

Supporting Information

Ferric Superoxide and Ferric Hydroxide Are Used in the Catalytic Mechanism of Hydroxyethylphosphonate Dioxygenase (HEPD): A Density Functional Theory Investigation

Hajime Hirao[†] and Keiji Morokuma^{*, †, §}

[†] *Fukui Institute for Fundamental Chemistry, Kyoto University, 34-4 Takano Nishihiraki-cho,
Sakyo, Kyoto 606-8103, Japan*

[§] *Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory
University, Atlanta, Georgia 30322*

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Complete list of the authors of Gaussian 09

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Table S1. Summary of energy data**(a) Protonated hydroxyl (R-OH)**

	B1			B2//B1		
	ΔE (kcal/mol)	E (Eh)	ZPE (Eh)	ΔE (kcal/mol)	E (Eh)	$\Delta(E+ZPE)$ (kcal/mol)
5RC (side-on)	5.7	-1795.404665	0.375837	5.7	-2935.761588	5.8
5RC (end-on)	6.8	-1795.403002	0.375573	5.3	-2935.762225	5.2
7RC (side-on)	0.0	-1795.413784	0.375603	0.0	-2935.770615	0.0
5TSh	33.8	-1795.359992	0.368191	30.3	-2935.722387	25.6
7TSh	34.8	-1795.358360	0.368027	31.5	-2935.720394	26.8
5Int-ooh	-5.5	-1795.422530	0.376559	-6.0	-2935.780178	-5.4
7Int-ooh	23.2	-1795.376827	0.372356	19.2	-2935.740089	17.1
5TSho	-1.8	-1795.416702	0.371486	-1.4	-2935.772885	-4.0
5Int-hooc	-30.5	-1795.462347	0.378377	-29.9	-2935.818293	-28.2
5TShoo	-17.8	-1795.442173	0.376247	-19.0	-2935.800960	-18.6
5Int-feoh2	-25.7	-1795.454725	0.374329	-28.7	-2935.816396	-29.5
5TSerie	17.9	-1795.385256	0.372566	15.9	-2935.745204	14.0
5Int-erie	-63.1	-1795.514313	0.376965	-65.5	-2935.874943	-64.6
5TSsoh	1.3	-1795.411766	0.374964	0.6	-2935.769603	0.2
5Int-coh	-18.4	-1795.443155	0.377255	-21.1	-2935.804307	-20.1
5Int-coh2(A)	-19.8	-1795.445396	0.377461	-16.7	-2935.797251	-15.5
5Int-coh2(B)	-31.2	-1795.463536	0.379149	-35.8	-2935.827718	-33.6
5TSoh(A)	-11.9	-1795.432788	0.370366	-15.8	-2935.795851	-19.1
5TSoh(B)	-9.4	-1795.428775	0.372062	-14.2	-2935.793320	-16.5
5Int-feoh(A)	-24.1	-1795.452261	0.373510	-27.7	-2935.814835	-29.1
5Int-feoh(B)	-13.4	-1795.435078	0.375453	-17.3	-2935.798258	-17.4
5TScc	-11.0	-1795.431349	0.370359	-15.5	-2935.795262	-18.8
5Int-hcooh	-33.8	-1795.467725	0.369572	-40.5	-2935.835144	-44.3
HCOOH		-189.751896	0.033931		-189.838926	
H2O		-76.407025	0.021146		-76.460542	
5Int-h2o		-1682.138358	0.361275		-2822.465967	
5Int-hcooh + H2O	-33.8	-1871.874750	0.390718	-40.5	-3012.295687	-44.3
5Int-h2o+HCOOH	-43.6	-1871.890254	0.395206	-46.3	-3012.304893	-47.2
5TSco + HCOOH	-36.7	-1871.879297	0.395381	-41.1	-3012.296691	-42.0
5Pro + HCOOH	-83.5	-1871.953810	0.400469	-85.0	-3012.366558	-82.6
5TSpt + HCOOH	-32.2	-1871.872201	0.392140	-34.4	-3012.285987	-37.3
5Int-pt + HCOOH	-45.8	-1871.893799	0.395341	-48.4	-3012.308345	-49.3
5TSco-pt+HCOOH	-40.0	-1871.884612	0.395783	-43.3	-3012.300126	-43.9
5Pro-pt+ HCOOH	-90.2	-1871.964531	0.401441	-90.4	-3012.375224	-87.5

(b) Deprotonated hydroxyl (R-O⁻)

	B1			B2//B1		
	ΔE (kcal/mol)	E (Eh)	ZPE (Eh)	ΔE (kcal/mol)	E (Eh)	$\Delta(E+ZPE)$ (kcal/mol)
5RC (side-on)	7.3	-1794.831943	0.360406	7.4	-2935.194259	6.9
7RC (side-on)	0.0	-1794.843616	0.361237	0.0	-2935.206070	0.0
5TSh	21.7	-1794.809028	0.355273	18.1	-2935.177287	14.3
7TSh	23.2	-1794.806605	0.355556	20.3	-2935.173750	16.7

(c) With the effect of Tyr98

	B1			B2//B1		
	ΔE (kcal/mol)	E (Eh)	ZPE (Eh)	ΔE (kcal/mol)	E (Eh)	$\Delta(E+ZPE)$ (kcal/mol)
5Int-ooH	0.0	-2142.224812	0.508102	0.0	-3282.710754	0.0
5TSho	5.9	-2142.215373	0.502903	7.2	-3282.699324	3.9
5Int-hooc	-22.9	-2142.261331	0.509956	-22.0	-3282.745754	-20.8
5TSooH	8.0	-2142.212031	0.506009	8.8	-3282.696745	7.5
5Int-coH	-13.1	-2142.245705	0.508673	-14.3	-3282.733617	-14.0

Figure S1. Relaxed scan calculations for the H-abstraction step (**RC** to **Int-ooH**). Relative energies are with respect to ⁷**RC**.

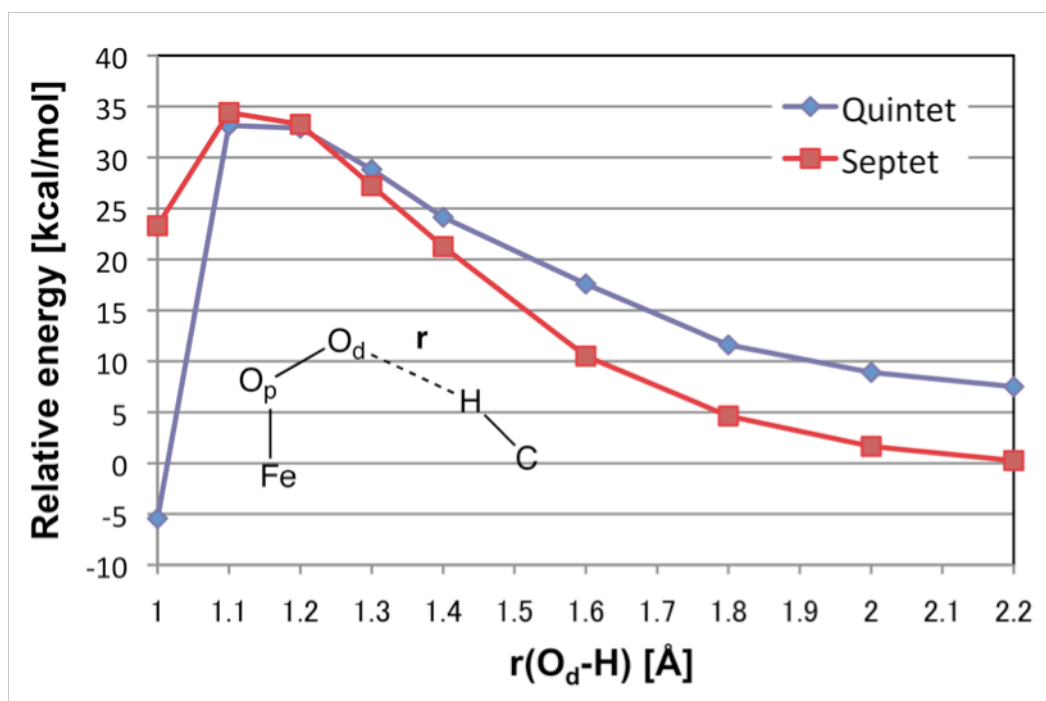


Figure S2. Relaxed scan calculations for the hydroperoxylation step (**Int-ooH** to **Int-hooc**). Relative energies are with respect to ⁵**Int-ooH**.

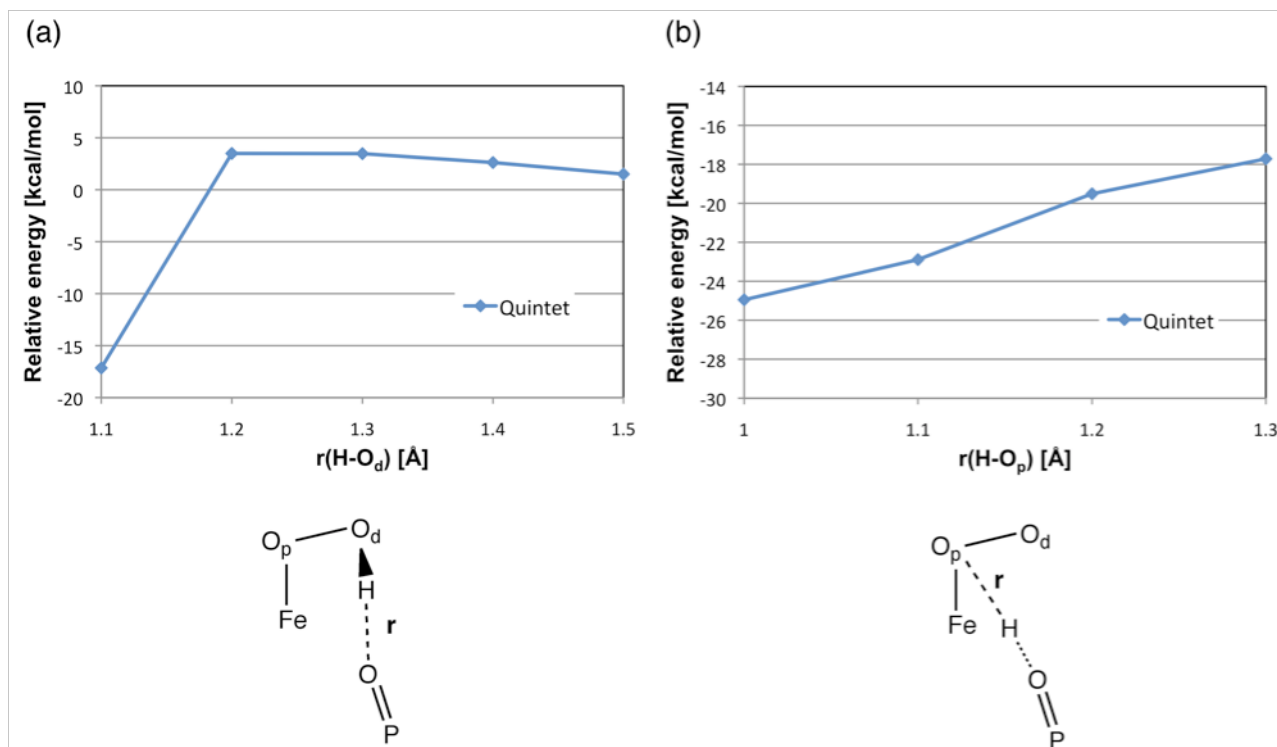


Figure S3. Relaxed scan calculations for the hydroxylation step (**Int-oooh** to **Int-coh**). Relative energies are with respect to $^5\text{Int-oooh}$.

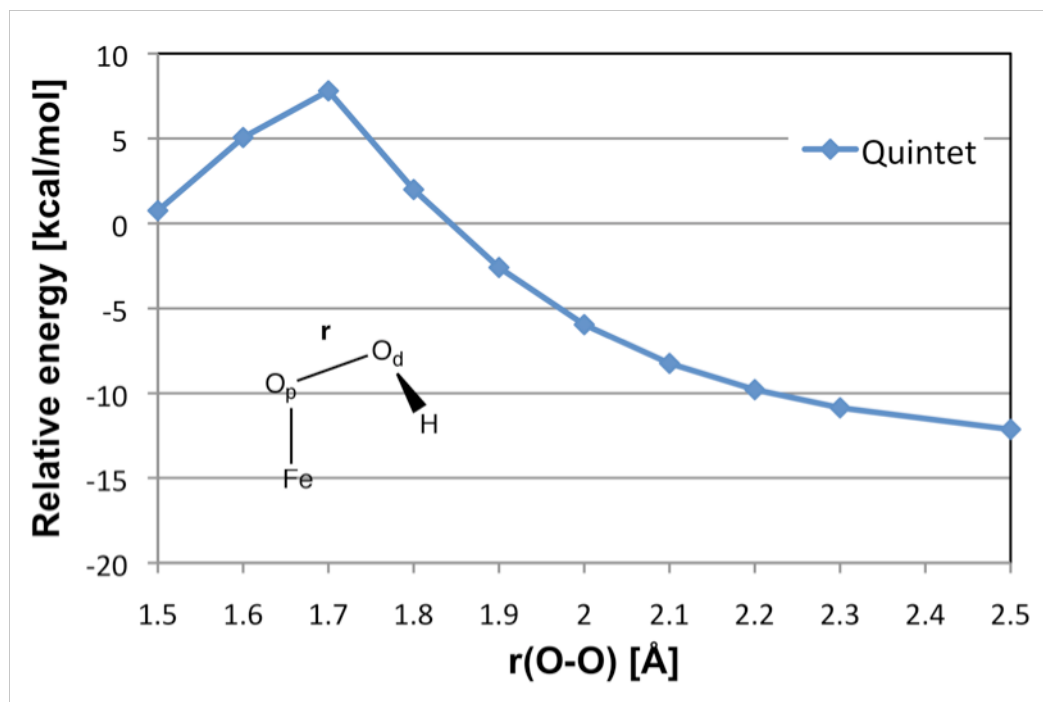


Figure S4. Relaxed scan calculations for the O-H bond activation step (**Int-coh2** to **Int-feoh**). Relative energies are with respect to $^5\text{Int-oooh}$.

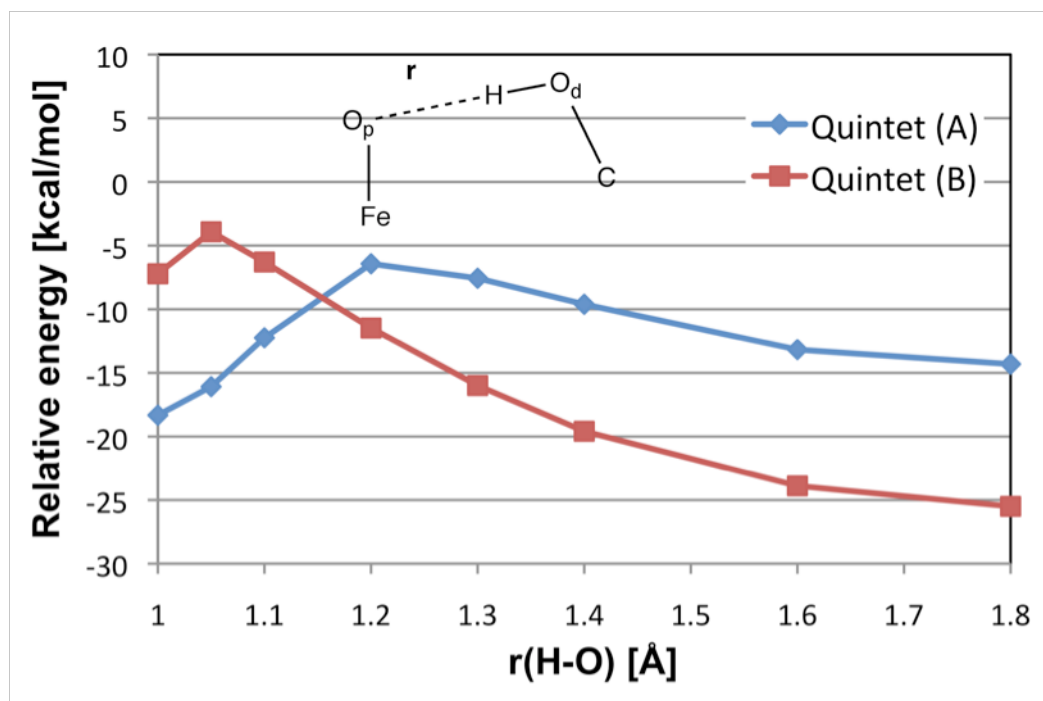


Figure S5. Relaxed scan calculations for the C-C bond cleavage step (**Int-feoh2** to **Int-hcooh**). Relative energies are with respect to ⁵**Int-feoh2**.

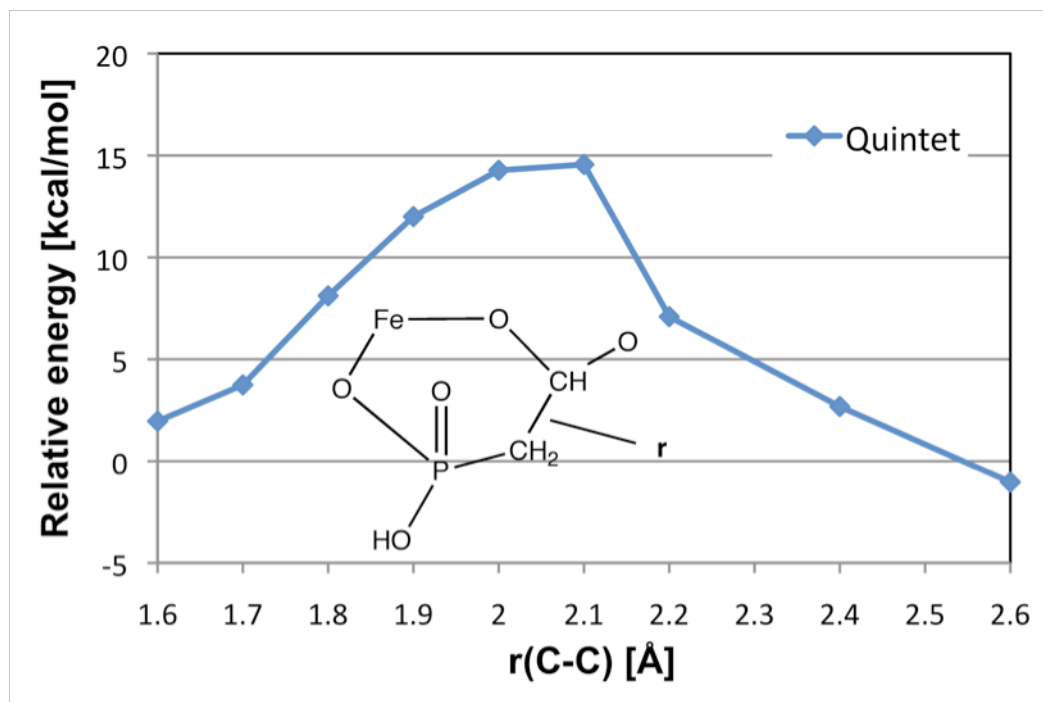


Figure S6. Relaxed scan calculations for the C-O bond formation step (**Int-h2o** to **Pro**). Relative energies are with respect to ⁵**Int-feoh2**.

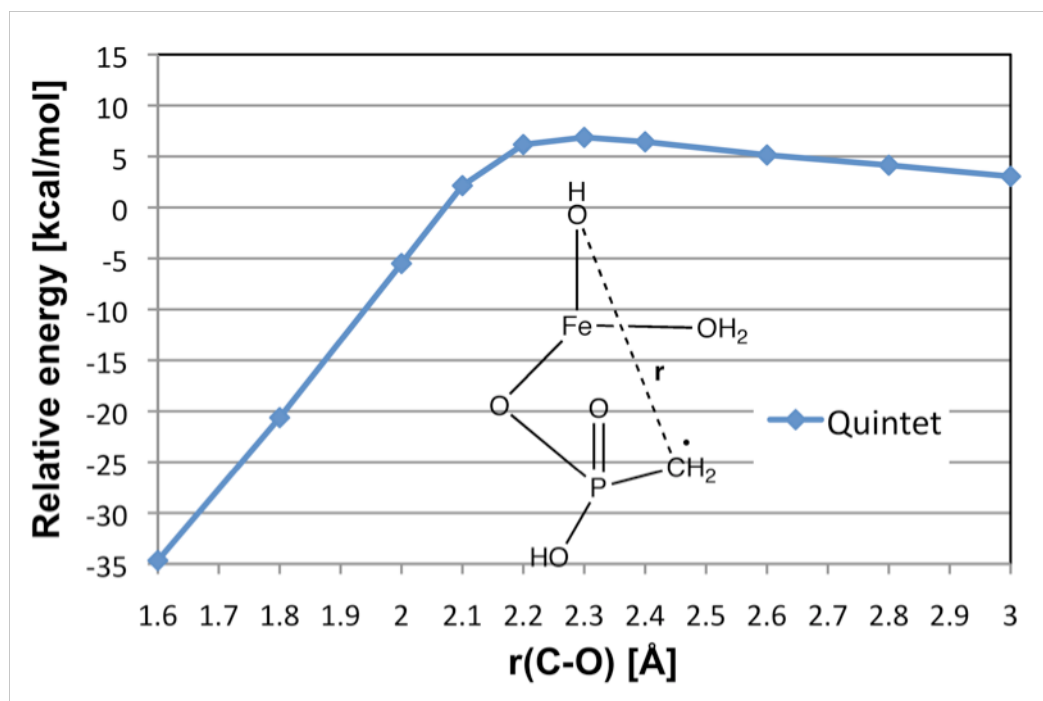


Figure S7. Relaxed scan calculations for the proton-transfer step (**Int-h2o** to **Int-pt**). Relative energies are with respect to ⁵**Int-feoh2**.

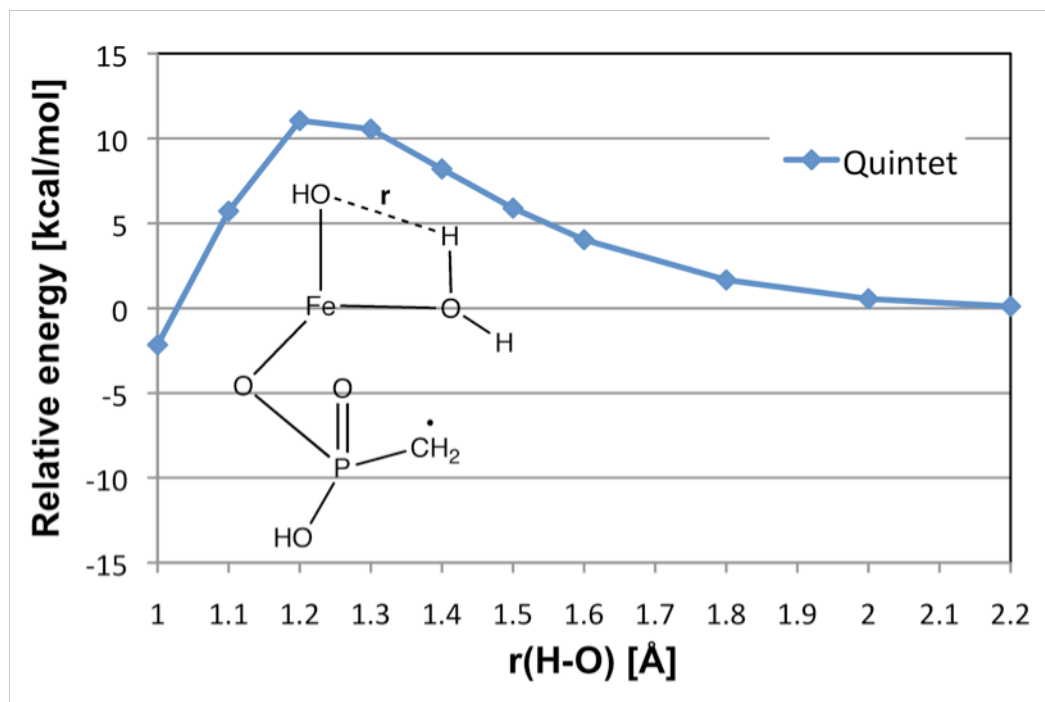


Figure S8. Relaxed scan calculations for the C-O bond formation step (**Int-pt** to **Pro-pt**). Relative energies are with respect to ⁵**Int-feoh2**.

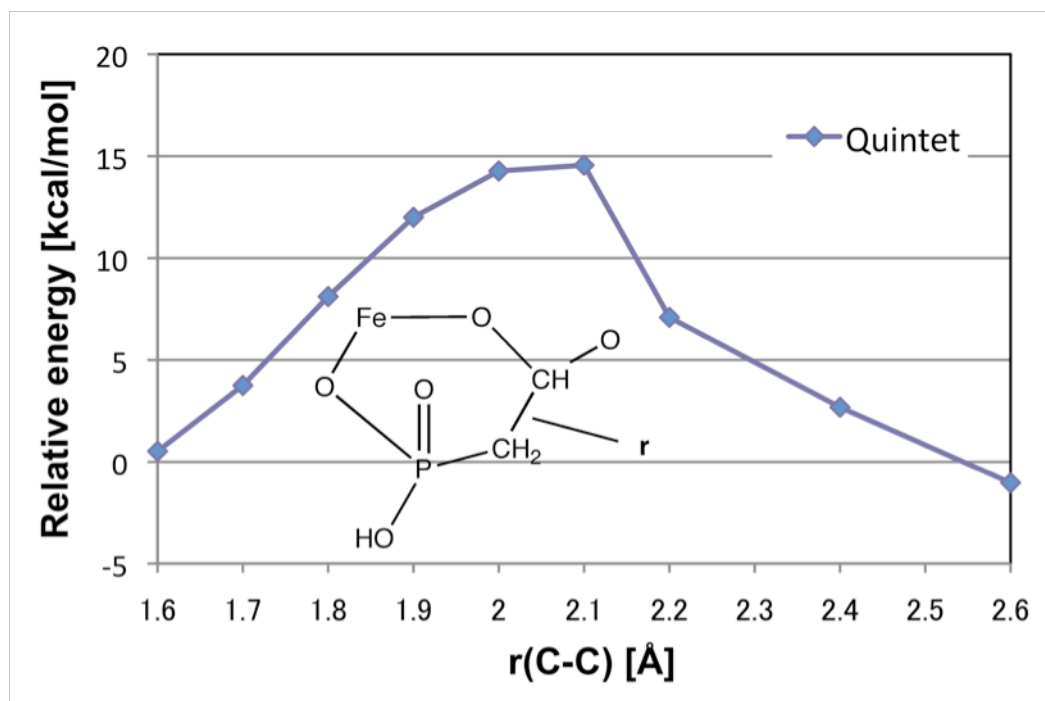
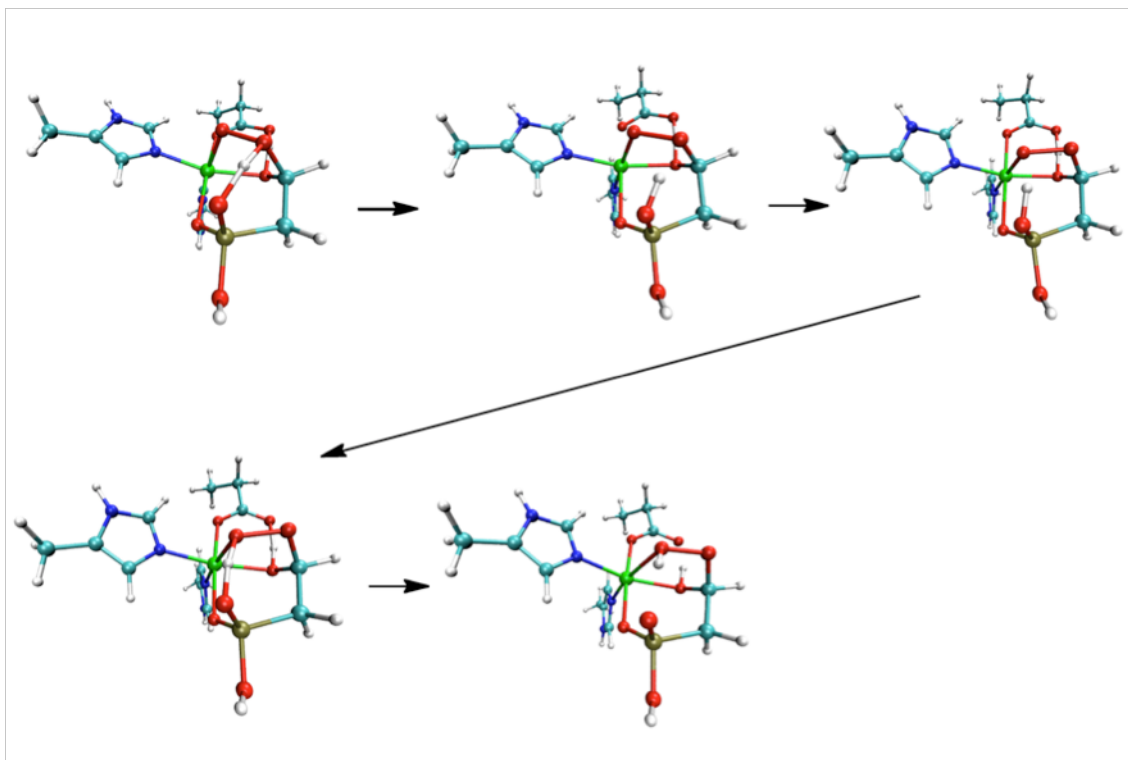
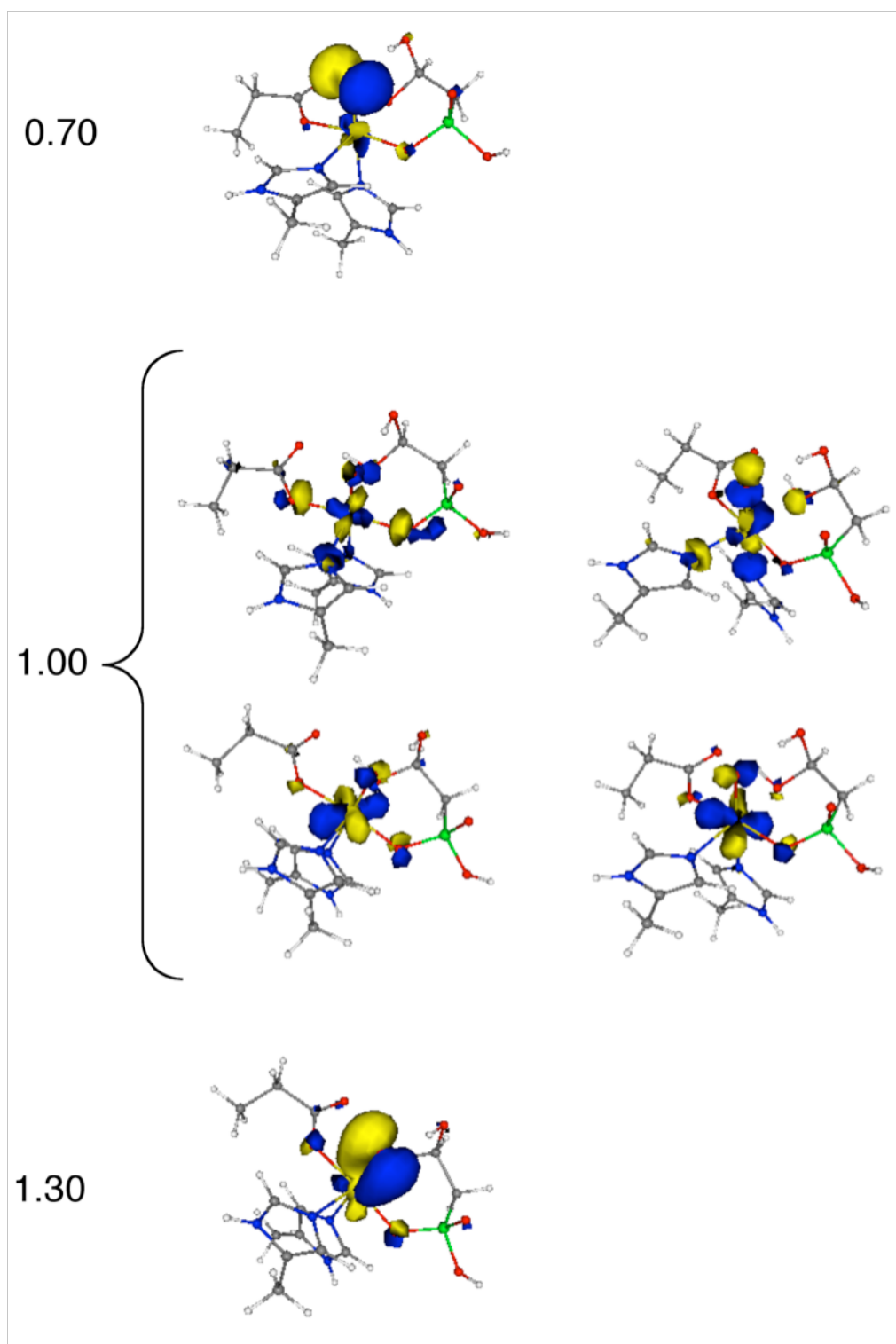


Figure S9. A few snapshot geometries generated during the geometry optimization started from a state slightly after **TSho**.



* **TSho** had an H---O distance of 1.24 Å. After slightly decreasing the distance to 1.23 Å, geometry optimization was performed using the `iop(1/8=5)` keyword with the three C_β atoms fixed.

Figure S10. Natural orbitals for **Int-coh2(A)**.



* The values are occupation numbers. Plotted with Molekel Ver 5.3.06 (Molekel ver.5.3; Swiss National Supercomputing Centre).

Figure S11. Energy change due to a Criegee-type rearrangement of **Int-hooc**. Relative energies are with respect to ⁵**Int-hooc**.

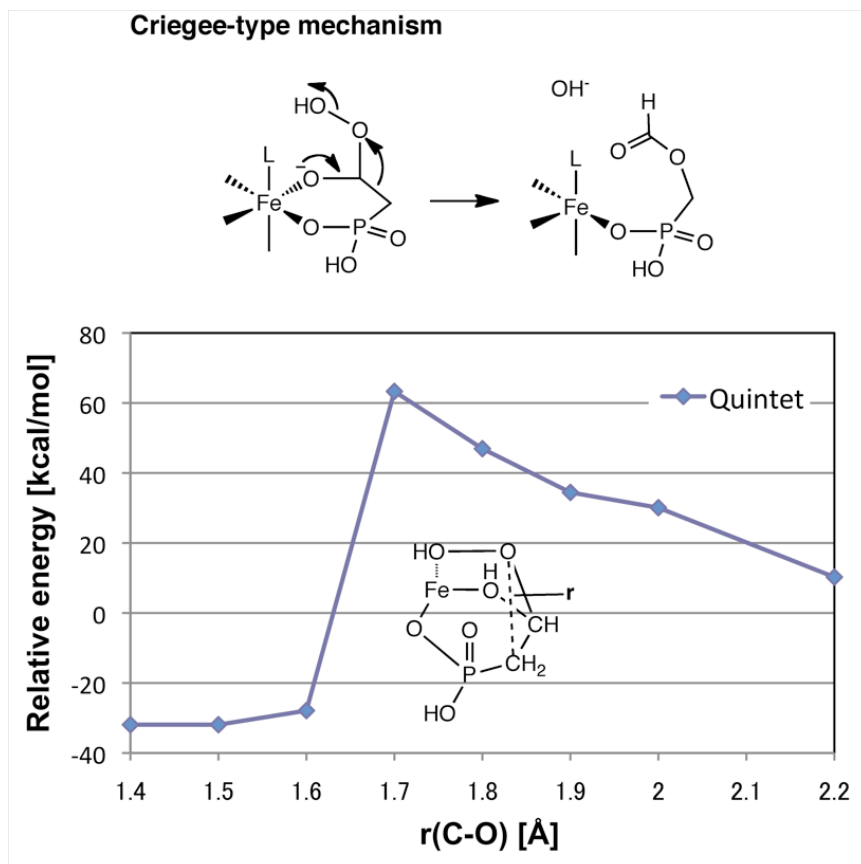
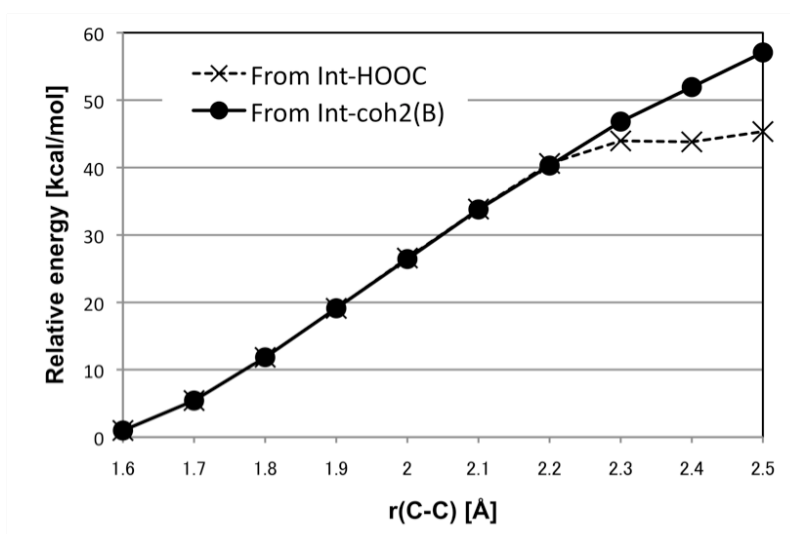


Figure S12. Energy change due to elongation of the C-C bond of **Int-hooc** and **Int-coh2(B)**.



XYZ coordinates of optimized geometries (in Å)

=== 5RC (side-on) ===

H	22.950400	28.549262	24.374890
C	23.079000	28.773000	25.442000
H	24.147021	28.678726	25.676725
H	22.798259	29.817940	25.598023
N	22.379042	26.511468	26.342262
H	23.037365	25.969258	25.801575
C	22.239955	27.892496	26.307989
C	21.497707	26.012981	27.247982
H	21.408962	24.969285	27.507424
N	20.798486	26.990853	27.787782
C	21.247289	28.163749	27.214944
H	20.833715	29.115095	27.515027
H	20.760239	21.098391	29.040814
C	20.224000	22.049000	29.138000
H	20.542996	22.707143	28.324399
H	19.155339	21.839861	29.006459
C	20.497428	22.692347	30.505466
H	20.181952	22.033669	31.319170
H	21.575929	22.867082	30.617410
C	19.793483	24.035387	30.680829
O	20.007451	24.891880	29.730266
O	19.072060	24.232605	31.674514
H	14.398433	23.838957	27.222910
C	15.392000	23.814000	26.757000
H	15.843953	22.847668	26.996432
H	15.250052	23.854625	25.669029
N	15.969342	26.263027	27.113555
H	15.146237	26.645902	26.670866
C	16.270011	24.915405	27.254423
C	16.958407	26.991054	27.697368
H	16.962762	28.070452	27.757265
N	17.877681	26.187982	28.200320
C	17.463133	24.900468	27.929122
H	18.047610	24.051158	28.245743
O	17.914735	26.503203	31.071360
C	17.629432	27.520377	32.040146
C	16.935246	28.682162	31.332423
O	18.912438	28.660132	29.420263
O	16.885367	30.138967	29.064056
P	18.002416	29.666555	30.199275
O	18.643231	30.855428	30.830976
H	16.958567	27.099281	32.799863
H	18.548932	27.849894	32.539123
H	16.084719	28.289540	30.764112
H	16.542802	29.384959	32.076016
H	18.281847	25.666574	31.496936
H	16.974032	31.101698	28.966580
Fe	19.524505	26.838134	29.589649
O	21.438166	27.393784	30.441917
O	20.625977	27.188060	31.425939

=== 5RC (end-on) ===

H	22.955373	28.502098	24.385298
C	23.079000	28.773000	25.442000
H	24.151341	28.734003	25.673190
H	22.754500	29.810411	25.558425
N	22.471487	26.519952	26.423327
H	23.145414	25.984777	25.894979
C	22.281598	27.892875	26.345390
C	21.610564	26.018631	27.346556
H	21.551624	24.980102	27.633733
N	20.877902	26.987898	27.859100
C	21.282618	28.157659	27.247289
H	20.832334	29.101748	27.516251
H	20.721704	21.080063	29.017423
C	20.224000	22.049000	29.138000
H	20.536226	22.700274	28.316495
H	19.144558	21.879610	29.042780
C	20.566613	22.673974	30.496811
H	20.259972	22.023448	31.320626
H	21.654979	22.805726	30.574972
C	19.927594	24.045060	30.712818
O	20.021619	24.859771	29.711173

O	19.375614	24.300785	31.799232
H	14.413240	23.747652	27.249566
C	15.392000	23.814000	26.757000
H	15.901590	22.858231	26.906081
H	15.214371	23.931700	25.679922
N	15.850827	26.255783	27.289073
H	14.992927	26.624987	26.904750
C	16.225849	24.919623	27.315691
C	16.821608	26.992062	27.892149
H	16.774531	28.064027	28.031436
N	17.799628	26.203659	28.301057
C	17.441534	24.917976	27.948107
H	18.082718	24.082677	28.182371
O	18.196851	26.587723	31.310613
C	18.147394	27.655462	32.266058
C	17.338264	28.804067	31.667034
O	19.002610	28.687393	29.474577
O	16.839367	30.014278	29.298639
P	18.150152	29.714871	30.282409
O	18.786889	31.002376	30.685122
H	17.649545	27.290504	33.173570
H	19.159284	27.979891	32.540483
H	16.381203	28.407044	31.311417
H	17.123208	29.548185	32.442089
H	18.604268	25.750006	31.696388
H	16.849935	30.967708	29.111192
Fe	19.507375	26.813319	29.556154
O	21.108287	27.170034	30.800911
O	21.483986	28.274127	31.254321

=== 7RC (side-on) ===

H	22.953092	28.526459	24.379608
C	23.079000	28.773000	25.442000
H	24.149372	28.705944	25.675613
H	22.776478	29.814586	25.578700
N	22.424392	26.514210	26.381443
H	23.089542	25.975301	25.845878
C	22.260204	27.891571	26.326021
C	21.553962	26.014381	27.297404
H	21.482282	24.973105	27.571475
N	20.839093	26.987621	27.825007
C	21.265374	28.158965	27.231934
H	20.834574	29.107332	27.517143
H	20.751337	21.094925	29.026418
C	20.224000	22.049000	29.138000
H	20.536735	22.710882	28.324979
H	19.152022	21.849217	29.019541
C	20.520217	22.680337	30.506306
H	20.209733	22.018491	31.319371
H	21.601712	22.844620	30.605568
C	19.829550	24.028457	30.699307
O	20.037657	24.888653	29.751711
O	19.124940	24.224840	31.705412
H	14.400664	23.826786	27.228159
C	15.392000	23.814000	26.757000
H	15.851953	22.848313	26.983490
H	15.244083	23.865392	25.670257
N	15.953733	26.262899	27.138086
H	15.125137	26.644630	26.704804
C	16.264888	24.916017	27.261811
C	16.942019	26.991354	27.723350
H	16.939701	28.070271	27.794798
N	17.870474	26.189366	28.210624
C	17.462783	24.902137	27.928154
H	18.055473	24.053526	28.231892
O	17.940989	26.490047	31.116428
C	17.650079	27.506402	32.082513
C	16.953033	28.664783	31.371709
O	18.935365	28.664642	29.464235
O	16.905529	30.144876	29.119203
P	18.022592	29.660208	30.249969
O	18.658727	30.843117	30.898537
H	16.979836	27.085579	32.843203
H	18.566756	27.842220	32.583811
H	16.110369	28.266023	30.796013

H	16.548578	29.362640	32.113570
H	18.318552	25.658671	31.540120
H	16.990848	31.109163	29.035849
Fe	19.519424	26.826330	29.591482
O	21.477922	27.419165	30.502355
O	20.676993	27.183350	31.465417

=== 5TSh ===

H	22.977354	28.493777	24.385225
C	23.079000	28.773000	25.442000
H	24.145183	28.729186	25.698720
H	22.758136	29.813086	25.542935
N	22.438175	26.530180	26.423973
H	23.123306	25.989766	25.915658
C	22.256767	27.904516	26.334080
C	21.559770	26.037581	27.332238
H	21.490477	25.002297	27.628065
N	20.821056	27.014636	27.822908
C	21.242590	28.180565	27.214035
H	20.795196	29.129302	27.471739
H	20.702429	21.065003	29.078782
C	20.224000	22.049000	29.138000
H	20.624182	22.673501	28.334230
H	19.152337	21.907868	28.953625
C	20.469322	22.690553	30.508923
H	20.080903	22.064617	31.317211
H	21.549835	22.798689	30.678755
C	19.854866	24.079412	30.647548
O	19.954501	24.851752	29.630449
O	19.298154	24.382186	31.734337
H	14.449550	23.666936	27.300413
C	15.392000	23.814001	26.757000
H	15.956335	22.879412	26.816655
H	15.143004	23.985007	25.701413
N	15.763799	26.242866	27.406353
H	14.868930	26.589556	27.091539
C	16.202900	24.927599	27.333443
C	16.729476	26.991541	28.000683
H	16.640454	28.048989	28.208139
N	17.765589	26.232484	28.312115
C	17.449498	24.951973	27.901033
H	18.140318	24.137797	28.052802
O	18.275125	26.621325	31.338478
C	18.416243	27.654229	32.238048
C	17.557197	28.846561	31.907236
O	18.765174	28.7110237	29.442203
O	16.530575	29.901676	29.613946
P	18.020593	29.737388	30.340106
O	18.614761	31.085435	30.569764
H	18.429226	27.320908	33.280821
H	19.785822	28.046688	32.071672
H	16.511211	28.524196	31.806560
H	17.608878	29.579928	32.717839
H	18.690401	25.694044	31.647396
H	16.410156	30.852525	29.453852
Fe	19.517550	26.890027	29.539304
O	21.010111	27.300668	30.687378
O	20.891423	28.101771	31.780325

=== 7TSh ===

H	22.975498	28.475910	24.390255
C	23.079000	28.773000	25.442000
H	24.147863	28.755529	25.690799
H	22.737148	29.807600	25.529794
N	22.491569	26.532571	26.461303
H	23.184623	25.998766	25.956870
C	22.281670	27.901266	26.352788
C	21.626377	26.035717	27.380523
H	21.576159	25.002712	27.688154
N	20.870566	27.004450	27.860874
C	21.266186	28.169382	27.233763
H	20.800669	29.112645	27.479265
H	20.679048	21.056058	29.048887
C	20.224000	22.049000	29.138000
H	20.601625	22.673961	28.323810
H	19.142824	21.931985	28.998040
C	20.539439	22.671056	30.503161

H	20.174077	22.044453	31.321866
H	21.628235	22.754185	30.630607
C	19.961401	24.071551	30.685026
O	19.975081	24.831907	29.654104
O	19.520081	24.393552	31.817575
H	14.451269	23.663089	27.302364
C	15.392000	23.814000	26.757000
H	15.958114	22.880171	26.811150
H	15.139723	23.988928	25.702832
N	15.762966	26.240741	27.417806
H	14.865844	26.587851	27.109947
C	16.203062	24.926076	27.335527
C	16.731896	26.987172	28.010189
H	16.646761	28.043173	28.226249
N	17.770336	26.227025	28.310108
C	17.452766	24.948131	27.896198
H	18.144892	24.133813	28.042803
O	18.459410	26.626616	31.465230
C	18.564332	27.685930	32.338779
C	17.669041	28.844055	31.983829
O	18.755548	28.682902	29.468726
O	16.573537	29.942097	29.747833
P	18.089061	29.727810	30.401968
O	18.737783	31.054043	30.615048
H	18.578609	27.381444	33.390708
H	19.960745	28.090002	32.102417
H	16.635326	28.480530	31.891118
H	17.692239	29.589753	32.784539
H	18.906856	25.719641	31.771473
H	16.466172	30.898710	29.615951
Fe	19.516144	26.857139	29.534089
O	21.113115	27.327949	30.681990
O	21.044260	28.115830	31.772479

=== 5Int-ooH ===

H	23.007833	28.419113	24.404885
C	23.079000	28.773000	25.442000
H	24.139305	28.759776	25.726458
H	22.747472	29.814737	25.459434
N	22.435701	26.601794	26.564853
H	23.148509	26.038331	26.124603
C	22.241211	27.962817	26.372226
C	21.526244	26.165270	27.474356
H	21.456619	25.149725	27.832076
N	20.758360	27.160947	27.871748
C	21.193223	28.283744	27.196512
H	20.727085	29.243340	27.366083
H	20.615194	21.026155	29.132241
C	20.224000	22.049000	29.138000
H	20.833357	22.653826	28.461402
H	19.204582	22.019592	28.737533
C	20.244146	22.621773	30.558472
H	19.640645	22.021884	31.246808
H	21.267152	22.615408	30.960013
C	19.756930	24.056590	30.612817
O	19.866681	24.808251	29.640296
O	19.218272	24.395869	31.761094
H	14.449400	23.606104	27.280309
C	15.392000	23.814001	26.757000
H	16.003284	22.908737	26.806795
H	15.151208	23.993481	25.700827
N	15.641718	26.248170	27.457749
H	14.745692	26.567495	27.118673
C	16.136118	24.953586	27.369156
C	16.570477	27.020187	28.083963
H	16.465147	28.075027	28.290466
N	17.628020	26.298595	28.403015
C	17.369835	25.017110	27.960158
H	18.092011	24.228333	28.097209
O	18.223475	26.817400	31.526926
C	18.396911	27.788443	32.306716
C	17.816658	29.147949	31.980771
O	18.444653	28.981005	29.318129
O	17.495055	31.187385	30.204247
P	18.558237	29.965472	30.490083
O	19.906178	30.537427	30.862846
H	18.651277	27.592539	33.354812
H	20.530650	29.059475	31.629023

H	16.743347	29.011046	31.797431
H	17.932709	29.823864	32.833849
H	18.905610	25.362028	31.736847
H	17.966798	32.022476	30.359352
Fe	19.366707	27.084838	29.553114
O	20.807494	27.297890	30.902909
O	20.458543	28.144671	32.021383

=== 7Int-ooH ===

H	23.038867	28.405606	24.408167
C	23.079000	28.773000	25.442000
H	24.135322	28.832832	25.734185
H	22.677679	29.789982	25.447716
N	22.575629	26.573859	26.588948
H	23.323227	26.051167	26.155922
C	22.291203	27.915064	26.375578
C	21.697704	26.088477	27.504958
H	21.699255	25.079136	27.887082
N	20.863324	27.035942	27.884672
C	21.219551	28.175313	27.192046
H	20.688297	29.103507	27.343318
H	20.751207	21.094884	29.024589
C	20.224000	22.049000	29.138000
H	20.542116	22.716251	28.331654
H	19.152710	21.851274	29.009767
C	20.509156	22.672254	30.510821
H	20.189208	22.010637	31.320547
H	21.590565	22.829902	30.625349
C	19.831336	24.026515	30.703907
O	19.960564	24.855175	29.725525
O	19.204221	24.246865	31.762435
H	14.425854	23.718914	27.269474
C	15.392000	23.814000	26.757000
H	15.922979	22.865662	26.875719
H	15.188452	23.949311	25.686570
N	15.821307	26.254662	27.322920
H	14.954031	26.616780	26.953391
C	16.218015	24.924047	27.320113
C	16.792472	26.990704	27.927927
H	16.746067	28.058141	28.084115
N	17.787427	26.214067	28.309107
C	17.442818	24.930831	27.935725
H	18.099026	24.100939	28.146013
O	18.107058	26.523567	31.379040
C	17.984852	27.462407	32.370634
C	17.462190	28.789972	31.937067
O	18.744885	28.707920	29.522873
O	17.704119	30.928038	30.272551
P	18.590332	29.634513	30.755472
O	19.873800	30.116835	31.398491
H	17.803457	27.083631	33.373381
H	20.998838	28.980217	31.354995
H	16.478286	28.705875	31.440294
H	17.336541	29.442707	32.806913
H	18.502849	25.632019	31.698549
H	18.237881	31.726319	30.420471
Fe	19.507359	26.846217	29.607963
O	21.103541	27.159615	30.778214
O	21.684966	28.228030	31.385335

=== 5TSooh ===

H	22.960299	28.467227	24.394156
C	23.078999	28.773000	25.442000
H	24.149642	28.733332	25.681445
H	22.763057	29.816771	25.519946
N	22.440926	26.559551	26.488725
H	23.114753	26.001641	25.984619
C	22.268068	27.931327	26.369142
C	21.566800	26.096147	27.419822
H	21.488401	25.067662	27.737285
N	20.842045	27.088332	27.898543
C	21.267032	28.233700	27.256910
H	20.829985	29.193085	27.491558
H	20.728933	21.081871	29.032444
C	20.224000	22.049000	29.138000
H	20.544968	22.696572	28.317178
H	19.147111	21.873970	29.025916

C	20.541035	22.685990	30.496618
H	20.224125	22.042394	31.322342
H	21.627485	22.821208	30.595830
C	19.900462	24.059868	30.688087
O	19.910518	24.836053	29.671535
O	19.411562	24.337548	31.813017
H	14.416030	23.719787	27.251135
C	15.392001	23.814001	26.757000
H	15.924900	22.869671	26.897655
H	15.208108	23.934274	25.681057
N	15.799339	26.262732	27.304267
H	14.937463	26.617916	26.916029
C	16.201803	24.933865	27.321563
C	16.758785	27.008734	27.916808
H	16.710522	28.077704	28.060940
N	17.751272	26.239904	28.321357
C	17.416519	24.951590	27.955569
H	18.074069	24.128175	28.185131
O	18.376618	26.611229	31.558152
C	18.727074	27.629749	32.407712
C	17.874595	28.867057	32.090434
O	18.573975	28.817180	29.432802
O	17.554747	30.982113	30.318325
P	18.589556	29.757470	30.643134
O	19.905747	30.306135	31.172833
H	18.667501	27.321892	33.456761
H	20.283913	28.952493	31.956826
H	16.849486	28.529559	31.916936
H	17.876486	29.558309	32.939840
H	18.814694	25.682102	31.789582
H	17.950076	31.807294	30.646250
Fe	19.489407	26.893662	29.598297
O	20.815135	27.376744	30.841260
O	20.196706	27.968800	32.267520

=== 5Int-coH ===

H	23.001784	28.442619	24.398033
C	23.079000	28.773000	25.442000
H	24.142668	28.784375	25.711979
H	22.715125	29.802527	25.492486
N	22.517031	26.551664	26.520746
H	23.230820	26.016872	26.046717
C	22.281390	27.912487	26.364157
C	21.648746	26.064362	27.439515
H	21.612785	25.042187	27.783270
N	20.862338	27.032838	27.871525
C	21.244580	28.187048	27.217466
H	20.753572	29.125337	27.427060
H	20.759270	21.099189	29.026562
C	20.224000	22.049000	29.138000
H	20.479961	22.689827	28.289138
H	19.150525	21.830880	29.082501
C	20.582299	22.724055	30.468228
H	20.325908	22.086101	31.318649
H	21.666452	22.899558	30.512556
C	19.902281	24.076388	30.672415
O	19.896399	24.853781	29.637224
O	19.405241	24.352281	31.780169
H	14.387917	23.822735	27.200670
C	15.392000	23.814001	26.757000
H	15.849703	22.850426	26.996441
H	15.273611	23.864189	25.666589
N	15.938093	26.266136	27.146403
H	15.122619	26.645193	26.686499
C	16.247251	24.918880	27.283868
C	16.910432	26.995013	27.754268
H	16.926934	28.072560	27.815767
N	17.826830	26.196599	28.270584
C	17.426107	24.907223	27.981769
H	18.014189	24.063446	28.303921
O	18.321445	26.656450	31.309830
C	18.097739	27.688459	32.304041
C	17.339758	28.820597	31.594628
O	18.735846	28.676692	29.257401
O	17.423848	30.786787	29.673717
P	18.420140	29.694834	30.393165
O	19.541852	30.366486	31.129392
H	17.472381	27.227168	33.075595

H	19.688541	28.810544	32.406391
H	16.453616	28.415211	31.097148
H	17.016548	29.548301	32.346327
H	18.712167	25.804141	31.708131
H	17.687501	31.671297	29.978031
Fe	19.558388	26.874907	29.592551
O	21.027456	27.328220	30.579334
O	19.262560	28.096618	32.933127

=== 5Int-coh2(A) ===

H	23.019054	28.447216	24.395458
C	23.079000	28.773000	25.442000
H	24.138531	28.790899	25.727320
H	22.706638	29.799458	25.492678
N	22.519921	26.543374	26.507124
H	23.246009	26.015725	26.043989
C	22.274723	27.901799	26.349137
C	21.641340	26.047483	27.412816
H	21.616922	25.025262	27.757219
N	20.840590	27.007150	27.836087
C	21.222402	28.164882	27.187320
H	20.723353	29.099988	27.392155
H	20.774491	21.105753	29.050511
C	20.224000	22.049000	29.138000
H	20.530167	22.701660	28.314611
H	19.158340	21.821773	29.012503
C	20.491005	22.711833	30.496922
H	20.181531	22.059929	31.318184
H	21.567453	22.899103	30.607785
C	19.774236	24.049332	30.660600
O	19.998916	24.911561	29.715714
O	19.035083	24.240071	31.641202
H	14.408002	23.788785	27.242647
C	15.392000	23.814000	26.757000
H	15.872902	22.848642	26.936175
H	15.227270	23.908248	25.675687
N	15.910727	26.255353	27.226935
H	15.068157	26.634848	26.819097
C	16.251708	24.910823	27.294281
C	16.891452	26.980562	27.823825
H	16.886599	28.054883	27.931974
N	17.844454	26.181382	28.267305
C	17.459389	24.896264	27.942095
H	18.074802	24.050026	28.203010
O	18.126486	26.646920	31.199773
C	18.073842	27.622547	32.268521
C	17.540341	28.934611	31.669882
O	18.805594	28.663456	29.264775
O	17.395010	30.716456	29.658637
P	18.540541	29.758814	30.363727
O	19.693367	30.568707	30.852558
H	17.342311	27.254467	32.997307
H	19.992127	27.869761	32.292981
H	16.546058	28.745766	31.249444
H	17.427359	29.653970	32.487617
H	18.398814	25.737824	31.555915
H	17.718753	31.631078	29.710694
Fe	19.545331	26.886798	29.574122
O	20.896218	27.429268	30.743896
O	19.273034	27.724351	32.951559

=== 5Int-coh2(B) ===

H	22.919180	28.626793	24.365719
C	23.079000	28.773000	25.442000
H	24.144178	28.606509	25.647601
H	22.858630	29.818745	25.671674
N	22.270273	26.497721	26.211182
H	22.893098	25.956087	25.629342
C	22.207767	27.884403	26.266657
C	21.372243	25.990884	27.094682
H	21.227934	24.939257	27.287740
N	20.733275	26.970873	27.701369
C	21.241958	28.152365	27.202138
H	20.887585	29.102769	27.571816
H	20.785427	21.111650	29.056019
C	20.224000	22.049000	29.138000
H	20.459408	22.665260	28.264949

H	19.156778	21.798694	29.099229
C	20.574144	22.779983	30.441184
H	20.351224	22.157667	31.312071
H	21.649665	23.002063	30.459880
C	19.835388	24.105651	30.615383
O	19.894134	24.895490	29.585336
O	19.234526	24.344953	31.674059
H	14.398061	23.798078	27.222341
C	15.392000	23.814000	26.757000
H	15.865165	22.848905	26.956742
H	15.250226	23.897272	25.671574
N	15.913847	26.258760	27.211183
H	15.082607	26.639947	26.782285
C	16.244829	24.912851	27.299884
C	16.884216	26.986044	27.818654
H	16.890676	28.060850	27.914448
N	17.822130	26.183763	28.289662
C	17.438059	24.895990	27.971927
H	18.045200	24.052186	28.255107
O	18.106538	26.665582	31.220788
C	18.138660	27.684004	32.241684
C	17.616155	28.988978	31.622314
O	18.741597	28.592410	29.172580
O	17.485071	30.726937	29.571040
P	18.604410	29.725918	30.258030
O	19.817804	30.484340	30.677770
H	17.446055	27.370265	33.031667
H	20.050132	27.952118	32.163400
H	16.604388	28.816317	31.238387
H	17.551126	29.738138	32.418061
H	18.475415	25.799457	31.588795
H	17.866371	31.620731	29.574169
Fe	19.482439	26.840060	29.489847
O	20.707721	27.299505	30.446810
O	19.378778	27.788080	32.857498

=== 5TSoh(A) ===

H	22.966934	28.498188	24.385179
C	23.079000	28.773000	25.442000
H	24.147321	28.726883	25.688920
H	22.760018	29.812764	25.551012
N	22.446641	26.526601	26.425792
H	23.128503	25.987029	25.911926
C	22.264019	27.901856	26.338365
C	21.575540	26.031332	27.337670
H	21.507766	24.996147	27.633978
N	20.838535	27.008966	27.831705
C	21.255273	28.177247	27.224023
H	20.809882	29.124279	27.489847
H	20.746659	21.088962	29.062235
C	20.224000	22.049000	29.138000
H	20.545810	22.680369	28.304363
H	19.151830	21.851806	29.018279
C	20.515113	22.722179	30.485414
H	20.200889	22.088691	31.319396
H	21.596997	22.884370	30.589053
C	19.839373	24.081380	30.646363
O	19.955133	24.883050	29.638336
O	19.232400	24.340664	31.704386
H	14.434813	23.698159	27.281715
C	15.392000	23.814000	26.757000
H	15.928874	22.864920	26.837035
H	15.170493	23.982240	25.694951
N	15.813801	26.237762	27.388163
H	14.935700	26.603148	27.048000
C	16.220577	24.910627	27.340465
C	16.785816	26.968541	27.991186
H	16.732424	28.031680	28.174937
N	17.795937	26.187414	28.332844
C	17.455894	24.910032	27.932943
H	18.122580	24.080784	28.107575
O	18.285824	26.706163	31.300242
C	18.477994	27.735885	32.287349
C	17.766261	29.006320	31.795943
O	18.775614	28.645444	29.256234
O	16.893727	30.286901	29.598259
P	18.348864	29.797994	30.230737
O	19.258389	30.966544	30.396171

H	17.963770	27.401284	33.205496
H	20.526598	27.501057	31.831239
H	16.703955	28.773435	31.667667
H	17.852564	29.765207	32.580031
H	18.605892	25.792358	31.631887
H	16.981558	31.233952	29.399161
Fe	19.553399	26.894366	29.554228
O	20.936974	27.378420	30.721573
O	19.797883	27.909365	32.636645

=== 5TSoh(B) ===

H	22.785890	28.927527	24.395205
C	23.079000	28.773000	25.442000
H	24.099122	28.367629	25.447047
H	23.110800	29.752480	25.926216
N	21.878381	26.570183	25.802295
H	22.312709	26.079495	25.034071
C	22.122522	27.887948	26.169957
C	20.975185	26.045021	26.671220
H	20.620052	25.026244	26.632127
N	20.624585	26.948052	27.563529
C	21.330078	28.097830	27.268748
H	21.222419	28.981489	27.881798
H	20.761513	21.096266	29.075059
C	20.224000	22.049000	29.138000
H	20.538249	22.675413	28.297971
H	19.154585	21.832324	29.024168
C	20.510085	22.745588	30.473538
H	20.219547	22.116589	31.319608
H	21.588321	22.936182	30.563352
C	19.808723	24.092401	30.635780
O	19.867016	24.864484	29.594359
O	19.246405	24.366584	31.709039
H	14.425865	23.700374	27.265208
C	15.392000	23.814000	26.757000
H	15.921592	22.861072	26.838372
H	15.189562	23.993060	25.693061
N	15.819517	26.230188	27.411375
H	14.951596	26.605249	27.056102
C	16.216867	24.900711	27.362428
C	16.783825	26.952218	28.032708
H	16.754584	28.015483	28.213621
N	17.780144	26.158503	28.384634
C	17.442023	24.883737	27.974095
H	18.099503	24.050427	28.159862
O	18.310617	26.778044	31.350367
C	18.771642	27.780352	32.278724
C	18.264562	29.156066	31.792975
O	18.740080	28.543809	29.169516
O	17.589282	30.709102	29.713623
P	18.867977	29.760164	30.158522
O	20.131251	30.553573	30.165621
H	18.272933	27.580125	33.250713
H	20.735050	27.420654	31.300917
H	17.171453	29.121343	31.737339
H	18.544050	29.902347	32.542936
H	18.612155	25.862616	31.659670
H	17.954548	31.580148	29.485318
Fe	19.471583	26.791942	29.424997
O	20.901450	27.284790	30.272448
O	20.096546	27.700984	32.538165

=== 5Int-feoh(A) ===

H	22.964229	28.501839	24.384426
C	23.079000	28.773000	25.442000
H	24.146388	28.710538	25.689658
H	22.775944	29.817549	25.551751
N	22.412994	26.535129	26.420786
H	23.088729	25.986998	25.908171
C	22.250128	27.912575	26.336262
C	21.533587	26.051214	27.331881
H	21.452307	25.016794	27.627599
N	20.810216	27.036847	27.827588
C	21.244589	28.199148	27.222559
H	20.812328	29.152555	27.487277
H	20.755940	21.096045	29.038945
C	20.224000	22.049000	29.138000

H	20.492392	22.682158	28.287343
H	19.150039	21.836015	29.073811
C	20.573281	22.732698	30.466490
H	20.308645	22.100901	31.318931
H	21.656743	22.909245	30.516541
C	19.889648	24.085196	30.647115
O	19.915338	24.864247	29.621993
O	19.350823	24.353610	31.743965
H	14.396314	23.788344	27.218775
C	15.392000	23.814000	26.757000
H	15.875403	22.855120	26.962752
H	15.251570	23.889027	25.670556
N	15.889829	26.266700	27.204811
H	15.056417	26.640307	26.773611
C	16.232259	24.924143	27.296809
C	16.859550	27.001061	27.812665
H	16.846260	28.077087	27.903543
N	17.804394	26.210222	28.287054
C	17.426168	24.921272	27.969307
H	18.039661	24.081518	28.253013
O	18.218113	26.585276	31.274599
C	18.028137	27.585552	32.265933
C	17.213385	28.749136	31.632490
O	18.707176	28.668877	29.340229
O	16.864294	30.381749	29.535004
P	18.138883	29.707232	30.347620
O	19.023107	30.760934	30.923360
H	17.398775	27.145222	33.069091
H	20.734348	27.732111	31.540246
H	16.316539	28.308357	31.187762
H	16.917219	29.443842	32.422605
H	18.646461	25.717163	31.637651
H	16.965257	31.346192	29.595549
Fe	19.574740	26.900164	29.591345
O	20.982497	27.316671	30.694175
O	19.134935	28.046622	32.869715

=== 5Int-feoh(B) ===

H	22.719379	29.502512	24.704590
C	23.079000	28.773000	25.442000
H	23.764116	28.086990	24.926889
H	23.658182	29.318982	26.191186
N	21.043936	27.262059	25.416609
H	21.047609	27.086963	24.422103
C	21.955793	28.050125	26.109157
C	20.150464	26.759951	26.307519
H	19.333013	26.107625	26.038951
N	20.437250	27.176717	27.525226
C	21.555872	27.977783	27.418194
H	21.979115	28.432788	28.300518
H	20.783106	21.119280	28.983579
C	20.224000	22.049000	29.138000
H	20.246590	22.620409	28.205058
H	19.182700	21.778290	29.351948
C	20.831354	22.864003	30.287765
H	20.844552	22.286683	31.216391
H	21.870021	23.123490	30.042839
C	20.092805	24.171525	30.559889
O	19.863470	24.905214	29.523774
O	19.752225	24.444699	31.730321
H	14.440571	23.644476	27.277389
C	15.392000	23.814000	26.757000
H	15.963749	22.883394	26.803745
H	15.162389	24.011855	25.701830
N	15.731250	26.229867	27.464441
H	14.842673	26.577633	27.133255
C	16.180117	24.918726	27.378336
C	16.676096	26.973971	28.093085
H	16.607425	28.031044	28.299830
N	17.707264	26.212273	28.413018
C	17.413366	24.934918	27.975511
H	18.106654	24.126269	28.141592
O	18.399956	26.595817	31.425953
C	18.469525	27.593238	32.424298
C	17.628294	28.816878	31.963520
O	18.530039	28.613509	29.391133
O	17.041780	30.548238	29.996407
P	18.358002	29.685833	30.504990

O	19.483451	30.591924	30.875992
H	17.993006	27.200864	33.349641
H	20.760034	27.601495	31.134864
H	16.626210	28.450793	31.721437
H	17.559281	29.531044	32.787975
H	18.915762	25.753622	31.701595
H	17.288450	31.487480	30.029932
Fe	19.423351	26.863152	29.413796
O	20.942738	27.360946	30.203906
O	19.709223	27.984103	32.782379

=== 5TSho ===

H	22.995875	28.434330	24.400689
C	23.079000	28.773000	25.442000
H	24.141387	28.743955	25.717583
H	22.759544	29.818140	25.476035
N	22.415944	26.592919	26.537002
H	23.115943	26.026097	26.080772
C	22.239231	27.959592	26.367593
C	21.509728	26.154939	27.449054
H	21.427441	25.135717	27.793662
N	20.760076	27.155182	27.869859
C	21.204666	28.281820	27.207950
H	20.755017	29.245604	27.396664
H	20.614589	21.025585	29.125522
C	20.224000	22.049000	29.138000
H	20.800357	22.645533	28.425887
H	19.187046	22.014773	28.784970
C	20.308745	22.640309	30.548303
H	19.739576	22.046883	31.270678
H	21.350036	22.637531	30.900229
C	19.821188	24.078144	30.617557
O	19.900567	24.812616	29.615790
O	19.339210	24.441082	31.765681
H	14.442695	23.615901	27.271895
C	15.392000	23.814000	26.757000
H	15.999440	22.907422	26.825435
H	15.164400	23.981393	25.695910
N	15.640299	26.255226	27.431285
H	14.746724	26.570685	27.082335
C	16.133208	24.958473	27.363812
C	16.564719	27.033313	28.056287
H	16.456030	28.089982	28.250487
N	17.618122	26.313968	28.392415
C	17.361606	25.026659	27.965230
H	18.081935	24.240098	28.123995
O	18.478141	26.742866	31.509466
C	18.835282	27.747150	32.298812
C	17.976578	29.018754	32.073222
O	18.404226	29.033545	29.338376
O	17.679085	31.254509	30.407298
P	18.565883	29.896369	30.578569
O	19.994201	30.333178	31.005327
H	18.910367	27.490620	33.364747
H	20.343860	29.294983	31.593562
H	16.932725	28.704932	31.988879
H	18.067308	29.707057	32.921583
H	19.000805	25.471102	31.728260
H	18.189313	32.006408	30.752727
Fe	19.367328	27.028842	29.556798
O	20.862029	27.506287	30.815739
O	20.351368	28.167430	32.019662

=== 5Int-hooc ===

H	23.052772	28.351172	24.428627
C	23.079000	28.773000	25.442000
H	24.132477	28.906081	25.720481
H	22.622080	29.765343	25.399580
N	22.702511	26.611283	26.704040
H	23.477300	26.109010	26.295376
C	22.344689	27.922762	26.424498
C	21.849336	26.123906	27.642732
H	21.895655	25.132430	28.066427
N	20.963282	27.042482	27.977253
C	21.260717	28.165041	27.229522
H	20.681500	29.069919	27.338804
H	20.703187	21.073142	28.998471

C	20.224000	22.049000	29.138000
H	20.554727	22.713318	28.333956
H	19.141811	21.903341	29.033404
C	20.568601	22.639625	30.511536
H	20.233536	21.982736	31.318976
H	21.658934	22.741745	30.602431
C	19.959914	24.023584	30.735735
O	20.156355	24.878549	29.794730
O	19.325393	24.237484	31.792930
H	14.445339	23.637020	27.284018
C	15.392000	23.814001	26.757000
H	15.961642	22.881037	26.780344
H	15.152529	24.030806	25.707639
N	15.740866	26.212901	27.511945
H	14.847818	26.564967	27.198594
C	16.190748	24.905506	27.389759
C	16.702594	26.941791	28.140379
H	16.626570	27.992877	28.376547
N	17.741213	26.180356	28.425109
C	17.435603	24.915683	27.964571
H	18.132205	24.100063	28.084857
O	18.554408	26.679581	31.622308
C	19.162138	27.584593	32.497633
C	18.630153	28.997741	32.214034
O	18.748303	28.746496	29.490254
O	18.169577	31.044140	30.477532
P	19.145779	29.734040	30.607240
O	20.593807	30.178529	30.675776
H	18.961317	27.313861	33.544143
H	21.193264	28.603572	31.017180
H	17.536535	28.956397	32.249531
H	18.970370	29.669571	33.009170
H	18.833035	25.711484	31.829046
H	18.734715	31.834511	30.480281
Fe	19.494601	26.825508	29.587434
O	21.083838	27.606305	31.117424
O	20.591385	27.480925	32.486096

=== 5TShoo ===

H	23.028695	28.415231	24.403288
C	23.079000	28.773000	25.440000
H	24.137720	28.822910	25.725203
H	22.684336	29.792312	25.458777
N	22.570740	26.567405	26.576650
H	23.312154	26.042754	26.135337
C	22.291813	27.912027	26.371907
C	21.695929	26.080843	27.494314
H	21.692917	25.069893	27.871754
N	20.868851	27.031798	27.883837
C	21.226748	28.174301	27.195356
H	20.702939	29.103976	27.360115
H	20.753095	21.093390	29.049602
C	20.224000	22.048999	29.138000
H	20.564155	22.704823	28.330590
H	19.156000	21.850267	28.986006
C	20.475736	22.689616	30.509718
H	20.133640	22.035600	31.316386
H	21.553763	22.849675	30.646645
C	19.788445	24.043718	30.670725
O	20.037151	24.904669	29.739246
O	19.045563	24.236811	31.653506
H	14.448570	23.674118	27.300483
C	15.392000	23.814000	26.757000
H	15.945694	22.872717	26.809976
H	15.144933	23.995619	25.702781
N	15.787841	26.233684	27.418594
H	14.898083	26.588668	27.098903
C	16.215945	24.914849	27.341009
C	16.760823	26.968565	28.018582
H	16.700890	28.026493	28.225402
N	17.789296	26.201479	28.326980
C	17.462708	24.925980	27.910874
H	18.145366	24.103971	28.059979
O	18.280494	26.701627	31.408011
C	18.833997	27.606384	32.372103
C	18.335426	29.026378	32.036751
O	18.709637	28.734013	29.350843

O	18.015548	31.038488	30.237160
P	19.003503	29.752926	30.486947
O	20.434571	30.209642	30.641272
H	18.451697	27.328352	33.370906
H	21.031048	28.494469	30.858272
H	17.242338	29.005488	31.970871
H	18.613927	29.691931	32.860557
H	18.523161	25.739839	31.650036
H	18.570770	31.835860	30.223597
Fe	19.503530	26.871691	29.593908
O	20.862484	27.511325	30.853791
O	20.196674	27.459668	32.522564

=== 5Int-feoh2 ===

H	23.032478	28.447335	24.394624
C	23.079001	28.773001	25.441999
H	24.134760	28.786149	25.741590
H	22.711088	29.801496	25.486265
N	22.495273	26.546795	26.498060
H	23.224583	26.015933	26.044116
C	22.258291	27.905896	26.338476
C	21.603283	26.055709	27.394933
H	21.572362	25.034328	27.741485
N	20.802726	27.017539	27.810811
C	21.197512	28.172215	27.165596
H	20.699932	29.110428	27.360889
H	20.776030	21.107438	29.040175
C	20.224000	22.048999	29.138000
H	20.500928	22.697487	28.301294
H	19.155969	21.816326	29.046695
C	20.528693	22.724263	30.482786
H	20.250522	22.077383	31.319224
H	21.606450	22.921248	30.559222
C	19.806715	24.057967	30.651936
O	19.964517	24.895942	29.678923
O	19.113536	24.258337	31.667648
H	14.404168	23.781791	27.234755
C	15.392000	23.814001	26.757000
H	15.881148	22.854741	26.946572
H	15.234506	23.898612	25.673661
N	15.887106	26.263927	27.216854
H	15.047234	26.635430	26.796658
C	16.237627	24.922398	27.293739
C	16.861061	26.997499	27.819053
H	16.848970	28.072121	27.921221
N	17.815295	26.209205	28.274531
C	17.440321	24.920704	27.951322
H	18.060488	24.080776	28.221002
O	18.072899	26.581401	31.229389
C	17.895496	27.513203	32.295218
C	17.392624	28.857730	31.709546
O	18.711645	28.701381	29.340641
O	17.725020	30.943629	30.030605
P	18.594624	29.655463	30.565377
O	19.855187	30.095400	31.249730
H	17.076492	27.117835	32.942415
H	20.856546	28.352932	31.032312
H	16.457401	28.677580	31.170613
H	17.195259	29.538138	32.542269
H	18.440102	25.690204	31.571711
H	18.208197	31.747828	30.284003
Fe	19.557320	26.886466	29.600347
O	20.904968	27.425633	30.713166
O	18.919144	27.650791	33.144533

=== 5TScrie ===

H	22.998401	28.414538	24.407374
C	23.079000	28.773000	25.442000
H	24.143119	28.774538	25.712015
H	22.732369	29.809696	25.460348
N	22.477722	26.595493	26.580008
H	23.180298	26.035848	26.118605
C	22.263879	27.953460	26.385824
C	21.586624	26.149695	27.504458
H	21.532207	25.133020	27.863154
N	20.815742	27.138603	27.913257
C	21.224322	28.265106	27.225797

H	20.737433	29.215461	27.392215
H	20.457336	20.979107	29.154154
C	20.224000	22.049000	29.138000
H	21.111935	22.587619	28.795099
H	19.428396	22.210270	28.403257
C	19.798465	22.522790	30.527982
H	18.922842	21.974455	30.892947
H	20.593534	22.338866	31.263582
C	19.479446	24.003772	30.579989
O	19.821434	24.774746	29.681305
O	18.816007	24.357695	31.660227
H	14.570103	23.432213	27.376981
C	15.392000	23.814000	26.757000
H	16.075651	22.981874	26.566653
H	14.964624	24.118132	25.792292
N	15.537798	26.126275	27.800345
H	14.570819	26.381851	27.661448
C	16.128655	24.927649	27.426262
C	16.477425	26.903837	28.403497
H	16.286340	27.890764	28.804240
N	17.637713	26.273849	28.440332
C	17.431926	25.050941	27.831443
H	18.235043	24.337474	27.730870
O	18.300231	26.932838	31.489521
C	18.900782	27.801975	32.230409
C	18.216759	29.529991	32.008143
O	18.639931	28.952135	29.310911
O	16.328438	29.705612	30.073960
P	17.968646	29.985197	30.225450
O	18.231018	31.446893	30.058921
H	18.864554	27.640568	33.322082
H	21.675906	27.678305	30.698130
H	17.293513	29.267722	32.533631
H	18.786371	30.275576	32.556537
H	18.624531	25.353940	31.659423
H	15.924181	30.573689	29.909237
Fe	19.411361	27.054688	29.593354
O	21.023951	27.014363	30.978225
O	19.941414	28.466425	31.760790

=== 5Int-crie ===

H	23.192374	28.235698	24.491188
C	23.079000	28.773000	25.442000
H	24.084068	29.022782	25.805993
H	22.562429	29.713296	25.231626
N	22.719796	26.748540	26.916939
H	23.571814	26.273039	26.656831
C	22.302325	27.985643	26.443686
C	21.805966	26.303449	27.817381
H	21.882042	25.373698	28.360279
N	20.825298	27.176569	27.946246
C	21.123024	28.227488	27.100763
H	20.475075	29.089870	27.042663
H	20.642420	21.037232	29.153375
C	20.224000	22.049000	29.138000
H	20.910082	22.699268	28.588857
H	19.279346	22.011800	28.583799
C	20.006955	22.562596	30.564645
H	19.307828	21.931487	31.121170
H	20.954289	22.546044	31.121559
C	19.503801	23.994388	30.595559
O	19.841716	24.814080	29.742016
O	18.692035	24.237099	31.604844
H	14.507757	23.514545	27.334731
C	15.392000	23.814001	26.757000
H	16.044742	22.940507	26.675870
H	15.055051	24.071118	25.744233
N	15.584322	26.190479	27.638141
H	14.649871	26.485119	27.393420
C	16.132810	24.935625	27.406891
C	16.515549	26.961134	28.257933
H	16.381804	27.990652	28.554931
N	17.629148	26.275396	28.442307
C	17.403070	25.019641	27.912427
H	18.171212	24.262725	27.929921
O	17.726738	26.704784	31.897603
C	18.460800	27.372769	32.630263
C	17.554683	29.471823	31.931107

O	18.338477	28.950773	29.336296
O	17.493547	31.260316	29.948268
P	18.497499	30.031992	30.418221
O	19.849652	30.555389	30.794464
H	19.176068	26.937544	33.330848
H	20.663594	28.319885	31.162611
H	16.652316	28.919017	31.658101
H	17.283881	30.348656	32.521634
H	18.371650	25.195065	31.636056
H	17.963375	32.093519	30.117499
Fe	19.359556	27.110174	29.534957
O	20.357021	27.395543	31.132741
O	18.373672	28.678207	32.822380

=== 5TScC ===

H	23.037792	28.437569	24.397496
C	23.079000	28.773000	25.442000
H	24.133628	28.795025	25.744985
H	22.704964	29.799675	25.475745
N	22.506524	26.553448	26.516845
H	23.241532	26.023686	26.070838
C	22.260589	27.909196	26.343510
C	21.614519	26.064159	27.414189
H	21.588480	25.045736	27.769261
N	20.805125	27.024179	27.817730
C	21.194383	28.175789	27.163481
H	20.688974	29.112058	27.347144
H	20.767251	21.100886	29.057388
C	20.224000	22.049000	29.138000
H	20.524133	22.688727	28.302744
H	19.155443	21.827575	29.027924
C	20.511083	22.728974	30.484104
H	20.209459	22.092611	31.320354
H	21.589359	22.913862	30.581286
C	19.805131	24.072038	30.627934
O	19.957942	24.892023	29.645322
O	19.119768	24.298476	31.648233
H	14.408781	23.765971	27.242798
C	15.392000	23.814000	26.757000
H	15.892991	22.858048	26.931673
H	15.224348	23.909017	25.676082
N	15.867275	26.264266	27.238987
H	15.021782	26.632698	26.827410
C	16.230431	24.925226	27.299014
C	16.838681	27.000144	27.841979
H	16.818498	28.073601	27.953464
N	17.803146	26.215852	28.282743
C	17.437504	24.927455	27.948012
H	18.067251	24.090301	28.203153
O	18.013706	26.541676	31.250192
C	17.818100	27.339615	32.378859
C	17.372083	29.197159	31.599269
O	18.720462	28.701636	29.330634
O	18.009015	31.077838	29.794318
P	18.692816	29.745909	30.482442
O	19.966729	30.094711	31.187750
H	16.758030	27.302273	32.689773
H	20.829352	28.295421	31.093691
H	16.421353	28.960627	31.122337
H	17.281329	29.732725	32.541255
H	18.471766	25.641315	31.535586
H	18.477909	31.858166	30.135624
Fe	19.546609	26.894568	29.595175
O	20.885627	27.383331	30.731322
O	18.707420	27.575197	33.199387

=== 5Int-hcooh ===

H	23.047309	28.396611	24.411227
C	23.079000	28.773000	25.442000
H	24.132450	28.829221	25.744883
H	22.682035	29.791549	25.434871
N	22.547385	26.583831	26.600167
H	23.291204	26.050101	26.173837
C	22.276254	27.927291	26.375214
C	21.662139	26.111603	27.512609
H	21.649254	25.105479	27.901747
N	20.833800	27.071358	27.878760

C	21.202711	28.206452	27.181436
H	20.681966	29.142323	27.325888
H	20.808204	21.127622	29.037905
C	20.224000	22.048999	29.138000
H	20.446512	22.691291	28.280092
H	19.163229	21.774700	29.091489
C	20.550484	22.760905	30.459951
H	20.319588	22.120406	31.315064
H	21.621323	22.999639	30.495275
C	19.778159	24.065142	30.617548
O	19.958433	24.936010	29.682802
O	19.010681	24.205901	31.594228
H	14.388743	23.825225	27.201683
C	15.392000	23.814000	26.757000
H	15.853812	22.856195	27.010762
H	15.275230	23.849908	25.666015
N	15.928002	26.272982	27.104107
H	15.113512	26.637847	26.631161
C	16.240353	24.930781	27.271113
C	16.884609	27.017202	27.717774
H	16.891964	28.095211	27.763608
N	17.796486	26.234580	28.265300
C	17.407627	24.938036	27.988766
H	17.990543	24.098962	28.332152
O	18.018977	26.487817	31.266853
C	16.694726	26.708639	31.259391
C	17.494661	30.907623	30.320274
O	18.655947	28.721439	29.298911
O	19.562646	30.958366	28.579591
P	19.031598	30.110978	29.896800
O	20.036653	30.161591	31.010978
H	16.490392	27.734115	30.912844
H	20.677704	28.391708	31.112432
H	16.865271	31.374521	29.568582
H	17.131336	30.871323	31.342544
H	18.306460	25.505162	31.524468
H	20.243960	31.580083	28.886596
Fe	19.519397	26.933719	29.612984
O	20.771674	27.452559	30.824716
O	15.846458	25.917803	31.591276

=== 5Int-h2o ===

H	23.168116	28.274502	24.467954
C	23.079000	28.773000	25.442000
H	24.093042	29.007196	25.791049
H	22.556502	29.719928	25.282305
N	22.742614	26.682715	26.836756
H	23.572740	26.202609	26.520085
C	22.325666	27.944627	26.431565
C	21.859626	26.209472	27.751673
H	21.938468	25.260136	28.258231
N	20.897213	27.089725	27.951417
C	21.173459	28.173635	27.139220
H	20.535220	29.044852	27.141459
H	20.812090	21.125425	29.095674
C	20.224000	22.049000	29.138000
H	20.526354	22.685727	28.299844
H	19.170496	21.778378	28.998053
C	20.431735	22.770990	30.478348
H	20.124412	22.131697	31.310445
H	21.494926	23.010574	30.605627
C	19.639158	24.074092	30.560136
O	20.000836	24.993898	29.726271
O	18.701134	24.166944	31.376304
H	14.450489	23.684141	27.306251
C	15.392000	23.814000	26.757000
H	15.947142	22.874775	26.828323
H	15.141909	23.973084	25.699839
N	15.780460	26.246676	27.363944
H	14.890661	26.590457	27.032383
C	16.214807	24.928454	27.316397
C	16.747636	26.998320	27.949852
H	16.681075	28.059831	28.130310
N	17.779232	26.244468	28.279859
C	17.459936	24.958627	27.889172
H	18.145537	24.142374	28.053173
C	17.442358	30.910497	30.028859
O	18.726522	28.778804	29.091140

O	19.517555	31.091997	28.329337
P	19.025635	30.203736	29.631674
O	20.049356	30.331204	30.731282
H	20.615501	28.561834	31.010987
H	17.229391	31.961707	29.863038
H	16.723593	30.327143	30.596579
H	20.333922	31.549749	28.591680
Fe	19.469649	26.977059	29.618746
O	20.599402	27.578577	30.936271
O	17.978621	26.661084	31.183520
H	18.505314	27.073364	31.892487
H	18.113790	25.663887	31.325385

=== 5TSpt ===

H	23.199397	28.231689	24.494605
C	23.079000	28.773000	25.442000
H	24.076921	29.081308	25.779515
H	22.504818	29.679857	25.234634
N	22.851642	26.738305	26.940568
H	23.711724	26.291620	26.656017
C	22.369670	27.954768	26.470614
C	21.987021	26.260129	27.868606
H	22.105667	25.336092	28.412432
N	20.975682	27.095620	28.018964
C	21.201028	28.153658	27.157866
H	20.513034	28.984232	27.113814
H	20.811007	21.127490	29.054150
C	20.224000	22.049000	29.138000
H	20.436088	22.670177	28.261240
H	19.163667	21.769938	29.111931
C	20.562034	22.798877	30.435784
H	20.352240	22.172345	31.306972
H	21.630770	23.049093	30.446799
C	19.766468	24.096328	30.588480
O	20.032450	25.000981	29.681196
O	18.939162	24.212099	31.498207
H	14.434867	23.680954	27.277473
C	15.392000	23.814000	26.757000
H	15.942341	22.872477	26.833121
H	15.173393	23.987107	25.695243
N	15.770067	26.238435	27.402853
H	14.886706	26.587425	27.059167
C	16.201472	24.918472	27.351499
C	16.727127	26.983989	28.007281
H	16.666154	28.045396	28.189944
N	17.750413	26.220367	28.346443
C	17.435615	24.936678	27.945584
H	18.118024	24.119789	28.117872
C	17.513738	30.642733	30.338052
O	18.813112	28.735670	29.010594
O	19.224499	31.150393	28.314137
P	19.059683	30.149749	29.613294
O	20.250666	30.315465	30.522423
H	20.720703	28.577053	31.020459
H	17.168171	31.671011	30.304145
H	16.987927	29.940979	30.978657
H	20.014870	31.693793	28.470854
Fe	19.438956	26.922301	29.575893
O	20.639674	27.595586	31.082926
O	18.428660	26.887108	31.343059
H	19.552085	27.312139	31.586917
H	18.410539	25.926489	31.583894

=== 5Int-pt ===

H	23.028364	28.447485	24.394510
C	23.079000	28.773000	25.442000
H	24.138259	28.809210	25.728275
H	22.690144	29.793794	25.489734
N	22.550741	26.534502	26.494437
H	23.283676	26.019217	26.028662
C	22.286457	27.889328	26.345794
C	21.675755	26.024500	27.398628
H	21.661180	24.997968	27.728915
N	20.862832	26.966997	27.832849
C	21.230512	28.130598	27.187108
H	20.714097	29.056233	27.392101
H	20.509697	20.992762	29.067192

C	20.224000	22.049000	29.138000
H	20.583713	22.561328	28.240949
H	19.129312	22.097779	29.132103
C	20.796163	22.679761	30.409501
H	20.439074	22.162100	31.306612
H	21.890635	22.577367	30.426791
C	20.493462	24.169286	30.593561
O	20.108126	24.801671	29.533405
O	20.655159	24.687423	31.715710
H	14.408467	23.803121	27.244177
C	15.392000	23.814000	26.757000
H	15.869945	22.851232	26.956375
H	15.226521	23.885673	25.674049
N	15.925926	26.263813	27.178559
H	15.085748	26.641542	26.764558
C	16.257360	24.917352	27.270523
C	16.913419	26.991956	27.761312
H	16.915191	28.067563	27.856459
N	17.858616	26.190852	28.213203
C	17.465195	24.902412	27.916434
H	18.080043	24.063356	28.201374
C	17.545781	29.766285	31.264844
O	19.036175	28.695008	29.299227
O	19.178449	31.219693	29.709867
P	19.118673	29.752380	30.444358
O	20.305683	29.617923	31.375875
H	21.004138	28.063791	31.169154
H	17.073487	30.690926	31.579739
H	17.137643	28.815571	31.592520
H	20.008075	31.645010	29.983861
Fe	19.458199	26.758992	29.590328
O	21.230119	27.192490	30.731120
O	18.420298	26.552302	31.117117
H	21.154329	26.458971	31.388650
H	18.846974	25.906559	31.711845

=== 5TSco-pt ===

H	23.003818	28.496161	24.382072
C	23.079000	28.773000	25.442000
H	24.140568	28.741207	25.719996
H	22.745379	29.809848	25.537304
N	22.442117	26.521832	26.398340
H	23.142837	25.991632	25.900815
C	22.248208	27.894090	26.314187
C	21.553639	26.017294	27.291415
H	21.493057	24.980514	27.583051
N	20.796503	26.981180	27.777505
C	21.216810	28.152456	27.180333
H	20.756487	29.095190	27.436720
H	20.437529	20.973538	29.114496
C	20.224000	22.049000	29.138000
H	20.731328	22.514385	28.287517
H	19.146125	22.177867	28.992934
C	20.679791	22.661495	30.463835
H	20.174239	22.186753	31.313173
H	21.751351	22.480426	30.624846
C	20.461169	24.171627	30.593623
O	20.097692	24.785913	29.520935
O	20.662698	24.716382	31.700378
H	14.424551	23.747071	27.271253
C	15.392000	23.814000	26.757000
H	15.910548	22.862863	26.903821
H	15.191143	23.921261	25.682985
N	15.853610	26.264538	27.258662
H	14.991131	26.629069	26.880214
C	16.232223	24.927707	27.288767
C	16.833937	27.002975	27.842197
H	16.802925	28.074276	27.976606
N	17.817065	26.217955	28.236697
C	17.457514	24.929530	27.900848
H	18.107148	24.102130	28.139059
C	17.768834	28.636001	31.895308
O	18.973348	28.725237	29.487827
O	18.419730	30.942427	30.555969
P	18.993050	29.435816	30.874859
O	20.321502	29.516939	31.592705
H	21.112746	28.020031	31.159230
H	17.978870	28.435407	32.939350

H	16.748815	28.501850	31.554269
H	18.923355	31.571023	31.099391
Fe	19.476595	26.770523	29.549969
O	21.282545	27.164729	30.671755
O	18.400742	26.589140	31.107708
H	21.222372	26.405141	31.304782
H	18.882380	26.099928	31.803202

=== 5Pro-pt ===

H	23.008913	28.404133	24.410166
C	23.079001	28.773001	25.442000
H	24.143171	28.816984	25.708078
H	22.694948	29.796698	25.453374
N	22.568151	26.585983	26.599533
H	23.299668	26.053040	26.152059
C	22.299913	27.930544	26.393941
C	21.695479	26.112390	27.527128
H	21.680168	25.098873	27.897419
N	20.880250	27.070115	27.923464
C	21.245743	28.204907	27.228441
H	20.735258	29.144112	27.385627
H	20.494199	20.988166	29.074035
C	20.224000	22.048999	29.138000
H	20.758251	22.585587	28.348514
H	19.152108	22.135034	28.929911
C	20.561939	22.611400	30.520676
H	20.041103	22.061698	31.312950
H	21.633101	22.490263	30.735420
C	20.236940	24.095134	30.703324
O	19.995527	24.761582	29.636854
O	20.244060	24.572071	31.867954
H	14.483442	23.584218	27.328946
C	15.392000	23.814000	26.757000
H	16.005264	22.909102	26.734756
H	15.087304	24.033965	25.725235
N	15.677432	26.215518	27.543609
H	14.757006	26.538806	27.282978
C	16.172388	24.930633	27.367206
C	16.641081	26.965364	28.147281
H	16.523352	28.002822	28.424828
N	17.719788	26.239788	28.362657
C	17.441576	24.976819	27.882044
H	18.171822	24.186580	27.962281
C	17.788447	27.433323	32.250741
O	18.751479	28.614631	30.044414
O	17.660846	30.127001	31.838707
P	18.705636	28.890927	31.568954
O	20.013157	29.149559	32.279753
H	21.038015	27.852858	31.538653
H	17.989829	27.311192	33.321150
H	16.712600	27.590639	32.121183
H	18.152092	30.836462	32.285408
Fe	19.478583	26.777017	29.581630
O	21.244416	27.053284	30.989621
O	18.144019	26.261086	31.508671
H	21.092475	26.272366	31.565377
H	18.862942	25.738101	31.941151

=== 5TSco ===

H	22.935536	28.428210	24.409520
C	23.079000	28.773000	25.442000
H	24.155587	28.746815	25.655561
H	22.755785	29.815875	25.492757
N	22.483467	26.596318	26.601211
H	23.144384	26.017957	26.102554
C	22.294121	27.962141	26.420435
C	21.634820	26.167260	27.566537
H	21.561496	25.154253	27.929995
N	20.907762	27.177536	28.014053
C	21.306311	28.302702	27.307494
H	20.874850	29.276429	27.511411
H	20.799543	21.121805	29.038747
C	20.224000	22.049000	29.138000
H	20.419677	22.667348	28.255346
H	19.160482	21.781586	29.137053
C	20.600543	22.795078	30.427198
H	20.406109	22.169232	31.302404

H	21.671418	23.035578	30.411314
C	19.820287	24.100144	30.589459
O	20.047030	25.001381	29.698235
O	19.010981	24.203117	31.537030
H	14.440103	23.684173	27.288063
C	15.392000	23.814000	26.757000
H	15.942711	22.872513	26.832926
H	15.161500	23.980007	25.696469
N	15.776665	26.242223	27.385764
H	14.890521	26.590065	27.048435
C	16.207996	24.922333	27.336757
C	16.736842	26.989761	27.985436
H	16.674959	28.050857	28.175895
N	17.763045	26.228671	28.321799
C	17.445925	24.944779	27.924104
H	18.128266	24.127329	28.096359
C	19.911464	29.962892	31.271241
O	18.613282	28.795384	29.225262
O	17.818634	31.064023	29.916334
P	19.184541	30.181036	29.650457
O	20.113537	30.892607	28.710316
H	21.427253	27.939957	30.678126
H	20.914043	30.321444	31.475888
H	19.294636	29.714845	32.128129
H	18.005845	31.978616	29.648158
Fe	19.396720	27.012847	29.612117
O	20.517016	27.774800	30.974241
O	18.093027	26.602716	31.276466
H	18.551059	27.113099	31.967110
H	18.349510	25.630834	31.465274

=== 5Pro ===

H	22.910477	28.399321	24.423330
C	23.079000	28.773000	25.442000
H	24.162986	28.783968	25.616738
H	22.727072	29.807263	25.478877
N	22.590077	26.610984	26.675031
H	23.253299	26.040169	26.170897
C	22.352925	27.963614	26.466189
C	21.780898	26.184217	27.679298
H	21.749719	25.176259	28.063494
N	21.034966	27.179353	28.126427
C	21.381840	28.293906	27.377033
H	20.931968	29.259400	27.572237
H	20.770760	21.114684	28.967178
C	20.224000	22.049000	29.138000
H	20.389844	22.702814	28.274570
H	19.155538	21.807177	29.183353
C	20.684764	22.729530	30.437638
H	20.521088	22.065630	31.291078
H	21.756690	22.953854	30.374198
C	19.925690	24.033304	30.686159
O	20.224898	25.009404	29.898369
O	19.062370	24.063012	31.588040
H	14.455862	23.632099	27.300828
C	15.392002	23.814000	26.757000
H	15.968330	22.884957	26.773810
H	15.133025	24.025519	25.711144
N	15.733629	26.216497	27.501546
H	14.832875	26.560449	27.201655
C	16.192770	24.913064	27.373669
C	16.695242	26.953318	28.119651
H	16.610969	28.001724	28.365025
N	17.744636	26.201509	28.390165
C	17.444946	24.934793	27.932129
H	18.146262	24.121601	28.043648
C	20.406465	29.350297	31.447144
O	18.693016	28.805558	29.477101
O	18.387362	31.021983	30.749510
P	19.467922	30.032172	30.002885
O	20.341952	30.815869	29.067256
H	21.624800	28.156035	30.438513
H	21.207409	30.024623	31.771248
H	19.729229	29.191802	32.290451
H	18.518851	31.916523	30.394553
Fe	19.387977	26.894350	29.671891
O	20.938626	28.046897	31.119349
O	18.137463	26.497079	31.451970

H	18.505003	26.963655	32.218532
H	18.389348	25.525469	31.593816

=== 5RC (side-on, deprotonated hydroxyl) ===

H	22.989799	28.478371	24.386203
C	23.079000	28.773000	25.442000
H	24.149293	28.776070	25.692892
H	22.720524	29.802922	25.528020
N	22.510595	26.525423	26.471902
H	23.220279	25.994763	25.989482
C	22.285690	27.892586	26.352025
C	21.634821	26.036819	27.400008
H	21.594809	25.008525	27.726621
N	20.868815	26.995476	27.865154
C	21.259702	28.151553	27.227207
H	20.777545	29.087007	27.470456
H	20.713564	21.130441	28.786445
C	20.224000	22.049000	29.138000
H	20.059674	22.705027	28.277381
H	19.240039	21.768402	29.535264
C	21.059784	22.762224	30.207822
H	21.219889	22.109749	31.072319
H	22.048431	23.006090	29.791242
C	20.423462	24.075465	30.719895
O	20.142153	24.913184	29.758632
O	20.249720	24.230252	31.923861
H	14.357652	24.022409	27.065207
C	15.392000	23.814000	26.757000
H	15.676119	22.853070	27.196212
H	15.389970	23.690331	25.664167
N	16.239497	26.205053	26.834754
H	15.515090	26.608207	26.259623
C	16.343479	24.871948	27.212420
C	17.249266	26.898167	27.438531
H	17.375408	27.969286	27.361237
N	17.990665	26.090251	28.163953
C	17.442484	24.835088	28.034454
H	17.871205	23.994163	28.558458
O	17.889787	26.764776	30.888851
C	17.508641	27.824347	31.700250
C	16.861254	28.962502	30.876267
O	19.055944	28.744216	29.224242
O	17.012197	30.027234	28.366548
P	18.014546	29.785240	29.703032
O	18.484171	31.140479	30.147223
H	16.759091	27.478402	32.437202
H	18.354790	28.229763	32.283068
H	16.033408	28.536630	30.296971
H	16.451411	29.743099	31.531131
H	17.108320	30.974114	28.173960
Fe	19.493006	26.835294	29.850673
O	21.414277	27.525449	30.545060
O	20.586889	27.442591	31.565292

=== 7RC (side-on, deprotonated hydroxyl) ===

H	22.955803	28.420829	24.407684
C	23.079000	28.773000	25.442000
H	24.156358	28.784322	25.659815
H	22.725275	29.807134	25.482629
N	22.530503	26.584995	26.605928
H	23.214778	26.021717	26.123899
C	22.310258	27.947361	26.421275
C	21.672566	26.145366	27.569089
H	21.605032	25.132089	27.935122
N	20.923209	27.135391	28.001129
C	21.305200	28.259635	27.300753
H	20.811483	29.200392	27.494218
H	20.799754	21.166409	28.826754
C	20.224000	22.049000	29.138000
H	19.998019	22.645525	28.247697
H	19.271282	21.693760	29.551602
C	20.983232	22.891838	30.170205
H	21.200424	22.298016	31.064196
H	21.945391	23.209249	29.740995
C	20.205474	24.156380	30.616874
O	19.928174	24.963359	29.634571
O	19.913955	24.283889	31.803565

H	14.341484	23.969443	27.041209
C	15.392000	23.814000	26.757000
H	15.715392	22.869635	27.204854
H	15.420865	23.688758	25.664750
N	16.112154	26.243870	26.838176
H	15.383473	26.604450	26.240561
C	16.277651	24.920296	27.228877
C	17.070478	26.994318	27.451740
H	17.161961	28.066127	27.353846
N	17.840665	26.231167	28.200385
C	17.360541	24.945564	28.071466
H	17.836540	24.136493	28.603399
O	18.201444	27.291121	31.084453
C	17.904533	28.506567	31.693569
C	17.060030	29.428256	30.787062
O	18.819148	28.879565	28.763385
O	16.695691	30.197040	28.197739
P	17.963418	30.036771	29.305596
O	18.560511	31.406729	29.474576
H	17.327397	28.316875	32.616873
H	18.823117	29.038333	31.999283
H	16.181375	28.865387	30.449333
H	16.705899	30.303218	31.348487
H	16.745438	31.127654	27.925813
Fe	19.439678	27.019866	29.723147
O	21.174357	27.096366	31.029299
O	20.932006	28.316519	30.644678

=== 5TSh (deprotonated hydroxyl) ===

H	22.998090	28.454318	24.392609
C	23.079000	28.773000	25.442000
H	24.147408	28.788156	25.700033
H	22.712801	29.801728	25.504039
N	22.519791	26.544990	26.521165
H	23.239519	26.008706	26.060394
C	22.285130	27.908187	26.365698
C	21.637464	26.069827	27.446518
H	21.593453	25.049204	27.795446
N	20.856819	27.035307	27.876806
C	21.246380	28.182152	27.218664
H	20.747706	29.115639	27.434397
H	20.779019	21.143706	28.856360
C	20.224000	22.049000	29.138000
H	20.101284	22.669374	28.243954
H	19.224748	21.735665	29.466898
C	20.940432	22.834486	30.244004
H	21.062952	22.214046	31.137746
H	21.944163	23.117655	29.894960
C	20.190713	24.122691	30.659087
O	20.001228	24.946498	29.666684
O	19.836872	24.262243	31.826182
H	14.367538	23.826111	27.155526
C	15.392000	23.814000	26.757000
H	15.835503	22.850516	27.025269
H	15.317494	23.849649	25.660427
N	15.922089	26.265920	27.144230
H	15.110995	26.639928	26.674688
C	16.229666	24.920398	27.309013
C	16.880680	27.005499	27.771576
H	16.877631	28.085965	27.828579
N	17.780573	26.214730	28.319131
C	17.389464	24.922897	28.041596
H	17.975092	24.090263	28.400078
O	18.163537	27.261283	31.125778
C	18.311140	28.376679	31.844897
C	17.661410	29.638607	31.274969
O	18.943859	28.861687	28.953845
O	16.704282	30.093825	28.746904
P	18.193543	30.064191	29.551586
O	18.764720	31.447835	29.421926
H	18.132135	28.236842	32.925706
H	19.662954	28.591018	31.850945
H	16.568771	29.513970	31.253235
H	17.883921	30.504167	31.910319
H	16.682336	30.978428	28.347131
Fe	19.469211	26.941549	29.732861
O	20.986600	27.552881	30.708259
O	20.852430	28.537110	31.655740

=== 7TSh (deprotonated hydroxyl) ===

H	23.137695	28.258823	24.471686
C	23.079000	28.773000	25.442000
H	24.108548	28.973917	25.770586
H	22.595057	29.739553	25.274898
N	22.678598	26.731247	26.890510
H	23.499814	26.221219	26.601851
C	22.302756	27.997379	26.453861
C	21.768288	26.318316	27.817389
H	21.810658	25.384254	28.355693
N	20.837725	27.231274	27.988617
C	21.157154	28.280794	27.152909
H	20.537061	29.164861	27.147166
H	20.915023	21.199513	29.054718
C	20.224000	22.049000	29.138000
H	20.159390	22.528848	28.152914
H	19.229776	21.667779	29.391044
C	20.674461	23.053531	30.209564
H	20.743806	22.541494	31.177806
H	21.663911	23.461775	29.973441
C	19.632617	24.186632	30.336138
O	20.040700	25.344486	29.945081
O	18.501672	23.874794	30.733998
H	14.315703	24.038211	26.778442
C	15.392000	23.814000	26.757000
H	15.562143	22.958931	27.417494
H	15.639331	23.496669	25.733332
N	16.222070	26.213418	26.603417
H	15.635769	26.501787	25.834708
C	16.225315	24.963885	27.215777
C	17.100308	27.014857	27.268397
H	17.274491	28.057749	27.047946
N	17.669268	26.350208	28.254196
C	17.129424	25.078807	28.238947
H	17.412855	24.358617	28.995400
O	17.953930	27.659566	31.119112
C	17.837117	28.912045	31.561871
C	17.112604	29.922179	30.667754
O	18.715777	29.020936	28.640244
O	16.591016	30.283948	27.997965
P	17.915061	30.272563	29.042602
O	18.542449	31.634931	28.952337
H	17.506959	28.985115	32.615055
H	19.267424	29.264583	31.582404
H	16.101530	29.541766	30.453208
H	17.000586	30.877947	31.194050
H	16.599475	31.181257	27.627506
Fe	19.233246	27.231296	29.641849
O	20.662049	28.101976	30.772897
O	20.414162	29.237777	31.472305

=== 5Int-ooH (with Tyr98) ===

H	22.994196	28.386504	24.417823
C	23.079000	28.773000	25.442000
H	24.141964	28.762483	25.715973
H	22.752879	29.816493	25.429841
N	22.442520	26.639346	26.634204
H	23.151233	26.064259	26.202263
C	22.246550	27.994590	26.406181
C	21.539332	26.225415	27.559232
H	21.468865	25.218178	27.939149
N	20.772229	27.230362	27.936928
C	21.203062	28.336101	27.229507
H	20.735352	29.299282	27.373167
H	20.667353	21.048028	29.121198
C	20.224000	22.049000	29.138000
H	20.751279	22.671611	28.410291
H	19.181582	21.958511	28.812394
C	20.313468	22.650408	30.545652
H	19.784456	22.037685	31.281471
H	21.361700	22.696215	30.872570
C	19.770114	24.065058	30.609647
O	19.876535	24.840052	29.654877
O	19.187342	24.363900	31.748163
H	14.435720	23.645451	27.269259
C	15.392000	23.814000	26.757000

H	15.984820	22.900588	26.856101
H	15.175731	23.954808	25.689826
N	15.671100	26.269668	27.362449
H	14.787944	26.589316	26.991086
C	16.144977	24.964714	27.337864
C	16.596519	27.051903	27.979168
H	16.499642	28.114611	28.145919
N	17.634952	26.327136	28.352318
C	17.365944	25.032610	27.954740
H	18.071472	24.238632	28.139566
O	18.047239	26.722900	31.482479
C	18.066431	27.687035	32.281132
C	17.384030	28.988798	31.934696
O	18.357209	29.012289	29.363497
O	17.004829	31.024555	30.175180
P	18.163888	29.951697	30.555642
O	19.385105	30.678012	31.120340
H	18.313184	27.509573	33.334203
H	20.213951	29.155379	31.760972
H	16.358978	28.748766	31.625409
H	17.331689	29.640265	32.812448
H	18.827630	25.311015	31.722384
H	17.291890	31.933552	30.426804
Fe	19.316736	27.122742	29.572755
O	20.648282	27.439853	30.991511
O	20.173773	28.228136	32.108623
H	16.241549	35.569090	36.406695
C	17.280000	35.763000	36.105000
H	17.392698	36.850868	36.024093
H	17.925684	35.421017	36.920971
C	17.623627	35.069732	34.803423
C	18.412799	33.913783	34.772022
H	18.805270	33.510067	35.703231
C	18.714944	33.260276	33.574310
H	19.329164	32.363540	33.570046
C	18.224441	33.766327	32.365894
O	18.487321	33.181185	31.156689
H	19.056957	32.367651	31.259869
C	17.144889	35.558986	33.578175
H	16.533564	36.459409	33.565110
C	17.435778	34.923568	32.374355
H	17.066953	35.313793	31.430207

=== 5TSho (with Tyr98) ===

H	22.974572	28.388446	24.418786
C	23.079000	28.773000	25.442000
H	24.147951	28.767008	25.692421
H	22.748319	29.815203	25.438400
N	22.472836	26.634678	26.642427
H	23.172862	26.060779	26.195073
C	22.270633	27.990201	26.421171
C	21.586742	26.217541	27.582722
H	21.517593	25.209101	27.960210
N	20.826348	27.221500	27.976311
C	21.242984	28.328820	27.264548
H	20.776008	29.290801	27.417643
H	20.643520	21.037221	29.134835
C	20.224000	22.049000	29.138000
H	20.787355	22.658198	28.426020
H	19.190436	21.982747	28.779150
C	20.283182	22.651607	30.547049
H	19.719066	22.050026	31.266120
H	21.322255	22.670077	30.905147
C	19.769379	24.082391	30.609006
O	19.915745	24.841337	29.631618
O	19.195472	24.415055	31.722263
H	14.429262	23.679345	27.267383
C	15.392000	23.814000	26.757000
H	15.967122	22.893740	26.890995
H	15.185390	23.922371	25.683974
N	15.706217	26.280125	27.284664
H	14.828885	26.599766	26.899998
C	16.160712	24.968368	27.304871
C	16.639125	27.066447	27.884565
H	16.553766	28.133797	28.022508
N	17.663743	26.338060	28.285892
C	17.378201	25.036040	27.927856
H	18.070774	24.239292	28.147340

O	18.268153	26.675771	31.415090
C	18.462643	27.697210	32.242884
C	17.517799	28.891889	31.936202
O	18.329344	29.048497	29.290095
O	17.220450	31.140611	30.302593
P	18.185290	29.877842	30.550587
O	19.519661	30.426650	31.202339
H	18.435349	27.431707	33.309357
H	19.893093	29.423638	31.743808
H	16.528064	28.485358	31.712212
H	17.431368	29.559159	32.801457
H	18.825781	25.441320	31.672499
H	17.645033	31.984634	30.598424
Fe	19.330422	27.053770	29.569768
O	20.631325	27.669848	30.965661
O	19.944117	28.236610	32.132442
H	16.219629	35.570652	36.317486
C	17.280000	35.763000	36.105000
H	17.396461	36.848803	36.007279
H	17.851713	35.443359	36.982663
C	17.736796	35.040883	34.856207
C	18.505486	33.873151	34.922944
H	18.802399	33.483061	35.894055
C	18.904696	33.189199	33.771189
H	19.500407	32.282713	33.846011
C	18.533299	33.677868	32.516837
O	18.883130	33.056925	31.340871
H	19.412247	32.237898	31.500499
C	17.383682	35.513653	33.582925
H	16.793064	36.423333	33.495708
C	17.772646	34.847997	32.424368
H	17.499808	35.222548	31.442219

=== 5Int-hooc (with Tyr98) ===

H	23.097559	28.202567	24.504306
C	23.079000	28.773000	25.442000
H	24.115484	29.025823	25.700047
H	22.549140	29.709784	25.249622
N	22.854424	26.796729	27.004925
H	23.675562	26.308848	26.677175
C	22.396265	28.021352	26.539542
C	22.019222	26.367520	27.986112
H	22.120585	25.436934	28.522880
N	21.049709	27.242440	28.179900
C	21.274516	28.276144	27.289553
H	20.615269	29.131254	27.256861
H	20.777830	21.111049	29.019858
C	20.224000	22.049000	29.138000
H	20.463336	22.698100	28.288962
H	19.154236	21.811163	29.097896
C	20.584947	22.733882	30.468239
H	20.342639	22.081660	31.311745
H	21.663603	22.934879	30.492295
C	19.850449	24.060964	30.663245
O	20.164432	25.004576	29.845078
O	18.992595	24.144662	31.570836
H	14.433580	23.752819	27.288701
C	15.392000	23.814000	26.757000
H	15.911739	22.863472	26.904679
H	15.172192	23.909459	25.685488
N	15.851690	26.265252	27.220046
H	14.981669	26.618880	26.848767
C	16.239345	24.933707	27.262334
C	16.831731	27.016978	27.788665
H	16.788239	28.087751	27.921454
N	17.827210	26.247715	28.187454
C	17.471228	24.953730	27.863820
H	18.120910	24.123370	28.095046
O	18.057282	26.516618	31.341351
C	18.297936	27.405542	32.390364
C	17.630573	28.748136	32.060315
O	18.567024	28.796392	29.473834
O	17.284017	30.831598	30.334831
P	18.399429	29.716153	30.698315
O	19.665526	30.384983	31.245004
H	17.901940	27.013253	33.337931
H	20.465692	28.815611	31.549054
H	16.586608	28.543319	31.802157

H	17.638732	29.383770	32.952159
H	18.381076	25.564767	31.562094
H	17.603193	31.727296	30.599817
Fe	19.394728	26.915169	29.595213
O	20.468540	27.814386	31.534109
O	19.689239	27.493125	32.725800
H	16.218323	35.602849	36.336367
C	17.280000	35.763000	36.105000
H	17.422289	36.843008	35.978670
H	17.856702	35.450821	36.982102
C	17.703019	34.998102	34.866762
C	18.502312	33.851217	34.943760
H	18.844944	33.503506	35.916169
C	18.877213	33.134434	33.802688
H	19.498410	32.246045	33.886932
C	18.450720	33.565787	32.543371
O	18.778123	32.920242	31.379066
H	19.344123	32.116019	31.529170
C	17.290497	35.411871	33.590246
H	16.673132	36.302677	33.491257
C	17.654050	34.713144	32.442841
H	17.334713	35.045185	31.459274

=== 5TSooH (with Tyr98) ===

H	22.944093	28.447154	24.402333
C	23.079000	28.773000	25.442000
H	24.150678	28.717818	25.673156
H	22.783173	29.823858	25.500568
N	22.417471	26.592997	26.536356
H	23.081637	26.019023	26.037456
C	22.260682	27.964321	26.393989
C	21.541294	26.155303	27.477202
H	21.452883	25.131590	27.805504
N	20.829548	27.162605	27.944578
C	21.266654	28.292967	27.281595
H	20.838115	29.260306	27.499208
H	20.683140	21.054918	29.125680
C	20.224000	22.049000	29.138000
H	20.733484	22.671848	28.397542
H	19.179355	21.937909	28.825567
C	20.320355	22.667204	30.538609
H	19.812408	22.050168	31.285111
H	21.373352	22.734327	30.845914
C	19.751460	24.073933	30.609820
O	19.924233	24.866933	29.660793
O	19.101910	24.357862	31.692986
H	14.447054	23.683946	27.300598
C	15.392000	23.814000	26.757000
H	15.958105	22.883401	26.853081
H	15.147572	23.945182	25.694577
N	15.760801	26.266327	27.314858
H	14.875833	26.604542	26.965090
C	16.197523	24.949129	27.297255
C	16.723016	27.029559	27.900334
H	16.652100	28.095025	28.060970
N	17.751193	26.283511	28.256728
C	17.436040	24.992716	27.882575
H	18.120698	24.179777	28.065814
O	18.196629	26.622955	31.350398
C	18.344698	27.611809	32.241645
C	17.493093	28.848281	31.895448
O	18.512476	28.924551	29.343078
O	17.169098	30.947553	30.120986
P	18.265636	29.837850	30.554649
O	19.471729	30.506306	31.229350
H	18.197185	27.286520	33.280508
H	19.921808	29.022521	32.065070
H	16.501093	28.486925	31.610046
H	17.383875	29.505621	32.765506
H	18.712640	25.375403	31.637733
H	17.443659	31.838127	30.446374
Fe	19.404331	27.043356	29.615341
O	20.644230	27.523490	30.912887
O	19.844052	28.048591	32.314186
H	16.194373	35.885365	36.208782
C	17.280000	35.763000	36.105000
H	17.719079	36.769162	36.120471
H	17.640055	35.233351	36.993281

C	17.639113	35.016844	34.837184
C	18.416206	33.853187	34.862185
H	18.769125	33.467505	35.816444
C	18.754699	33.167736	33.691731
H	19.357320	32.264029	33.733122
C	18.312280	33.647941	32.455594
O	18.609971	33.031033	31.269620
H	19.168813	32.216644	31.404652
C	17.205014	35.477584	33.584028
H	16.598656	36.379649	33.527337
C	17.532697	34.810541	32.407588
H	17.196294	35.177034	31.442087

C	17.444850	34.705991	32.427282
H	17.115303	35.064477	31.456360

=== 5Int-coh (with Tyr98) ===

H	22.980413	28.438268	24.401432
C	23.078999	28.773000	25.442000
H	24.143997	28.745097	25.704863
H	22.754609	29.815822	25.488058
N	22.446385	26.577801	26.528654
H	23.137071	26.020589	26.046194
C	22.255955	27.946032	26.376416
C	21.571429	26.116537	27.453336
H	21.504464	25.095475	27.795491
N	20.820597	27.108725	27.897379
C	21.236092	28.252245	27.241478
H	20.778701	29.206933	27.454203
H	20.784005	21.116571	29.005170
C	20.224000	22.049000	29.138000
H	20.390406	22.677098	28.257378
H	19.158295	21.792165	29.172480
C	20.659841	22.768322	30.421829
H	20.496766	22.138525	31.300541
H	21.735102	22.989689	30.373291
C	19.935989	24.092569	30.652567
O	19.897109	24.890487	29.633340
O	19.430899	24.328651	31.766289
H	14.391496	23.796558	27.207970
C	15.392001	23.814000	26.757000
H	15.870280	22.855798	26.976758
H	15.265596	23.881724	25.668610
N	15.891364	26.270931	27.189064
H	15.063550	26.640992	26.743875
C	16.230452	24.927971	27.298174
C	16.852749	27.010281	27.801382
H	16.843125	28.086801	27.882715
N	17.792012	26.223530	28.294926
C	17.416192	24.930238	27.985693
H	18.025000	24.093874	28.288232
O	18.292230	26.598253	31.339283
C	18.032926	27.574171	32.377433
C	17.227707	28.705847	31.722720
O	18.641492	28.714744	29.383043
O	17.243111	30.759551	29.885707
P	18.249837	29.670049	30.543405
O	19.358534	30.344269	31.333550
H	17.429184	27.056767	33.130122
H	19.589420	28.738364	32.520502
H	16.350971	28.289511	31.217778
H	16.885900	29.393133	32.503832
H	18.704614	25.739213	31.707579
H	17.411879	31.647691	30.280027
Fe	19.513049	26.911607	29.626954
O	20.977261	27.379138	30.613488
O	19.184650	27.996879	33.022743
H	16.222658	35.667011	36.387007
C	17.280000	35.763000	36.105000
H	17.481005	36.832939	35.972204
H	17.877478	35.414431	36.954033
C	17.598635	34.977192	34.849260
C	18.323100	33.779884	34.895941
H	18.676322	33.406377	35.854899
C	18.611312	33.047090	33.741641
H	19.175920	32.120086	33.801193
C	18.174130	33.512741	32.497234
O	18.445004	32.853156	31.327553
H	19.004039	32.044797	31.487902
C	17.166008	35.420525	33.589697
H	16.603724	36.349451	33.514695