800
H	1.28292300	-2.94715800	-0.64607600
O	-0.36763600	-0.41215900	0.78928800
H	3.16516400	1.50031800	-0.17639400
H	1.35554700	3.14689600	-0.30001700
H	-1.60125800	0.93808400	1.49074100
O	-3.34417000	0.23731500	-0.78535700
H	-2.99312300	-0.30685800	-1.50558100
C	-4.11505400	-0.60473800	0.08543900
H	-4.94165000	-1.08138600	-0.45509700
H	-3.49204100	-1.38038700	0.54706700
H	-4.52710400	0.03621600	0.86839200
O	3.02390100	-1.11824700	-0.39750800
H	3.89262300	-0.72614500	-0.22058900
H	-0.44418100	1.54825400	-1.16602400
H	0.98734300	-2.70725100	1.09053400

Scan Point for comp9-c5oh_alpha_3.3Å

C	1.33766800	2.15362800	0.11985100
C	-0.18933900	1.92464600	-0.08567900
C	2.02368400	-0.34871400	0.15328000
C	-0.70957000	0.88851600	0.81673800
C	0.62961300	-0.95044100	-0.11331300
H	2.06602400	0.96931700	-1.53870900
H	1.54224000	2.30517400	1.18534300
H	2.17350200	-0.31787600	1.24214600
H	-0.74857600	2.84180200	0.10498100
H	0.25759600	-0.68479000	-1.10657200
C	0.49562200	-2.43315400	0.14966700
H	-0.55336700	-2.73200900	0.06744900
H	1.06623600	-2.98254600	-0.60222800
O	-0.34394600	-0.31907200	0.85603300
H	3.26973000	1.32794300	-0.29650700
H	1.57266600	3.09385200	-0.38686700
H	-1.44975900	1.12430700	1.58317900
O	-3.45822800	0.21612500	-0.88113500

H	-3.28347500	-0.37282800	-1.62963000
C	-4.18828100	-0.51973100	0.11242200
H	-5.14399700	-0.88272500	-0.28478300
H	-3.60761900	-1.37091800	0.48809300
H	-4.38823700	0.16787000	0.93752400
O	2.94672300	-1.27522200	-0.43280100
H	3.84295000	-0.92742300	-0.30639100
H	-0.37287900	1.61265800	-1.12440200
H	0.87166100	-2.69825500	1.14231300

Scan Point for comp9-c5oh_alpha_3.5Å

C	1.40038000	2.14582800	0.09027600
C	-0.13726600	1.94340500	-0.05215600
C	2.03624600	-0.36783300	0.13043300
C	-0.64786500	0.91989100	0.86957700
C	0.62613700	-0.94942700	-0.09462700
H	2.04660700	0.92851300	-1.57905200
H	1.64807900	2.30690600	1.14511400
H	2.21114000	-0.32369400	1.21518900
H	-0.67160000	2.87192000	0.15450300
H	0.23039300	-0.68169100	-1.07817900
C	0.47473800	-2.42749700	0.18312900
H	-0.58169300	-2.70751600	0.13874800
H	1.00963700	-2.99240800	-0.58332300
O	-0.31072500	-0.29587700	0.89740900
H	3.29977200	1.27698400	-0.38386000
H	1.63224300	3.07499600	-0.43781200
H	-1.36641300	1.16966400	1.65255500
O	-3.56474000	0.21050600	-0.93003800
H	-3.43814900	-0.39844900	-1.67219600
C	-4.24936600	-0.49143200	0.11853300
H	-5.22433300	-0.86127100	-0.22168300
H	-3.65479700	-1.33426000	0.49149100
H	-4.40693200	0.22080500	0.93192100
O	2.93162800	-1.31690400	-0.46221900
H	3.83575400	-0.98317100	-0.35467300
H	-0.36707900	1.62999200	-1.08172900
H	0.87921100	-2.69218400	1.16463000

Scan Point for comp9-c5oh_alpha_3.6Å

C	1.42787000	2.13275800	0.04484600
C	-0.12029200	1.96978100	-0.01627700
C	1.99686900	-0.39701900	0.09940800
C	-0.60569100	0.98113400	0.95463100
C	0.56145100	-0.94219400	-0.04046800
H	1.95141400	0.86897400	-1.63233300
H	1.73199000	2.30334300	1.08339500
H	2.23170600	-0.33962100	1.17225000
H	-0.61884500	2.91691200	0.19513500
H	0.12431900	-0.67952300	-1.00745000
C	0.38535100	-2.40997200	0.27473900
H	-0.67780600	-2.66608400	0.27728200
H	0.87764500	-3.00332700	-0.49864300
O	-0.30542000	-0.24406500	0.98573300
H	3.27573400	1.20121600	-0.51167500
H	1.65785700	3.04633300	-0.51040200
H	-1.26883300	1.26714900	1.77357000
O	-3.47984500	0.14814200	-1.04669300
H	-3.50757200	-0.49607200	-1.76923400
C	-4.10335700	-0.43515700	0.10768400
H	-5.14353200	-0.71349200	-0.10095600
H	-3.55612400	-1.31961400	0.45520600
H	-4.09301300	0.32358000	0.89376700
O	2.83144500	-1.38119800	-0.52394400
H	3.74595900	-1.06025300	-0.49369900
H	-0.41011300	1.63745700	-1.02459100
H	0.82209300	-2.66304200	1.24544800

Scan Point for comp9-c5oh_alpha_3.8Å

C	1.38159900	2.14897200	0.01425900
C	-0.16396000	1.94954200	0.01982200
C	2.01312600	-0.36761200	0.07064800
C	-0.58249500	0.95808800	1.01842300
C	0.58622100	-0.94496800	-0.01475000
H	1.87449300	0.88089600	-1.66937700
H	1.72317600	2.34007700	1.03750400
H	2.28342100	-0.29420700	1.13407100
H	-0.67419700	2.88698900	0.24568100
H	0.10779900	-0.69524700	-0.96558300
C	0.45013800	-2.41477600	0.30947700
H	-0.60733100	-2.69124100	0.34687600
H	0.92778600	-2.99993800	-0.47923100
O	-0.25355600	-0.25993700	1.04269800

H	3.22928100	1.25704500	-0.60028000
H	1.56641700	3.06070500	-0.56053500
H	-1.21493900	1.23453000	1.86469200
O	-3.58022400	0.05950700	-1.13705300
H	-3.59505900	-0.68546400	-1.75540400
C	-4.07209200	-0.39692700	0.13220900
H	-5.09294300	-0.78878300	0.04598100
H	-3.42424200	-1.17268900	0.55808600
H	-4.08235200	0.46640500	0.80182300
O	2.84949800	-1.33739200	-0.57206500
H	3.75844900	-0.99967300	-0.56496700
H	-0.49004300	1.60148400	-0.97211800
H	0.92317000	-2.65782900	1.26569100

Scan Point for comp9-c5oh_alpha_4.0Å

C	1.22749000	2.17585700	-0.07036500
C	-0.29807200	1.91927700	0.11759000
C	1.96528300	-0.31297100	-0.01804300
C	-0.55649700	0.95432400	1.19324100
C	0.56455000	-0.94520800	0.10055600
H	1.57569700	0.87356300	-1.76251000
H	1.67601400	2.41365800	0.90031100
H	2.36952400	-0.19930800	0.99821200
H	-0.81836400	2.84520100	0.36673000
H	-0.03790700	-0.76194800	-0.79349900
C	0.54081400	-2.40212900	0.50325800
H	-0.48882900	-2.72262100	0.68517200
H	0.94747800	-3.00452300	-0.31181600
O	-0.17086100	-0.24690900	1.22443000
H	3.02802800	1.33556900	-0.86856200
H	1.30884600	3.07464400	-0.68784800
H	-1.09850300	1.24049400	2.09712800
O	-3.43993100	-0.21544800	-1.32020100
H	-3.68590000	-1.04769900	-1.74988900
C	-3.79354100	-0.29937300	0.06838200
H	-4.86923000	-0.47114300	0.19699100
H	-3.23979700	-1.09899100	0.57491000
H	-3.53493700	0.66002700	0.52330700
O	2.74159600	-1.27605100	-0.74158000
H	3.62199600	-0.90077800	-0.89614200
H	-0.72055800	1.51931400	-0.81679300
H	1.13873500	-2.57538100	1.40307700

Scan Point for comp9-c5oh_alpha_4.4Å

C	0.77095400	2.21513500	0.11200200
C	-0.62706000	1.56146800	0.32221500
C	2.11977000	0.00907700	-0.09223600
C	-0.57674800	0.46883000	1.30221700
C	0.93635900	-0.97371600	0.00262100
H	1.33861800	1.18830600	-1.70682800
H	1.19846800	2.47398100	1.08682400
H	2.52740800	0.14327000	0.92025900
H	-1.34853800	2.29729000	0.67957000
H	0.26052400	-0.87740300	-0.85205700
C	1.30098600	-2.41769800	0.26085200
H	0.39475500	-3.00381600	0.43854800
H	1.80229600	-2.82277800	-0.62079500
O	0.10487600	-0.58893600	1.20725900
H	2.67516600	1.93672800	-0.82741200
H	0.58801800	3.15428300	-0.41745700
H	-1.13092700	0.52214800	2.24150000
O	-4.03991400	-0.27526400	-1.30790700
H	-4.06521500	-1.16302600	-1.69372900
C	-4.03366900	-0.40080300	0.12223500
H	-4.92503200	-0.93131700	0.47882100
H	-3.13834900	-0.92832600	0.47492700
H	-4.03965100	0.61198300	0.53128700
O	3.08599700	-0.65395000	-0.91694300
H	3.84121100	-0.05750200	-1.03535100
H	-0.98405000	1.15433800	-0.63613800
H	1.96893000	-2.51309300	1.12228200

Scan Point for comp9-c5oh_beta_1.4Å

C	0.17646900	-2.07175600	-0.28804300
C	-0.78718800	-1.55945800	0.79617300
C	1.78385300	-0.01870000	-0.43887200
C	-1.34079100	-0.15299500	0.55910600
C	0.86106000	0.90116100	0.38134600
H	1.96896000	-1.71389000	0.86047100
H	-0.22499100	-1.87244500	-1.29109400
H	1.57800100	0.18674900	-1.49988700
H	-1.64698400	-2.22884900	0.91100600
H	0.88513700	0.61760600	1.44038100

C	1.18951600	2.37994800	0.24238000
H	0.45282700	2.97633400	0.79002400
H	2.17916400	2.59386000	0.65386300
O	-0.48702200	0.72188000	-0.13596400
H	1.17735900	2.68566500	-0.80996200
H	2.26125700	-2.05996300	-0.84451800
H	0.23149500	-3.16142100	-0.19308500
H	-0.27772400	-1.54676000	1.76538300
H	-1.68822000	0.29945100	1.49419400
O	-2.49180200	-0.24082300	-0.23301800
H	-2.34973700	-0.72037400	-1.07835700
C	-3.32481300	0.98276700	-0.44539800
H	-2.76604100	1.68021900	-1.06496500
H	-4.22804600	0.61980300	-0.93011300
H	-3.52439200	1.36877800	0.55170900
O	3.13724000	0.37175500	-0.13759200
H	3.73804700	-0.22689800	-0.60671500

Scan Point for comp9-c5oh_beta_1.5Å

C	-0.16613900	2.07710200	-0.26288500
C	0.77782000	1.54929500	0.83137400
C	-1.76614600	0.02441600	-0.45923900
C	1.31706200	0.14546400	0.60552500
C	-0.88235800	-0.89293300	0.40502000
H	-1.99089800	1.71826800	0.83482200
H	0.25534000	1.89335700	-1.26073400
H	-1.51439700	-0.18456900	-1.50947600
H	1.64202900	2.20904800	0.96502700
H	-0.93250700	-0.59055800	1.45731700
C	-1.21797000	-2.37036700	0.28238600
H	-0.50480900	-2.96174700	0.86525600
H	-2.22185200	-2.56606400	0.66746600
O	0.48997700	-0.74190500	-0.07313500
H	-1.17632800	-2.69696500	-0.76266800
H	-2.23324300	2.06548300	-0.87787000
H	-0.22186400	3.16518900	-0.15262800
H	0.25646300	1.53275500	1.79541300
H	1.73680700	-0.29269900	1.51635100
O	2.53311300	0.25008200	-0.26641300
H	2.33555900	0.69957800	-1.11603100
C	3.31251200	-0.99403200	-0.50319700
H	2.71449700	-1.68230800	-1.09663500
H	4.21010400	-0.66799500	-1.02497000

H	3.54362700	-1.38513500	0.48535200
O	-3.13139200	-0.36337900	-0.21553500
H	-3.70928300	0.23306900	-0.71533800

Scan Point for comp9-c5oh_beta_1.6Å

C	0.09421400	2.14978900	0.01528200
C	0.93050200	1.39481700	1.05930200
C	-1.46526300	0.15793900	-0.55517600
C	1.33434300	-0.02741200	0.73790300
C	-1.04349500	-0.79665900	0.58414400
H	-1.92168100	1.80455800	0.73267600
H	0.62512600	2.15888700	-0.94430800
H	-0.85843300	-0.07665400	-1.44392500
H	1.86224700	1.93854300	1.24279800
H	-1.32961300	-0.36428800	1.54948300
C	-1.60854700	-2.20305000	0.46006400
H	-1.18767500	-2.83539500	1.24777600
H	-2.69414600	-2.18923100	0.57553600
O	0.40984800	-1.01389700	0.62803100
H	-1.36438300	-2.64249800	-0.51291900
H	-1.80724600	2.22916600	-0.97655400
H	0.04176300	3.19471400	0.33866300
H	0.40230700	1.34506800	2.02073700
H	2.15561100	-0.37920600	1.36325100
O	2.11284500	0.04352100	-0.65812800
H	1.47123200	0.02158300	-1.39797700
C	3.13287800	-1.00320000	-0.87371600
H	2.67482100	-1.98510500	-0.75209700
H	3.50548600	-0.85403900	-1.88599700
H	3.91327600	-0.82020900	-0.13793100
O	-2.84327500	-0.14208600	-0.84406100
H	-3.15461500	0.49498600	-1.50532000

Scan Point for comp9-c5oh_beta_1.7Å

C	0.10031300	2.15021100	0.00928800
C	0.92634100	1.40765200	1.07016700
C	-1.45388600	0.15557700	-0.56276100
C	1.30594500	-0.02381300	0.79127700
C	-1.06085500	-0.79160300	0.59135900
H	-1.92290900	1.81087200	0.71057300

H	0.64150900	2.14706600	-0.94403500
H	-0.83148800	-0.08696900	-1.43787400
H	1.86378000	1.94304500	1.24593000
H	-1.36951400	-0.35488800	1.54730500
C	-1.60959800	-2.20261500	0.45981900
H	-1.20924400	-2.82653100	1.26461400
H	-2.69822400	-2.19522500	0.54172600
O	0.39770300	-0.99808700	0.68407000
H	-1.33234000	-2.64591500	-0.50234700
H	-1.79076900	2.22370900	-1.00025000
H	0.04598600	3.19842100	0.32131400
H	0.39302200	1.38324400	2.03130500
H	2.15733600	-0.37771300	1.37190100
O	2.13609000	0.04608200	-0.69060500
H	1.48860900	0.01979700	-1.42254900
C	3.11819600	-1.02781100	-0.88841100
H	2.63567000	-1.99814900	-0.76042800
H	3.50949300	-0.91009500	-1.89881700
H	3.90244100	-0.86775900	-0.15048300
O	-2.82665600	-0.14595000	-0.87193600
H	-3.12937800	0.49073100	-1.53758100

Scan Point for comp9-c5oh_beta_2.0Å

C	0.08788900	2.15539200	-0.02734300
C	0.88563800	1.46751600	1.09174600
C	-1.42501400	0.13653000	-0.58302000
C	1.21940100	0.02081000	0.95135900
C	-1.10805600	-0.78022500	0.61530600
H	-1.95177200	1.82161700	0.63531100
H	0.65914800	2.10491700	-0.96043400
H	-0.74296500	-0.12025700	-1.40761100
H	1.83141100	1.99034900	1.25254600
H	-1.47787100	-0.33112900	1.54249400
C	-1.59999200	-2.20846300	0.47495300
H	-1.24241000	-2.80486600	1.31944100
H	-2.69146400	-2.22806800	0.48046700
O	0.35866400	-0.93811300	0.82451000
H	-1.24391600	-2.66043800	-0.45642600
H	-1.77538300	2.18636000	-1.08269000
H	0.02519400	3.21568700	0.23746500
H	0.32999500	1.51974300	2.04355800
H	2.13398600	-0.33053000	1.42265600
O	2.23759000	0.05245100	-0.76977100

H	1.58815100	0.03270300	-1.49468600
C	3.10728400	-1.10056400	-0.90604100
H	2.53419600	-2.02867200	-0.82942500
H	3.61024600	-1.04325700	-1.87446500
H	3.84402400	-1.03825600	-0.10440400
O	-2.77115800	-0.19273200	-0.96390400
H	-3.04771000	0.42776100	-1.65565300

Scan Point for comp9-c5oh_beta_2.5Å

C	0.08525100	2.11252700	-0.02547000
C	0.71550100	1.48480800	1.23635700
C	-1.41558200	0.10603100	-0.66422700
C	1.04372600	0.04737200	1.18369900
C	-1.22107100	-0.75447500	0.59907200
H	-2.02768800	1.86412900	0.39962200
H	0.77346400	1.97559100	-0.86492500
H	-0.67105300	-0.20550400	-1.41163400
H	1.63189800	2.01312700	1.50617300
H	-1.63835200	-0.25571400	1.47933800
C	-1.70554700	-2.18504400	0.49708100
H	-1.42245000	-2.73658600	1.39831400
H	-2.79449400	-2.19501200	0.41887700
O	0.24539400	-0.90046600	0.91000200
H	-1.28451800	-2.68653200	-0.37986100
H	-1.63295300	2.13557000	-1.29984400
H	0.02766100	3.18859800	0.16362700
H	0.01881900	1.58294400	2.08895200
H	2.00364400	-0.31248100	1.54723600
O	2.52166100	0.07300300	-0.83249800
H	1.90543700	0.03981700	-1.58030600
C	3.33051300	-1.11599200	-0.86067400
H	2.72054400	-2.01558700	-0.71839300
H	3.87148100	-1.19144500	-1.81054100
H	4.05292900	-1.03417500	-0.04576800
O	-2.73109300	-0.21915800	-1.13556700
H	-2.94533700	0.38179700	-1.86563000

Scan Point for comp9-c5oh_beta_3.0Å

C	0.00380000	2.06383800	0.04684300
C	0.48610100	1.41621200	1.37457700

C	-1.49725000	0.10106900	-0.72892000
C	0.85193300	-0.00268300	1.25075700
C	-1.37169500	-0.77664400	0.53095200
H	-2.13857100	1.86934000	0.29989900
H	0.76267400	1.89806700	-0.72432700
H	-0.72797200	-0.21976500	-1.44618400
H	1.35433500	1.94761700	1.76722600
H	-1.80612300	-0.28027600	1.40308600
C	-1.86834200	-2.19866600	0.39807400
H	-1.62665400	-2.76213600	1.30398100
H	-2.95395000	-2.19061000	0.28092600
O	0.09346700	-0.93672600	0.86538600
H	-1.42366600	-2.69759600	-0.46835600
H	-1.60475300	2.13984200	-1.36186300
H	-0.03349700	3.14104900	0.23196400
H	-0.32133700	1.47276900	2.12399500
H	1.84615900	-0.35913800	1.51942600
O	2.99627200	0.14610600	-0.84201000
H	2.57471200	0.09134600	-1.71206400
C	3.84982500	-0.99808200	-0.68189000
H	3.27326000	-1.93118600	-0.68568800
H	4.60768400	-1.03787300	-1.47351800
H	4.35267800	-0.89149300	0.28222100
O	-2.79839700	-0.18846900	-1.25701900
H	-2.96506700	0.41845800	-1.99460300

Scan Point for comp9-c5oh_beta_3.3Å

C	-0.01256400	2.00961200	0.13524400
C	0.41763000	1.28435900	1.44316200
C	-1.59740800	0.15458900	-0.73899400
C	0.74473100	-0.13186300	1.22838600
C	-1.49973100	-0.79717200	0.46904800
H	-2.16149800	1.89925300	0.37443600
H	0.74581600	1.83689300	-0.63579700
H	-0.84731700	-0.16043900	-1.47877100
H	1.29332400	1.76479400	1.88188700
H	-1.91740300	-0.34152000	1.37080900
C	-2.03682000	-2.19346900	0.25211700
H	-1.80026900	-2.82040700	1.11667000
H	-3.12314000	-2.14806600	0.15097800
O	-0.03695300	-1.01785400	0.78373900
H	-1.61653500	-2.64753300	-0.65035300
H	-1.61205000	2.22389300	-1.27255200

H	0.00174200	3.07887600	0.36400300
H	-0.40737400	1.32809100	2.17265300
H	1.73871500	-0.52601800	1.44500400
O	3.30725300	0.16325400	-0.82986300
H	3.00092100	0.08609200	-1.74525300
C	4.27412200	-0.87111300	-0.58931700
H	3.82869400	-1.86753600	-0.69939500
H	5.12912300	-0.78099700	-1.27025800
H	4.62603900	-0.74959800	0.43794300
O	-2.91284400	-0.05306000	-1.26913800
H	-3.04751900	0.57532500	-1.99508900

Scan Point for comp9-c5oh_beta_3.5Å

C	-0.04878700	2.00802100	0.13796900
C	0.34425900	1.29684600	1.46516500
C	-1.60791500	0.14321300	-0.76116700
C	0.67742300	-0.12145500	1.27482000
C	-1.54450200	-0.79571300	0.45912500
H	-2.20361600	1.89922600	0.31743700
H	0.73113900	1.82743000	-0.60942300
H	-0.83699600	-0.17922700	-1.47592100
H	1.20714200	1.78224300	1.92339000
H	-1.98769300	-0.33073200	1.34378200
C	-2.07502400	-2.19445000	0.24176600
H	-1.86321200	-2.81210900	1.11931800
H	-3.15801300	-2.15056200	0.10914000
O	-0.09122600	-1.01243000	0.81759000
H	-1.62906800	-2.65787700	-0.64346200
H	-1.60782700	2.20676400	-1.31667700
H	-0.04106200	3.07965600	0.35567800
H	-0.50105600	1.34796000	2.17054200
H	1.66488200	-0.51288800	1.52379100
O	3.45626100	0.16741600	-0.83340400
H	3.17587000	0.08087400	-1.75624000
C	4.41591200	-0.86422100	-0.55514800
H	3.97377700	-1.86182700	-0.66774000
H	5.28986700	-0.78074300	-1.21246500
H	4.73858600	-0.73223700	0.48039000
O	-2.90767300	-0.07062300	-1.32636200
H	-3.02191900	0.55041100	-2.06208200

Scan Point for comp9-c5oh_beta_3.6Å

C	-0.03160000	1.99036500	0.17672500
C	0.33802400	1.25322700	1.49804200
C	-1.62364700	0.16471700	-0.75629900
C	0.66831900	-0.15796400	1.26259500
C	-1.56085000	-0.79833900	0.44568400
H	-2.18836200	1.91686000	0.34445700
H	0.75080200	1.80614700	-0.56734900
H	-0.86694800	-0.15805500	-1.48589600
H	1.19933400	1.72274400	1.97509600
H	-1.99331600	-0.34838600	1.34321500
C	-2.10304600	-2.18839300	0.20285600
H	-1.88616300	-2.82674500	1.06421300
H	-3.18697300	-2.13504600	0.08172600
O	-0.10505500	-1.03275000	0.78378200
H	-1.66873100	-2.63458400	-0.69697400
H	-1.58075400	2.23580500	-1.28310100
H	-0.00648200	3.05852000	0.40957000
H	-0.51575300	1.29724600	2.19201600
H	1.66372000	-0.55384900	1.47377100
O	3.47966900	0.12462200	-0.96819600
H	3.30451600	-0.09801100	-1.89404700
C	4.45394300	-0.79817600	-0.45730900
H	4.07855700	-1.82855900	-0.48080000
H	5.39091400	-0.74252700	-1.02469100
H	4.65192400	-0.51498300	0.57931400
O	-2.93351800	-0.01817600	-1.30825300
H	-3.04124900	0.60608400	-2.04213800

Scan Point for comp9-c5oh_beta_3.8Å

C	0.13970500	1.82526000	0.42725400
C	0.48593400	0.83860000	1.58218100
C	-1.68566200	0.35885800	-0.69123600
C	0.63827900	-0.53920300	1.09995200
C	-1.68580300	-0.79311600	0.33269700
H	-2.00182400	1.94322300	0.72041800
H	0.86010700	1.69369700	-0.38712900
H	-0.99735000	0.08702000	-1.50439100
H	1.41707200	1.12688200	2.07162600
H	-2.02436900	-0.45746400	1.31662400
C	-2.39464300	-2.05718600	-0.09745700
H	-2.22177300	-2.84873700	0.63745800

H	-3.46892300	-1.86663900	-0.14543500
O	-0.25237100	-1.23414800	0.53746400
H	-2.05072400	-2.39416900	-1.08008800
H	-1.43731000	2.47374300	-0.86690900
H	0.29397200	2.82931000	0.83220700
H	-0.32444000	0.85614400	2.32769000
H	1.58921500	-1.06963700	1.18131700
O	3.65931700	0.21450300	-1.07840400
H	3.64829700	-0.04052600	-2.01248100
C	4.54241500	-0.67349000	-0.37604400
H	4.19230200	-1.71149800	-0.43025600
H	5.56321500	-0.61624500	-0.77328800
H	4.55269400	-0.35373200	0.66862100
O	-3.02674500	0.41279300	-1.19434400
H	-3.08974000	1.16453400	-1.80402300

Scan Point for comp9-c5oh_beta_4.0Å

C	-0.13116500	-1.78289200	0.46926600
C	-0.46580200	-0.74875900	1.58628000
C	1.73471000	-0.39361300	-0.67996200
C	-0.59083700	0.61080600	1.04815600
C	1.74492800	0.79623400	0.29962300
H	2.00357200	-1.93077300	0.79257300
H	-0.84079700	-1.66479600	-0.35666300
H	1.06144700	-0.13962200	-1.51136800
H	-1.40532600	-1.00122700	2.07958000
H	2.06715000	0.49362100	1.29972200
C	2.47996400	2.02993400	-0.17273400
H	2.31026900	2.85401000	0.52619000
H	3.55147700	1.82061900	-0.19868200
O	0.31721500	1.26902200	0.46974700
H	2.15385900	2.33052200	-1.17305600
H	1.44864500	-2.50850700	-0.78146100
H	-0.31105400	-2.76838200	0.90781100
H	0.33988600	-0.75560600	2.33647500
H	-1.53723500	1.15424100	1.08826800
O	-3.89255500	-0.32029100	-1.00894800
H	-3.92791800	-0.17761900	-1.96602200
C	-4.66691500	0.70487200	-0.36782500
H	-4.24116400	1.69965800	-0.54828200
H	-5.70824300	0.69099600	-0.71164400
H	-4.64624700	0.49762700	0.70481300
O	3.08035100	-0.49033700	-1.16394800

H	3.13225900	-1.25500400	-1.75830100

Scan Point for comp9-c5oh_beta_4.4Å

C	-0.04764100	-1.79632600	0.46085800
C	-0.40495900	-0.75923100	1.56839600
C	1.80693100	-0.39084600	-0.68591900
C	-0.54578700	0.59436200	1.01951100
C	1.79163900	0.80743500	0.28322900
H	2.08645300	-1.91090700	0.80241100
H	-0.75126300	-1.69348500	-0.37209100
H	1.13639200	-0.15424800	-1.52464700
H	-1.34393100	-1.02168400	2.05748900
H	2.11048300	0.51847400	1.28839700
C	2.51197100	2.04786100	-0.19424500
H	2.32257900	2.87614000	0.49456100
H	3.58681100	1.85494400	-0.20744000
O	0.35580500	1.26023400	0.43969700
H	2.19146700	2.33296600	-1.20085100
H	1.55238100	-2.51045600	-0.77059200
H	-0.21817000	-2.78115300	0.90454200
H	0.39590800	-0.74941800	2.32372900
H	-1.49969900	1.12534700	1.05035300
O	-4.31729900	-0.39034000	-1.02157200
H	-4.54148600	-0.23913700	-1.95133300
C	-4.73098200	0.75666900	-0.26395400
H	-4.18556300	1.65717600	-0.57222100
H	-5.80797600	0.93626800	-0.36851900
H	-4.51006000	0.54439200	0.78479900
O	3.15736000	-0.47209100	-1.15904500
H	3.22270100	-1.23651500	-1.75244500

Scan Point for comp9-c7oh_alpha_1.4Å

C	-0.31068500	2.44635700	-0.44739500
C	0.96183600	1.81348100	0.13941700
C	-1.97609500	0.51666000	0.07117800
C	1.25582700	0.41226100	-0.39798100
C	-0.88368200	-0.47040400	0.48458700
H	-1.51990900	2.22035000	1.31903700
H	-0.36384600	2.25012800	-1.52662900
H	-2.24102200	0.31353400	-0.97335500

H	1.83972500	2.42161700	-0.10131800
H	-0.46885300	-0.20866400	1.46651800
C	-1.36148400	-1.91638000	0.58901200
H	-0.52192100	-2.55693000	0.88719900
H	-2.13076000	-1.97479200	1.36422100
O	0.18295600	-0.46918900	-0.51711600
H	-2.86949300	0.30327100	0.67152200
H	-2.43734000	2.60458600	-0.13036700
H	-0.21940000	3.53252700	-0.33511900
H	1.69868600	0.46390700	-1.39452400
O	2.26911600	-0.13699200	0.39673100
H	2.05928300	-0.18041900	1.35464300
C	2.96773400	-1.37386800	-0.05814600
H	3.76857100	-1.52422800	0.66193700
H	2.25090100	-2.19213700	-0.06696500
H	3.35121500	-1.14070900	-1.04911900
H	0.88872000	1.78367400	1.23472700
O	-1.96314500	-2.41693300	-0.61064100
H	-1.28098200	-2.47599400	-1.29655300

Scan Point for comp9-c7oh_alpha_1.5Å

C	-0.42686400	2.44805800	-0.42783300
C	0.86964200	1.85002300	0.14684600
C	-1.99371200	0.43104000	0.06210800
C	1.20223700	0.48418900	-0.43593800
C	-0.85761700	-0.50340400	0.48003400
H	-1.63510200	2.14557200	1.32739200
H	-0.46998400	2.27575600	-1.51158000
H	-2.23798000	0.22253000	-0.98631900
H	1.72416000	2.49606500	-0.07638000
H	-0.44315700	-0.21595600	1.45401500
C	-1.26508300	-1.96926200	0.59152200
H	-0.39006700	-2.57084800	0.86752400
H	-2.00936100	-2.06126200	1.38767900
O	0.20798700	-0.45564600	-0.52829000
H	-2.88080400	0.16743600	0.65131100
H	-2.56068800	2.49453800	-0.12600800
H	-0.37851200	3.53374700	-0.28891700
H	1.66887900	0.55070600	-1.41937500
O	2.33526500	-0.04030800	0.39541700
H	2.10832200	-0.09861400	1.34687000
C	3.01669300	-1.27617600	-0.05675000
H	3.83287700	-1.42860800	0.64664300

H	2.30430300	-2.09917800	-0.04643000
H	3.38622800	-1.06120500	-1.05738700
H	0.79516100	1.78263100	1.23992000
O	-1.87641600	-2.49615200	-0.59110500
H	-1.20872300	-2.54296200	-1.29191200

Scan Point for comp9-c7oh_alpha_1.6Å

C	-0.56275200	2.43577000	-0.41836000
C	0.77213000	1.89533900	0.13113400
C	-2.01620400	0.33360300	0.07087200
C	1.14248500	0.55565600	-0.47287400
C	-0.83297900	-0.54152000	0.48188200
H	-1.73430100	2.05369800	1.34684900
H	-0.61168600	2.27784600	-1.50393400
H	-2.25488800	0.11713600	-0.97708000
H	1.59183500	2.58050900	-0.10284400
H	-0.42372200	-0.23164900	1.45049800
C	-1.15604500	-2.02797300	0.58708600
H	-0.24544200	-2.58180700	0.84683200
H	-1.88150400	-2.16558000	1.39390200
O	0.22646700	-0.43480700	-0.53586600
H	-2.88442500	0.02001800	0.66341600
H	-2.69211700	2.36599400	-0.09393000
H	-0.56606900	3.52004000	-0.26223700
H	1.63619400	0.62574500	-1.44179900
O	2.39023600	0.07041400	0.40328700
H	2.14148000	-0.00647200	1.34672400
C	3.07118100	-1.15700300	-0.04645500
H	3.89797900	-1.30995600	0.64559900
H	2.36960000	-1.99007300	-0.02997500
H	3.43280700	-0.94868200	-1.05181900
H	0.71579300	1.81661000	1.22371400
O	-1.75456000	-2.57923500	-0.59014200
H	-1.09094400	-2.60413400	-1.29595900

Scan Point for comp9-c7oh_alpha_1.7Å

C	-0.63455600	2.43067700	-0.41069400
C	0.71860500	1.91006400	0.11848200
C	-2.02975000	0.28947800	0.07031500
C	1.09350500	0.58559100	-0.50127200

C	-0.83176300	-0.56104600	0.48731700
H	-1.78299200	2.00420800	1.35987700
H	-0.69114000	2.28805400	-1.49788000
H	-2.25796900	0.07299000	-0.97981000
H	1.52327100	2.60916600	-0.12399900
H	-0.42874900	-0.24136100	1.45474300
C	-1.11948700	-2.05470700	0.58584300
H	-0.19588200	-2.58878900	0.84026600
H	-1.83796500	-2.21022600	1.39560000
O	0.23471300	-0.43260300	-0.52811500
H	-2.89257300	-0.04908700	0.65669800
H	-2.75841400	2.30512000	-0.07163800
H	-0.65611300	3.51199400	-0.23740100
H	1.61292400	0.64592200	-1.45658100
O	2.45254900	0.12686300	0.41117800
H	2.19969300	0.03036200	1.35047600
C	3.12867400	-1.09139700	-0.04659300
H	3.96838700	-1.25334100	0.62907200
H	2.43447600	-1.93182600	-0.02687900
H	3.47823600	-0.88468100	-1.05708500
H	0.67601100	1.82331800	1.21048900
O	-1.71051800	-2.61320200	-0.59094600
H	-1.04685800	-2.63220200	-1.29695000

Scan Point for comp9-c7oh_alpha_1.8Å

C	-0.65936500	2.43300900	-0.40222900
C	0.69803100	1.90284900	0.11279000
C	-2.04219600	0.28178700	0.06396500
C	1.05341700	0.58911600	-0.52541400
C	-0.84698900	-0.56692000	0.49032800
H	-1.80491200	1.98824400	1.36585800
H	-0.72082300	2.30698100	-1.49109400
H	-2.26087200	0.06905600	-0.98884000
H	1.50327100	2.60037500	-0.13017200
H	-0.44366500	-0.24299700	1.45560100
C	-1.12789100	-2.06120600	0.58736600
H	-0.20169200	-2.59168700	0.83961600
H	-1.84279500	-2.21741300	1.40016100
O	0.22892800	-0.43752400	-0.52319400
H	-2.90782400	-0.06416400	0.64155700
H	-2.78176300	2.29441600	-0.06385900
H	-0.67671900	3.51140800	-0.21191700
H	1.60392100	0.63095600	-1.46352900

O	2.50752900	0.13325700	0.43257900
H	2.23850900	-0.01022800	1.35999900
C	3.20377200	-1.05134300	-0.05937900
H	4.03930700	-1.24083300	0.61588800
H	2.52371700	-1.90466100	-0.08833300
H	3.56702300	-0.80367100	-1.05629200
H	0.66333000	1.80186800	1.20351100
O	-1.72126000	-2.62016500	-0.58704000
H	-1.05752300	-2.64694300	-1.29273800

Scan Point for comp9-c7oh_alpha_1.9Å

C	0.70814900	-2.43048200	-0.39352200
C	-0.66404200	-1.90747400	0.09601100
C	2.05570200	-0.25709600	0.07027900
C	-1.00885700	-0.60526300	-0.55824900
C	0.85150200	0.57981300	0.49267400
H	1.82903900	-1.95640700	1.38313700
H	0.78288800	-2.31816700	-1.48290500
H	2.27388000	-0.04714300	-0.98307300
H	-1.46002100	-2.61132900	-0.15715100
H	0.44349400	0.25096100	1.45383900
C	1.11047500	2.07775600	0.58508800
H	0.17585900	2.59632800	0.83040700
H	1.81750500	2.24428600	1.40274300
O	-0.22370600	0.43530900	-0.52740400
H	2.91511900	0.10389300	0.64774900
H	2.82395700	-2.26001500	-0.03474300
H	0.73107800	-3.50588800	-0.18825100
H	-1.58720700	-0.63252100	-1.47933100
O	-2.56174400	-0.16387000	0.44360600
H	-2.28205300	-0.00227400	1.36328900
C	-3.26852700	1.00450200	-0.05425900
H	-4.10645500	1.20374200	0.61681300
H	-2.59956200	1.86713300	-0.09987300
H	-3.63505200	0.74606500	-1.04779400
H	-0.64832700	-1.79679400	1.18597800
O	1.70422500	2.63957300	-0.58686500
H	1.04225900	2.66537100	-1.29430400

Scan Point for comp9-c7oh_alpha_2.0Å

C	0.74670200	-2.42963000	-0.38658000
C	-0.64068500	-1.90965500	0.06920600
C	2.06736000	-0.24315400	0.08552700
C	-0.96744500	-0.61414800	-0.59522100
C	0.85730700	0.59025700	0.49575900
H	1.82955200	-1.93337400	1.40825100
H	0.84367600	-2.32753100	-1.47502700
H	2.29295500	-0.03839700	-0.96717100
H	-1.42805800	-2.61602900	-0.20155500
H	0.43905400	0.26257800	1.45264400
C	1.10442000	2.09036500	0.57943000
H	0.16410000	2.60419000	0.81208900
H	1.80151300	2.26569400	1.40376400
O	-0.21492900	0.43606700	-0.53337400
H	2.91906200	0.12793400	0.66787400
H	2.85303200	-2.24026500	0.01132300
H	0.76839200	-3.50264700	-0.16966900
H	-1.57059600	-0.62253600	-1.50008900
O	-2.61857000	-0.18672800	0.44933600
H	-2.33022200	-0.02241700	1.36447500
C	-3.32980300	0.97652200	-0.03985800
H	-4.18096300	1.16770100	0.61835600
H	-2.67256300	1.84978600	-0.07072100
H	-3.68267900	0.72981700	-1.04178100
H	-0.64974500	-1.79449800	1.15875000
O	1.70660500	2.64691900	-0.58996000
H	1.04911500	2.67337100	-1.30158300

Scan Point for comp9-c7oh_alpha_2.1Å

C	0.81195400	-2.42418000	-0.37680400
C	-0.59795400	-1.92417400	0.03488900
C	2.07506100	-0.21048900	0.11330400
C	-0.92006500	-0.63795600	-0.63927600
C	0.84897500	0.60888600	0.50249000
H	1.83408900	-1.89454000	1.44413700
H	0.93885200	-2.32951700	-1.46258900
H	2.31257600	-0.00982200	-0.93747100
H	-1.36573900	-2.64264400	-0.25826500
H	0.41962300	0.28333100	1.45501500
C	1.07174300	2.11342000	0.56944600
H	0.12018100	2.61582400	0.77989800
H	1.75250600	2.30884800	1.40280100
O	-0.21548900	0.43186200	-0.53855900

H	2.91143200	0.18002900	0.70505300
H	2.90129600	-2.19174000	0.07778700
H	0.84258600	-3.49464500	-0.14924400
H	-1.53612000	-0.63762400	-1.53522300
O	-2.70193700	-0.25768700	0.40491100
H	-2.47050600	-0.20119300	1.34749600
C	-3.35108700	0.97076400	0.00813800
H	-4.26274200	1.10170600	0.59801400
H	-2.68754300	1.82883200	0.15047500
H	-3.60829100	0.86665000	-1.04698400
H	-0.63959100	-1.80548200	1.12361500
O	1.68503400	2.66230100	-0.59722100
H	1.03771000	2.67502000	-1.31853500

Scan Point for comp9-c7oh_alpha_2.2Å

C	0.91470900	-2.40583800	-0.36584900
C	-0.52225700	-1.95083300	0.00958000
C	2.08743400	-0.14509000	0.12964900
C	-0.86818100	-0.67970200	-0.67469000
C	0.83042300	0.63337800	0.50082200
H	1.88130500	-1.82582200	1.47014800
H	1.06193700	-2.31816600	-1.44942900
H	2.32982100	0.05671500	-0.91976300
H	-1.25868500	-2.69539300	-0.29810900
H	0.39619200	0.29479500	1.44656300
C	0.99727600	2.14484300	0.56331200
H	0.02591100	2.61295100	0.76175700
H	1.66081500	2.36664400	1.40392400
O	-0.21836700	0.41533600	-0.55407900
H	2.90221100	0.27917100	0.72819800
H	2.98402600	-2.09590300	0.12630800
H	0.97434800	-3.47214700	-0.12548800
H	-1.50671900	-0.68656700	-1.55506100
O	-2.74913400	-0.33451300	0.41290400
H	-2.49364700	-0.26537600	1.34745800
C	-3.40380400	0.88963000	0.02163300
H	-4.27463800	1.06173900	0.66163200
H	-2.72036500	1.74208200	0.09176100
H	-3.73131200	0.75966700	-1.01125800
H	-0.59118100	-1.82864800	1.09672400
O	1.60342200	2.71044800	-0.59848300
H	0.96216500	2.70302200	-1.32533900

Scan Point for comp9-c7oh_alpha_2.3Å

C	0.96488600	-2.40037800	-0.35946900
C	-0.48131400	-1.95664300	0.00171600
C	2.10292000	-0.12146100	0.13019200
C	-0.82948000	-0.69378800	-0.68917300
C	0.83899700	0.64360800	0.50403900
H	1.91489800	-1.79817500	1.47819700
H	1.11872100	-2.32081900	-1.44258300
H	2.33947600	0.07936900	-0.92070000
H	-1.20812000	-2.70937000	-0.30823900
H	0.40698200	0.29951900	1.44873900
C	0.98762500	2.15674500	0.56393200
H	0.01089900	2.61403800	0.76069100
H	1.64701000	2.38627700	1.40576600
O	-0.21284200	0.41271300	-0.55022100
H	2.91378500	0.31605800	0.72440200
H	3.02670200	-2.05951500	0.13992800
H	1.03164100	-3.46371700	-0.10864800
H	-1.48616000	-0.69930300	-1.55632200
O	-2.82041300	-0.36540500	0.41461700
H	-2.57896500	-0.29346500	1.35185900
C	-3.47490500	0.85440400	0.01627500
H	-4.35237800	1.03200300	0.64654200
H	-2.79402000	1.70965100	0.08653100
H	-3.79457400	0.72228600	-1.01911200
H	-0.55706700	-1.82818700	1.08782700
O	1.58940900	2.72715400	-0.59731800
H	0.94829200	2.71557200	-1.32427300

Scan Point for comp9-c7oh_alpha_2.4Å

C	0.94627400	-2.41358800	-0.35439900
C	-0.49786100	-1.93834300	-0.02291900
C	2.11833300	-0.15639300	0.14542100
C	-0.80727300	-0.66893800	-0.71398400
C	0.86905500	0.63791500	0.50616500
H	1.87476300	-1.82247500	1.49801500
H	1.12177500	-2.34269100	-1.43465000
H	2.36862700	0.03475900	-0.90403700
H	-1.23414100	-2.67545700	-0.34716300
H	0.41863700	0.30540200	1.44625800

C	1.04861600	2.14770500	0.55925900
H	0.07814300	2.62668600	0.73473300
H	1.69690400	2.36830600	1.41202900
O	-0.18465400	0.42722000	-0.55485200
H	2.93257100	0.26744800	0.74488000
H	3.00451900	-2.11141500	0.18035000
H	0.98452600	-3.47677600	-0.09737400
H	-1.48041100	-0.64767700	-1.56854100
O	-2.89800700	-0.32980300	0.41465100
H	-2.68010700	-0.26990500	1.35792600
C	-3.56736600	0.88208400	0.02260600
H	-4.49759400	1.00238800	0.58874000
H	-2.92873800	1.75828700	0.17998200
H	-3.80313900	0.78872700	-1.03940600
H	-0.59210900	-1.80648200	1.06195400
O	1.68460300	2.69666500	-0.59367000
H	1.05879900	2.69039100	-1.33387800

Scan Point for comp9-c7oh_alpha_2.5Å

C	0.98135700	-2.41297500	-0.34568500
C	-0.47215500	-1.94245000	-0.04708800
C	2.12919100	-0.14672500	0.15968300
C	-0.77735600	-0.67483600	-0.73940800
C	0.87368800	0.64404800	0.50429200
H	1.87066500	-1.80380400	1.52036900
H	1.17751300	-2.34945300	-1.42267700
H	2.38885600	0.03851500	-0.88850700
H	-1.19836500	-2.68342000	-0.38489900
H	0.41182000	0.31123500	1.43871500
C	1.04566200	2.15457500	0.55293600
H	0.06928100	2.63036100	0.70299700
H	1.67273700	2.38228000	1.41958600
O	-0.17297400	0.42619200	-0.56586600
H	2.93511000	0.28605900	0.76396200
H	3.02668800	-2.09573300	0.22615400
H	1.01787400	-3.47389900	-0.07955600
H	-1.46408600	-0.64735600	-1.58350700
O	-2.96671400	-0.34321100	0.42108400
H	-2.75251700	-0.28316700	1.36475900
C	-3.62891000	0.87050100	0.02662600
H	-4.56357700	0.99700200	0.58480600
H	-2.98833000	1.74502900	0.18799000
H	-3.85749500	0.78006600	-1.03738900

H	-0.58927800	-1.80852500	1.03591400
O	1.70693200	2.69924200	-0.58741600
H	1.10162800	2.67907000	-1.34420500

Scan Point for comp9-c7oh_alpha_2.6Å

C	1.10089100	-2.38724200	-0.33513700
C	-0.37309700	-1.97058000	-0.05144200
C	2.14955000	-0.06882800	0.15327600
C	-0.72421400	-0.71966600	-0.74910600
C	0.86258600	0.66640300	0.50269000
H	1.96296600	-1.72464900	1.52575200
H	1.29873900	-2.33111500	-1.41211000
H	2.39470700	0.12167900	-0.89747800
H	-1.06717400	-2.74160500	-0.38962400
H	0.41586500	0.30835600	1.43531400
C	0.96393900	2.18275800	0.55903500
H	-0.03148200	2.60972800	0.72834500
H	1.59312200	2.43407800	1.41764400
O	-0.17596700	0.40684900	-0.56790400
H	2.93888100	0.40211100	0.75072700
H	3.13021700	-1.97775300	0.23320300
H	1.17605700	-3.44195900	-0.05332400
H	-1.42413100	-0.71694400	-1.58347000
O	-3.02356500	-0.43359100	0.43036300
H	-2.82540300	-0.36459300	1.37651500
C	-3.68996500	0.77070000	0.01700800
H	-4.63226800	0.89895800	0.56230800
H	-3.05744000	1.65201400	0.17482200
H	-3.90638100	0.66810900	-1.04860200
H	-0.50410300	-1.83309900	1.03003600
O	1.57890400	2.76529000	-0.58839000
H	0.95575900	2.73672100	-1.33039000

Scan Point for comp9-c7oh_alpha_2.7Å

C	1.15642500	-2.37789400	-0.32851400
C	-0.32643200	-1.98065000	-0.06112100
C	2.16399400	-0.04112300	0.15602000
C	-0.69187700	-0.73600700	-0.75999600
C	0.86561400	0.67480900	0.50187100
H	1.99655300	-1.69336000	1.53464400

H	1.36184200	-2.32597400	-1.40418000
H	2.40788700	0.14945900	-0.89499200
H	-1.00567000	-2.76270800	-0.40395000
H	0.42041600	0.30823600	1.43194800
C	0.94159400	2.19246900	0.55949800
H	-0.06190000	2.60225500	0.72344000
H	1.56130700	2.45326400	1.42219000
O	-0.16870500	0.39963200	-0.57149100
H	2.94470900	0.44445700	0.75298300
H	3.17520500	-1.93362200	0.24984900
H	1.24312200	-3.42952700	-0.03880600
H	-1.40244800	-0.73959200	-1.58603800
O	-3.09536600	-0.46802300	0.44059800
H	-2.91933100	-0.39609200	1.39060100
C	-3.74201400	0.73893700	0.00670000
H	-4.69404300	0.88235200	0.53143900
H	-3.10390100	1.61553500	0.16958100
H	-3.93914900	0.63126200	-1.06227900
H	-0.47035200	-1.84149200	1.01897300
O	1.55334800	2.78577100	-0.58391400
H	0.93412400	2.74923800	-1.32883200

Scan Point for comp9-c7oh_alpha_2.8Å

C	1.21309000	-2.36605700	-0.32838300
C	-0.27526500	-1.99546900	-0.05134000
C	2.17689900	-0.00857900	0.13950200
C	-0.67112100	-0.75770400	-0.74404800
C	0.87074500	0.68199400	0.50578900
H	2.06018800	-1.65990100	1.52402600
H	1.40737500	-2.31394100	-1.40606900
H	2.39967400	0.18458800	-0.91576000
H	-0.94160100	-2.79054800	-0.38943200
H	0.44486400	0.30370000	1.44026100
C	0.91813400	2.20054300	0.56743500
H	-0.09118200	2.59076300	0.74235900
H	1.54081700	2.46969800	1.42544500
O	-0.17482600	0.38874100	-0.55393300
H	2.95764300	0.49373000	0.72227000
H	3.22831900	-1.87936500	0.22590800
H	1.32095600	-3.41476400	-0.03542900
H	-1.39934000	-0.77127400	-1.55507200
O	-3.19170000	-0.51523100	0.45089500
H	-3.08097500	-0.44993600	1.41103100

C	-3.74681600	0.71963800	-0.02711600
H	-4.72083200	0.91890400	0.43560300
H	-3.07471200	1.56321300	0.17042400
H	-3.88374500	0.61453300	-1.10574000
H	-0.41507500	-1.85775000	1.02987400
O	1.50789000	2.80893700	-0.57945900
H	0.88183000	2.76472200	-1.31823700

Scan Point for comp9-c7oh_alpha_2.9Å

C	1.22272900	-2.36955600	-0.32685100
C	-0.26715600	-1.99413700	-0.06553700
C	2.18861200	-0.01476400	0.14541300
C	-0.65631100	-0.75273000	-0.75425400
C	0.88413300	0.68100200	0.50718600
H	2.05585700	-1.66314800	1.53185700
H	1.42684900	-2.32030100	-1.40274200
H	2.41585100	0.17590500	-0.90931800
H	-0.93229300	-2.78646600	-0.41236200
H	0.45325900	0.30345500	1.43966400
C	0.93645600	2.19932500	0.56819500
H	-0.07206000	2.59302900	0.73997800
H	1.55746800	2.46661800	1.42799500
O	-0.16206800	0.39228100	-0.55499900
H	2.96875700	0.48611600	0.73022900
H	3.23426100	-1.88834300	0.24396100
H	1.32375200	-3.41801300	-0.03065200
H	-1.39034900	-0.75830200	-1.56082200
O	-3.27396800	-0.51655700	0.47134600
H	-3.11231500	-0.41421200	1.42079800
C	-3.77631700	0.72690800	-0.04103900
H	-4.70242300	1.01974400	0.46785300
H	-3.03828700	1.53111200	0.06497900
H	-3.98881900	0.57371300	-1.10161100
H	-0.41850500	-1.85850200	1.01495500
O	1.53179000	2.80478900	-0.57721500
H	0.90765000	2.76298900	-1.31776600

Scan Point for comp9-c7oh_alpha_3.0Å

C	1.26087500	-2.36355700	-0.32012100
C	-0.23644600	-1.99987200	-0.08520600

C	2.19900700	-0.00012700	0.16341600
C	-0.62633400	-0.76170200	-0.77798000
C	0.88414900	0.68614300	0.50521000
H	2.05741800	-1.64696600	1.55060100
H	1.48225600	-2.31492300	-1.39252700
H	2.44090700	0.19085800	-0.88793700
H	-0.88893500	-2.79799100	-0.44261600
H	0.44251100	0.30600900	1.43158900
C	0.92256400	2.20498500	0.56370600
H	-0.09200000	2.59005900	0.71863300
H	1.52734200	2.47929300	1.43283700
O	-0.14722200	0.38760100	-0.57034300
H	2.96606000	0.50771900	0.75952400
H	3.25860600	-1.86462800	0.28257200
H	1.36495100	-3.41051900	-0.01977700
H	-1.35669500	-0.77116000	-1.58851400
O	-3.33835000	-0.53409900	0.48422800
H	-3.18324300	-0.42655600	1.43409700
C	-3.82131400	0.71118800	-0.04200800
H	-4.74711400	1.02028900	0.45780400
H	-3.07357600	1.50684800	0.06147900
H	-4.02839500	0.55122800	-1.10274000
H	-0.40771700	-1.86448100	0.99272900
O	1.53093100	2.81302300	-0.57329700
H	0.91969800	2.76273600	-1.32396800

Scan Point for comp9-c7oh_alpha_3.1Å

C	1.31508000	-2.35236900	-0.31515400
C	-0.18770600	-2.01004800	-0.08100400
C	2.21788400	0.02618800	0.16077400
C	-0.59552600	-0.77851600	-0.77397200
C	0.89433600	0.69312900	0.50711900
H	2.10506400	-1.61921700	1.55218100
H	1.53406300	-2.30318100	-1.38804200
H	2.45213600	0.21846200	-0.89211500
H	-0.82790700	-2.81808800	-0.43826900
H	0.46102600	0.30602100	1.43456700
C	0.90907500	2.21224000	0.56521300
H	-0.11146900	2.58134500	0.71986600
H	1.50937300	2.49586000	1.43449800
O	-0.13634000	0.37824900	-0.56538000
H	2.98014800	0.54675500	0.75212100
H	3.30602400	-1.82168600	0.28138700

H	1.43442300	-3.39686500	-0.01200000
H	-1.32934100	-0.79886600	-1.58156700
O	-3.42832800	-0.56854900	0.46745600
H	-3.32727400	-0.49080200	1.42747600
C	-3.88270100	0.69293000	-0.04571700
H	-4.83013400	0.99159300	0.41876400
H	-3.13859800	1.48253100	0.11556400
H	-4.04074100	0.56396600	-1.11902300
H	-0.36203100	-1.87548500	0.99681200
O	1.50827700	2.82933200	-0.57171400
H	0.89837400	2.76875500	-1.32270400

Scan Point for comp9-c7oh_alpha_3.2Å

C	1.43248700	-2.31340800	-0.30533200
C	-0.08855600	-2.03990200	-0.10020400
C	2.22389200	0.10105800	0.18480100
C	-0.53878900	-0.82541700	-0.79559600
C	0.86799900	0.71314400	0.50568100
H	2.15106300	-1.54586300	1.57735400
H	1.66881100	-2.25055100	-1.37386500
H	2.47042100	0.30133900	-0.86374900
H	-0.68535800	-2.87404100	-0.47224200
H	0.43640000	0.31207800	1.42806600
C	0.81857800	2.23161100	0.55358700
H	-0.21869900	2.55990100	0.68802100
H	1.39150600	2.54475400	1.43119000
O	-0.13447000	0.35005800	-0.58016600
H	2.95162500	0.65461400	0.78989300
H	3.38556900	-1.69899400	0.33217500
H	1.59332100	-3.35231900	-0.00213200
H	-1.26480100	-0.87575300	-1.60930900
O	-3.47113000	-0.63941900	0.47199200
H	-3.43284000	-0.58007800	1.43783600
C	-3.93912800	0.61687200	-0.04153800
H	-4.93922500	0.85412700	0.34088600
H	-3.25306800	1.43373100	0.21333900
H	-3.98997800	0.52026400	-1.12852300
H	-0.29047300	-1.91654900	0.97455800
O	1.41267400	2.86531800	-0.57671300
H	0.82368200	2.76698500	-1.34023200

Scan Point for comp9-c7oh_alpha_3.3Å

C	1.45768700	-2.30957200	-0.30898500
C	-0.06512200	-2.04432500	-0.10816100
C	2.23556700	0.10742300	0.18700800
C	-0.52240500	-0.82893100	-0.79678200
C	0.87749900	0.71379700	0.50902600
H	2.16668000	-1.54171500	1.57732300
H	1.69667300	-2.24309200	-1.37668700
H	2.48128800	0.30974300	-0.86134300
H	-0.65664200	-2.87993100	-0.48531500
H	0.44789600	0.31034300	1.43135000
C	0.82209600	2.23200700	0.55731700
H	-0.21651800	2.55618400	0.69154000
H	1.39365500	2.54715000	1.43509100
O	-0.12602000	0.34788900	-0.57568500
H	2.96081800	0.66364800	0.79263200
H	3.40563600	-1.68707200	0.33560300
H	1.62265700	-3.34831300	-0.00745700
H	-1.25332600	-0.87854300	-1.60655800
O	-3.53903700	-0.62902900	0.52608000
H	-3.57886700	-0.51830800	1.48739400
C	-3.96790200	0.59436800	-0.09148900
H	-4.98954200	0.85467400	0.21071700
H	-3.29560700	1.42484800	0.15620500
H	-3.95135400	0.43086200	-1.17157900
H	-0.27115400	-1.92650800	0.96677100
O	1.41408100	2.86804300	-0.57275400
H	0.82594300	2.76709100	-1.33659700

Scan Point for comp9-c7oh_alpha_3.5Å

C	1.50297500	-2.30661000	-0.30321300
C	-0.02308500	-2.04767000	-0.12061300
C	2.26488100	0.11342400	0.20110500
C	-0.47875900	-0.83302800	-0.81123500
C	0.90167200	0.71488500	0.51022000
H	2.18731400	-1.53571300	1.59102900
H	1.75400400	-2.23917500	-1.36806600
H	2.51988700	0.31630000	-0.84491400
H	-0.60657400	-2.88517500	-0.50598100
H	0.46485800	0.30995900	1.42852900
C	0.84033500	2.23289000	0.55742700
H	-0.20062400	2.55343400	0.68183300

H	1.40254500	2.55030600	1.44040100
O	-0.09127600	0.34531800	-0.58343900
H	2.98209600	0.67272700	0.81342800
H	3.44073800	-1.67609700	0.36333800
H	1.66853000	-3.34465800	0.00034300
H	-1.20403700	-0.88398400	-1.62617900
O	-3.70098100	-0.63611700	0.54099100
H	-3.75717900	-0.50351300	1.49863800
C	-4.06739500	0.58950900	-0.11152100
H	-5.08449700	0.89592900	0.16152100
H	-3.36929800	1.39888700	0.13454500
H	-4.03318500	0.40207800	-1.18732300
H	-0.24275300	-1.93231400	0.95209300
O	1.44065900	2.87059100	-0.56726600
H	0.86022400	2.76709400	-1.33663900

Scan Point for comp9-c7oh_alpha_3.6Å

C	1.52633500	-2.30229700	-0.27592700
C	-0.01074400	-2.06109100	-0.21894800
C	2.22930800	0.11997100	0.28164800
C	-0.44193900	-0.83815400	-0.91172800
C	0.84733900	0.71971100	0.49531200
H	2.04882900	-1.52491900	1.66832100
H	1.86195400	-2.22986600	-1.31649700
H	2.55443200	0.31743800	-0.74573400
H	-0.54966000	-2.89772900	-0.66655700
H	0.35413800	0.32233400	1.38828400
C	0.78105800	2.23814200	0.52695500
H	-0.26620400	2.55822100	0.57506400
H	1.28013700	2.56174400	1.44490700
O	-0.07998600	0.34108300	-0.65112100
H	2.90098400	0.68606800	0.93758000
H	3.39859400	-1.66112700	0.54749700
H	1.67669700	-3.33973000	0.03760900
H	-1.13577700	-0.88400400	-1.75410600
O	-3.69369300	-0.63145500	0.61906600
H	-3.75664800	-0.44103500	1.56640300
C	-3.98602900	0.57266600	-0.10560000
H	-4.98573000	0.95156100	0.13905900
H	-3.24496200	1.35426700	0.10161100
H	-3.95455300	0.32330200	-1.16891400
H	-0.32353000	-1.97457700	0.83409400
O	1.45809400	2.87062000	-0.55661800

H	0.92772000	2.77133900	-1.36164300

Scan Point for comp9-c7oh_alpha_3.7Å

C	-1.50319200	-2.31873300	0.27501600
C	0.02960600	-2.05158600	0.21548700
C	-2.24637800	0.09201500	-0.28193200
C	0.44145000	-0.82327800	0.91022600
C	-0.87343800	0.71157400	-0.49708200
H	-2.04444600	-1.55095500	-1.66759100
H	-1.83772100	-2.25350800	1.31635600
H	-2.57391200	0.28615700	0.74529200
H	0.58313500	-2.88039200	0.65981800
H	-0.37433900	0.31892300	-1.38879600
C	-0.82962900	2.23076800	-0.53279800
H	0.21254900	2.56631000	-0.58449300
H	-1.33593400	2.54450800	-1.45024200
O	0.05886700	0.34972100	0.65077600
H	-2.92667800	0.64697300	-0.93853600
H	-3.38823300	-1.70773300	-0.54230500
H	-1.63637600	-3.35823400	-0.03948500
H	1.13707600	-0.85829200	1.75173800
O	3.81858500	-0.62339100	-0.58809000
H	3.83552300	-0.45611200	-1.54181200
C	3.98518400	0.62809400	0.09581600
H	4.93039800	1.11015400	-0.18159200
H	3.15509700	1.31260600	-0.11753800
H	4.00003300	0.40829200	1.16601100
H	0.33907300	-1.95709600	-0.83799800
O	-1.51305300	2.85561300	0.55119300
H	-0.97768000	2.76845600	1.35431100

Scan Point for comp9-c7oh_alpha_3.8Å

C	1.44854400	-2.34593200	-0.32061900
C	-0.05657000	-2.02702500	-0.06962200
C	2.32061000	0.04418900	0.14423500
C	-0.49768400	-0.79442500	-0.73710100
C	0.99767900	0.69178900	0.52518300
H	2.25639200	-1.60353500	1.53629100
H	1.65137800	-2.29091600	-1.39637600
H	2.52526600	0.23981800	-0.91426100

H	-0.68782700	-2.84136800	-0.42849000
H	0.59071600	0.29348000	1.45979700
C	0.99259300	2.21028100	0.59077000
H	-0.03024400	2.56507300	0.76286200
H	1.60229700	2.49693500	1.45251900
O	-0.05775000	0.36771200	-0.52291200
H	3.09018800	0.57636200	0.71541300
H	3.43931900	-1.78650400	0.24574100
H	1.58651300	-3.38911100	-0.02108000
H	-1.26436500	-0.81464800	-1.51514100
O	-4.05427700	-0.54391000	0.57736400
H	-4.12992100	-0.28811000	1.50815300
C	-4.07806400	0.64582900	-0.22599900
H	-5.00468400	1.21212200	-0.07234900
H	-3.22052700	1.29415700	-0.00830000
H	-4.03060400	0.32775100	-1.27015100
H	-0.22458700	-1.90471800	1.01180800
O	1.56671800	2.84060600	-0.55162300
H	0.94604100	2.77746100	-1.29353500

Scan Point for comp9-c7oh_alpha_3.9Å

C	1.39309700	-2.37064900	-0.32754400
C	-0.09899300	-2.00056200	-0.07134500
C	2.35012500	-0.01423600	0.14127600
C	-0.50181000	-0.75040100	-0.73063700
C	1.05180200	0.67758200	0.52838800
H	2.23068600	-1.66221200	1.52930800
H	1.59513300	-2.32045300	-1.40359000
H	2.55883600	0.17703400	-0.91718000
H	-0.75973200	-2.79119100	-0.43027100
H	0.63512500	0.29051900	1.46353000
C	1.09933900	2.19515200	0.59859900
H	0.09107800	2.58398700	0.78278300
H	1.72755800	2.45805800	1.45456100
O	-0.01926400	0.39443400	-0.51543200
H	3.13857900	0.48938500	0.71244300
H	3.40369100	-1.88386700	0.23572100
H	1.49513800	-3.41873400	-0.03087500
H	-1.27702400	-0.74030600	-1.50065100
O	-4.16712300	-0.49191200	0.57650700
H	-4.23001100	-0.22849000	1.50608800
C	-4.16587800	0.69289700	-0.23446900
H	-5.07772600	1.28243800	-0.08006700

H	-3.29172100	1.32153300	-0.02491100
H	-4.13038600	0.36691000	-1.27667300
H	-0.25865400	-1.87711900	1.01150900
O	1.68204300	2.80960700	-0.54819800
H	1.04948200	2.77504200	-1.28195900

Scan Point for comp9-c7oh_alpha_4.0Å

C	1.35455000	-2.38553000	-0.33636800
C	-0.12624700	-1.97864300	-0.07181700
C	2.37795800	-0.05893900	0.13987900
C	-0.50008200	-0.71427000	-0.72062400
C	1.10056400	0.66699100	0.53370800
H	2.21556400	-1.70886600	1.52153900
H	1.55399300	-2.33428900	-1.41278100
H	2.58939000	0.13075400	-0.91829200
H	-0.80989500	-2.74913600	-0.43170100
H	0.67811700	0.29008800	1.47045300
C	1.19007100	2.18261900	0.60405000
H	0.19491700	2.59919200	0.79854800
H	1.83409800	2.42771100	1.45350200
O	0.01569000	0.41560400	-0.50404200
H	3.18092000	0.42093200	0.71146100
H	3.37899800	-1.95768100	0.22434900
H	1.43054400	-3.43768100	-0.04635000
H	-1.28241600	-0.67874700	-1.48275000
O	-4.27543900	-0.45309100	0.57490000
H	-4.33019200	-0.18271600	1.50300300
C	-4.25742100	0.72635000	-0.24360500
H	-5.15973100	1.33084800	-0.09091200
H	-3.37324700	1.34277100	-0.03989100
H	-4.22874700	0.39316800	-1.28375600
H	-0.27735500	-1.85775700	1.01273100
O	1.77777000	2.78130900	-0.54855400
H	1.13657000	2.76631600	-1.27548100

Scan Point for comp9-c7oh_alpha_4.1Å

C	1.34813300	-2.39039800	-0.34088500
C	-0.12746000	-1.96765500	-0.07455800
C	2.40090600	-0.07860500	0.14107400
C	-0.48897600	-0.69659400	-0.71695100

C	1.13296500	0.66257600	0.53791400
H	2.21607900	-1.72910200	1.51899800
H	1.54774500	-2.33796500	-1.41715400
H	2.61448700	0.11116000	-0.91660300
H	-0.81992500	-2.72941100	-0.43570700
H	0.70825100	0.28920500	1.47512400
C	1.24281000	2.17710100	0.60750300
H	0.25488800	2.60734000	0.80889600
H	1.89600300	2.41409800	1.45226000
O	0.04126700	0.42624000	-0.49675000
H	3.20977300	0.38935700	0.71413800
H	3.37773700	-1.99015200	0.22307800
H	1.41179200	-3.44432200	-0.05451700
H	-1.27721900	-0.64692500	-1.47246500
O	-4.36903400	-0.43299600	0.58135500
H	-4.43837100	-0.14729000	1.50380200
C	-4.33370100	0.73305900	-0.25616900
H	-5.23235500	1.34718500	-0.12137300
H	-3.44605100	1.34506600	-0.05443300
H	-4.29790300	0.38244000	-1.29027700
H	-0.27667300	-1.84804500	1.01070100
O	1.82929900	2.76737100	-0.55014900
H	1.18194600	2.76282700	-1.27160000

Scan Point for comp9-c7oh_alpha_4.2Å

C	1.46422700	-2.36082000	-0.31628600
C	-0.03538800	-2.01459600	-0.06974000
C	2.37816800	0.01310300	0.15064700
C	-0.45425800	-0.77345500	-0.73583000
C	1.06635500	0.68379200	0.52986100
H	2.28083300	-1.63302000	1.54243300
H	1.67104100	-2.31059900	-1.39145200
H	2.58822300	0.20526200	-0.90739800
H	-0.68020400	-2.81741200	-0.43054100
H	0.65091600	0.29132900	1.46326700
C	1.08764000	2.20208900	0.59786700
H	0.07135700	2.57401500	0.77267800
H	1.70375500	2.47680400	1.45892500
O	0.00662100	0.38015700	-0.52004300
H	3.15584700	0.53118800	0.72362600
H	3.46347100	-1.83770200	0.25482700
H	1.58200200	-3.40610900	-0.01557200
H	-1.22304600	-0.77867200	-1.51232700

O	-4.39858000	-0.42880100	0.66540700
H	-4.41889400	-0.00670300	1.53653300
C	-4.19827800	0.58741700	-0.32815400
H	-5.00025700	1.33524300	-0.30299800
H	-3.23317200	1.09219700	-0.19667300
H	-4.21208700	0.08948400	-1.30053800
H	-0.20394700	-1.89033700	1.01163300
O	1.66998600	2.82455000	-0.54469900
H	1.04538800	2.77616700	-1.28446200

Scan Point for comp9-c7oh_alpha_4.3Å

C	1.44787000	-2.37230200	-0.31788800
C	-0.04472700	-2.00600700	-0.05836100
C	2.39887700	-0.01193700	0.14378900
C	-0.45232300	-0.75837800	-0.71938900
C	1.09958000	0.67639100	0.53383500
H	2.28944900	-1.65794500	1.53495200
H	1.64651900	-2.32366400	-1.39463800
H	2.60351900	0.17825600	-0.91566200
H	-0.70382700	-2.79937600	-0.41425100
H	0.68656700	0.28914400	1.47051800
C	1.14247000	2.19417500	0.60245500
H	0.13319000	2.58003700	0.78737800
H	1.77074000	2.45973200	1.45755600
O	0.02693400	0.38833300	-0.50704800
H	3.18770700	0.49505400	0.71141500
H	3.45867400	-1.87802400	0.23770000
H	1.55374500	-3.41947400	-0.01938200
H	-1.22822500	-0.75208100	-1.48879200
O	-4.54832700	-0.45487300	0.55365500
H	-4.69718600	-0.14169000	1.45768600
C	-4.19062800	0.67103400	-0.26187500
H	-4.97879300	1.43383700	-0.25543100
H	-3.24930700	1.12507700	0.07153100
H	-4.06898600	0.30006300	-1.28230200
H	-0.20197900	-1.88091000	1.02467700
O	1.72216000	2.80945100	-0.54539300
H	1.08941400	2.77138900	-1.27882700

Scan Point for comp9-c7oh_alpha_4.4Å

C	1.43684500	-2.37970700	-0.31961500
C	-0.05136600	-1.99524300	-0.06148900
C	2.41820100	-0.03285800	0.14760300
C	-0.44267800	-0.74125000	-0.72018300
C	1.12723500	0.67183900	0.53598100
H	2.28346600	-1.67928700	1.53611300
H	1.63801400	-2.33175300	-1.39589200
H	2.62787400	0.15617700	-0.91105200
H	-0.72038300	-2.77937800	-0.41936500
H	0.70812700	0.28948100	1.47198300
C	1.18953700	2.18891700	0.60463700
H	0.18572000	2.58767000	0.79186500
H	1.82314700	2.44649100	1.45823500
O	0.05179200	0.39860600	-0.50601800
H	3.21193200	0.46314700	0.71815600
H	3.45276000	-1.91315600	0.24136900
H	1.52900600	-3.42867600	-0.02287800
H	-1.21896400	-0.72357200	-1.48904500
O	-4.64057200	-0.42644400	0.55986700
H	-4.78370700	-0.09472800	1.45821100
C	-4.24539900	0.67495100	-0.27197400
H	-5.00854100	1.46277700	-0.27685400
H	-3.28948100	1.10209600	0.05565100
H	-4.13500000	0.28499100	-1.28662000
H	-0.20795900	-1.87028400	1.02174000
O	1.77425800	2.79673200	-0.54468000
H	1.13854700	2.76869800	-1.27599000

Scan Point for comp9-c7oh_alpha_4.5Å

C	1.43502100	-2.38389000	-0.32195800
C	-0.04915500	-1.98854000	-0.05767300
C	2.43792000	-0.04633100	0.14523700
C	-0.43363500	-0.73005000	-0.71172000
C	1.15429200	0.66881400	0.53846000
H	2.29303100	-1.69325400	1.53229100
H	1.63279600	-2.33514300	-1.39881300
H	2.64606600	0.14206200	-0.91382300
H	-0.72595400	-2.76650100	-0.41443000
H	0.73563900	0.28979500	1.47604000
C	1.22956100	2.18531200	0.60684300
H	0.23013500	2.59263400	0.79910100
H	1.86963500	2.43741200	1.45724000
O	0.07196400	0.40510000	-0.49893400

H	3.23732700	0.44254200	0.71409100
H	3.45639000	-1.93563100	0.23379400
H	1.52013500	-3.43420100	-0.02788400
H	-1.21493100	-0.70450900	-1.47528400
O	-4.73846300	-0.40396400	0.55795500
H	-4.87407400	-0.05927700	1.45263800
C	-4.29711600	0.67400000	-0.28129700
H	-5.02871500	1.49105900	-0.29615800
H	-3.32609200	1.06527900	0.04700800
H	-4.19713700	0.27138400	-1.29213000
H	-0.20059100	-1.86476300	1.02650000
O	1.81371100	2.78821500	-0.54534600
H	1.17414600	2.76593700	-1.27351300

Scan Point for comp9-c7oh_alpha_4.6Å

C	1.50160100	-2.36784300	-0.30685000
C	0.00655000	-2.00987800	-0.04916700
C	2.43744400	0.00018200	0.14745400
C	-0.40786400	-0.76709300	-0.71501800
C	1.13359700	0.68112900	0.53544800
H	2.33906200	-1.64225100	1.54353300
H	1.70017000	-2.32176100	-1.38374300
H	2.64071800	0.18857300	-0.91258300
H	-0.64720800	-2.80856800	-0.40302000
H	0.72248400	0.29333500	1.47272500
C	1.16648100	2.19932100	0.60086700
H	0.15427400	2.57895500	0.78272300
H	1.79102800	2.47073500	1.45687100
O	0.06387000	0.38334700	-0.50578900
H	3.22319500	0.51379000	0.71337800
H	3.50929200	-1.85874400	0.24660700
H	1.61386000	-3.41328200	-0.00460800
H	-1.18229200	-0.76816600	-1.48587900
O	-4.78292000	-0.35264700	0.64404100
H	-4.89664600	0.14290200	1.46818400
C	-4.28167900	0.54328100	-0.35921500
H	-4.97451100	1.37554700	-0.53377500
H	-3.29978800	0.94555400	-0.08076400
H	-4.18467900	-0.03337500	-1.28213400
H	-0.15232100	-1.88208400	1.03328700
O	1.74481000	2.81598000	-0.54689100
H	1.11459300	2.77102000	-1.28209000

Scan Point for comp9-c7oh_beta_1.4Å

C	1.49464300	1.88829700	-0.31315200
C	1.67601400	0.91751400	0.86657500
C	-0.96456400	1.23471800	-0.74228600
C	1.12448400	-0.50181200	0.72297900
C	-1.21182100	0.39937700	0.51992100
H	-0.26198000	2.98585300	0.29594600
H	1.89488700	1.44067100	-1.23411500
H	-0.66793500	0.57540200	-1.56851000
H	2.74523900	0.79457300	1.06990900
H	-1.17115400	1.04768200	1.40557000
C	-2.57220600	-0.29020400	0.54714700
H	-2.67479100	-0.85590000	1.48184300
H	-3.35269600	0.47510000	0.52104500
O	-0.26060700	-0.69014200	0.72003700
H	-1.92438700	1.68052900	-1.02926400
H	0.04418500	3.01064200	-1.43571700
H	2.12975100	2.75908200	-0.11374900
H	1.23088300	1.33054100	1.77887300
O	-2.80735300	-1.14648900	-0.57669400
H	-2.20057700	-1.89968600	-0.51754000
O	1.67520900	-1.09580400	-0.41889500
H	1.41905800	-0.67055500	-1.26536600
H	1.51602700	-1.11565400	1.53783400
C	1.64066900	-2.58337800	-0.54854500
H	2.16335300	-2.79519100	-1.47859000
H	2.18191500	-2.96150100	0.31566600
H	0.60147000	-2.90494500	-0.57085400

Scan Point for comp9-c7oh_beta_1.5Å

C	-1.58802200	-1.81538500	-0.32448600
C	-1.72561500	-0.85972300	0.87527300
C	0.88578200	-1.25328400	-0.76583600
C	-1.08836300	0.52262400	0.78215900
C	1.19197900	-0.46774500	0.51400000
H	0.12769000	-2.99432000	0.24766200
H	-1.97590900	-1.33004500	-1.23074900
H	0.60297100	-0.55841800	-1.56807000
H	-2.78747400	-0.68187700	1.07439600
H	1.13260700	-1.13726400	1.38165500

C	2.57878200	0.16164600	0.54108100
H	2.71565200	0.69927900	1.48770900
H	3.32394500	-0.63723400	0.49404100
O	0.28223700	0.65197000	0.77240800
H	1.82227000	-1.72646700	-1.08497600
H	-0.19382400	-2.97522700	-1.48087100
H	-2.25824200	-2.66284800	-0.13920200
H	-1.30848800	-1.31569100	1.78102500
O	2.84098000	1.02772700	-0.56772200
H	2.30864200	1.82888300	-0.46479600
O	-1.65629900	1.19877200	-0.43038900
H	-1.43429000	0.74135800	-1.26789600
H	-1.47237400	1.16755600	1.57425400
C	-1.43466600	2.66177100	-0.56978200
H	-1.95375300	2.94553300	-1.48328700
H	-1.88949300	3.11815500	0.30770700
H	-0.36386100	2.85112500	-0.63137400

Scan Point for comp9-c7oh_beta_1.6Å

C	-1.59520900	-1.80558100	-0.31436200
C	-1.70894800	-0.86977400	0.90528900
C	0.87163100	-1.22904300	-0.79579800
C	-1.05526100	0.49786900	0.83780900
C	1.20112300	-0.48478400	0.50119100
H	0.13704600	-2.99636400	0.17841300
H	-2.00959300	-1.30937500	-1.20254300
H	0.57227000	-0.50831900	-1.56833000
H	-2.76472300	-0.68776700	1.12701000
H	1.14047900	-1.17190300	1.35322400
C	2.58708600	0.14544000	0.53146100
H	2.73995100	0.65640900	1.48992200
H	3.32782000	-0.65385000	0.45441900
O	0.29036000	0.63041500	0.80288700
H	1.79975300	-1.68967100	-1.15630800
H	-0.22880600	-2.92415900	-1.54042300
H	-2.25632000	-2.65826600	-0.12601100
H	-1.27798200	-1.34717800	1.79603600
O	2.83360100	1.03877600	-0.55775200
H	2.29874100	1.83600700	-0.42887300
O	-1.68194400	1.20988300	-0.45071800
H	-1.42710700	0.75335200	-1.27559400
H	-1.45006700	1.18534000	1.58724500
C	-1.43669600	2.65937200	-0.57747300

H	-1.95947900	2.97701500	-1.47895800
H	-1.87298000	3.11218000	0.31038100
H	-0.36316700	2.83891200	-0.64795300

Scan Point for comp9-c7oh_beta_1.7Å

C	-1.80597500	-1.60941400	-0.37028600
C	-1.85350300	-0.68130300	0.85535500
C	0.72766900	-1.34871400	-0.77082700
C	-0.99632200	0.56264500	0.87579100
C	1.15090800	-0.65298200	0.52232300
H	-0.25229400	-2.99323600	0.21427900
H	-2.10664900	-1.05363300	-1.26652300
H	0.53902700	-0.60913100	-1.55883700
H	-2.88083400	-0.34086600	1.01659500
H	1.08097900	-1.35230100	1.36478700
C	2.57668100	-0.10983600	0.50043400
H	2.79833100	0.37295700	1.45999700
H	3.26306600	-0.95094700	0.37110200
O	0.33686700	0.52108000	0.90188100
H	1.59724300	-1.92945300	-1.09940900
H	-0.54760800	-2.91527100	-1.51817300
H	-2.57986000	-2.36961300	-0.21782500
H	-1.56078400	-1.23262000	1.76054900
O	2.82844700	0.79431800	-0.57960100
H	2.36349400	1.62534400	-0.39935400
O	-1.46698300	1.42936000	-0.50886900
H	-1.16509300	0.97311700	-1.31750700
H	-1.34632300	1.31343900	1.58177700
C	-1.00804900	2.82251800	-0.54131200
H	-1.41661500	3.26316200	-1.45022700
H	-1.42234500	3.30406100	0.34298100
H	0.08176800	2.85336400	-0.54056700

Scan Point for comp9-c7oh_beta_1.8Å

C	1.35650300	1.96584700	-0.34254900
C	1.59054300	1.08382200	0.89553400
C	-1.04486100	1.13313700	-0.78443700
C	1.05005500	-0.31976700	0.90596400
C	-1.29943700	0.36178700	0.50904200
H	-0.48271000	2.97315200	0.18238800

H	1.79583700	1.48006600	-1.22206800
H	-0.69154500	0.44879500	-1.56532700
H	2.66392500	0.99575800	1.08547600
H	-1.35992400	1.05257800	1.35849900
C	-2.57400300	-0.47227900	0.50692200
H	-2.65172900	-1.02457500	1.45098500
H	-3.42286500	0.21343900	0.44008800
O	-0.23547600	-0.60928100	0.86646300
H	-2.02371200	1.49868100	-1.11711800
H	-0.13795300	2.93278800	-1.54180200
H	1.93143700	2.88537700	-0.18632400
H	1.15173000	1.55407000	1.78904500
O	-2.68061900	-1.36472800	-0.60566200
H	-2.07474600	-2.10774400	-0.46673100
O	1.80543200	-1.04226200	-0.55944000
H	1.27403500	-0.80077200	-1.34174500
H	1.56884800	-1.00711200	1.57145900
C	1.92839700	-2.49649400	-0.49764600
H	2.35912100	-2.82642500	-1.44406800
H	2.60808800	-2.71541200	0.32495500
H	0.94994000	-2.95300300	-0.33491800

Scan Point for comp9-c7oh_beta_1.9Å

C	1.34310800	1.97027400	-0.35403900
C	1.57666900	1.11632700	0.90402800
C	-1.04529700	1.11018700	-0.80072100
C	1.03089300	-0.27864400	0.95667000
C	-1.31483100	0.36612900	0.50367900
H	-0.50815200	2.97256000	0.13903600
H	1.79108600	1.46641800	-1.21838100
H	-0.67410600	0.41176400	-1.56020200
H	2.64917500	1.03007600	1.09761400
H	-1.39190000	1.06974900	1.34083500
C	-2.57612100	-0.48711200	0.49987000
H	-2.65406300	-1.03142900	1.44838600
H	-3.43275300	0.18768900	0.42092500
O	-0.23667400	-0.58299400	0.89770000
H	-2.02253400	1.45893600	-1.15547100
H	-0.14801400	2.90412900	-1.58121800
H	1.91184700	2.89597200	-0.21284600
H	1.13699200	1.60934000	1.78640600
O	-2.66266100	-1.38900700	-0.60593500
H	-2.05485200	-2.12778300	-0.45379500

O	1.84456700	-1.05351300	-0.57549000
H	1.30296700	-0.81815700	-1.35058000
H	1.56622600	-0.97958000	1.59314100
C	1.94031100	-2.50279800	-0.49116300
H	2.35409100	-2.86912800	-1.43277200
H	2.62289400	-2.72469700	0.32906700
H	0.95657400	-2.94238000	-0.30850800

Scan Point for comp9-c7oh_beta_2.0Å

C	1.32611200	1.97572200	-0.36109900
C	1.55383800	1.15349300	0.91941700
C	-1.04855100	1.08530700	-0.82155000
C	1.00847200	-0.23414300	1.00756300
C	-1.33346500	0.36887800	0.49364700
H	-0.54044500	2.97219700	0.08611000
H	1.78837700	1.45290000	-1.20596400
H	-0.65985500	0.37309500	-1.55887700
H	2.62466400	1.07372600	1.12323000
H	-1.42925200	1.08635400	1.31665700
C	-2.57965100	-0.50580700	0.48906800
H	-2.66265000	-1.03273600	1.44680600
H	-3.44529900	0.15401700	0.38505700
O	-0.24223000	-0.55663900	0.92462700
H	-2.02353200	1.41686500	-1.19818300
H	-0.15572100	2.86976800	-1.62695700
H	1.88583000	2.90888400	-0.23477600
H	1.10544400	1.66777600	1.78648500
O	-2.63506300	-1.42862400	-0.60065000
H	-2.02441400	-2.15921300	-0.42287600
O	1.88169400	-1.05793500	-0.59207800
H	1.32329600	-0.83764200	-1.35797900
H	1.55959200	-0.94719000	1.61574300
C	1.97137000	-2.50107600	-0.48211100
H	2.34909700	-2.90141600	-1.42596900
H	2.67893900	-2.71372000	0.31981800
H	0.99315000	-2.93348500	-0.25306600

Scan Point for comp9-c7oh_beta_2.1Å

C	1.32264800	1.97567700	-0.36538800
C	1.53373000	1.18385400	0.93749500

C	-1.04548800	1.07786600	-0.84543400
C	0.97790000	-0.19209900	1.05669200
C	-1.35573600	0.38565400	0.47590100
H	-0.54976300	2.98053400	0.03713200
H	1.79442000	1.43010300	-1.18987700
H	-0.64637600	0.35206200	-1.56347700
H	2.60145500	1.10334600	1.15542600
H	-1.47449000	1.11591400	1.28430300
C	-2.58742100	-0.50924400	0.46059600
H	-2.70547100	-0.98987000	1.43856100
H	-3.45742100	0.12983200	0.28556800
O	-0.26034200	-0.52135400	0.94858200
H	-2.01431700	1.40346300	-1.24264300
H	-0.13955500	2.84706700	-1.66771900
H	1.88248900	2.91045000	-0.25342800
H	1.07720700	1.72245900	1.78647400
O	-2.57550200	-1.48479900	-0.58289800
H	-1.98274900	-2.20732200	-0.32836200
O	1.90471400	-1.07655900	-0.60726300
H	1.33184300	-0.86715800	-1.36425500
H	1.53568500	-0.91965300	1.64106000
C	1.97863800	-2.51410000	-0.46853800
H	2.32544000	-2.95036800	-1.40921200
H	2.70370000	-2.72058200	0.31996400
H	1.00271500	-2.93141300	-0.20107100

Scan Point for comp9-c7oh_beta_2.2Å

C	-1.32386400	-1.97740900	-0.37698500
C	-1.52224400	-1.21769200	0.94773000
C	1.03382300	-1.06234800	-0.86753400
C	-0.95974000	0.14810700	1.10200300
C	1.36467600	-0.40204300	0.46431800
H	0.55576800	-2.98685900	-0.02122000
H	-1.80631900	-1.41093800	-1.18087700
H	0.61872300	-0.32081300	-1.56014600
H	-2.58759200	-1.13962600	1.17694200
H	1.49638700	-1.14827200	1.25571000
C	2.58783500	0.50400100	0.45236900
H	2.71412400	0.96450200	1.43895900
H	3.46058900	-0.12432200	0.25340800
O	0.26666200	0.48801700	0.97294500
H	1.99720100	-1.37350600	-1.28880100
H	0.12242800	-2.81548200	-1.71692700

H	-1.88189800	-2.91485700	-0.28074800
H	-1.05972900	-1.78079000	1.77838500
O	2.55349900	1.50009300	-0.57034200
H	1.95175900	2.20864000	-0.29771700
O	-1.94610400	1.11608800	-0.60975000
H	-1.40644400	0.88513300	-1.38372900
H	-1.52481900	0.88138500	1.67232900
C	-1.93784900	2.55132000	-0.45850100
H	-2.29390300	3.02249000	-1.37951900
H	-2.62073000	2.79000000	0.35855700
H	-0.93236500	2.91578400	-0.22234000

Scan Point for comp9-c7oh_beta_2.3Å

C	1.01212300	2.11399600	-0.36164000
C	1.28360500	1.40523800	0.98115800
C	-1.20436600	0.91220500	-0.87930700
C	0.91771200	-0.02318400	1.12414300
C	-1.44617700	0.20940600	0.44888300
H	-0.98322800	2.88322000	-0.03132100
H	1.56454900	1.58930400	-1.14810200
H	-0.69164300	0.23366300	-1.57132900
H	2.34238300	1.48208800	1.23777100
H	-1.66458900	0.92759200	1.24651300
C	-2.54084100	-0.84722300	0.44079000
H	-2.59562500	-1.32692800	1.42492500
H	-3.48910900	-0.33425400	0.25764000
O	-0.23493800	-0.53597000	0.94365700
H	-2.19868600	1.09669600	-1.30268300
H	-0.50997500	2.76550500	-1.72159800
H	1.45515700	3.11203200	-0.27727100
H	0.72246200	1.90465000	1.79177000
O	-2.39111200	-1.82317100	-0.58985100
H	-1.68358300	-2.43590100	-0.33906900
O	2.15028800	-0.83801000	-0.63847200
H	1.55024500	-0.80054000	-1.40067100
H	1.58236200	-0.69217400	1.66555100
C	2.52278200	-2.21180600	-0.41400700
H	3.00901500	-2.61942200	-1.30631000
H	3.23235600	-2.21866700	0.41568800
H	1.64995900	-2.82375800	-0.16047100

Scan Point for comp9-c7oh_beta_2.4Å

C	0.97257900	2.13078200	-0.36592600
C	1.22515200	1.46085000	1.00187400
C	-1.21016800	0.87536800	-0.90489200
C	0.88650900	0.03038500	1.16464400
C	-1.46526000	0.19475500	0.43211600
H	-1.04347600	2.86893900	-0.09792100
H	1.55421900	1.59695800	-1.12454500
H	-0.67166300	0.19246600	-1.57237700
H	2.27477700	1.56733300	1.28387300
H	-1.71264500	0.92287000	1.21196100
C	-2.53348800	-0.88852700	0.42653900
H	-2.59885000	-1.34418500	1.42132100
H	-3.48926500	-0.40342500	0.20985400
O	-0.24329700	-0.51399300	0.96066900
H	-2.19945200	1.03279800	-1.35054800
H	-0.53009800	2.72134300	-1.77389700
H	1.39452600	3.13879400	-0.29455500
H	0.63004900	1.96795000	1.78326700
O	-2.33643800	-1.88587600	-0.57504800
H	-1.62648800	-2.48013900	-0.28835900
O	2.21031000	-0.82228300	-0.64657300
H	1.60579200	-0.79727000	-1.40510600
H	1.57088700	-0.62907000	1.69410100
C	2.57522100	-2.19168800	-0.39654400
H	3.05506900	-2.62564000	-1.28046500
H	3.28845400	-2.18691000	0.43033800
H	1.70056200	-2.79370400	-0.12447600

Scan Point for comp9-c7oh_beta_2.5Å

C	0.85155800	2.17339100	-0.36840200
C	1.11683500	1.53929600	1.01548200
C	-1.26622200	0.81195200	-0.92014200
C	0.85484500	0.09601700	1.18608800
C	-1.49187900	0.12961000	0.42077500
H	-1.19980600	2.81853200	-0.13323400
H	1.46767500	1.65432000	-1.10953600
H	-0.69853700	0.14920400	-1.58332700
H	2.15368000	1.70715800	1.31456700
H	-1.77478600	0.84984600	1.19554100
C	-2.50316500	-1.00659300	0.42352500
H	-2.54111100	-1.46050600	1.42043300

H	-3.48313500	-0.57063700	0.20992300
O	-0.23296500	-0.51331100	0.95515600
H	-2.26167700	0.92230100	-1.36626100
H	-0.65936900	2.67738200	-1.80114900
H	1.22518000	3.20078700	-0.30809600
H	0.47925200	2.02551800	1.77662700
O	-2.26156200	-1.99657000	-0.57548000
H	-1.53100600	-2.56401100	-0.28588400
O	2.34537200	-0.73252700	-0.64198300
H	1.77799100	-0.72455200	-1.42814200
H	1.57681700	-0.53085200	1.70533300
C	2.73523500	-2.09066800	-0.37497800
H	3.25642300	-2.51885600	-1.23848900
H	3.41877800	-2.06687000	0.47652000
H	1.86731100	-2.71395400	-0.12937300

Scan Point for comp9-c7oh_beta_2.6Å

C	0.77808100	2.19109500	-0.37577100
C	1.01719100	1.60674000	1.03671400
C	-1.28485700	0.75249900	-0.94690500
C	0.81579500	0.15650500	1.22180000
C	-1.50969600	0.09201500	0.40533800
H	-1.29582700	2.78165900	-0.21748800
H	1.43123800	1.66842100	-1.08184300
H	-0.69039500	0.09165000	-1.58792700
H	2.03197000	1.83029000	1.37220500
H	-1.82065500	0.81852100	1.16307200
C	-2.48683400	-1.07308200	0.41973200
H	-2.51405400	-1.51552700	1.42223000
H	-3.47846300	-0.66792300	0.19923100
O	-0.23468800	-0.50226900	0.96493900
H	-2.27688100	0.82508100	-1.40796900
H	-0.70439000	2.60811400	-1.86501000
H	1.11958700	3.23032600	-0.33475300
H	0.32380100	2.08103400	1.75497200
O	-2.21576300	-2.06631800	-0.56771000
H	-1.45801500	-2.59803100	-0.28039400
O	2.45962000	-0.67471800	-0.61311400
H	1.91924800	-0.64418500	-1.41704200
H	1.56368800	-0.44105800	1.73953300
C	2.83307600	-2.04078000	-0.36806500
H	3.37159100	-2.45658600	-1.22734000
H	3.49545400	-2.04255800	0.50041000

H	1.95558900	-2.66336900	-0.15620200

Scan Point for comp9-c7oh_beta_2.7Å

C	0.69258200	2.21963000	-0.39832300
C	0.91993900	1.69348400	1.03969700
C	-1.30831400	0.69280100	-0.96130800
C	0.78231300	0.24102800	1.25289800
C	-1.52547600	0.04734100	0.39943400
H	-1.40181900	2.73908000	-0.28341000
H	1.37542000	1.69414900	-1.07380300
H	-0.68291900	0.04154700	-1.58216000
H	1.91254200	1.97488900	1.39682800
H	-1.88639600	0.76781100	1.14085900
C	-2.43698200	-1.16987500	0.41428900
H	-2.45509700	-1.60091300	1.42201600
H	-3.44600800	-0.82350100	0.17339200
O	-0.22851200	-0.47203000	0.98939000
H	-2.29692200	0.71884600	-1.43434900
H	-0.78232800	2.54345700	-1.91842500
H	0.99925700	3.27024100	-0.38727600
H	0.18156900	2.15502300	1.71983300
O	-2.09546700	-2.15727300	-0.55631800
H	-1.30055200	-2.62605600	-0.26066300
O	2.52801500	-0.62619700	-0.61537500
H	1.97295400	-0.61055900	-1.40935700
H	1.55992000	-0.31677300	1.77258900
C	2.89262000	-1.98880000	-0.34303900
H	3.40924400	-2.43471900	-1.20101000
H	3.57330700	-1.97539000	0.51118500
H	2.01385000	-2.59686500	-0.09609900

Scan Point for comp9-c7oh_beta_2.8Å

C	0.59637900	2.23657700	-0.39055300
C	0.81498200	1.73079500	1.05828300
C	-1.35219400	0.64659600	-0.96927200
C	0.74687100	0.27224700	1.25546400
C	-1.54695300	-0.00531500	0.39205400
H	-1.51295500	2.69370900	-0.30576900
H	1.30451800	1.72441200	-1.05004400
H	-0.70800400	0.01349100	-1.58945400

H	1.78373300	2.06113200	1.43767700
H	-1.92653300	0.70228800	1.13690700
C	-2.41589900	-1.25260000	0.40885400
H	-2.41611300	-1.68502900	1.41606400
H	-3.43677800	-0.94013000	0.17129300
O	-0.22684600	-0.48206600	0.97221400
H	-2.34123300	0.64318100	-1.44196600
H	-0.86786600	2.50551400	-1.93175600
H	0.87183100	3.29573200	-0.38442500
H	0.03586800	2.15697200	1.71449700
O	-2.04352500	-2.22673900	-0.56371000
H	-1.23900900	-2.67650200	-0.26465700
O	2.65861400	-0.53677700	-0.62355600
H	2.14858200	-0.54089100	-1.44706400
H	1.55616800	-0.26097400	1.75282600
C	3.02857600	-1.88839900	-0.31012200
H	3.62610100	-2.33045400	-1.11614100
H	3.63227600	-1.85299200	0.59972900
H	2.14566300	-2.51407200	-0.13159200

Scan Point for comp9-c7oh_beta_2.9Å

C	0.37753600	2.30036200	-0.38828800
C	0.66746400	1.79726500	1.05066800
C	-1.44533900	0.56476900	-0.95454700
C	0.72455100	0.33612300	1.22533000
C	-1.55271600	-0.12074600	0.39925800
H	-1.75953000	2.57993600	-0.25008500
H	1.11115800	1.85590700	-1.06930700
H	-0.76555000	-0.00227600	-1.60003100
H	1.61386100	2.20190000	1.41438300
H	-1.96991000	0.54294600	1.16386800
C	-2.31489300	-1.43628300	0.41810800
H	-2.25692300	-1.87909900	1.41907400
H	-3.36280000	-1.20588700	0.20576800
O	-0.18407600	-0.49335300	0.94054400
H	-2.44211800	0.48594000	-1.40438100
H	-1.13838700	2.47326100	-1.89254500
H	0.56766600	3.37802100	-0.37227400
H	-0.12934500	2.15066100	1.72849300
O	-1.88343100	-2.36459000	-0.57484100
H	-1.04771300	-2.76331900	-0.28899500
O	2.78106900	-0.39072400	-0.68580200
H	2.34296800	-0.49965700	-1.54266100

H	1.58805800	-0.13697800	1.69197300
C	3.23241600	-1.68041000	-0.24389900
H	3.91538200	-2.13066300	-0.97410800
H	3.77023900	-1.52965000	0.69501400
H	2.38986400	-2.36103700	-0.07067400

Scan Point for comp9-c7oh_beta_3.0Å

C	0.31104800	2.30979200	-0.38690700
C	0.60134800	1.81776700	1.05709100
C	-1.46707200	0.53165900	-0.96005400
C	0.69495100	0.35864100	1.22869700
C	-1.56704600	-0.15231200	0.39485600
H	-1.83294500	2.54144600	-0.26434000
H	1.05825800	1.87832700	-1.06133300
H	-0.76831500	-0.02103800	-1.59787700
H	1.53483000	2.24613300	1.42685700
H	-2.00105000	0.50361100	1.15679700
C	-2.30143700	-1.48350500	0.41396200
H	-2.23102800	-1.92691200	1.41390000
H	-3.35452100	-1.27342000	0.20599800
O	-0.19046900	-0.49315300	0.93888000
H	-2.45795600	0.42738400	-1.41761500
H	-1.19758100	2.44372400	-1.90200000
H	0.47839500	3.39116500	-0.37297700
H	-0.20966600	2.15309800	1.72679200
O	-1.85590500	-2.40100100	-0.58261600
H	-1.01186100	-2.78498000	-0.30118400
O	2.88117700	-0.34228300	-0.70239600
H	2.48265500	-0.47432200	-1.57509100
H	1.57526400	-0.09519600	1.68439600
C	3.31886500	-1.61767900	-0.20957000
H	4.03024100	-2.08582800	-0.90038500
H	3.82097700	-1.44021800	0.74440300
H	2.47238200	-2.29663500	-0.04909400

Scan Point for comp9-c7oh_beta_3.1Å

C	0.27213000	2.31173000	-0.39013800
C	0.53660800	1.84316200	1.06762000
C	-1.46754800	0.49983100	-0.97606500
C	0.65825800	0.38788600	1.24885400

C	-1.57958800	-0.17020500	0.38472500
H	-1.87686200	2.51293500	-0.31415500
H	1.03983100	1.88140800	-1.04189900
H	-0.74928100	-0.04969200	-1.59471600
H	1.45202200	2.29444700	1.45466000
H	-2.03564600	0.48624400	1.13312100
C	-2.29387600	-1.51224300	0.40691000
H	-2.22466600	-1.94792600	1.41032500
H	-3.34833900	-1.31852800	0.19003300
O	-0.20436000	-0.48327100	0.94985900
H	-2.44848700	0.37506800	-1.44964000
H	-1.20688800	2.40331700	-1.93733800
H	0.42422900	3.39535200	-0.38709700
H	-0.29815000	2.16919600	1.71184000
O	-1.82884700	-2.42969200	-0.58062100
H	-0.98160200	-2.80078700	-0.29189200
O	2.96106200	-0.31161100	-0.70506600
H	2.58076500	-0.45034800	-1.58474300
H	1.54722100	-0.04675600	1.70771200
C	3.37268300	-1.58501000	-0.18577900
H	4.09737300	-2.06890700	-0.85156000
H	3.85113000	-1.40033200	0.77896600
H	2.51557600	-2.25359500	-0.03881800

Scan Point for comp9-c7oh_beta_3.2Å

C	0.11909600	2.34808100	-0.42002200
C	0.28626000	1.97717500	1.08215700
C	-1.40281900	0.35258200	-1.03826400
C	0.55871700	0.55221100	1.32386500
C	-1.54784900	-0.25902800	0.34629400
H	-2.03528900	2.35315200	-0.53376500
H	0.97930700	1.96285700	-0.97743700
H	-0.60290300	-0.16284100	-1.58114600
H	1.10120500	2.54745500	1.53084900
H	-2.10811800	0.38772400	1.02920600
C	-2.13954500	-1.65786200	0.39774600
H	-2.09801500	-2.03485800	1.42628800
H	-3.19094400	-1.57226000	0.10820200
O	-0.18595200	-0.41531100	1.00660900
H	-2.33722100	0.12090400	-1.56312300
H	-1.22082800	2.21779100	-2.08807200
H	0.17011200	3.44015500	-0.46495400
H	-0.64424300	2.22334100	1.62035500

O	-1.53382000	-2.57717000	-0.50778400
H	-0.67123400	-2.84294600	-0.15529100
O	2.94462900	-0.19366300	-0.67390700
H	2.60037100	-0.32270100	-1.56975000
H	1.46754600	0.22952900	1.83464500
C	3.37229300	-1.46708800	-0.16798700
H	4.13930100	-1.91349900	-0.81244000
H	3.80157400	-1.29265400	0.82145200
H	2.53039700	-2.16434900	-0.07581300

Scan Point for comp9-c7oh_beta_3.3Å

C	0.05038300	2.35105600	-0.42337100
C	0.19428800	2.00011300	1.08648500
C	-1.39968500	0.30676100	-1.05588000
C	0.50226300	0.58599000	1.34724100
C	-1.55775500	-0.29640800	0.33108500
H	-2.10036300	2.29287600	-0.58653000
H	0.93391700	1.98558500	-0.95737300
H	-0.57379900	-0.19069800	-1.57615400
H	0.98314500	2.59751600	1.54635500
H	-2.15268400	0.33850500	0.99564800
C	-2.10464300	-1.71343000	0.38178700
H	-2.07740200	-2.07940000	1.41481000
H	-3.14989800	-1.66637600	0.06326300
O	-0.20576400	-0.40579000	1.02193800
H	-2.31558900	0.04378200	-1.59826100
H	-1.24613900	2.16610400	-2.12011900
H	0.07097300	3.44371400	-0.47800000
H	-0.75419500	2.22612500	1.60096800
O	-1.44384200	-2.61943300	-0.49835500
H	-0.57417000	-2.83791500	-0.13051100
O	3.01385600	-0.12741800	-0.67091400
H	2.68719500	-0.26438600	-1.57206300
H	1.41174000	0.29407300	1.87589800
C	3.43164900	-1.39564400	-0.14418400
H	4.21883600	-1.84312200	-0.76300900
H	3.83099600	-1.21205500	0.85608800
H	2.59018300	-2.09561000	-0.07111400

Scan Point for comp9-c7oh_beta_3.5Å

C	-0.00729500	2.34447400	-0.42128400
C	0.09894700	2.00782000	1.09539000
C	-1.41084900	0.27471400	-1.07676000
C	0.42519900	0.60092400	1.37157000
C	-1.59402500	-0.32122500	0.31024700
H	-2.15151900	2.25461300	-0.64281300
H	0.89581100	1.98748800	-0.92780300
H	-0.56556400	-0.21470000	-1.57303100
H	0.86427600	2.62195100	1.57261000
H	-2.21469600	0.30861100	0.95580200
C	-2.11929800	-1.74645400	0.35712400
H	-2.10964400	-2.10617800	1.39265200
H	-3.15775100	-1.71784400	0.01492800
O	-0.25707400	-0.40445600	1.03361000
H	-2.30937600	-0.00506700	-1.63942800
H	-1.25386900	2.12766100	-2.15134200
H	-0.00032700	3.43681500	-0.48440800
H	-0.86751600	2.22082200	1.58075000
O	-1.42488900	-2.64663600	-0.50280500
H	-0.55940500	-2.84765100	-0.11564100
O	3.18583500	-0.07296200	-0.67165500
H	2.86255600	-0.23289400	-1.57021700
H	1.32867600	0.32673100	1.92014600
C	3.56889300	-1.33189100	-0.09811300
H	4.34766300	-1.82014600	-0.69637600
H	3.96750500	-1.12255400	0.89743300
H	2.70948000	-2.00707500	-0.00416600

Scan Point for comp9-c7oh_beta_3.6Å

C	0.06768100	2.33306500	-0.41285900
C	0.15161400	1.99397400	1.10541400
C	-1.40848800	0.31613300	-1.07673400
C	0.43854300	0.57740600	1.37259900
C	-1.60755900	-0.27960700	0.30828700
H	-2.07740000	2.32141500	-0.64025800
H	0.95953500	1.94130700	-0.91433300
H	-0.58337500	-0.20151900	-1.57822200
H	0.93109000	2.58459100	1.58928100
H	-2.20749400	0.36536900	0.95843900
C	-2.17462900	-1.68894900	0.34884100
H	-2.16972600	-2.05608100	1.38179800
H	-3.21370400	-1.62717600	0.01292400
O	-0.27102100	-0.40604900	1.02696900

H	-2.31855400	0.07127700	-1.63712600
H	-1.18144800	2.16402100	-2.14673500
H	0.11629800	3.42424700	-0.47677800
H	-0.81205100	2.23344600	1.58315200
O	-1.51282400	-2.60343300	-0.52162700
H	-0.64873900	-2.82863200	-0.14475000
O	3.29236800	-0.14112200	-0.70089900
H	3.05642300	-0.29160300	-1.62800600
H	1.33839600	0.27394100	1.91206300
C	3.44854500	-1.41531200	-0.05775700
H	4.21602600	-2.02105600	-0.55456400
H	3.76651600	-1.21853100	0.96884900
H	2.50430500	-1.97352200	-0.04085000

Scan Point for comp9-c7oh_beta_3.7Å

C	0.10889200	2.31276200	-0.39635000
C	0.17410000	1.96318000	1.12102500
C	-1.42791200	0.34564600	-1.07661600
C	0.42644100	0.53742100	1.37272000
C	-1.64285000	-0.25264300	0.30513700
H	-2.03412600	2.36922300	-0.63175300
H	0.99060700	1.89633400	-0.89607200
H	-0.62040900	-0.19451500	-1.58300900
H	0.96566700	2.53002900	1.61355700
H	-2.22150600	0.40678700	0.96011100
C	-2.25492400	-1.64326200	0.33900800
H	-2.25858000	-2.01680800	1.36954800
H	-3.29299400	-1.54441300	0.00824700
O	-0.30877100	-0.42366700	1.01818500
H	-2.34611100	0.13382000	-1.63718000
H	-1.13804200	2.19098800	-2.13575200
H	0.19162300	3.40215600	-0.45459600
H	-0.78614900	2.22286100	1.59447600
O	-1.62818100	-2.57415400	-0.53992600
H	-0.78217400	-2.84958400	-0.15608100
O	3.33600500	-0.21291300	-0.78631500
H	3.04707000	-0.49826300	-1.66514600
H	1.32293200	0.20512600	1.90107200
C	3.59029300	-1.38072200	0.00890500
H	4.35756200	-2.01546800	-0.45083400
H	3.95430000	-1.03484900	0.97933400
H	2.67753400	-1.97061100	0.15743800

Scan Point for comp9-c7oh_beta_3.8Å

C	0.05692800	2.32705200	-0.40971000
C	0.10117400	2.00295000	1.11405900
C	-1.39758700	0.29963800	-1.09121200
C	0.39219400	0.59048500	1.39554900
C	-1.62511400	-0.28597000	0.29390400
H	-2.08186800	2.30717700	-0.68911500
H	0.96192100	1.93178300	-0.88473800
H	-0.56001700	-0.21953400	-1.56987500
H	0.86337200	2.60270200	1.61390400
H	-2.24171200	0.36081700	0.92642700
C	-2.18538900	-1.69806500	0.33267100
H	-2.19850600	-2.05886200	1.36779200
H	-3.21794500	-1.64436500	-0.02402600
O	-0.30281700	-0.39987500	1.04063000
H	-2.29415400	0.04770000	-1.66983700
H	-1.14942500	2.13843800	-2.17182300
H	0.10512200	3.41763700	-0.48305500
H	-0.87706800	2.23938100	1.56227500
O	-1.50163400	-2.61413400	-0.51914700
H	-0.64062000	-2.82739800	-0.12831900
O	3.32917200	-0.23523700	-0.86991600
H	3.13726100	-0.64097800	-1.72789700
H	1.28499800	0.29641300	1.95175700
C	3.52028400	-1.28015700	0.09529000
H	4.33388000	-1.95341500	-0.20094800
H	3.79050200	-0.79932000	1.03839200
H	2.60410900	-1.86603100	0.23860700

Scan Point for comp9-c7oh_beta_3.9Å

C	0.11648100	2.30108200	-0.39296600
C	0.15125600	1.96014400	1.12768800
C	-1.43004200	0.34728000	-1.08902700
C	0.38940300	0.53365800	1.38719600
C	-1.66991400	-0.24375600	0.29201500
H	-2.02197200	2.37905300	-0.66158900
H	1.00094000	1.87024300	-0.87595800
H	-0.62093400	-0.20263500	-1.58211800
H	0.93824700	2.52315900	1.63179700
H	-2.25173000	0.42324900	0.93643600

C	-2.29434800	-1.62898400	0.32235000
H	-2.31286000	-2.00012900	1.35356800
H	-3.32780900	-1.52178400	-0.02014800
O	-0.34690200	-0.42312300	1.02364200
H	-2.34233900	0.14264500	-1.66167600
H	-1.10496300	2.18515600	-2.15088100
H	0.21385100	3.38893400	-0.45663600
H	-0.81546700	2.22900600	1.58219300
O	-1.66647700	-2.56757500	-0.54759700
H	-0.82795500	-2.85123800	-0.15351100
O	3.46163300	-0.28342500	-0.87195700
H	3.26740900	-0.69654200	-1.72581900
H	1.27656900	0.19668900	1.92798500
C	3.62268800	-1.31903000	0.10859700
H	4.42999500	-2.00824600	-0.16751200
H	3.88616000	-0.83057500	1.04973100
H	2.69542500	-1.88883400	0.24532400

Scan Point for comp9-c7oh_beta_4.0Å

C	0.09661300	2.29066700	-0.38352200
C	0.13640100	1.93751100	1.13405900
C	-1.46901500	0.35549200	-1.08832200
C	0.36369500	0.50702200	1.38083800
C	-1.70684700	-0.24534500	0.28885300
H	-2.04246300	2.38800500	-0.63922900
H	0.97461900	1.85584600	-0.87460000
H	-0.66684000	-0.19646300	-1.59041200
H	0.93077600	2.48958200	1.63869100
H	-2.28085700	0.42087900	0.94103100
C	-2.34158400	-1.62611300	0.31144400
H	-2.36148500	-2.00330200	1.34043200
H	-3.37473400	-1.50919500	-0.02885800
O	-0.38235300	-0.44059500	1.01329200
H	-2.38596600	0.16323100	-1.65783300
H	-1.13533100	2.20039800	-2.13542200
H	0.20341800	3.37804600	-0.43953800
H	-0.82567000	2.21062900	1.59594700
O	-1.72130500	-2.56381700	-0.56481900
H	-0.88604800	-2.85805300	-0.17153300
O	3.58773200	-0.25681700	-0.86017400
H	3.42238900	-0.66702600	-1.72151000
H	1.25033900	0.15823400	1.91504200
C	3.75861800	-1.29688200	0.11389400

H	4.59279200	-1.95852900	-0.14969800
H	3.98376300	-0.81022900	1.06587200
H	2.84643400	-1.89605700	0.22423600

Scan Point for comp9-c7oh_beta_4.1Å

C	0.06196500	2.28836300	-0.38203100
C	0.10313300	1.93320900	1.13514000
C	-1.49696900	0.34838700	-1.08892400
C	0.33813700	0.50337900	1.37778100
C	-1.73034400	-0.25694600	0.28702100
H	-2.07757200	2.37808500	-0.63570800
H	0.94143700	1.85748300	-0.87397100
H	-0.69345300	-0.19939700	-1.59346900
H	0.89476700	2.48825300	1.64080100
H	-2.30731800	0.40424100	0.94170400
C	-2.35707700	-1.64141300	0.30617500
H	-2.37343700	-2.02185900	1.33404200
H	-3.39129900	-1.52950100	-0.03251600
O	-0.40370300	-0.44711800	1.00923700
H	-2.41402100	0.15376100	-1.65749000
H	-1.17121500	2.19621700	-2.13308100
H	0.16478300	3.37619000	-0.43655300
H	-0.86040000	2.20090800	1.59682400
O	-1.73261900	-2.57276400	-0.57381200
H	-0.89348500	-2.86079500	-0.18418200
O	3.69579800	-0.23173000	-0.85733100
H	3.52897400	-0.64821500	-1.71532100
H	1.22897800	0.15777500	1.90719400
C	3.84972000	-1.26404400	0.12787000
H	4.67923800	-1.93606600	-0.12387200
H	4.07289000	-0.77023800	1.07666300
H	2.93078600	-1.85297300	0.23735800

Scan Point for comp9-c7oh_beta_4.2Å

C	-0.03831900	2.29801300	-0.38109500
C	0.05085100	1.92434900	1.12908700
C	-1.57158800	0.33375600	-1.07386400
C	0.31940100	0.49661700	1.34813400
C	-1.75922800	-0.29604600	0.29776000
H	-2.18540800	2.34304600	-0.57487500

H	0.83647200	1.89288100	-0.90188600
H	-0.76774100	-0.18851800	-1.60435300
H	0.84489200	2.48858800	1.62060800
H	-2.33698600	0.34130100	0.97491400
C	-2.35020200	-1.69613900	0.31040400
H	-2.33729000	-2.08920000	1.33369600
H	-3.39295300	-1.60756100	-0.00804100
O	-0.41245900	-0.46465900	0.98780700
H	-2.49716400	0.12525300	-1.62351000
H	-1.31679500	2.20298200	-2.09926800
H	0.03969900	3.38844400	-0.42352900
H	-0.90495600	2.16819700	1.61889800
O	-1.71768400	-2.60002300	-0.59205400
H	-0.85702900	-2.85724700	-0.22836300
O	3.84146100	-0.15493600	-0.84516700
H	3.72096000	-0.56618200	-1.71336600
H	1.23042700	0.16232600	1.85003600
C	4.02033200	-1.19326500	0.12946300
H	4.89074200	-1.81751900	-0.10684200
H	4.18795400	-0.70336800	1.09167900
H	3.13047800	-1.83065600	0.20281800

Scan Point for comp9-c7oh_beta_4.3Å

C	-0.10985200	2.28226300	-0.38898200
C	-0.02358400	1.91601000	1.12299700
C	-1.63447400	0.31086800	-1.07785900
C	0.24583800	0.49012900	1.35293300
C	-1.82521500	-0.31468100	0.29518400
H	-2.25680000	2.31981700	-0.58782300
H	0.76707900	1.87658900	-0.90582700
H	-0.82674200	-0.21033100	-1.60343400
H	0.76789400	2.48442100	1.61387800
H	-2.40931200	0.32206300	0.96746500
C	-2.40839300	-1.71813300	0.30943000
H	-2.39807900	-2.10790800	1.33404900
H	-3.44994400	-1.63718500	-0.01472700
O	-0.48161700	-0.47488000	0.99377600
H	-2.55733100	0.09671400	-1.62996100
H	-1.38413600	2.17703900	-2.10967100
H	-0.03425900	3.37268000	-0.43632100
H	-0.98107000	2.16064000	1.60949500
O	-1.76575000	-2.62088400	-0.58705100
H	-0.90011300	-2.86246500	-0.22412200

O	3.88245300	-0.17452200	-0.84325900
H	3.95817400	-0.59684100	-1.71130300
H	1.15213100	0.16098900	1.86643400
C	4.44385500	-1.05697300	0.14034400
H	5.50186800	-1.26129900	-0.06430700
H	4.36056200	-0.55172300	1.10567600
H	3.89498600	-2.00561100	0.18593500

Scan Point for comp9-c7oh_beta_4.4Å

C	-0.11926600	2.27448900	-0.40756000
C	-0.03913900	1.92262700	1.10850100
C	-1.64959100	0.30182000	-1.08122400
C	0.22676200	0.49831500	1.35167500
C	-1.84489400	-0.30859400	0.29788100
H	-2.26527000	2.31833000	-0.61461400
H	0.75799000	1.86091500	-0.91763800
H	-0.84317000	-0.22807000	-1.60006500
H	0.75185900	2.49406000	1.59661600
H	-2.42648500	0.33793700	0.96294600
C	-2.43595000	-1.70846600	0.32624200
H	-2.42499100	-2.08917500	1.35423900
H	-3.47802400	-1.62381100	0.00461200
O	-0.50254400	-0.46777600	0.99923400
H	-2.57236700	0.08593100	-1.63274700
H	-1.38780200	2.15596400	-2.13169100
H	-0.03979900	3.36414100	-0.46505700
H	-0.99783600	2.17359800	1.58942800
O	-1.80214600	-2.62326300	-0.56426100
H	-0.93889600	-2.87087300	-0.19987400
O	3.90744600	-0.31317600	-0.91857600
H	3.94758400	-0.92176400	-1.67069400
H	1.13155300	0.17130100	1.86917600
C	4.56651100	-0.92807000	0.19869400
H	5.61505200	-1.15370200	-0.03090900
H	4.53136900	-0.21109400	1.02258700
H	4.05782600	-1.85026700	0.50549000

X.4: Hartree-Fock Optimized Stationary Points and Energetics for Septanoside Hydrolysis.

Compound 1 (Alpha) - Anti Reactant Complex

C	-1.11812700	1.41900900	0.17255200
C	0.19652500	1.72893700	-0.54638500
C	1.39430300	0.94318700	-0.01183000
C	-1.66016100	0.01146200	-0.04015200
C	1.43794200	-0.43891100	-0.67040000
C	-0.66486600	-1.09251400	0.33634900
H	-0.98048000	1.58401400	1.24711600
H	0.07967300	1.51693200	-1.61796400
H	-1.91960000	-0.11194000	-1.09716900
H	2.28847700	1.47622900	-0.34552600
H	1.86752100	-0.38613200	-1.67158300
H	-0.15990900	-0.87908000	1.28139100
O	1.35547600	0.88402200	1.39704800
H	2.23910600	1.03305500	1.75149400
O	0.51737800	3.09635400	-0.35504500
H	-0.28727200	3.60879200	-0.51028000
O	-2.04830300	2.36534800	-0.33981000
H	-2.85695200	2.30981100	0.18358700
O	-2.82648600	-0.06923700	0.76559100
H	-3.39872900	-0.76191800	0.41299900
C	-1.32209500	-2.45016400	0.43989500
H	-0.54249200	-3.21495400	0.50796200
H	-1.92407300	-2.48317100	1.35229600
O	-2.13339200	-2.64813400	-0.71098200
H	-2.51769800	-3.53053400	-0.66916200
O	0.30351000	-1.17436800	-0.73748400
O	2.42305800	-1.26845800	0.13620700
H	2.26350200	-2.21258000	-0.06419700
C	3.84505500	-0.92971000	-0.00359900
H	4.09551900	-0.90703600	-1.06266400
H	3.98651700	0.03582700	0.47363000
H	4.38550500	-1.70932500	0.52528600

Compound 1 (Alpha) - Gauche Reactant Complex

C	1.85852200	0.02433200	0.14683800
C	1.38690700	-1.25211400	-0.55414200

C	0.08311800	-1.82708700	0.00195100
C	0.97255200	1.24465800	-0.06399200
C	-1.12229900	-1.10102400	-0.61304300
C	-0.48317000	1.00903100	0.35216600
H	1.93680500	-0.17023800	1.22274500
H	1.25965200	-1.04619800	-1.62544500
H	0.98244300	1.51176400	-1.12601900
H	0.02091800	-2.86112900	-0.34651500
H	-1.36698700	-1.50632000	-1.59508700
H	-0.55118100	0.45911500	1.29432700
O	0.07836500	-1.79221400	1.41396500
H	-0.12179100	-2.67064400	1.75448600
O	2.35810800	-2.26821200	-0.36723900
H	3.22575700	-1.88140500	-0.54564400
O	3.15138300	0.28185900	-0.38652600
H	3.53005500	1.02856300	0.09374900
O	1.56088700	2.27969400	0.70847400
H	1.27153800	3.12943300	0.35271000
C	-1.26215400	2.29567100	0.49881600
H	-2.32553400	2.05645100	0.59737800
H	-0.93258000	2.80351900	1.40968700
O	-1.02379500	3.10589700	-0.64531500
H	-1.53680300	3.91706300	-0.55945100
O	-1.09619200	0.24625200	-0.71349900
O	-2.31633100	-1.43940800	0.26569200
H	-2.37632000	-2.39353700	0.47100900
C	-3.60888800	-0.93137800	-0.21564900
H	-3.53412900	0.15067600	-0.20217600
H	-3.78391800	-1.32185000	-1.21646900
H	-4.34483600	-1.28873500	0.49864600

Compound 1 (Alpha) - Transition State for Anti-Gauche Interconversion

C	1.42862700	-1.19861100	0.10765400
C	0.15813200	-1.79086900	-0.50677200
C	-1.14822700	-1.25796700	0.07736900
C	1.64632300	0.30035500	-0.10048600
C	-1.50393500	0.09727700	-0.53097000
C	0.48939200	1.17458000	0.39710000
H	1.42918200	-1.40097300	1.17285600
H	0.16081000	-1.60199400	-1.57699600
H	1.79505700	0.49199500	-1.15647600
H	-1.93249800	-1.93550400	-0.23532600
H	-1.89164600	-0.02305600	-1.52877400

H	0.15057700	0.85350700	1.37205200
O	-1.07321100	-1.22805700	1.47433100
H	-1.93281700	-1.34517100	1.85335600
O	0.13798100	-3.17966000	-0.27713900
H	0.95702700	-3.55756000	-0.56777400
O	2.49076400	-1.90209400	-0.50000100
H	3.29686200	-1.72636100	-0.03515500
O	2.82360000	0.60151000	0.61435000
H	3.29880400	1.30212900	0.19107100
C	0.83046500	2.64631300	0.50127200
H	-0.07066900	3.18811500	0.76787800
H	1.55777000	2.78405700	1.29195100
O	1.33847000	3.11021900	-0.72886500
H	1.55354200	4.02941100	-0.65682600
O	-0.57877700	1.07633100	-0.55720300
O	-2.67705300	0.60490100	0.25654200
H	-2.48949300	1.44761800	0.67351400
C	-4.01360900	0.56093900	-0.34868100
H	-4.02259600	1.22299900	-1.19942100
H	-4.18435500	-0.46524600	-0.62464900
H	-4.69275800	0.87872500	0.42368100

Compound 1 (Alpha) - Transition State for MeOH Dissociation (Anti)

C	1.48393000	-1.22666300	0.18219300
C	0.26371500	-1.82970000	-0.51910600
C	-1.07003700	-1.19157100	-0.11781400
C	1.74523800	0.26247500	-0.07530500
C	-1.19224300	0.14354000	-0.81901800
C	0.61911700	1.19372300	0.39887600
H	1.38794100	-1.37958900	1.25089900
H	0.38768100	-1.72506100	-1.59437300
H	1.91517800	0.42129400	-1.13321500
H	-1.86579000	-1.81292000	-0.50466400
H	-1.85920100	0.25271900	-1.65615300
H	0.20642200	0.89052200	1.34638600
O	-1.14674600	-1.06809500	1.26380300
H	-2.01599700	-0.76921500	1.50328900
O	0.14492500	-3.18571000	-0.18397300
H	0.95110300	-3.63597600	-0.39897900
O	2.57727100	-1.96726200	-0.30461200
H	3.33408800	-1.82676600	0.24723200
O	2.90178700	0.56854400	0.65892600
H	3.42303700	1.21666500	0.20613400

C	0.98190900	2.65789600	0.46010500
H	0.07981000	3.22843300	0.65033200
H	1.66044100	2.79994700	1.29187900
O	1.57539900	3.04910900	-0.75244900
H	1.78766800	3.97148500	-0.71940200
O	-0.47327300	1.12461900	-0.59904100
O	-3.27597000	0.64003800	0.43445200
H	-3.23055400	1.53682700	0.73727600
C	-4.51462900	0.41133200	-0.21345000
H	-4.61738500	1.04404600	-1.08809600
H	-4.53355900	-0.62577300	-0.51873400
H	-5.34002100	0.59722400	0.46447700

Compound 1 (Alpha) - Transition State for MeOH Dissociation (Gauche)

C	1.84627100	-0.56421800	0.13115200
C	0.97807400	-1.63304600	-0.54040300
C	-0.46844600	-1.68160100	-0.03234200
C	1.41428700	0.89236300	-0.06773300
C	-1.22941900	-0.55344100	-0.70459600
C	-0.01027700	1.20394400	0.41081200
H	1.88923600	-0.76780600	1.19463200
H	0.97005600	-1.45867600	-1.61359100
H	1.49336600	1.14406000	-1.11813400
H	-0.91396800	-2.59845200	-0.38920800
H	-1.77616700	-0.78247800	-1.59995300
H	-0.22792000	0.74450100	1.36159000
O	-0.49213400	-1.62072700	1.35715700
H	-1.19886900	-2.15196600	1.69717100
O	1.50920200	-2.90415500	-0.27260600
H	2.42030700	-2.92526800	-0.53417700
O	3.12590700	-0.73556900	-0.43296200
H	3.77480600	-0.29436600	0.09715100
O	2.32279200	1.65508900	0.68635200
H	2.47831700	2.49300700	0.27332900
C	-0.34088300	2.67600500	0.49949900
H	-1.39930600	2.77770600	0.71146900
H	0.21706000	3.10164200	1.32427000
O	-0.01217300	3.30965700	-0.71280500
H	-0.25105100	4.22487700	-0.66913400
O	-0.93602700	0.66463000	-0.58644400
O	-2.97268400	-0.78142300	0.33364300
H	-2.88818000	-0.43371900	1.21354100
C	-4.13505900	-0.24237500	-0.29132400
H	-4.01941500	0.82178700	-0.45566800

H	-4.25646000	-0.75149600	-1.23616700
H	-4.99817900	-0.42915500	0.33380600

Compound 1 (Alpha) - Product Complex (Gauche)

C	1.76818100	-0.86152800	0.15937500
C	0.74517000	-1.77087800	-0.52915400
C	-0.70603300	-1.52585900	-0.10102600
C	1.60992800	0.64555900	-0.07840300
C	-1.19670800	-0.26850500	-0.78821700
C	0.27705300	1.22912700	0.41328400
H	1.74037800	-1.04498100	1.22741500
H	0.81891100	-1.63073300	-1.60461100
H	1.71997700	0.85700400	-1.13496200
H	-1.30821900	-2.33743000	-0.48401600
H	-1.87535700	-0.34387500	-1.61956600
H	-0.02810000	0.81697400	1.36086300
O	-0.78844800	-1.44140700	1.28356500
H	-1.68381700	-1.58090300	1.56270400
O	1.00760200	-3.10979700	-0.20657800
H	1.89717300	-3.32644100	-0.45301500
O	3.01173400	-1.26953400	-0.35873600
H	3.71381300	-0.90669300	0.16339600
O	2.64767700	1.24558700	0.65233000
H	2.95811400	2.02596000	0.21419900
C	0.22307500	2.73624600	0.48854100
H	-0.79910100	3.03309000	0.69464500
H	0.84541900	3.05316700	1.31601300
O	0.67047000	3.28758100	-0.72436000
H	0.62986100	4.23270100	-0.67906700
O	-0.76081500	0.86911000	-0.57853100
O	-3.34455800	-0.26779400	0.45100400
H	-3.26468000	0.29675400	1.20770100
C	-4.48452500	0.10932000	-0.30037700
H	-4.37062900	1.11212200	-0.69826200
H	-4.58145700	-0.59084000	-1.11859400
H	-5.37843300	0.06325400	0.31146800

Compound 1 (Alpha) - Product Complex (Anti)

C	1.48393000	-1.22666300	0.18219300
C	0.26371500	-1.82970000	-0.51910600
C	-1.07003700	-1.19157100	-0.11781400
C	1.74523800	0.26247500	-0.07530500

C	-1.19224300	0.14354000	-0.81901800
C	0.61911700	1.19372300	0.39887600
H	1.38794100	-1.37958900	1.25089900
H	0.38768100	-1.72506100	-1.59437300
H	1.91517800	0.42129400	-1.13321500
H	-1.86579000	-1.81292000	-0.50466400
H	-1.85920100	0.25271900	-1.65615300
H	0.20642200	0.89052200	1.34638600
O	-1.14674600	-1.06809500	1.26380300
H	-2.01599700	-0.76921500	1.50328900
O	0.14492500	-3.18571000	-0.18397300
H	0.95110300	-3.63597600	-0.39897900
O	2.57727100	-1.96726200	-0.30461200
H	3.33408800	-1.82676600	0.24723200
O	2.90178700	0.56854400	0.65892600
H	3.42303700	1.21666500	0.20613400
C	0.98190900	2.65789600	0.46010500
H	0.07981000	3.22843300	0.65033200
H	1.66044100	2.79994700	1.29187900
O	1.57539900	3.04910900	-0.75244900
H	1.78766800	3.97148500	-0.71940200
O	-0.47327300	1.12461900	-0.59904100
O	-3.27597000	0.64003800	0.43445200
H	-3.23055400	1.53682700	0.73727600
C	-4.51462900	0.41133200	-0.21345000
H	-4.61738500	1.04404600	-1.08809600
H	-4.53355900	-0.62577300	-0.51873400
H	-5.34002100	0.59722400	0.46447700

Compound 2 (Beta) - Reactant Complex (Gauche)

C	1.85852200	0.02433200	0.14683800
C	1.38690700	-1.25211400	-0.55414200
C	0.08311800	-1.82708700	0.00195100
C	0.97255200	1.24465800	-0.06399200
C	-1.12229900	-1.10102400	-0.61304300
C	-0.48317000	1.00903100	0.35216600
H	1.93680500	-0.17023800	1.22274500
H	1.25965200	-1.04619800	-1.62544500
H	0.98244300	1.51176400	-1.12601900
H	0.02091800	-2.86112900	-0.34651500
H	-1.36698700	-1.50632000	-1.59508700
H	-0.55118100	0.45911500	1.29432700
O	0.07836500	-1.79221400	1.41396500
H	-0.12179100	-2.67064400	1.75448600

O	2.35810800	-2.26821200	-0.36723900
H	3.22575700	-1.88140500	-0.54564400
O	3.15138300	0.28185900	-0.38652600
H	3.53005500	1.02856300	0.09374900
O	1.56088700	2.27969400	0.70847400
H	1.27153800	3.12943300	0.35271000
C	-1.26215400	2.29567100	0.49881600
H	-2.32553400	2.05645100	0.59737800
H	-0.93258000	2.80351900	1.40968700
O	-1.02379500	3.10589700	-0.64531500
H	-1.53680300	3.91706300	-0.55945100
O	-1.09619200	0.24625200	-0.71349900
O	-2.31633100	-1.43940800	0.26569200
H	-2.37632000	-2.39353700	0.47100900
C	-3.60888800	-0.93137800	-0.21564900
H	-3.53412900	0.15067600	-0.20217600
H	-3.78391800	-1.32185000	-1.21646900
H	-4.34483600	-1.28873500	0.49864600

Compound 2 (Beta) - Reactant Complex (Anti)

C	0.23799400	1.62897300	-0.11875700
C	1.53283700	0.83272800	-0.14781900
C	1.59963200	-0.37025400	0.78729300
C	-1.01187500	0.79937100	-0.40031600
C	0.66109600	-1.53077900	0.46387700
C	-1.35764800	-0.14340400	0.76869800
H	0.12254500	2.10463800	0.86389900
H	1.69354100	0.49028700	-1.17733000
H	-0.88862900	0.22528500	-1.32549600
H	2.61877800	-0.76415300	0.70670400
H	1.01468300	-2.45648200	0.91852300
H	-1.11726100	0.33552300	1.72122600
O	1.31234300	-0.04705200	2.13143400
H	2.02048000	0.51925900	2.46384800
O	2.61344200	1.66010700	0.25745600
H	2.58228700	2.47334600	-0.26261400
O	0.40660600	2.62408600	-1.11713000
H	-0.39618400	3.16011400	-1.14203300
O	-2.05051600	1.75413100	-0.55796100
H	-2.79632600	1.32508300	-0.99698200
C	-2.82331500	-0.51895500	0.77701700
H	-2.97548700	-1.32666700	1.49786700
H	-3.41171100	0.34640000	1.09092300
O	-3.18510000	-0.92932900	-0.53705900

H	-4.10265600	-1.22372100	-0.52741800
O	-0.65985600	-1.41210000	0.71736700
O	0.77561800	-1.78347700	-1.03838300
H	-0.01252600	-2.29305900	-1.31674100
C	2.01355000	-2.40544100	-1.53163300
H	1.81278100	-2.67654300	-2.56407300
H	2.78964600	-1.64772200	-1.47068200
H	2.23210700	-3.27593900	-0.91557800

Compound 2 (Beta) - Transition State for MeOH Dissociation (Gauche)

C	-0.91093300	-1.48590300	-0.23834300
C	-1.78865100	-0.23954700	-0.28631900
C	-1.51235300	0.83938600	0.75430600
C	0.58787200	-1.22129300	-0.39951100
C	-0.15343800	1.51605800	0.72461600
C	1.20742600	-0.51999500	0.81971000
H	-1.07288800	-2.01341600	0.69647300
H	-1.68207500	0.20811800	-1.26649800
H	0.77007100	-0.64465900	-1.29861000
H	-2.24193800	1.62028100	0.59840600
H	-0.12483000	2.53106400	1.07175000
H	0.79138800	-0.91112200	1.73734400
O	-1.60897900	0.32106200	2.05388100
H	-2.04914000	0.93494600	2.62686000
O	-3.13337900	-0.59480600	-0.07886700
H	-3.40916300	-1.19740100	-0.75598000
O	-1.36564000	-2.27547200	-1.31130000
H	-0.96287600	-3.13167600	-1.27253700
O	1.18120300	-2.49059500	-0.51251200
H	1.96632100	-2.44564300	-1.04046900
C	2.71488200	-0.61832000	0.90003400
H	3.05241200	-0.01261700	1.73304300
H	2.98780200	-1.64768000	1.09174200
O	3.27653200	-0.16166000	-0.30728500
H	4.22117300	-0.16272600	-0.24077800
O	0.95575000	0.91971500	0.83658500
O	-0.20420900	2.19944500	-1.12624400
H	0.18527900	1.57367200	-1.72642900
C	0.38762700	3.48616200	-1.32186800
H	0.29848400	3.76070500	-2.36396800
H	-0.16380600	4.18705800	-0.71322200
H	1.42898100	3.47029900	-1.02694700

Compound 2 (Beta) - Product Complex (Gauche)

C	-0.22672900	-1.68704100	-0.42970000
C	-1.52414400	-0.91276800	-0.21044500
C	-1.59428100	-0.06527400	1.05754300
C	1.03442600	-0.82690600	-0.53852400
C	-0.66337700	1.13352600	1.07542300
C	1.40367300	-0.12108500	0.77447000
H	-0.09135400	-2.40346300	0.37408200
H	-1.68247900	-0.25835100	-1.05925400
H	0.91425900	-0.09250500	-1.32557200
H	-2.59846700	0.32635100	1.12475300
H	-1.05262400	2.10464600	1.32235200
H	1.21764800	-0.74415600	1.63579800
O	-1.27295400	-0.82089100	2.19055800
H	-1.81509200	-0.56621100	2.92600100
O	-2.59713300	-1.81135200	-0.09609000
H	-2.64825700	-2.34289100	-0.87915100
O	-0.42486700	-2.36930500	-1.64394100
H	0.28189000	-2.98415500	-1.78410700
O	2.07129100	-1.71871300	-0.85422500
H	2.71770300	-1.29873400	-1.40462600
C	2.81801600	0.40398400	0.84491200
H	2.91989500	0.99824700	1.74558600
H	3.48777600	-0.44341600	0.91473400
O	3.08759600	1.17413600	-0.29934100
H	3.96806600	1.51953600	-0.25186200
O	0.56439100	1.08668400	0.96049800
O	-1.43639300	2.26965300	-1.12305000
H	-1.04817800	1.93172600	-1.91786700
C	-1.33781400	3.68069200	-1.10941700
H	-1.82534100	4.10898700	-1.97851300
H	-1.83879900	4.03316900	-0.21780300
H	-0.30072000	3.99875800	-1.08539300

Compound 2 (Beta) - Product Complex (Anti)

C	-0.22672900	-1.68704100	-0.42970000
C	-1.52414400	-0.91276800	-0.21044500
C	-1.59428100	-0.06527400	1.05754300
C	1.03442600	-0.82690600	-0.53852400
C	-0.66337700	1.13352600	1.07542300
C	1.40367300	-0.12108500	0.77447000
H	-0.09135400	-2.40346300	0.37408200

H	-1.68247900	-0.25835100	-1.05925400
H	0.91425900	-0.09250500	-1.32557200
H	-2.59846700	0.32635100	1.12475300
H	-1.05262400	2.10464600	1.32235200
H	1.21764800	-0.74415600	1.63579800
O	-1.27295400	-0.82089100	2.19055800
H	-1.81509200	-0.56621100	2.92600100
O	-2.59713300	-1.81135200	-0.09609000
H	-2.64825700	-2.34289100	-0.87915100
O	-0.42486700	-2.36930500	-1.64394100
H	0.28189000	-2.98415500	-1.78410700
O	2.07129100	-1.71871300	-0.85422500
H	2.71770300	-1.29873400	-1.40462600
C	2.81801600	0.40398400	0.84491200
H	2.91989500	0.99824700	1.74558600
H	3.48777600	-0.44341600	0.91473400
O	3.08759600	1.17413600	-0.29934100
H	3.96806600	1.51953600	-0.25186200
O	0.56439100	1.08668400	0.96049800
O	-1.43639300	2.26965300	-1.12305000
H	-1.04817800	1.93172600	-1.91786700
C	-1.33781400	3.68069200	-1.10941700
H	-1.82534100	4.10898700	-1.97851300
H	-1.83879900	4.03316900	-0.21780300
H	-0.30072000	3.99875800	-1.08539300

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