

Supporting Information

Roles of base in the Pd-catalyzed Annulative Chlorophenylene Dimerization

Li-Ping Xu,^{a,b} Brandon E. Haines,^c Manjaly J. Ajitha,^a Kei Murakami,^d Ken Itami, ^{,d} and Djamaladdin G. Musaev^{*,a}*

^a Cherry L. Emerson Center for Scientific Computation, Emory University, Atlanta, Georgia 30322, USA.

^b School of Chemistry and Chemical Engineering, Shandong University of Technology, Zibo, 255000, China

^c Westmont College, Department of Chemistry, Santa Barbara CA, 93108, USA

^d Institute of Transformative Bio-Molecules (WPI-ITbM) and Graduate School of Science, and JST-ERATO, Itami Molecular Nanocarbon Project, Nagoya University, Chikusa, Nagoya 464-8602, Japan

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1. Validating the used basis sets by recalculating energies of some intermediates and transition states with a larger basis sets.

Table S1. The calculated relative energies of pre-reaction complex, intermediates, and transition states of the active catalyst generation and first C–Cl bond activation steps by using a larger basis sets.

Method ^a	PdP2	PdP	INT1	TS1	INT2
[B3LYP-D3BJ]/BS1	0.0 ^b	21.1	14.0	26.1	-3.4
[B3LYP-D3BJ]/BS2	0.0	20.0	14.9	26.0	-6.4

^aBS1: 6-31G(d,p) + Lanl2dz (Pd, Cs); BS2: 6-311+G(d,p) + SDD (Pd, Cs)

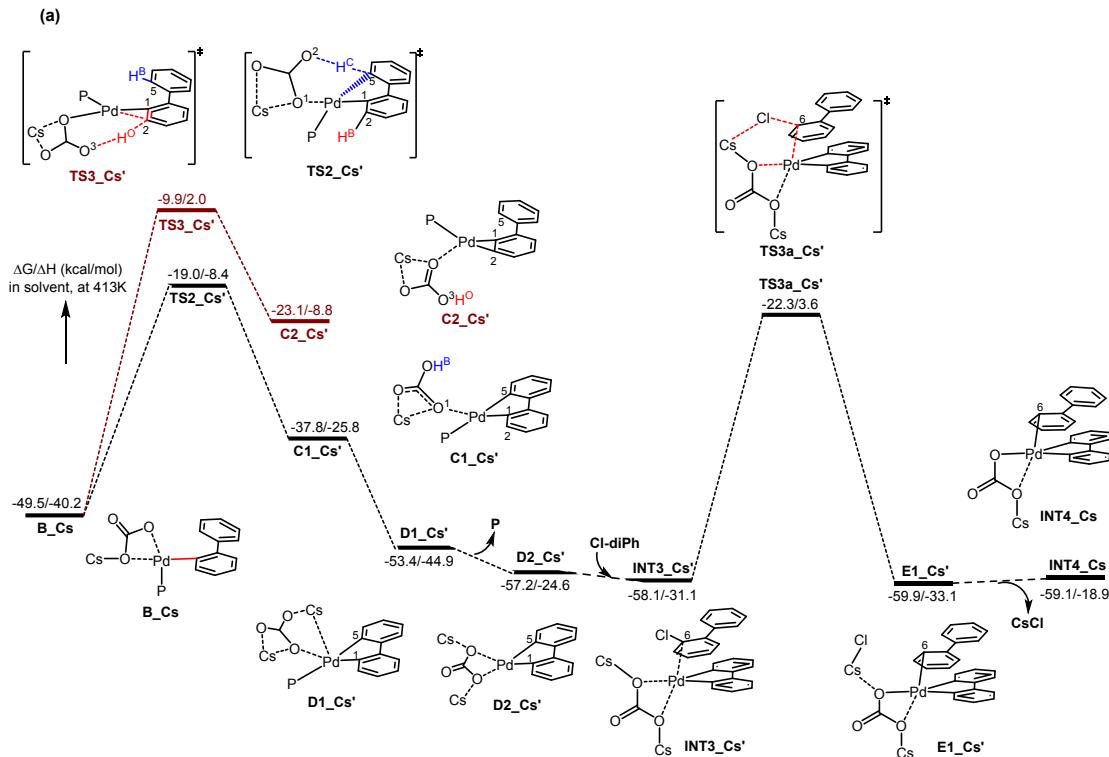
^bΔG in kcal/mol

2. Ligand effects on the calculated energies of the first C–Cl oxidative addition.

Table S2. Ligand effects on the calculated energies of the first C–Cl oxidative addition.

Ligand	PdP2	PdP	INT1	TS1	INT2
PBu(Ad) ₂	0.0	21.1	14.0	26.1	-3.4
PBu ₃	0.0	20.9	15.1	26.2	-9.3

3. Reaction pathway initiated from **B_Cs** and following without the Cs-cluster formation.



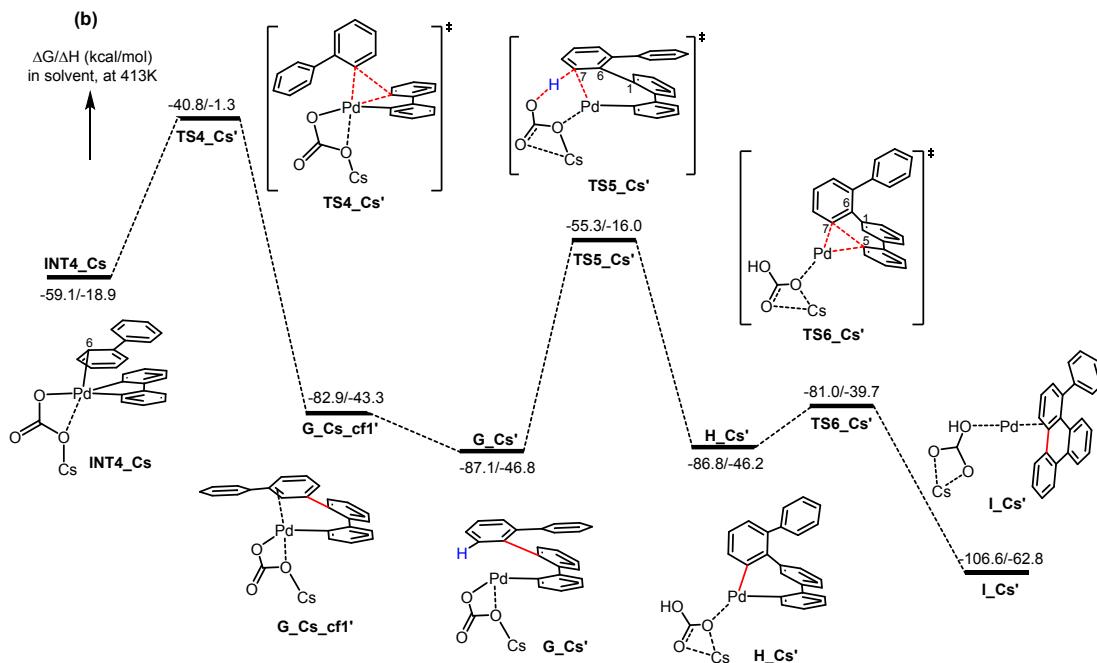


Figure S1. Potential energy surface of the reaction proceeding via without the formation of Cs-cluster complex: (a) from **B_Cs** to **INT4_Cs**, including palladacycle or Pd-aryne formation, and the second C-Cl addition steps; and (b) from **INT4_Cs** to the product **I_Cs'**, including the first C-C coupling, second C-H activation, and second C-C coupling steps.

Briefly, from **B_Cs**, the first C-H activation can proceed through transition states **TS2_Cs'** and **TS3_Cs'** leading to the palladacycle and Pd-aryne intermediates, respectively (Figure S1 (a)). It is found that both the transition state and product of the Pd-aryne pathway lie energetically higher than those of the palladacycle formation pathway. Therefore, here we did not pursue the investigation of the reactions initiated from the Pd-aryne complex. For the palladacycle formation pathway, we found that the barrier for the first C-H activation is 30.5 kcal/mol at the transition state **TS2_Cs'**, which is close to that of the same step of the “Cs-cluster complex” pathway (i.e., 31.4 kcal/mol). After the C - H activation, the thermodynamically favorable CsHCO_3 -to- Cs_2CO_3 ligand exchange leads to intermediates **D1_Cs'** and **D2_Cs'**. It should be mentioned that from **D1_Cs'** to **INT4_Cs**, these two pathways (i.e. with and without “Cs-cluster complex” formation pathways) are overlapped.

From **INT4_Cs** (Figure S1 (b)), the first C-C coupling takes place through transition state **TS4_Cs'** and generates intermediate **G_Cs_cf1'**, which later isomerizes to **G_Cs'**. This step of the reaction has a barrier of 18.3 kcal/mol and is exergonic by 28.0 kcal/mol. Subsequent second C - H activation (at the transition state **TS5_Cs'**) and second C-C coupling (through transition state **TS6_Cs'**) lead to the PAH product, **I_Cs'**: overall reaction is highly exergonic.

To summarize, the reaction proceeding via the without “Cs-cluster complex” formation mechanism, is comparable to that proceeding via the “Cs-cluster complex” formation (which was discussed in the main text). Indeed, (a) the rate-determining steps of both reactions are same (second C - Cl addition), and (b) both pathways lead to the thermodynamically stable PAH product.

4. The C–Cl bond activation of the second equivalent substrate **1a** (or **Cl-diPh**) by intermediate **C_Cs**.

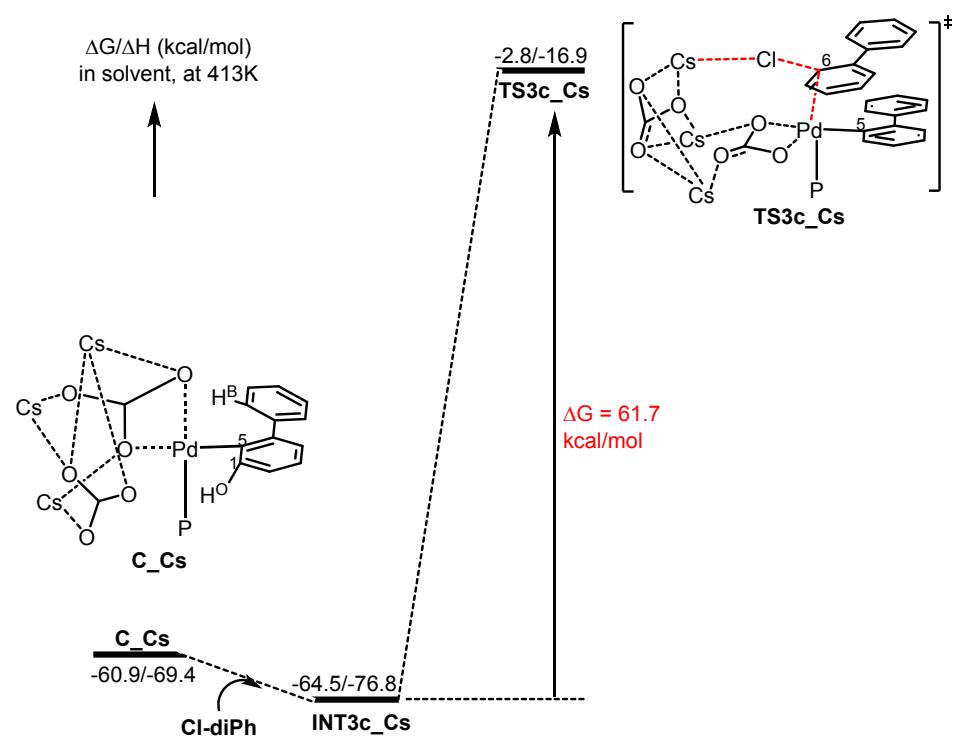


Figure S2. The C–Cl bond activation of the second equivalent substrate **1a** (i.e. **Cl-diPh**) by intermediate **C_Cs**.

5. Structure of the intermediate **C1_Cs_cf1**.

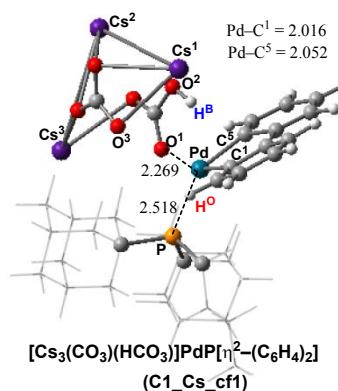


Figure S3. Structure of the intermediate **C1_Cs_cf1**

6. The second C–Cl bond activation by intermediate **C1_Cs**.

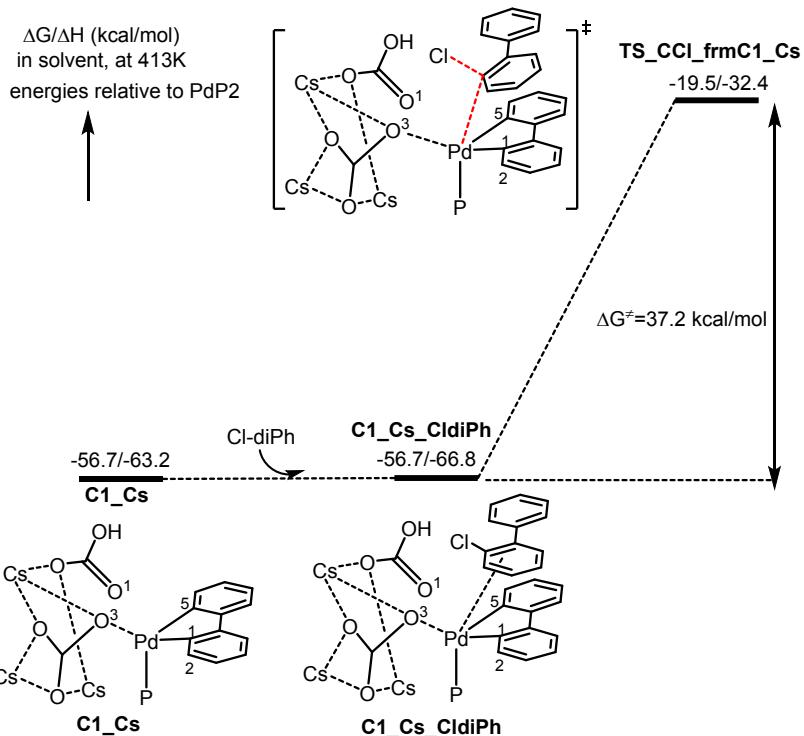
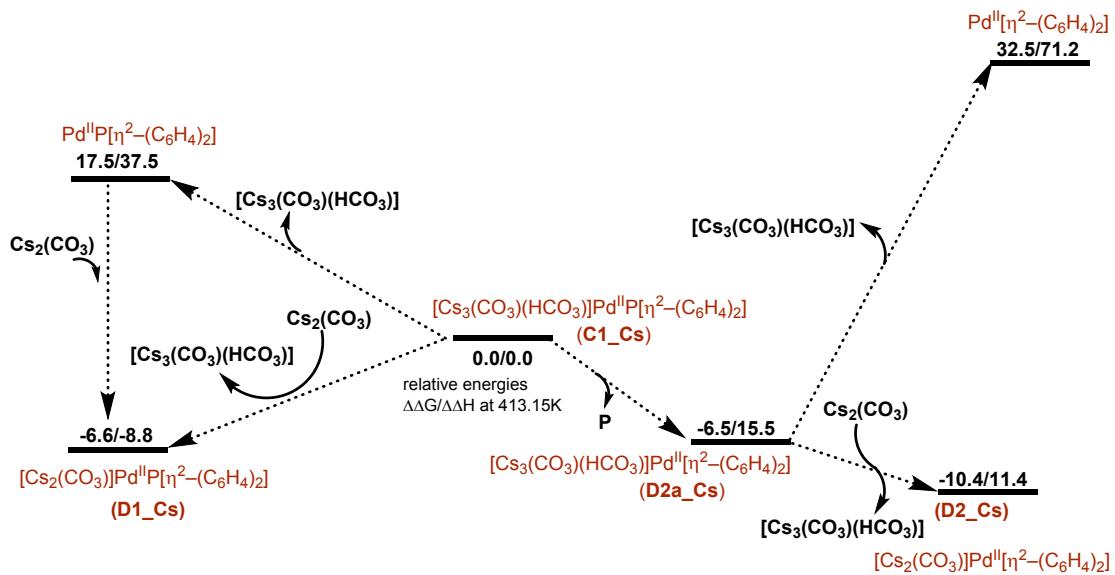


Figure S4. The second C-Cl bond activation by intermediate **C1_Cs**.

7. Transformations connecting intermediate **C1_Cs** with the energetically more favorable **D1_Cs** and **D2_Cs** products.

Scheme S1. The Identified Transformations Connecting Intermediate **C1_Cs** with the Energetically More Favorable **D1_Cs** and **D2_Cs** Products.



8. The calculated Pd-aryne intermediates **D1_Cs_benz** and **D2_Cs_benz** with their important geometry parameters (distances are in Å).

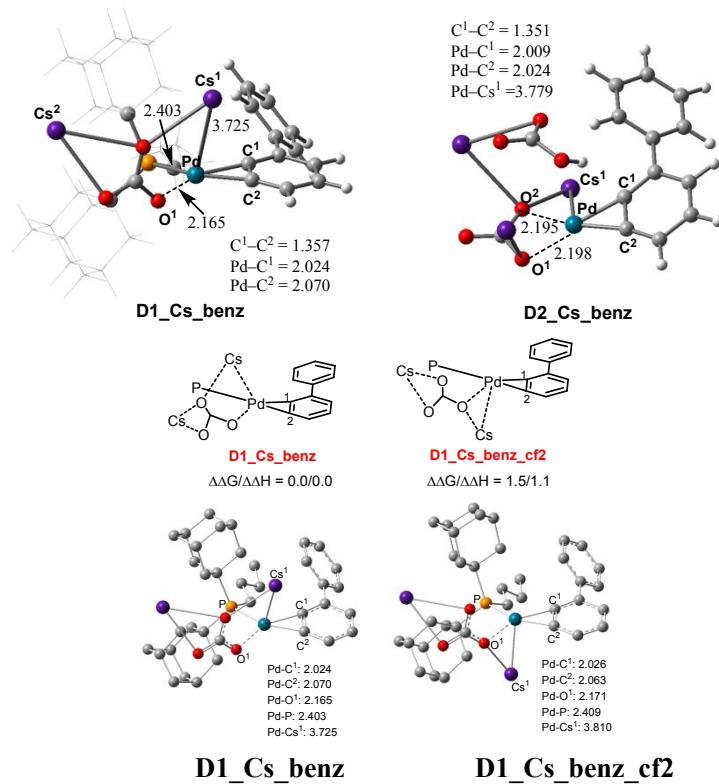


Figure S5. The calculated Pd-aryne intermediates **D1_Cs_benz**, **D2_Cs_benz** and **D1_Cs_benz_cf2** with their important geometry parameters (distances are in Å).

9. Structures and important geometry parameters (distances are in Å) of key intermediate **C_Cs** and the palladacycle and Pd-aryne formation transition states, and distortion interaction analysis for the palladacycle transition state (**TS2_Cs**).

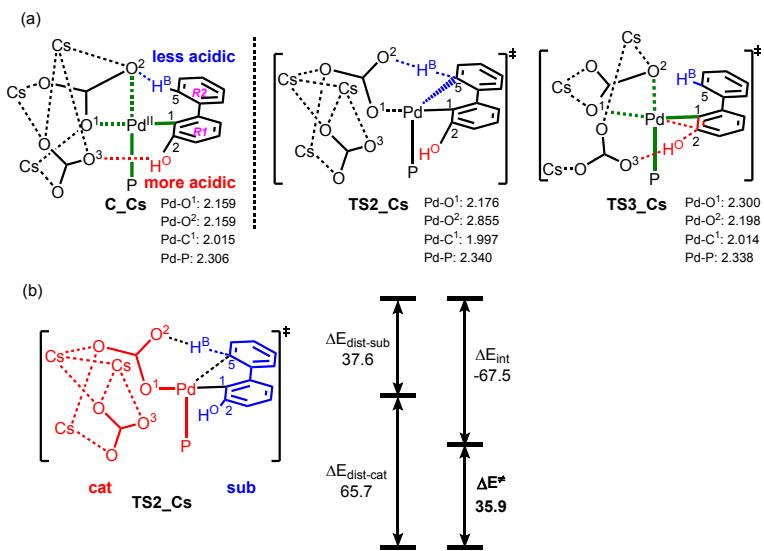


Figure S6. (a) Structures and important geometry parameters (distances are in Å) of key intermediate **C_Cs** and the palladacycle and Pd-aryne formation transition states, and (b) Distortion interaction analysis for the palladacycle transition state (**TS2_Cs**).

We have performed the distortion/interaction analysis of the C-H^B activation in **TS2_Cs**. Calculations show the large distortion energies from both catalyst, 65.7 kcal/mol, and substrate, 37.6 kcal/mol, which are only partly compensated by the catalyst-substrate interaction energy of 67.5 kcal/mol. Thus, the calculated relatively high C–H activation barrier is, mostly, result of the geometry distortion of both fragments.

10. The studied isomers of the intermediate **INT3_Cs**.

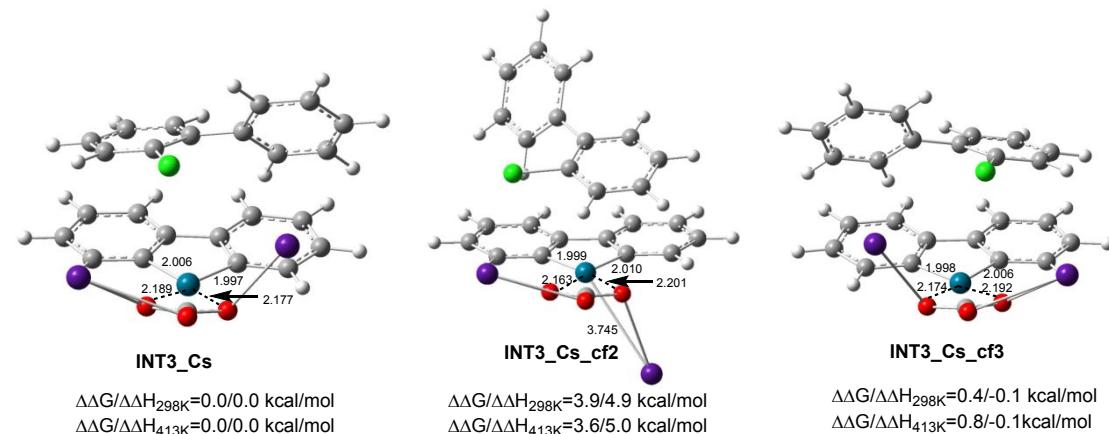


Figure S7. The studied isomers of the intermediate **INT3_Cs**

11. The second C–Cl activation step initiated from the intermediate **D1_Cs**.

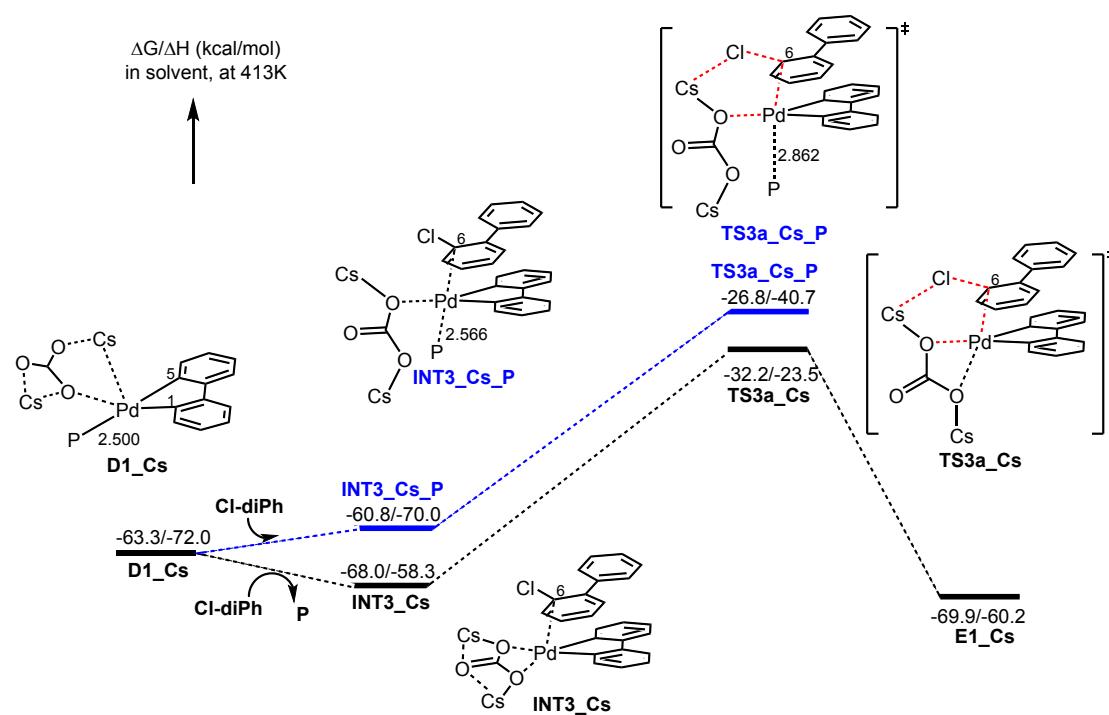


Figure S8. The second C-Cl activation step initiated from the intermediate **D1_Cs**.

12. The second C–Cl activation by the intermediate **D2a_Cs**.

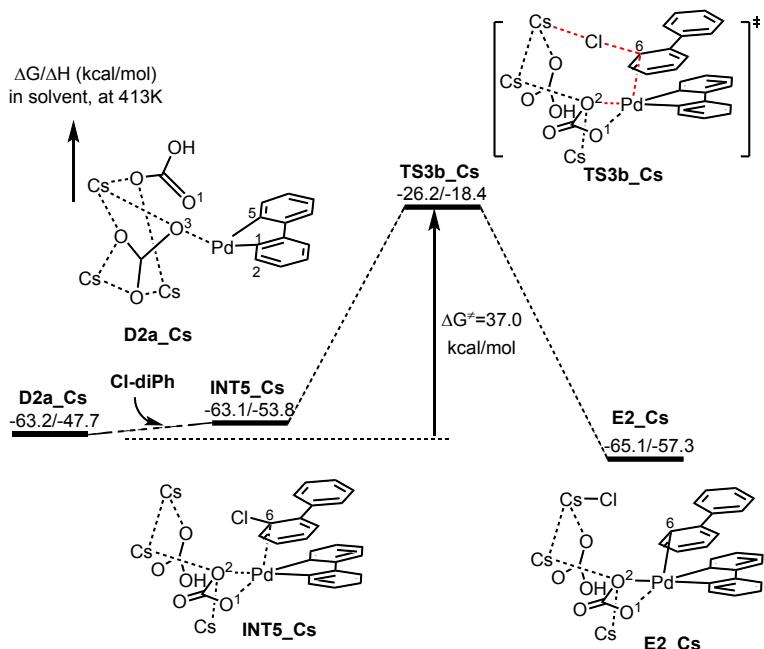


Figure S9. The second C-Cl bond activation by the intermediate **D2a_Cs**.

13. The second C-Cl activation step on the Pd-aryne pathway from the intermediate **D1_Cs_benz**.

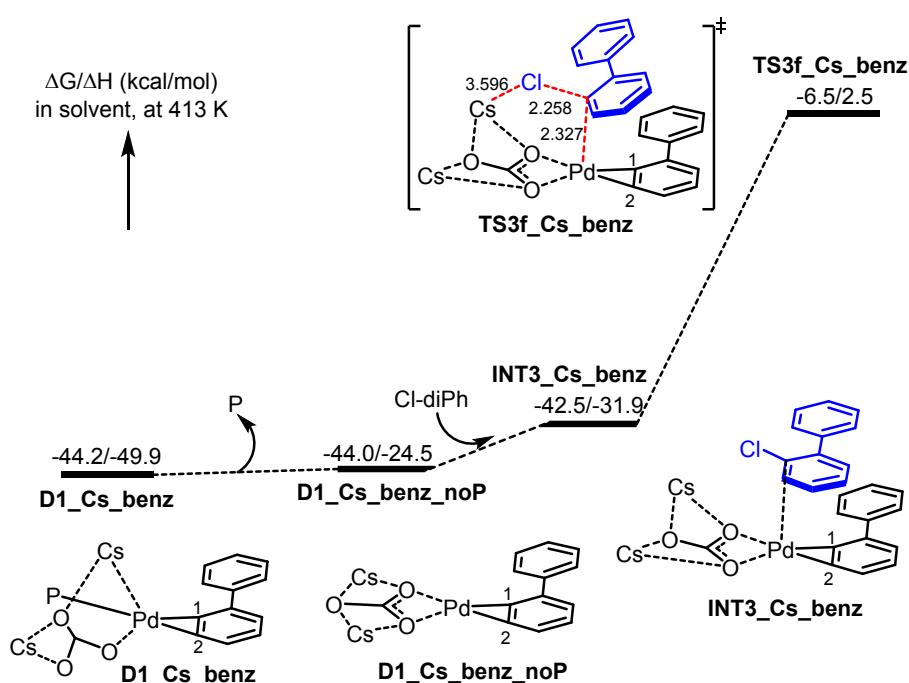


Figure S10. The second C-Cl activation step on the Pd-aryne pathway from the intermediate **D1_Cs_benz**.

14. Potential energy surface of the PAH formation from intermediate **F_Cs**.

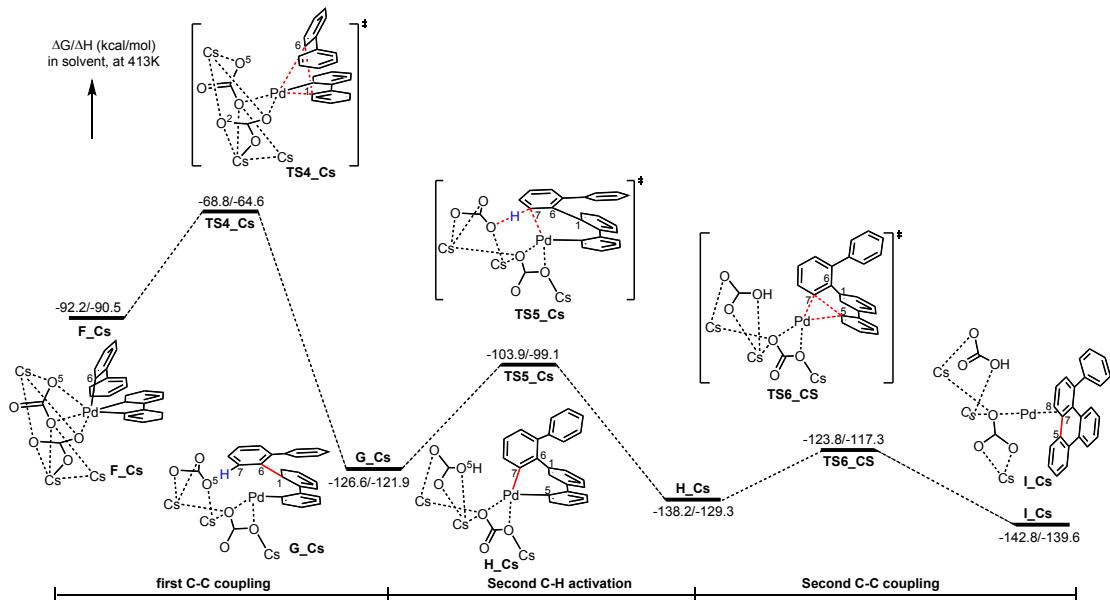


Figure S11. Potential energy surface of the PAH formation from intermediate **F_Cs**.

15. PAH and COT formation initiated from the complex **INT4_Cs** with no “Cs-cluster”.

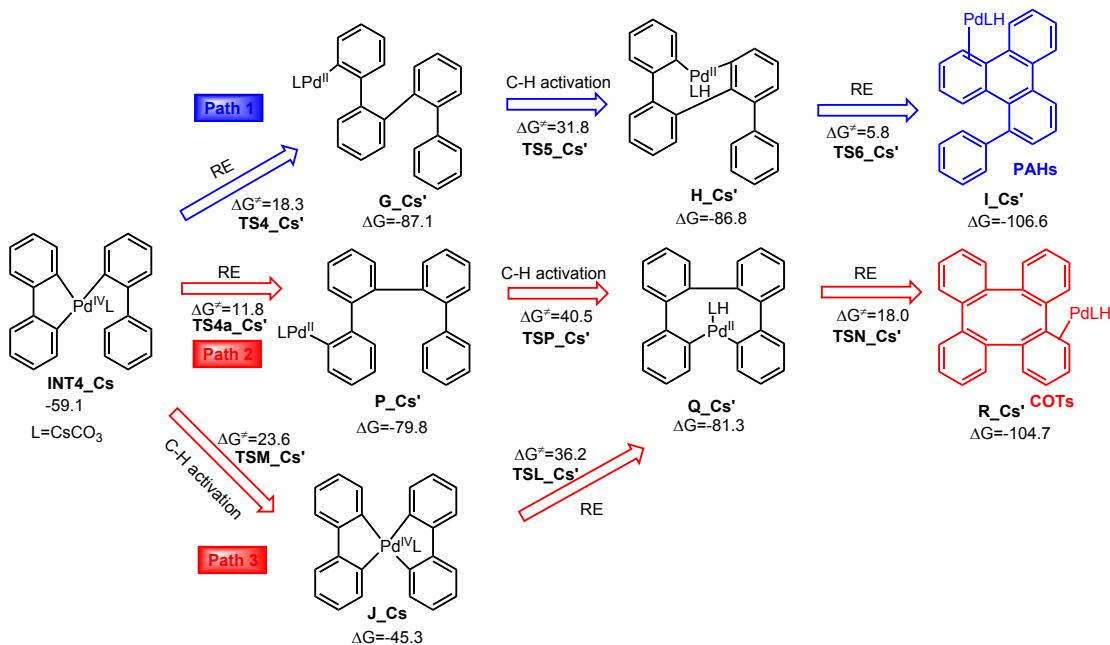


Figure S12. PAH and COT formation initiated from the complex **INT4_Cs** with no “Cs-cluster”.

16. Comparison of the PAH and COT formation from intermediate **F_Cs**.

For **Path 2**, which leads to COT product, the rate-determining step is the second C-H activation at the bay-position of the second diphenyl moiety which requires 43.1 kcal/mol free energy barrier at the transition state **TSP_Cs**. This barrier is higher than the second C-H activation at the transition state **TS5_Cs** of the **Path 1** leading to PAH product. As it can be seen from the calculated structures of the pre-reaction complex **P_Cs** and transition state **TSP_Cs** (**Figure S12**), upon the second C-H activation one of the CO_3 moieties moves away from the Pd center to perform the C-H bond deprotonation, which destabilizes the calculated transition state.

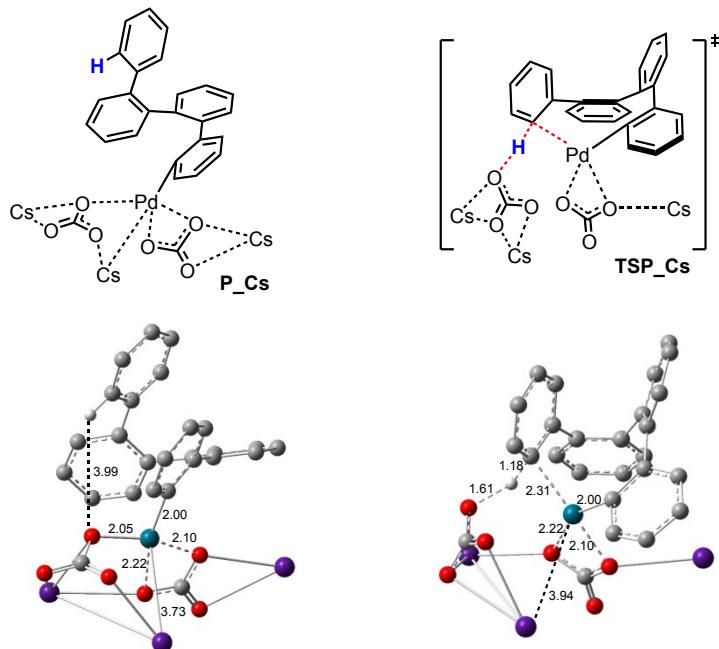


Figure S13. Geometries for pre-reaction complex **P_Cs** and the reductive elimination transition state **TSP_Cs**. Hydrogen atoms are omitted for clarity and bond distances are given in Å.

For **Path 3**, which also leads to COT product, the calculated activation free energy of the first C-C reductive elimination transition state **TSL_Cs** is 37.8 kcal/mol. The **TSL_Cs** is highly unstable compared to the pre-reaction complex (**J_Cs**) because during this reaction the favorable in-plane π -conjugation interaction of the two Pd-bound diphenyl rings has to be broken (**Figure S13**). This can be seen clearly from the changes of the relevant dihedral angles (-3.69° to 17.45° and -1.86° to 16.47° for $\angle 1345$ and $\angle 6789$, respectively).

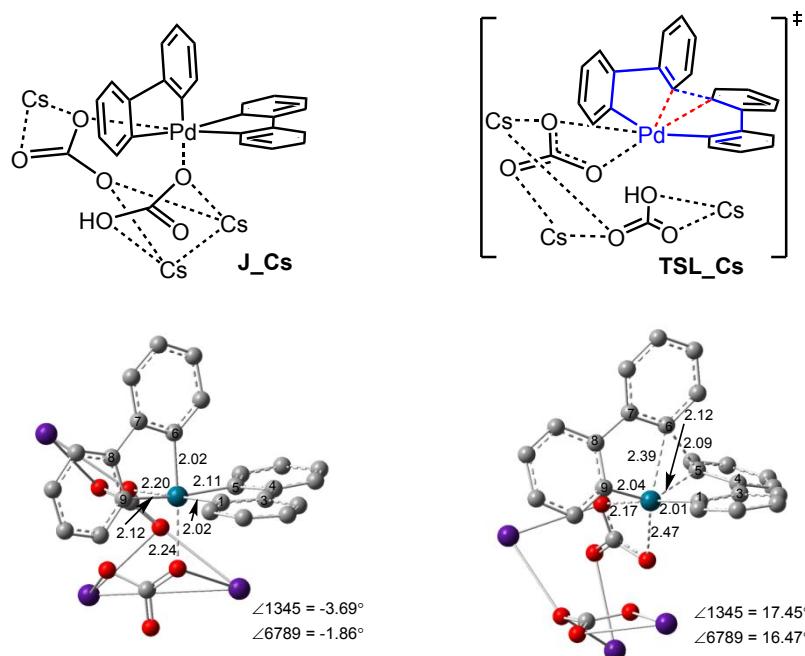


Figure S14. Structures and important geometry parameters (distances are in Å, and angles are in deg.) of the pre-reaction complex **J_Cs** and C-C reductive elimination transition state **TSL_Cs**. Hydrogen atoms are omitted for clarity.

In summary, our calculations show that the formation of COT through either Path 2 or Path 3 is kinetically and thermodynamically unfavorable compared to the formation of PAH (i.e. Path-1). This conclusion is consistent with the available experiments.

17. Potential energy surface of ligand exchange and first C-Cl bond activation steps of the Na_2CO_3 mediated Pd-catalyzed annulative chlorophenylene dimerization reaction

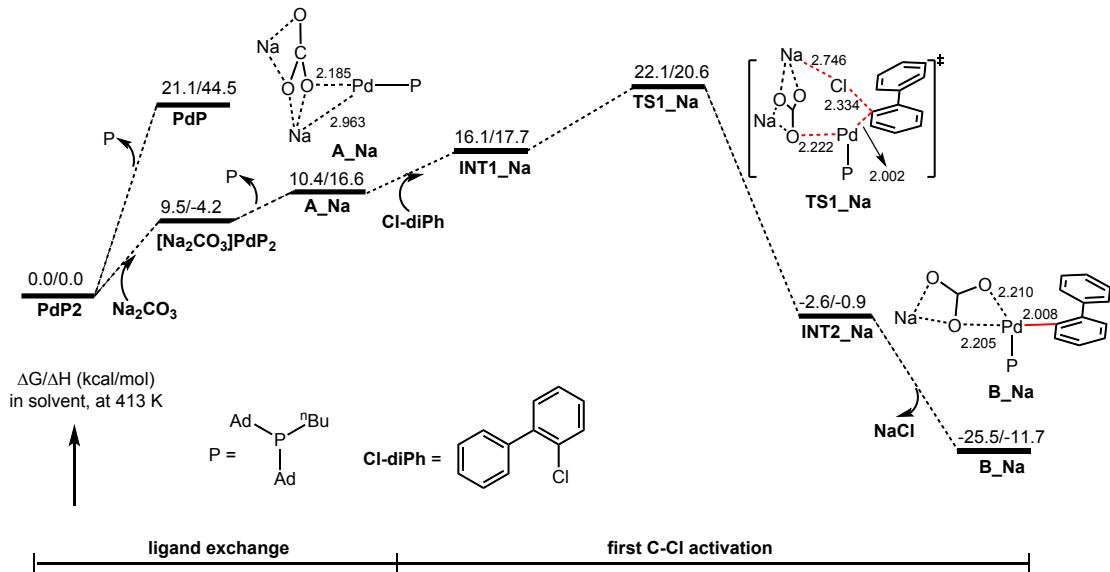


Figure S15. Potential energy surface of ligand exchange and first C-Cl bond activation steps of the Na_2CO_3 mediated Pd-catalyzed annulative chlorophenylene dimerization reaction

18. Reaction pathway initiated from **B_Na** and following without the Na-cluster formation (i.e., without the coordination of Na_2CO_3 to NaCO_3).

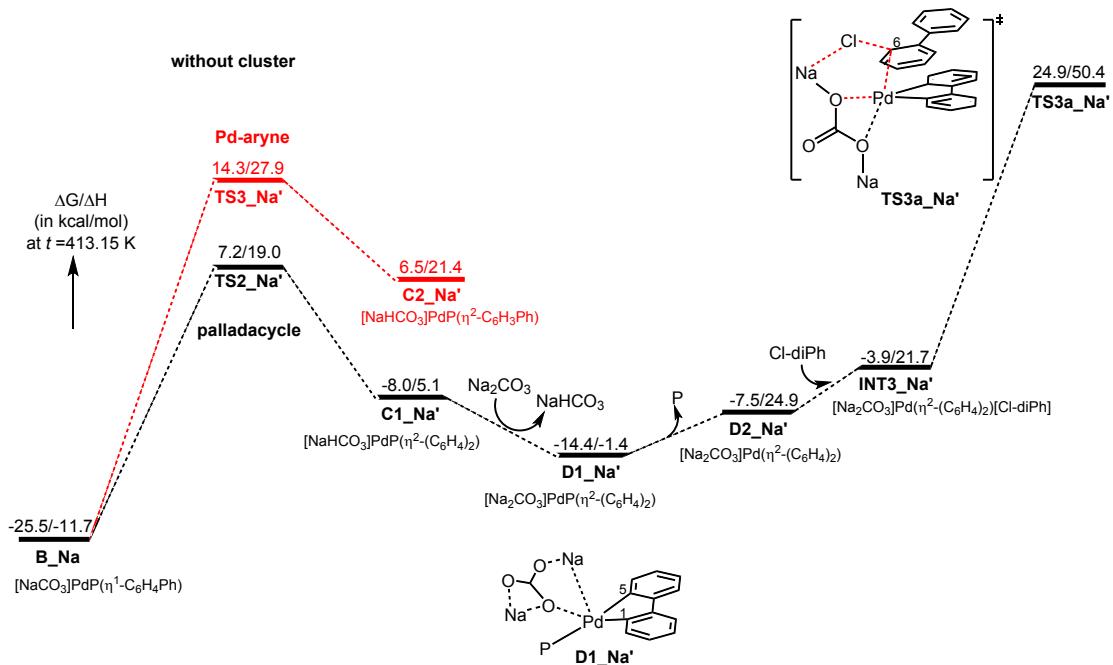
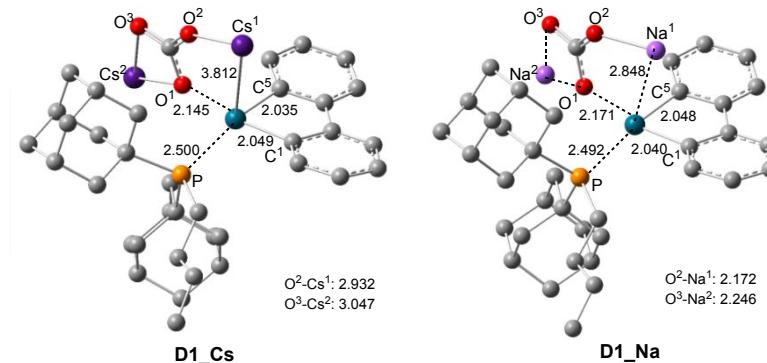


Figure S16. Reaction pathway initiated from **B_Cs** and following without the formation of Na-cluster (i.e., without the coordination of Na_2CO_3 to NaCO_3).

19. Comparison of the intermediates **D1_Cs** and **D1_Na**.



	D1_Cs	D1_Na
<i>Mulliken charges</i>	Pd: -0.363 O ¹ : -0.633 $\Delta_{\text{Chg}} = 0.270$	Pd: -0.404 O ¹ : -0.603 $\Delta_{\text{Chg}} = 0.199$
<i>Bond distance</i>	Pd-O ¹ : 2.145	Pd-O ¹ : 2.171
<i>NBO second-order perturbation (E2)</i>	10.5 [Cs(5S) to Pd (P*)]	7.4 [Na(2S) to Pd (P*)]
<i>base dissociation</i>	+23.0	+9.5

Figure S17. Comparison of the intermediates **D1_Cs** and **D1_Na**.

20. Second C-Cl bond activation initiated by intermediates **C1_Na**, **D1_Na**, and **D2_Na**.

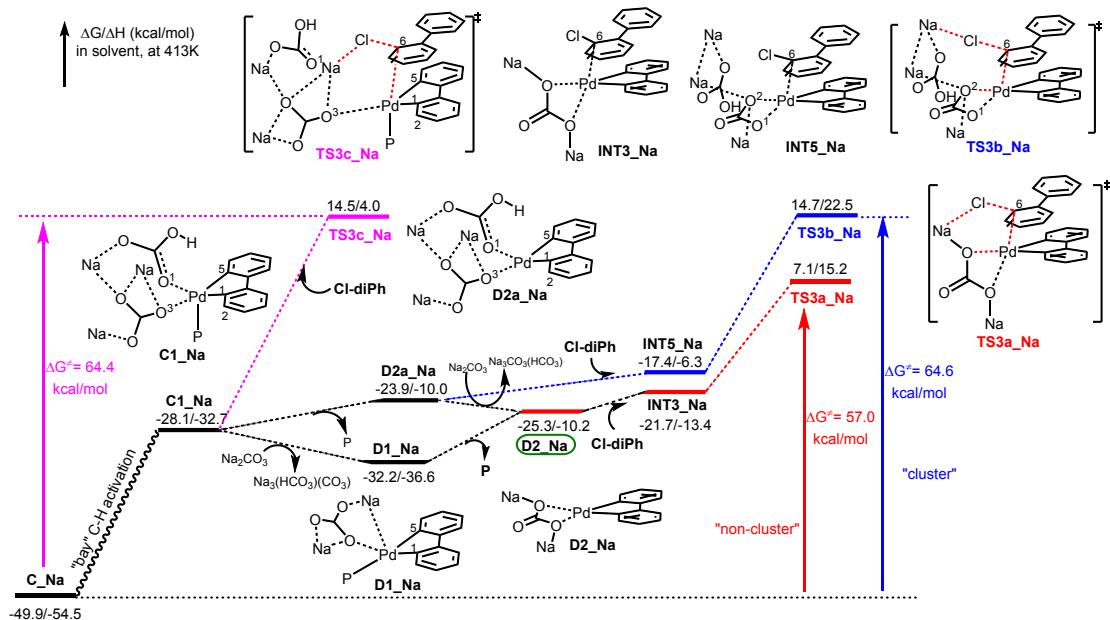


Figure S18. Second C-Cl activation initiated by intermediates **C1_Na**, **D1_Na**, and **D2a_Na**. The calculated activation barriers are 64.4, 57.0 and 64.6 kcal/mol, respectively, relative to the most stable species, **C_Na**.

21. Electronic energies, thermal correction to enthalpy and entropy at 413.15K, and imaginary frequencies, for all reported intermediates and transition states.

Structure	Electronic Energy	Thermal correction to enthalpy	thermal correction to free energy	imaginary frequency
A_Cs	-1710.187859	0.673695	0.495209	
A_Na	-1995.042426	0.673545	0.50512	
B_Cs	-2153.025268	0.860616	0.662449	
B_Na	-2295.445976	0.862123	0.663363	
C_Cs	-2456.775001	0.893095	0.652379	
C_Na	-2884.093042	0.893163	0.664077	
C1_Cs	-2456.76551	0.893491	0.649551	
C1_Cs_cfl	-2456.743725	0.892455	0.649096	
C1_Cs_Cl-diPh	-3379.746973	1.088679	0.793673	
C1_Cs'	-2153.003685	0.862004	0.659598	
C1_Na	-2884.058372	0.89324	0.664218	
C2_Cs	-2456.739588	0.891437	0.648283	
C2_Cs'	-2152.976129	0.861553	0.655426	
C2_Na	-2884.015281	0.892801	0.661522	
Cl_diPh	-922.952695	0.172105	0.115281	
Cs2CO3	-303.698911	0.028238	-0.042764	
Cs2CO3_PdP2	-2989.858986	1.314301	1.045219	
Cs3_CO3_HCO3	-588.127665	0.068364	-0.034471	
CsCl	-480.204119	0.005903	-0.037564	
D1_Cs	-2172.348046	0.85072	0.642029	
D1_Cs_benz	-2172.314568	0.852386	0.638972	
D1_Na	-2457.198774	0.852858	0.648622	
D2_Cs	-1177.110809	0.249916	0.096807	
D2_Cs_benz	-1177.072716	0.250088	0.09386	
D2_Na	-1604.393375	0.250769	0.118202	
E1_Cs	-1815.678087	0.405295	0.236495	
E2_Cs	-2100.102095	0.445364	0.247582	
F_Cs	-1639.221785	0.42818	0.244677	
G_Cs	-1639.23808	0.429028	0.241694	
G_Cs_cfl'	-1335.489899	0.399091	0.253455	
G_Cs'	-1335.494614	0.398252	0.251337	
H_Cs	-1639.284818	0.429423	0.234329	
H_Cs'	-1335.494107	0.39866	0.251454	
I_Cs	-1639.30137	0.429596	0.243603	
I_Cs'	-1335.521636	0.399688	0.247361	
INT1	-2329.410783	0.836967	0.649125	
INT1_Cs	-2633.163247	0.867281	0.644147	

INT1_Na	-2918.01525	0.867569	0.64962	
INT1_PBu3	-1864.785983	0.60422	0.432379	
INT2	-2329.442649	0.838572	0.653278	
INT2_Cs	-2633.199634	0.866913	0.64298	
INT2_Na	-2918.046218	0.868855	0.650793	
INT2_PBu3	-1864.825902	0.604909	0.433359	
INT3_Cs	-1815.674668	0.404984	0.236076	
INT3_Cs_cf2	-1815.666866	0.40501	0.234006	
INT3_Cs_cf3	-1815.674829	0.40496	0.237426	
INT3_Cs_P	-3095.322605	1.047905	0.783218	
INT3c_Cs	-3379.76237	1.088077	0.796638	
INT3_Na	-2100.508826	0.405557	0.250345	
INT4_Cs	-1335.449319	0.397286	0.250775	
INT5_Cs	-2100.09636	0.445095	0.245071	
INT5_Na	-2527.363199	0.445998	0.260881	
J_Cs	-1639.219402	0.42796	0.243714	
Na2CO3	-588.5763779	0.028588	-0.031049	
Na3_CO3_HCO3	-1015.442096	0.06897	-0.015958	
NaCl	-622.6166909	0.005964	-0.032643	
P_Cs	-1639.272909	0.429441	0.243885	
P_nBu_2Ad	-1279.624673	0.638312	0.512366	
PBu3	-815.007268	0.405288	0.295048	
Pd_2P	-2686.115017	1.281131	1.056203	
Pd_2PBu3	-1756.863529	0.818162	0.610985	
Pd_P	-1406.418753	0.642144	0.505929	
Pd_P2_Na2CO3	-3274.701877	1.313543	1.050762	
Pd_PBu3	-941.796949	0.409706	0.289993	
Q_Cs	-1639.272377	0.429453	0.241907	
R_Cs	-1639.292677	0.429533	0.243432	
TS_CCl_frmC1_Cs	-3379.688719	1.085229	0.794631	-292.71
TS1	-2329.396803	0.836144	0.654413	-208.59
TS1_Cs	-2633.159225	0.866246	0.643412	-168.79
TS1_Na	-2918.00991	0.866813	0.653837	-153.46
TS1_PBu3	-1864.771402	0.602641	0.435443	-180.45
TS2_Cs	-2456.717796	0.88617	0.645218	-1590.53
TS2_Cs'	-2152.969922	0.855935	0.655747	-1491.77
TS2_Na	-2884.033261	0.886968	0.662806	-1505.05
TS2a_Cs	-2152.96056	0.855732	0.655801	-1489.74
TS3_Cs	-2456.731313	0.885322	0.64596	-290.99
TS3_Cs'	-2152.952815	0.855487	0.653055	-1440.02
TS3a_Cs	-1815.616726	0.402356	0.235109	-219.01
TS3a_Cs_P	-3095.273226	1.04516	0.787973	-288.19

TS3a_Na	-2100.460862	0.403229	0.248247	-264.67
TS3b_Cs	-2100.037671	0.44284	0.245156	-290.95
TS3c_Cs	-3379.664015	1.085306	0.796599	-105.44
TS3b_Na	-2527.314959	0.443642	0.263799	-295.24
TS3c_Na	-3806.974214	1.087067	0.810535	-190.99
TS4_Cs	-1639.178624	0.426324	0.238738	-386.86
TS4_Cs'	-1335.419431	0.395511	0.250027	-332.23
TS4a_Cs	-1639.189599	0.426055	0.243593	-348.98
TS5_Cs	-1639.230517	0.423259	0.234664	-637.79
TS5_Cs'	-1335.439717	0.392402	0.247185	-527.29
TS6_Cs	-1639.263824	0.42759	0.236279	-333.53
TS6_Cs'	-1335.48226	0.397089	0.248721	-304.53
TSL_Cs	-1639.155192	0.425517	0.239785	-332.47
TSM_Cs	-1639.164982	0.422473	0.235916	-1455.91
TSN_Cs	-1639.224442	0.425516	0.242576	-353.86
TSP_Cs	-1639.201395	0.424714	0.241176	-114.96
TS4a_Cs'	-1335.430751	0.39547	0.251027	-211.65
P_Cs'	-1335.48206	0.398147	0.250424	
TSP_Cs'	-1335.413094	0.391312	0.246124	-1642.15
Q_Cs'	-1335.482022	0.398088	0.248132	
TSN_Cs'	-1335.455908	0.396496	0.250584	-338.10
R_Cs'	-1335.523041	0.398974	0.25171	
TSM_Cs'	-1335.408253	0.391537	0.247275	-1099.37
J_Cs'	-1335.424823	0.397272	0.248228	
TSL_Cs'	-1335.36834	0.395354	0.249391	-321.28
TS2_Na'	-2295.390707	0.8558	0.660115	-1519.75
C1_Na'	-2295.4191	0.862048	0.664391	
TS3_Na'	-2295.376527	0.855855	0.657322	-1466.87
C2_Na'	-2295.392473	0.861451	0.660872	
D1_Cs_benz_noP	-892.645231	0.209959	0.082296	
INT3_Cs_benz	-1815.632806	0.405151	0.234772	
TS3f_Cs_benz	-1815.575389	0.40249	0.234782	-311.13

BS2 method single point calculation ^a	Single point energy	BS2 method single point calculation	Single point energy
Cl_diPh_BS2	-923.0961099	INT1_BS2	-2330.954378
INT2_BS2	-2330.992397	Pd_2P_BS2	-2687.742711
Pd_P_BS2	-1407.822069	TS1_BS2	-2330.941875
P_nBu_2Ad_BS2	-1279.850784		

^aSee Table S1 for more details.

Cartesian coordinates (in Å) of all calculated species.

A_Cs				A_Na			
Pd	0.566744	0.910338	1.176241	H	-4.234955	-5.503333	-0.056252
P	-0.509510	-0.227759	-0.420197	H	-4.909921	-3.960292	-0.600087
C	-1.837270	0.838510	-1.263759	H	-3.708714	-4.797246	-1.591539
C	-2.971985	1.017168	-0.219275	Cs	2.947821	3.656008	-1.019474
C	-2.438262	0.296204	-2.580525	O	3.512594	2.257369	1.614947
C	-1.253801	2.249837	-1.541928	O	1.516349	2.099873	2.677943
H	-3.423731	0.053491	0.029613	C	2.488084	2.837405	2.115485
H	-2.541404	1.415547	0.707968	O	2.328725	4.113077	2.082577
C	-4.065472	1.960600	-0.750353	Cs	-0.713017	4.199244	2.645110
H	-2.860895	-0.700452	-2.433816				
H	-1.654993	0.204379	-3.339594	Pd	0.789664	0.888637	1.035641
C	-3.534287	1.248932	-3.102165	P	-0.332444	-0.336976	-0.465476
H	-0.813405	2.634889	-0.614723	C	-1.622314	0.818932	-1.249744
H	-0.443579	2.190052	-2.273160	C	-2.714067	1.052425	-0.170385
C	-2.339157	3.203396	-2.072841	C	-2.294876	0.337743	-2.554406
H	-4.856991	2.047911	0.004432	C	-0.954346	2.195250	-1.519258
C	-4.650297	1.379134	-2.050622	H	-3.223421	0.116908	0.075082
C	-3.460970	3.345735	-1.031863	H	-2.232479	1.407368	0.749003
H	-3.948944	0.836682	-4.030346	C	-3.753882	2.078907	-0.652984
C	-2.924275	2.634382	-3.378401	H	-2.780120	-0.630610	-2.408416
H	-1.886111	4.184096	-2.266642	H	-1.542692	0.205620	-3.338535
H	-5.449384	2.029444	-2.428562	C	-3.338783	1.371717	-3.029316
H	-5.098314	0.396722	-1.853955	H	-0.478907	2.533690	-0.591458
H	-3.064597	3.778159	-0.104158	H	-0.160339	2.098562	-2.263436
H	-4.235570	4.030256	-1.400518	C	-1.987736	3.225170	-2.007276
H	-2.137273	2.553383	-4.139252	H	-4.515790	2.204440	0.126521
H	-3.690867	3.311847	-3.775729	C	-4.413816	1.562668	-1.944516
C	0.692932	-0.961422	-1.704744	C	-3.060682	3.424640	-0.924377
C	1.254869	0.171698	-2.590524	H	-3.806080	1.003096	-3.950709
C	0.147086	-2.084814	-2.613881	C	-2.645656	2.718318	-3.303104
C	1.874258	-1.552349	-0.886554	H	-1.474620	4.176531	-2.201620
H	0.459569	0.605532	-3.202994	H	-5.174368	2.274164	-2.290367
H	1.636721	0.966464	-1.941114	H	-4.925311	0.611443	-1.749180
C	2.367063	-0.347734	-3.517244	H	-2.597288	3.797559	-0.000920
H	-0.704945	-1.734277	-3.202797	H	-3.795956	4.172614	-1.247772
H	-0.202652	-2.919230	-1.999335	H	-1.886784	2.598055	-4.086740
C	1.253447	-2.599650	-3.559858	H	-3.376873	3.450407	-3.669012
H	2.271405	-0.776852	-0.221624	C	0.788978	-1.126819	-1.779308
H	1.514189	-2.365066	-0.243724	C	1.399643	-0.022053	-2.673329
C	2.979917	-2.083808	-1.815451	C	0.143999	-2.205625	-2.678654
H	2.737213	0.484242	-4.129920	C	1.949932	-1.799095	-0.995933
C	1.782385	-1.443236	-4.426871	H	0.615208	0.462603	-3.262139
C	3.516781	-0.927428	-2.676534	H	1.856141	0.748710	-2.039908
H	0.830513	-3.380149	-4.204284	C	2.445526	-0.612909	-3.636197
C	2.407453	-3.183103	-2.726289	H	-0.700125	-1.793240	-3.238430
H	3.790973	-2.494934	-1.201992	H	-0.241289	-3.020930	-2.059401
H	2.551501	-1.811765	-5.117340	C	1.185241	-2.785393	-3.659387
H	0.970373	-1.027983	-5.037696	H	2.419504	-1.053812	-0.343223
H	3.943049	-0.146843	-2.032753	H	1.556150	-2.589563	-0.344976
H	4.322021	-1.282912	-3.332031	C	2.990033	-2.397971	-1.960576
H	2.045749	-4.022962	-2.119589	H	2.853980	0.195709	-4.254761
H	3.191288	-3.574894	-3.387114	C	1.764621	-1.660718	-4.534868
C	-1.412389	-1.734939	0.241425	C	3.577388	-1.275016	-2.832715
C	-2.506168	-2.490022	-0.529910	H	0.692688	-3.532055	-4.294461
H	-1.815830	-1.414456	1.207411	C	2.319265	-3.450376	-2.860400
H	-0.600245	-2.429031	0.490045	H	3.788891	-2.867117	-1.373202
C	-2.873669	-3.809293	0.160849	H	2.488033	-2.074846	-5.248536
H	-3.407959	-1.873499	-0.606704	H	0.965077	-1.189177	-5.120778
H	-2.196792	-2.703533	-1.555900	H	4.074953	-0.528974	-2.200118
C	-3.994489	-4.561569	-0.560047	H	4.335914	-1.681903	-3.513475
H	-1.979502	-4.444273	0.219020	H	1.918104	-4.268657	-2.248818
H	-3.171258	-3.604453	1.197883	H	3.057406	-3.888147	-3.544390

C	-1.289622	-1.785171	0.242560	C	-3.891080	-1.563489	1.614942
C	-2.452275	-2.469279	-0.493351	H	-4.534082	-2.162590	-2.231012
H	-1.642055	-1.435632	1.218251	C	-5.005996	-0.888352	-0.537720
H	-0.513926	-2.527264	0.468271	H	-4.982419	0.281924	1.294401
C	-2.897646	-3.750691	0.221820	H	-4.500053	-3.579485	-0.168388
H	-3.308014	-1.789492	-0.558995	H	-2.942287	-3.642694	-1.000242
H	-2.181438	-2.714470	-1.522896	H	-3.408312	-1.195184	2.527598
C	-4.084634	-4.427920	-0.467049	H	-4.774392	-2.139813	1.919168
H	-2.050377	-4.447711	0.270048	H	-5.319720	-0.042153	-1.162642
H	-3.158143	-3.513135	1.261851	H	-5.912402	-1.447505	-0.273165
H	-4.384018	-5.342381	0.055047	C	-1.208258	2.254291	-1.513108
H	-4.953625	-3.760912	-0.499191	C	-2.315619	2.329195	-2.572608
H	-3.837168	-4.697943	-1.499974	H	-0.308713	2.762861	-1.876846
Na	0.186184	5.413954	0.338823	H	-1.510425	2.826711	-0.632680
O	1.933982	4.103949	0.928453	C	-2.498194	3.767980	-3.071242
O	1.537523	2.423370	2.398682	H	-2.104388	1.679689	-3.426017
C	1.203330	3.569531	1.827212	H	-3.263871	1.982321	-2.150518
O	0.091589	4.141069	2.212531	C	-3.634197	3.897945	-4.087931
Na	-0.597574	2.264691	3.263323	H	-2.689135	4.424582	-2.212199
B_Cs				H	-1.557266	4.114660	-3.518496
Pd	0.713195	0.851528	1.059195	H	-3.743396	4.929580	-4.437143
P	-0.575172	0.644823	-0.835532	H	-3.451373	3.265297	-4.963881
C	0.553031	-0.074026	-2.171425	H	-4.590492	3.589322	-3.650778
C	1.875708	0.738296	-2.106728	C	0.546483	2.858597	1.010799
C	0.008709	0.022001	-3.614875	C	-0.461948	3.580910	1.691201
C	0.881515	-1.549527	-1.840356	C	1.500092	3.586378	0.280457
H	1.679585	1.794902	-2.322270	C	-0.493925	4.985402	1.599911
H	2.280754	0.690225	-1.089800	C	1.461542	4.980972	0.197137
C	2.903667	0.183020	-3.108074	H	2.279862	3.052699	-0.255554
H	-0.178791	1.069042	-3.871342	C	0.452750	5.686187	0.855683
H	-0.939482	-0.514057	-3.709951	H	-1.266578	5.530872	2.135675
C	1.036316	-0.556546	-4.610458	H	2.211932	5.511678	-0.383663
H	1.257706	-1.613941	-0.814434	C	0.409543	6.770146	0.800866
H	-0.025472	-2.157782	-1.903964	C	1.958392	-0.771173	2.587226
C	1.914442	-2.105567	-2.837173	O	1.961278	0.536615	2.778404
H	3.820261	0.781137	-3.038983	O	1.278595	-1.155714	1.515220
C	2.335292	0.264011	-4.534950	Cs	1.313267	-4.155676	1.736821
C	3.211088	-1.282684	-2.754549	C	-1.520107	2.893458	2.475889
H	0.616583	-0.494902	-5.621745	C	-2.862901	3.285943	2.351584
C	1.336024	-2.025238	-4.261260	C	-1.215148	1.830488	3.345534
H	2.123232	-3.152028	-2.580915	C	-3.874135	2.627320	3.052263
H	3.067391	-0.120835	-5.255904	H	-3.117210	4.093188	1.671153
H	2.135672	1.309565	-4.801634	C	-2.226846	1.170945	4.044174
H	3.630703	-1.344330	-1.742378	H	-0.182581	1.520556	3.469209
H	3.961832	-1.688468	-3.444317	C	-3.560772	1.561190	3.897506
H	0.417679	-2.622851	-4.326822	H	-4.907372	2.937607	2.926292
H	2.047471	-2.444049	-4.983925	H	-1.971188	0.349949	4.708235
C	-2.077373	-0.442995	-0.475695	H	-4.346494	1.040371	4.436370
C	-1.677173	-1.640143	0.425528	B_Na			
C	-2.789039	-0.991885	-1.733084	Pd	1.142638	0.812689	0.799871
C	-3.059611	0.433656	0.343176	P	-0.152867	0.578835	-1.086283
H	-0.974307	-2.287734	-0.102131	C	0.978993	-0.131091	-2.422809
H	-1.156518	-1.277268	1.314836	C	2.282238	0.713504	-2.395993
C	-2.921394	-2.456189	0.823609	C	0.409076	-0.071719	-3.859159
H	-2.112032	-1.646584	-2.291059	C	1.346678	-1.593243	-2.072437
H	-3.077047	-0.179731	-2.404339	H	2.058653	1.761210	-2.627330
C	-4.040874	-1.794580	-1.323116	H	2.707295	0.691792	-1.386442
H	-2.556125	0.795540	1.240633	C	3.306449	0.164941	-3.405665
H	-3.370580	1.313135	-0.225583	H	0.198314	0.966727	-4.130714
C	-4.307867	-0.375490	0.734136	H	-0.529859	-0.626835	-3.931282
H	-2.600676	-3.300091	1.448256	C	1.432655	-0.645433	-4.861592

H	1.740662	-1.639311	-1.051514	C	2.385720	-0.759361	2.467357
H	0.453075	-2.222952	-2.109700	O	2.420289	0.539660	2.582207
C	2.376420	-2.141307	-3.077707	O	1.741339	-1.222391	1.400607
H	4.208985	0.786216	-3.361756	O	2.896926	-1.556768	3.298456
C	2.712663	0.206701	-4.823854	Na	1.905076	-3.318888	2.195162
C	3.654259	-1.286603	-3.032958	C	-1.075204	2.876673	2.162950
H	0.993506	-0.610714	-5.865826	C	-2.416788	3.264594	2.016452
C	1.771865	-2.100173	-4.492450	C	-0.774994	1.839541	3.064337
H	2.614274	-3.177381	-2.806976	C	-3.432288	2.623824	2.727400
H	3.441818	-0.174556	-5.549527	H	-2.666042	4.053729	1.313295
H	2.483894	1.242032	-5.106539	C	-1.790983	1.197938	3.773392
H	4.094196	-1.321005	-2.028188	H	0.257763	1.538865	3.208379
H	4.401212	-1.686819	-3.729767	C	-3.123930	1.582372	3.604764
H	0.867040	-2.720096	-4.531816	H	-4.464873	2.928809	2.585211
H	2.480844	-2.515087	-5.219640	H	-1.539293	0.397492	4.463355
C	-1.625661	-0.536368	-0.691151	H	-3.913178	1.075994	4.151985
C	-1.184858	-1.696933	0.239373	C_Cs			
C	-2.329649	-1.135763	-1.930373	Pd	-0.609436	0.425604	0.178540
C	-2.627671	0.333155	0.112167	P	-1.735193	0.083859	-1.805220
H	-0.458524	-2.338700	-0.263535	C	-0.473021	-0.480915	-3.089891
H	-0.679343	-1.291720	1.118889	C	0.710584	0.521276	-3.025043
C	-2.402808	-2.538254	0.664338	C	-0.972116	-0.529957	-4.552343
H	-1.639221	-1.784829	-2.477586	C	0.048160	-1.876865	-2.684396
H	-2.646566	-0.348629	-2.618693	H	0.362966	1.521642	-3.310646
C	-3.555287	-1.963336	-1.489673	H	1.129979	0.592715	-2.016885
H	-2.129651	0.731283	0.997292	C	1.842501	0.082870	-3.971133
H	-2.966722	1.188502	-0.476692	H	-1.293013	0.467344	-4.867504
C	-3.849986	-0.500966	0.532531	H	-1.830708	-1.198574	-4.657068
H	-2.053193	-3.356382	1.307255	C	0.166791	-0.997519	-5.484905
C	-3.093568	-3.117271	-0.582534	H	0.360505	-1.836152	-1.637885
C	-3.394061	-1.654850	1.439450	H	-0.756055	-2.615271	-2.757369
H	-4.043230	-2.367805	-2.384728	C	1.201058	-2.309397	-3.607907
C	-4.541180	-1.064833	-0.721002	H	2.653918	0.815035	-3.894986
H	-4.538890	0.151536	1.081064	C	1.327732	0.009063	-5.417178
H	-3.953662	-3.731550	-0.287754	C	2.355924	-1.296394	-3.521835
H	-2.400650	-3.769817	-1.129322	H	-0.222270	-1.050913	-6.509255
H	-2.917438	-1.250638	2.340197	C	0.669953	-2.385725	-5.050576
H	-4.258869	-2.248415	1.762541	H	1.550423	-3.305592	-3.303180
H	-4.882083	-0.243883	-1.364899	H	2.133465	-0.299725	-6.095857
H	-5.429345	-1.642618	-0.435889	C	0.985536	0.998300	-5.748001
C	-0.824175	2.171696	-1.762045	H	2.743900	-1.221892	-2.497693
C	-1.936256	2.213665	-2.818588	H	3.180853	-1.622351	-4.170124
H	0.060173	2.704141	-2.128145	H	-0.144719	-3.119393	-5.112445
H	-1.144260	2.734712	-0.882066	H	1.464075	-2.723738	-5.728154
C	-2.183714	3.652251	-3.289181	C	-3.125272	-1.164656	-1.518231
H	-1.695246	1.590325	-3.683037	C	-2.648605	-2.321661	-0.601021
H	-2.867239	1.816004	-2.403282	C	-3.719510	-1.781683	-2.804710
C	-3.324291	3.751154	-4.304153	C	-4.227153	-0.393478	-0.744103
H	-2.405530	4.282064	-2.417539	H	-1.864643	-2.901836	-1.093793
H	-1.259507	4.050741	-3.727970	H	-2.200248	-1.916738	0.308157
H	-3.482242	4.784441	-4.628871	C	-2.956684	-2.376281	-3.317253
H	-3.111608	3.148910	-5.194627	H	-4.045152	-1.006405	-3.501441
H	-4.264732	3.387288	-3.875190	C	-4.909892	-2.696982	-2.450160
C	0.990294	2.812230	0.693744	H	-3.802930	0.012364	0.175991
C	-0.011473	3.545789	1.370040	H	-4.596742	0.453817	-1.325674
C	1.953806	3.516416	-0.043997	C	-5.406009	-1.320124	-0.407572
C	-0.025642	4.949236	1.266389	H	-3.451592	-4.064949	0.381661
C	1.931676	4.911066	-0.134564	C	-4.418155	-3.842903	-1.548757
H	2.725401	2.968269	-0.575908	C	-4.912230	-2.463958	0.491822
C	0.930851	5.632134	0.518265	H	-5.324361	-3.107858	-3.378953
H	-0.792737	5.506974	1.797067	C	-5.992610	-1.890423	-1.710192
H	2.689334	5.428272	-0.717539				
H	0.900904	6.715926	0.455522				

H	-6.165047	-0.732791	0.122011	H	-1.321806	0.589476	-4.897067
H	-5.248959	-4.519422	-1.310760	H	-1.882197	-1.075550	-4.736246
H	-3.658368	-4.434226	-2.076225	C	0.107487	-0.873684	-5.586600
H	-4.507279	-2.051415	1.424072	H	0.322084	-1.882711	-1.776312
H	-5.746095	-3.125725	0.759703	H	-0.815458	-2.579776	-2.916348
H	-6.355443	-1.073458	-2.347559	C	1.137958	-2.279296	-3.774138
H	-6.853314	-2.534554	-1.489713	H	2.651139	0.831218	-3.965957
C	-2.527127	1.612893	-2.501833	C	1.282931	0.113788	-5.491791
C	-3.565118	1.572433	-3.630611	C	2.314297	-1.291946	-3.678507
H	-1.679664	2.240834	-2.794891	H	-0.292641	-0.877936	-6.607453
H	-2.964932	2.120196	-1.639307	C	0.589335	-2.287286	-5.213047
C	-3.931077	2.992514	-4.080046	H	1.473548	-3.287085	-3.499623
H	-3.204801	1.005118	-4.492390	H	2.076365	-0.174639	-6.192291
H	-4.475739	1.069614	-3.290261	H	0.951206	1.121219	-5.773361
C	-5.010002	3.007924	-5.164753	H	2.734124	-1.271608	-2.666062
H	-4.271517	3.567173	-3.208348	H	3.117867	-1.605882	-4.356392
H	-3.027575	3.497938	-4.445841	H	-0.239245	-3.002104	-5.294885
H	-5.255181	4.029527	-5.472113	H	1.369195	-2.613263	-5.911992
H	-4.680337	2.460327	-6.054991	C	-3.091584	-1.143357	-1.523344
H	-5.932110	2.534948	-4.808259	C	-2.548649	-2.251394	-0.582840
C	-0.905531	2.409834	-0.008133	C	-3.692964	-1.812343	-2.781448
C	-2.008495	3.089339	0.560226	C	-4.205131	-0.390461	-0.748692
C	0.046029	3.162128	-0.717862	H	-1.748915	-2.813569	-1.070178
C	-2.132640	4.480808	0.384983	H	-2.109647	-1.798066	0.309222
C	-0.089559	4.543959	-0.889828	C	-3.678901	-3.220233	-0.186660
H	0.909917	2.653211	-1.134992	H	-2.922792	-2.380504	-3.312383
C	-1.189028	5.207715	-0.339339	H	-4.078060	-1.063299	-3.477284
H	-2.978392	4.995371	0.834184	C	-4.830901	-2.771254	-2.371863
H	0.660354	5.096358	-1.451480	H	-3.778994	0.059580	0.149318
H	-1.306865	6.280473	-0.464198	H	-4.619717	0.422596	-1.348718
C	0.642067	-1.003252	1.903820	C	-5.338507	-1.354524	-0.359694
O	0.489444	0.303317	2.033141	H	-3.258909	-3.995684	0.465620
O	0.043366	-1.520269	0.848764	C	-4.269590	-3.868736	-1.451010
O	1.308099	-1.695153	2.707088	C	-4.780241	-2.450832	0.560952
Cs	2.259098	-3.479451	-0.040061	H	-5.247122	-3.225282	-3.279227
C	-3.072719	2.362546	1.301150	C	-5.929893	-1.988945	-1.630491
C	-4.426416	2.626431	1.037007	H	-6.109190	-0.782432	0.169330
C	-2.759176	1.382473	2.260279	H	-5.065039	-4.573441	-1.178072
C	-5.438171	1.921254	1.690555	H	-3.495566	-4.441363	-1.977955
H	-4.684410	3.368240	0.286769	H	-4.372848	-1.996321	1.472025
C	-3.771064	0.677329	2.912742	H	-5.581484	-3.136217	0.865232
H	-1.719446	1.168771	2.485085	H	-6.342929	-1.209369	-2.283576
C	-5.114282	0.938579	2.627797	H	-6.755656	-2.662140	-1.368212
H	-6.478140	2.129603	1.456652	C	-2.566613	1.635926	-2.575781
H	-3.508981	-0.079524	3.646842	C	-3.642774	1.549942	-3.666490
H	-5.899121	0.381721	3.130685	H	-1.735777	2.260920	-2.920222
Cs	2.329178	2.827768	1.894034	H	-2.975989	2.163037	-1.711223
Cs	4.342625	-1.113821	3.019958	C	-4.016926	2.949582	-4.169602
O	3.702338	-0.866674	-0.116051	H	-3.313835	0.941249	-4.512024
C	3.738769	0.432279	-0.003851	H	-4.542200	1.067739	-3.271863
O	4.546625	0.980610	0.861246	C	-5.128256	2.919140	-5.220679
O	2.956399	1.181382	-0.720147	H	-4.328863	3.566472	-3.316426
C_Na							
Pd	-0.584761	0.522396	0.085204	H	-5.377742	3.926706	-5.567938
P	-1.744053	0.129604	-1.869959	H	-4.827692	2.328729	-6.093534
C	-0.495703	-0.438492	-3.166765	H	-6.041067	2.469047	-4.814524
C	0.711785	0.533442	-3.073576	C	-0.905215	2.490883	-0.101689
C	-1.011836	-0.423319	-4.623978	C	-1.981290	3.147141	0.537703
C	0.002035	-1.859967	-2.822580	C	0.025766	3.263136	-0.813439
H	0.386713	1.555606	-3.297683	C	-2.086647	4.546633	0.441854
H	1.105082	0.531210	-2.051440	C	-0.084912	4.655943	-0.891719
C	1.823869	0.116686	-4.052634	H	0.837509	2.774101	-1.343878
				C	-1.149685	5.301576	-0.262450

H	-2.913087	5.044578	0.941886	C	-2.894068	-3.072663	-0.610368
H	0.649847	5.226352	-1.453739	H	-2.238348	0.325842	1.255042
H	-1.250831	6.381256	-0.317336	H	-3.285438	0.237389	-0.161384
C	0.714335	-0.736290	1.948876	C	-3.501105	-1.432117	1.191699
O	0.529828	0.573030	1.930604	H	-0.828093	-3.398674	2.153951
O	0.232116	-1.374805	0.903504	C	-2.013798	-3.841507	0.391271
O	1.313728	-1.316746	2.883867	C	-2.626001	-2.200653	2.194354
Na	2.166661	-2.139292	-0.104644	H	-3.287364	-3.765149	-1.364791
C	-3.037896	2.398490	1.268056	C	-4.060435	-2.404463	0.139079
C	-4.391950	2.664314	1.009909	H	-4.327763	-0.941453	1.719849
C	-2.717795	1.408385	2.213430	H	-2.599980	-4.629549	0.881244
C	-5.399839	1.948078	1.657040	H	-1.185733	-4.333192	-0.136378
H	-4.652690	3.419048	0.273738	H	-2.237225	-1.513972	2.956817
C	-3.726354	0.693284	2.860547	H	-3.220876	-2.963044	2.713458
H	-1.676673	1.202870	2.437899	H	-4.701426	-1.864315	-0.569327
C	-5.070434	0.954976	2.581385	H	-4.684187	-3.166411	0.623548
H	-6.440905	2.157417	1.429719	C	-1.509643	1.536023	-2.019826
H	-3.460907	-0.070145	3.586208	C	-2.718242	1.035718	-2.820541
H	-5.852521	0.390321	3.079550	H	-0.799255	2.018835	-2.701814
Na	2.274832	1.743991	0.984367	H	-1.838816	2.332702	-1.353619
Na	3.530177	-1.139011	3.292551	C	-3.350077	2.170074	-3.636709
O	4.058123	-1.623529	1.084303	H	-2.439765	0.221952	-3.495608
C	3.794717	-0.370861	0.853685	H	-3.477148	0.628328	-2.144570
O	4.054909	0.523470	1.761796	C	-4.579640	1.716822	-4.426811
O	3.178548	-0.029097	-0.239393	H	-3.625320	2.989723	-2.959818
				H	-2.598190	2.580457	-4.324097
C1_Cs							
Pd	0.682816	1.848337	0.793035	H	-5.012685	2.540823	-5.003030
P	-0.419051	0.425095	-0.977967	H	-4.321842	0.916091	-5.129275
C	0.793475	-0.242230	-2.297919	H	-5.357294	1.331827	-3.757378
C	1.866615	0.866543	-2.468433	C	1.703844	3.217993	1.904695
C	0.149294	-0.507410	-3.680902	C	1.002741	4.405830	2.230889
C	1.510783	-1.533961	-1.840747	C	3.049194	3.126676	2.274864
H	1.395707	1.801059	-2.800993	C	1.654155	5.459432	2.887256
H	2.326657	1.040724	-1.494204	H	3.702994	4.177479	2.939636
C	2.931075	0.438850	-3.495871	H	7.165741	3.387060	3.051903
H	-0.337673	0.396984	-4.055026	C	3.002145	5.347108	3.240295
H	-0.618283	-1.283690	-3.608059	H	1.116225	6.372761	3.130154
C	1.219272	-0.938153	-4.706849	H	4.741711	4.064991	3.233921
H	2.004944	-1.376241	-0.881229	H	3.499238	6.167875	3.751136
H	0.788261	-2.348132	-1.734137	C	2.696232	-0.450515	1.236704
C	2.573103	-1.963438	-2.871628	O	2.020074	-0.746963	2.286834
H	3.673215	1.242518	-3.593811	O	2.468532	0.674242	0.577652
C	2.266124	0.179522	-4.857915	O	3.624367	-1.212726	0.772029
C	3.620190	-0.848028	-3.006005	Cs	2.442323	-3.815628	1.772935
H	0.726676	-1.114619	-5.671355	C	-0.417242	4.381888	1.850698
C	1.908420	-2.227257	-4.230586	C	-1.327355	5.399351	2.165021
H	3.057730	-2.879493	-2.508948	C	-0.832219	3.194770	1.173484
H	3.019230	-0.108960	-5.602927	C	-2.681422	5.268325	1.850433
H	1.785063	1.096994	-5.221065	H	-0.984448	6.296644	2.674455
H	4.075003	-0.690700	-2.023687	C	-2.204530	3.089152	0.905247
H	4.413298	-1.145839	-3.704536	C	-3.120918	4.100548	1.231280
H	1.172129	-3.036901	-4.140604	H	-3.381114	6.061426	2.100029
H	2.656824	-2.549498	-4.966478	H	-2.600173	2.199497	0.437258
C	-1.478351	-0.992707	-0.289440	Cs	3.207074	0.577239	4.784417
C	-0.618605	-1.779706	0.732346	Cs	5.477878	1.194543	-0.060120
C	-2.052893	-1.990946	-1.320935	O	6.938133	2.578932	2.570404
C	-2.646762	-0.354207	0.501484	C	6.236609	1.783078	3.504662
H	0.210084	-2.258913	0.210064	O	5.855317	0.684035	3.042735
H	-0.162740	-1.102439	1.459258	O	6.068237	2.287540	4.637035
C	-1.461491	-2.858471	1.437509	H	3.588886	2.214358	2.048399
H	-1.240992	-2.473636	-1.871753				
H	-2.675082	-1.474785	-2.055036				

C1_Cs'

Pd	0.223527	1.316068	0.966483	H	-2.296718	2.405280	-6.516155
P	-0.403364	0.762145	-1.405596	H	-3.650283	3.039687	-5.571526
C	0.927191	-0.197147	-2.355300	C	-0.257879	3.279445	1.074906
C	2.254758	0.544590	-2.036111	C	-0.602063	3.756078	2.371883
C	0.754705	-0.230238	-3.890852	C	-0.184948	4.212055	0.036712
C	1.046766	-1.650253	-1.838352	C	-0.967998	5.093589	2.562470
H	2.197859	1.580779	-2.393862	C	-0.530484	5.557655	0.236920
H	2.400472	0.589145	-0.953611	H	0.155872	3.909802	-0.945208
C	3.448126	-0.168650	-2.697564	C	-0.949180	5.993083	1.493248
H	0.702274	0.788407	-4.286713	H	-1.243036	5.445815	3.553518
H	-0.177891	-0.736004	-4.161677	H	-0.471326	6.257620	-0.592786
C	1.947162	-0.954811	-4.550110	H	-1.232044	7.030273	1.649679
H	1.163892	-1.632285	-0.754144	C	2.460899	-0.779238	1.443243
H	0.134960	-2.208173	-2.073644	O	3.099727	0.419594	1.650042
C	2.244729	-2.360777	-2.495291	O	1.196056	-0.739000	1.222392
H	4.366589	0.379551	-2.454787	O	3.158557	-1.804187	1.482335
C	3.247558	-0.200331	-4.222621	Cs	0.722863	-3.802867	1.665733
C	3.542204	-1.606705	-2.156809	C	-0.440787	2.761260	3.441085
H	1.791152	-0.969146	-5.635804	C	-0.747825	2.946209	4.794507
C	2.040845	-2.395709	-4.019316	C	0.110697	1.534041	2.993261
H	2.301927	-3.385565	-2.105608	C	-0.507222	1.922397	5.715406
H	4.100397	-0.693078	-4.706174	H	-1.177138	3.884436	5.137586
H	3.197337	0.822537	-4.617475	C	0.337887	0.519333	3.926534
H	3.692640	-1.596995	-1.071261	H	2.405808	1.110878	1.656571
H	4.402682	-2.120074	-2.605215	C	0.036286	0.711332	5.283317
H	1.123882	-2.947706	-4.263888	H	-0.745681	2.071208	6.764996
H	2.874454	-2.920576	-4.502888	H	0.742998	-0.431807	3.595523
C	-1.997608	-0.229632	-1.178271	H	0.224739	-0.085591	5.999070
C	-1.817573	-1.230453	-0.007596				
C	-2.493617	-1.010379	-2.416598	C1_Cs_cf1			
C	-3.083965	0.793088	-0.743504	Pd	0.001452	1.463929	1.210412
H	-1.052473	-1.962732	-0.269310	P	-0.410215	0.778930	-1.189396
H	-1.461240	-0.697756	0.880423	C	1.006448	0.214119	-2.309373
C	-3.139899	-1.952797	0.305240	C	2.135192	1.264188	-2.127287
H	-1.748308	-1.754506	-2.713920	C	0.699656	0.099525	-3.819979
H	-2.632105	-0.340750	-3.266976	C	1.529892	-1.141425	-1.791235
C	-3.824858	-1.722102	-2.098392	H	1.794755	2.238073	-2.502635
H	-2.734775	1.335908	0.142931	H	2.414250	1.371213	-1.072728
H	-3.254643	1.535377	-1.527664	C	3.395780	0.842350	-2.904765
C	-4.410029	0.073963	-0.437538	H	0.374619	1.070516	-4.206488
H	-2.973471	-2.657994	1.129742	H	-0.108381	-0.613058	-4.007421
C	-3.614490	-2.716346	-0.943210	C	1.965693	-0.343157	-4.586294
C	-4.202426	-0.919781	0.716458	H	1.732151	-1.036829	-0.721852
H	-4.159750	-2.260340	-2.993384	H	0.767013	-1.916082	-1.915517
C	-4.883605	-0.680318	-1.693216	C	2.799088	-1.561557	-2.554367
H	-5.158685	0.822595	-0.151771	H	4.166781	1.607849	-2.754350
H	-4.549975	-3.247950	-0.728232	C	3.073857	0.707825	-4.401587
H	-2.869590	-3.470825	-1.228298	C	3.894195	-0.502364	-2.346760
H	-3.877828	-0.385699	1.618400	H	1.715726	-0.438103	-5.650447
H	-5.146897	-1.423506	0.957750	C	2.455749	-1.698542	-4.047653
H	-5.050783	0.026715	-2.515808	H	3.146019	-2.534434	-2.179878
H	-5.841800	-1.176692	-1.494580	H	3.970276	0.409918	-4.961397
C	-0.852339	2.175665	-2.533566	H	2.744913	1.673908	-4.806512
C	-1.718965	2.023935	-3.793901	H	4.115278	-0.397800	-1.277772
H	0.114427	2.613939	-2.812116	H	4.813437	-0.810292	-2.863506
H	-1.324953	2.913048	-1.881458	H	1.679671	-2.462872	-4.186935
C	-1.707163	3.312423	-4.625689	H	3.340003	-2.026461	-4.608679
H	-1.385826	1.193846	-4.420332	C	-1.789796	-0.519494	-1.046527
H	-2.752043	1.800173	-3.510357	C	-1.389054	-1.623689	-0.033733
C	-2.609015	3.224547	-5.858673	C	-2.199128	-1.212035	-2.365657
H	-2.021755	4.153796	-3.994239	C	-3.010921	0.228824	-0.442388
H	-0.676053	3.529842	-4.934482	H	-0.531380	-2.186560	-0.409474
H	-2.582013	4.150536	-6.441791	H	-1.072423	-1.177443	0.909360

C	-2.558275	-2.597577	0.205618	O	3.671182	1.647845	0.589765	
H	-1.351314	-1.783296	-2.757223					
H	-2.474345	-0.482427	-3.128719	C1_Cs_ClдиPh				
C	-3.382306	-2.171426	-2.122783	Pd	-1.556696	0.456192	1.758252	
H	-2.712589	0.688538	0.507965	C	-0.832154	2.263686	1.148967	
H	-3.339527	1.038470	-1.098548	C	-1.724826	3.359239	1.237968	
C	-4.183773	-0.740707	-0.215084	C	0.468452	2.503829	0.697958	
H	-2.232311	-3.364694	0.919525	C	-1.297782	4.653745	0.909130	
C	-2.962166	-3.261355	-1.121923	C	0.896887	3.797325	0.361157	
C	-3.759863	-1.830485	0.782379	H	1.152100	1.667276	0.603752	
H	-3.662864	-2.632663	-3.077774	C	0.012109	4.874039	0.477882	
C	-4.579015	-1.386728	-1.555619	H	-1.988034	5.491568	0.969530	
H	-5.033903	-0.177244	0.188637	H	1.920244	3.951267	0.025582	
H	-3.789035	-3.964520	-0.959345	H	0.336629	5.879509	0.221024	
H	-2.119561	-3.836787	-1.527016	C	1.381155	-0.213399	2.613987	
H	-3.488285	-1.374002	1.742731	O	0.490190	-0.407878	1.657550	
H	-4.593983	-2.518295	0.971871	O	1.144683	0.570650	3.598089	
H	-4.893394	-0.612427	-2.267409	O	2.502113	-0.854220	2.512852	
H	-5.434233	-2.059205	-1.411873	C	-3.097400	2.978116	1.594402	
C	-1.166249	2.214424	-2.120427	C	-4.164022	3.881663	1.680511	
C	-2.106730	2.046560	-3.322021	C	-3.301332	1.572940	1.752224	
H	-0.305491	2.808668	-2.440061	C	-5.472791	3.426751	1.853905	
H	-1.658728	2.822904	-1.357212	H	-3.979945	4.948077	1.578605	
C	-2.413472	3.401384	-3.972418	C	-4.630213	1.156106	1.904561	
H	-1.674386	1.380299	-4.073020	C	-5.706233	2.056039	1.944292	
H	-3.050615	1.587945	-3.011816	H	-6.296306	4.133954	1.903432	
C	-3.383415	3.284197	-5.150159	H	-4.865016	0.106592	2.014134	
H	-2.829493	4.078437	-3.214516	H	-6.719573	1.678507	2.059920	
H	-1.474095	3.859670	-4.309488	Cl	-0.282253	0.543822	-2.430617	
H	-3.586652	4.260614	-5.601535	C	-1.878240	-0.193526	-2.254096	
H	-2.975858	2.632373	-5.931176	C	-1.917615	-1.577663	-2.087293	
H	-4.340891	2.857686	-4.830038	C	-3.043560	0.592761	-2.240042	
C	-0.010168	3.466620	0.942449	C	-3.139584	-2.216284	-1.887187	
C	-0.476974	4.248349	2.037964	H	-0.995687	-2.146513	-2.104143	
C	0.576860	4.133679	-0.138519	C	-4.256528	-0.084787	-2.014279	
C	-0.398870	5.646991	1.995654	C	-4.313304	-1.463718	-1.838127	
C	0.667317	5.533726	-0.168442	H	-3.167197	-3.293670	-1.760595	
H	0.996778	3.567163	-0.960543	H	-5.170584	0.499315	-1.997754	
C	0.166074	6.292557	0.891902	H	-5.268596	-1.949369	-1.669350	
H	-0.756189	6.236081	2.836757	C	-3.071306	2.063248	-2.441742	
H	1.129745	6.024993	-1.021004	C	-3.826482	2.863561	-1.572201	
H	0.227894	7.376974	0.868363	C	-2.403439	2.674472	-3.515400	
C	1.472697	-0.670364	3.059478	C	-3.889552	4.244238	-1.754765	
O	1.841532	0.511767	3.662511	H	-4.329916	2.408505	-0.728061	
O	0.701212	-0.603380	2.043499	C	-2.473466	4.054040	-3.700027	
O	1.933816	-1.707361	3.572145	H	-1.839853	2.066618	-4.214161	
Cs	2.959252	-3.053206	1.004214	C	-3.212420	4.845146	-2.816241	
C	-0.949670	3.455873	3.180026	H	-4.456857	4.845145	-1.051886	
C	-1.608393	3.950020	4.312945	H	-1.953703	4.510845	-4.536945	
C	-0.698459	2.066627	3.043443	H	-3.258562	5.921075	-2.955740	
C	-2.041712	3.072562	5.310506	Cs	2.490492	-1.254391	-0.605671	
H	-1.802472	5.015222	4.414041	Cs	2.349012	-1.425204	5.617412	
C	-1.161948	1.202146	4.041537	P	-2.446361	-1.783335	2.607309	
H	1.325771	1.220364	3.226106	C	-1.305877	-3.300708	2.357302	
C	-1.826897	1.699344	5.171201	C	-0.718399	-3.153331	0.929470	
H	-2.555971	3.458858	6.186139	C	-2.020605	-4.672171	2.435448	
H	-1.000434	0.132303	3.945426	C	-0.124446	-3.292600	3.353037	
H	-2.174694	1.014109	5.940468	H	-1.524165	-3.173198	0.189627	
Cs	3.765485	4.073675	2.401740	H	-0.219222	-2.184552	0.869209	
Cs	4.801286	-0.493791	4.392031	C	0.271568	-4.294099	0.627655	
O	4.316170	-0.410160	1.270063	H	-2.829758	-4.717537	1.701323	
C	4.435273	0.884633	1.316675	H	-2.467256	-4.829703	3.420560	
O	5.312885	1.429057	2.110411	C	-1.029577	-5.816710	2.136340	

H	0.401572	-2.341982	3.258604	C	0.909418	-0.023232	-2.215299
H	-0.488681	-3.396433	4.378059	C	2.180896	0.774599	-1.820749
C	0.852334	-4.446962	3.057744	C	0.787000	-0.009930	-3.756367
H	0.665862	-4.163189	-0.389669	C	1.098293	-1.484819	-1.742065
C	-0.454814	-5.646308	0.719285	H	2.080064	1.824304	-2.128419
C	1.426286	-4.259072	1.645830	H	2.291127	0.761992	-0.733278
H	-1.566465	-6.771025	2.204585	C	3.433064	0.160859	-2.472071
C	0.115466	-5.791096	3.161843	H	0.682461	1.016758	-4.119832
H	1.669888	-4.419414	3.790577	H	-0.103509	-0.563383	-4.072002
H	0.236697	-6.468082	0.491995	C	2.039997	-0.635355	-4.402875
H	-1.264332	-5.687541	-0.020974	H	1.192643	-1.503956	-0.654481
H	1.945124	-3.295193	1.620295	H	0.227181	-2.085126	-2.019108
H	2.156012	-5.047608	1.419414	C	2.350496	-2.102318	-2.395257
H	-0.283982	-5.924764	4.175814	H	4.307045	0.752696	-2.174814
H	0.810079	-6.619758	2.973947	C	3.282776	0.179451	-4.002679
C	-2.879833	-1.615210	4.453153	C	3.591340	-1.291324	-1.985590
C	-1.689191	-0.891277	5.137717	H	1.918915	-0.613501	-5.492882
C	-3.170999	-2.932950	5.205816	C	2.198602	-2.088325	-3.924918
C	-4.104484	-0.677368	4.598530	H	2.453843	-3.135787	-2.042036
H	-0.783164	-1.490869	5.051006	H	4.178154	-0.243455	-4.475533
H	-1.482841	0.045951	4.613324	H	3.185422	1.213028	-4.359342
C	-1.987663	-0.624858	6.623263	H	3.683047	-1.320728	-0.894548
H	-2.315456	-3.608788	5.140977	H	4.497473	-1.737174	-2.416337
H	-4.022752	-3.448101	4.753619	H	1.323188	-2.679961	-4.222425
C	-3.470901	-2.650675	6.692043	H	3.076168	-2.546869	-4.398181
H	-3.896597	0.269702	4.097066	C	-2.033571	-0.280258	-1.116828
H	-4.984919	-1.109745	4.115650	C	-1.795860	-1.279765	0.047066
C	-4.422099	-0.412091	6.082512	C	-2.447769	-1.074427	-2.377696
H	-1.118718	-0.129748	7.076120	C	-3.204933	0.648342	-0.691270
C	-2.257839	-1.959229	7.340335	H	-0.961886	-1.945312	-0.180723
C	-3.221094	0.284516	6.743486	H	-1.518199	-0.725773	0.950456
H	-3.666588	-3.604003	7.198572	C	-3.063483	-2.109536	0.318963
C	-4.706295	-1.741359	6.801966	H	-1.644053	-1.751916	-2.680259
H	-5.304093	0.237639	6.139365	H	-2.630152	-0.401284	-3.217159
H	-2.449069	-1.784088	8.406752	C	-3.723313	-1.894386	-2.093365
H	-1.375112	-2.609344	7.271479	H	-2.916417	1.204709	0.208591
H	-3.026707	1.245696	6.251143	H	-3.418010	1.385177	-1.470678
H	-3.437243	0.495481	7.798698	C	-4.476384	-0.176687	-0.418986
H	-5.576066	-2.235765	6.350562	H	-2.853999	-2.812313	1.134730
H	-4.949145	-1.557286	7.856308	C	-3.453030	-2.887772	-0.950042
C	-3.954946	-2.337900	1.650978	C	-4.212049	-1.171137	0.723855
C	-5.072018	-3.197925	2.251089	H	-3.998489	-2.442142	-3.002881
H	-3.524809	-2.862298	0.792263	C	-4.868050	-0.946484	-1.693294
H	-4.386414	-1.436293	1.215937	H	-5.285390	0.507871	-0.136458
C	-6.080913	-3.621842	1.176395	H	-4.346017	-3.496690	-0.760529
H	-4.664375	-4.091604	2.731815	H	-2.645420	-3.574981	-1.232699
H	-5.603544	-2.645193	3.032117	H	-3.947916	-0.628592	1.640667
C	-7.232757	-4.456342	1.740194	H	-5.119026	-1.750480	0.937856
H	-6.479232	-2.724689	0.683857	H	-5.076505	-0.242568	-2.509187
H	-5.557145	-4.191033	0.396495	H	-5.786849	-1.520134	-1.518271
H	-7.937179	-4.750096	0.955396	C	-1.036066	2.218145	-2.433468
H	-6.859754	-5.370855	2.215066	C	-1.861933	2.010266	-3.712808
H	-7.791199	-3.894682	2.497664	H	-0.096502	2.723058	-2.691312
H	2.630736	2.575933	-1.817026	H	-1.576085	2.916894	-1.790786
Cs	3.877837	2.100381	2.782302	C	-1.924525	3.299055	-4.541757
O	3.076784	1.735777	-1.637611	H	-1.455459	1.208250	-4.331833
C	4.026712	2.020624	-0.632794	H	-2.882106	1.712269	-3.451767
O	4.635607	1.013496	-0.208606	C	-2.789812	3.149830	-5.794919
O	4.107588	3.219293	-0.275549	H	-2.313587	4.113319	-3.916217
C1_Na							
Pd	-0.066433	1.420061	1.067993	H	-0.905287	3.591812	-4.827379
P	-0.515162	0.830832	-1.302442	H	-2.817325	4.077406	-6.375424
				H	-2.403796	2.357933	-6.446661
				H	-3.820943	2.888574	-5.531707

C	-0.527701	3.393831	1.130123	C	-2.099379	-1.460176	-1.460915
C	-0.853824	3.908824	2.419473	C	-2.243836	-0.170355	0.697246
C	-0.384204	4.309885	0.080357	H	0.179782	-2.415304	-0.293248
C	-1.098204	5.275845	2.596247	H	0.152373	-1.498915	1.186378
C	-0.608979	5.683989	0.269946	C	-1.455380	-2.975170	0.990470
H	-0.079993	3.972358	-0.901879	H	-1.434978	-1.943574	-2.183730
C	-0.984827	6.164363	1.523222	H	-2.670464	-0.705047	-2.004058
H	-1.356197	5.657256	3.580650	C	-3.065055	-2.513998	-0.880234
H	-0.493996	6.367276	-0.567329	H	-1.656112	0.275777	1.507313
H	-1.173664	7.223433	1.671884	H	-2.812024	0.636295	0.229454
C	2.288862	-0.388675	1.842099	C	-3.216131	-1.217076	1.266400
O	2.454754	0.600547	2.800803	H	-0.871155	-3.750078	1.504696
O	1.123420	-0.526644	1.360062	C	-2.262956	-3.610100	-0.156145
O	3.313604	-1.039980	1.559379	C	-2.415995	-2.311777	1.990715
Na	5.173270	0.103802	0.854605	H	-3.638272	-2.958527	-1.703202
C	-0.852091	2.907846	3.493817	C	-4.026302	-1.840074	0.115137
C	-1.273246	3.113261	4.812469	H	-3.894854	-0.722595	1.972370
C	-0.390077	1.633389	3.080436	H	-2.942394	-4.378005	0.235542
C	-1.255229	2.056043	5.727690	H	-1.584435	-4.106609	-0.862738
H	-1.631895	4.088846	5.130331	H	-1.848692	-1.873295	2.821703
C	-0.410131	0.579370	4.001221	H	-3.095184	-3.060367	2.418781
H	1.592078	1.061831	2.890796	H	-4.611455	-1.063932	-0.394614
C	-0.831967	0.788741	5.323203	H	-4.738523	-2.576287	0.509008
H	-1.583802	2.220817	6.749842	C	-1.086328	1.990978	-1.468757
H	-0.082088	-0.409733	3.692783	C	-2.378660	1.858938	-2.283321
H	-0.831214	-0.036917	6.030100	H	-0.357431	2.590162	-2.029893
Na	2.438209	3.199089	0.769735	H	-1.305785	2.574522	-0.575310
Na	3.992815	1.785925	4.143629	C	-2.828817	3.227951	-2.808282
O	5.530507	1.710855	2.442103	H	-2.265097	1.168613	-3.123361
C	4.703224	2.473857	1.793462	H	-3.172646	1.451342	-1.648334
O	3.989980	3.351258	2.436478	C	-4.222810	3.193662	-3.436428
O	4.521113	2.297093	0.516824	H	-2.821245	3.946397	-1.981029
C2_Cs							
Pd	1.231365	1.486970	0.948097	H	-4.510733	4.174758	-3.828352
P	-0.073070	0.549521	-0.844292	H	-4.270860	2.475546	-4.263320
C	0.928850	0.021773	-2.372693	H	-4.973467	2.898154	-2.694681
C	2.161286	0.964403	-2.390070	C	0.306108	3.104285	1.729544
C	0.179220	0.169398	-3.717498	C	-0.584371	4.162249	1.943835
C	1.450980	-1.428589	-2.253752	C	1.529227	3.036432	2.306138
H	1.835032	2.009580	-2.467674	C	-0.111215	5.179503	2.810866
H	2.684920	0.848385	-1.437591	C	2.003738	4.013971	3.180429
C	3.088821	0.623078	-3.571011	H	3.634298	2.926685	1.606982
H	-0.173275	1.197553	-3.841749	C	1.145214	5.107066	3.415331
H	-0.701214	-0.480776	-3.743442	H	-0.759852	6.025456	3.026496
C	1.112469	-0.178743	-4.896319	H	2.988715	3.958226	3.638744
H	2.015946	-1.543178	-1.326168	C	1.460689	5.908758	4.079955
H	0.612995	-2.131417	-2.247588	C	3.127911	-1.046008	0.842454
C	2.374411	-1.774715	-3.437685	O	2.443503	-1.651389	1.744932
H	3.944625	1.311996	-3.565551	O	3.018944	0.262534	0.685355
C	2.320485	0.774364	-4.895608	O	3.959279	-1.666170	0.074288
C	3.583455	-0.827503	-3.421560	Cs	2.510435	-4.356235	0.250941
H	0.553119	-0.063703	-5.833086	C	-1.941171	4.263826	1.355847
C	1.603571	-1.629414	-4.758831	C	-2.397265	5.455334	0.768447
H	2.719891	-2.810734	-3.322438	C	-2.813265	3.165229	1.390558
H	2.977850	0.547368	-5.744840	C	-3.678315	5.537672	0.220548
H	1.980455	1.810989	-5.015279	H	-1.733198	6.313756	0.726678
H	4.104550	-0.962857	-2.468206	C	-4.091443	3.242024	0.838960
H	4.278828	-1.078374	-4.233293	H	-2.473486	2.251009	1.860268
H	0.750178	-2.320080	-4.777122	C	-4.530025	4.430344	0.249488
H	2.250443	-1.890124	-5.606478	H	-4.008902	6.465019	-0.238354
C	-1.275441	-0.811151	-0.325979	H	-4.746641	2.376187	0.875053
C	-0.491203	-1.923982	0.411377	Cs	-5.523818	4.493245	-0.183120
				Cs	2.980534	0.256444	4.093949

Cs	5.765501	0.834065	-0.585806	C	-0.552125	1.705639	-4.097072				
O	4.537968	3.079710	1.270811	H	-1.180640	-0.188392	-3.289481				
C	5.444969	2.720077	2.282524	H	-1.898475	1.197921	-2.496108				
O	6.632851	2.655594	1.898668	C	-1.664119	1.858341	-5.136435				
O	4.956124	2.495669	3.420254	H	-0.260667	2.693893	-3.719094				
C2_Cs'											
Pd	1.426302	0.387236	1.418268	H	-1.962969	0.883977	-5.539361				
P	0.099873	-0.400541	-0.406923	H	-2.553445	2.319922	-4.692595				
C	0.753807	-2.009586	-1.159342	C	1.075504	2.308482	1.864713				
C	2.287589	-1.805160	-1.311398	C	0.418253	3.535231	1.939652				
C	0.189396	-2.401787	-2.543209	C	1.989534	1.874219	2.758415				
C	0.519100	-3.171100	-0.167833	C	0.788216	4.329956	3.051871				
H	2.488186	-0.987928	-2.014459	C	2.380163	2.649987	3.845669				
H	2.709613	-1.525219	-0.343881	H	3.543740	0.258097	2.532593				
C	2.960183	-3.093308	-1.819495	C	1.748993	3.904605	3.973423				
H	0.393719	-1.608745	-3.268926	H	0.315077	5.300555	3.180896				
H	-0.895591	-2.533167	-2.500139	H	3.114837	2.329275	4.581448				
C	0.854035	-3.706101	-3.037075	H	2.005296	4.554002	4.807286				
H	0.921683	-2.873991	0.801971	C	3.534417	-1.648548	2.438586				
H	-0.552697	-3.361287	-0.057506	O	4.190460	-0.469267	2.673421				
C	1.202134	-4.456773	-0.665611	O	2.330812	-1.572723	1.990985				
H	4.037538	-2.912824	-1.919059	O	4.140398	-2.703086	2.685804				
C	2.369059	-3.484421	-3.184742	Cs	1.452132	-4.174659	3.539225				
C	2.716335	-4.220383	-0.800724	C	-0.623108	3.979888	0.983676				
H	0.422008	-3.973238	-4.009281	C	-1.900169	4.347693	1.433951				
C	0.603543	-4.842389	-2.029581	C	-0.365354	4.010699	-0.394278				
H	1.015767	-5.264423	0.054947	C	-2.901780	4.700717	0.528732				
H	2.848547	-4.398230	-3.558280	H	-2.111976	4.324167	2.498883				
H	2.563396	-2.692570	-3.919328	C	-1.363295	4.367396	-1.301323				
H	3.144254	-3.940024	0.169549	H	0.630508	3.760467	-0.745760				
H	3.213134	-5.142434	-1.129188	C	-2.639503	4.703784	-0.843307				
H	-0.474016	-5.024816	-1.926209	H	-3.889602	4.965801	0.894319				
H	1.056860	-5.772626	-2.394722	H	-1.144946	4.386873	-2.364800				
C	-1.683129	-0.549808	0.193928	H	-3.419758	4.973347	-1.548563				
C	-1.685596	-1.249384	1.581026	C2_Na							
C	-2.655449	-1.301882	-0.741635	Pd	1.175437	1.524112	0.923162				
C	-2.195152	0.897271	0.423244	P	-0.115450	0.636296	-0.876247				
H	-1.317249	-2.274389	1.497945	C	0.917487	0.132411	-2.388465				
H	-1.000777	-0.714302	2.249817	C	2.070364	1.169560	-2.460885				
C	-3.105484	-1.268781	2.176671	C	0.151274	0.169779	-3.732000				
H	-2.322634	-2.336009	-0.877464	C	1.549423	-1.267862	-2.213000				
H	-2.677802	-0.837549	-1.730538	H	1.662127	2.179720	-2.590919				
C	-4.075991	-1.303535	-0.140629	H	2.609095	1.160588	-1.510496				
H	-1.517954	1.412531	1.108466	C	3.020224	0.849243	-3.629978				
H	-2.193953	1.469775	-0.506628	H	-0.278541	1.162690	-3.892857				
C	-3.618071	0.884792	1.007074	H	-0.675991	-0.546579	-3.723226				
H	-3.073940	-1.783757	3.145244	C	1.101944	-0.154450	-4.903585				
C	-4.053074	-2.017914	1.222345	H	2.115264	-1.310479	-1.280005				
C	-3.604923	0.172187	2.369419	H	0.766763	-2.030996	-2.174042				
H	-4.747768	-1.835619	-0.825404	C	2.489911	-1.590733	-3.390103				
C	-4.562656	0.145026	0.043659	H	3.821956	1.598058	-3.651789				
H	-3.948248	1.922474	1.130662	C	2.233638	0.887860	-4.952008				
H	-5.064327	-2.053652	1.646941	C	3.622975	-0.553780	-3.438475				
H	-3.717486	-3.055649	1.095919	H	0.529929	-0.121644	-5.838984				
H	-2.947510	0.708603	3.065590	C	1.701047	-1.557836	-4.709225				
H	-4.611225	0.168571	2.807536	H	2.913677	-2.591297	-3.234139				
H	-4.587684	0.658875	-0.925878	H	2.901623	0.677965	-5.796840				
H	-5.586329	0.149195	0.439290	H	1.814388	1.889459	-5.110818				
C	0.123029	0.795508	-1.832502	H	4.197975	-0.609110	-2.507220				
C	-0.962826	0.816074	-2.917694	H	4.312710	-0.782228	-4.260964				
H	1.104283	0.638212	-2.295954	H	0.901375	-2.309657	-4.689316				
H	0.173711	1.779942	-1.368203								

H	2.359510	-1.806844	-5.551088	H	-4.705929	2.548557	0.759934
C	-1.245697	-0.761974	-0.311377	H	-5.416172	4.693886	-0.286928
C	-0.397552	-1.790845	0.478152	Na	2.660265	0.372788	3.223270
C	-2.018708	-1.502454	-1.425046	Na	4.983249	0.463080	-0.195683
C	-2.256652	-0.141509	0.684902	O	4.524844	2.603825	1.278497
H	0.328455	-2.259343	-0.187532	C	5.100355	1.711730	2.182525
H	0.182759	-1.285770	1.255424	O	6.100794	1.103826	1.730935
C	-1.296636	-2.881143	1.088045	O	4.552729	1.603766	3.311750
H	-1.319114	-1.968191	-2.125553				
H	-2.632047	-0.803229	-1.997865				
C	-2.918623	-2.593652	-0.808607	Cl_diPh			
H	-1.701040	0.363535	1.483008	C	-0.406148	-0.140898	0.009149
H	-2.869385	0.615420	0.189976	C	0.897039	-0.112972	-0.518269
C	-3.166440	-1.226924	1.286168	C	1.644764	1.060346	-0.572195
H	-0.664834	-3.596290	1.631496	C	1.100390	2.252099	-0.092309
C	-2.051612	-3.606904	-0.039815	C	-0.184896	2.258502	0.447006
C	-2.305959	-2.242239	2.056570	C	-0.918719	1.073553	0.494470
H	-3.456960	-3.105050	-1.615939	H	1.311302	-1.038355	-0.905341
C	-3.926835	-1.943525	0.155710	H	2.645164	1.044528	-0.992214
H	-3.880470	-0.750288	1.968936	H	1.670102	3.174841	-0.130472
H	-2.682127	-4.403214	0.375811	H	-0.617363	3.171864	0.839156
H	-1.336602	-4.083411	-0.724032	Cl	-2.513375	1.143237	1.250894
H	-1.774743	-1.739130	2.874661	C	-1.148038	-1.427835	0.030779
H	-2.942443	-3.014564	2.506833	C	-2.415360	-1.553396	-0.558386
H	-4.555977	-1.226378	-0.386950	C	-0.553091	-2.562372	0.602687
H	-4.593498	-2.707129	0.575706	C	-3.072993	-2.782414	-0.567873
C	-1.180802	2.024840	-1.522289	H	-2.878143	-0.688474	-1.020972
C	-2.471716	1.807793	-2.320853	C	-1.213359	-3.791305	0.596305
H	-0.482072	2.633425	-2.110287	H	0.425384	-2.473339	1.064702
H	-1.416086	2.625951	-0.644214	C	-2.475878	-3.904697	0.011693
C	-2.979641	3.130238	-2.908151	H	-4.050474	-2.864949	-1.033297
H	-2.333880	1.083675	-3.128138	H	-0.742204	-4.657910	1.050042
H	-3.245620	1.397097	-1.663582	H	-2.990614	-4.860577	0.005508
C	-4.372246	3.004939	-3.528369				
H	-3.000870	3.887559	-2.116353	Cs₂CO₃			
H	-2.263781	3.485359	-3.661824	C	-0.001553	1.272571	-0.044509
H	-4.703272	3.951964	-3.966890	O	-0.021389	-0.031122	-0.206887
H	-4.389636	2.245492	-4.318572	O	1.132452	1.902740	-0.034560
H	-5.108415	2.712645	-2.770786	O	-1.117106	1.918914	0.101409
C	0.327008	3.157011	1.726496	Cs	-3.010620	-0.281527	-0.592747
C	-0.536415	4.232680	1.942710	Cs	2.948137	-0.386990	-0.649778
C	1.527265	3.017750	2.332872				
C	-0.044756	5.208815	2.846273	Cs₂CO₃_PdP2			
C	2.012842	3.950866	3.246163	Pd	1.104420	1.975089	0.426665
H	3.606421	2.764291	1.576276	P	-0.361552	0.409670	-0.492877
C	1.191948	5.073387	3.481262	C	-1.883387	1.301826	-1.173476
H	-0.666440	6.072819	3.068486	C	-2.735328	1.697108	0.063298
H	2.973252	3.843270	3.744245	C	-2.762959	0.523816	-2.177383
H	1.518427	5.844784	4.174803	C	-1.422501	2.624799	-1.840103
C	3.176106	-1.061480	1.029946	H	-3.087200	0.807382	0.591853
O	2.612432	-1.608166	2.046857	H	-2.107254	2.262087	0.764261
O	2.941577	0.209301	0.754618	C	-3.950642	2.541280	-0.360392
O	4.021454	-1.670390	0.272006	H	-3.108730	-0.418613	-1.744830
Na	2.546527	-4.299827	0.513116	H	-2.179769	0.273190	-3.069640
C	-1.877267	4.375275	1.329475	C	-3.978571	1.379499	-2.591437
C	-2.295109	5.583402	0.749453	H	-0.807631	3.178054	-1.122992
C	-2.769481	3.291747	1.329134	H	-0.789968	2.420029	-2.707338
C	-3.560916	5.696827	0.172033	C	-2.630135	3.473532	-2.273796
H	-1.614478	6.429679	0.736238	H	-4.539795	2.785713	0.531988
C	-4.033415	3.401511	0.751370	C	-4.812546	1.731037	-1.346125
H	-2.457119	2.362469	1.789085	C	-3.469131	3.835094	-1.037384
C	-4.434205	4.606077	0.167742	H	-4.592023	0.803927	-3.295395
H	-3.862989	6.635998	-0.282177	C	-3.491306	2.673722	-3.267033
			H	-2.262711	4.389488	-2.753237	

H	-5.696343	2.312075	-1.638152	C	-0.008940	6.896741	0.653764	
H	-5.173298	0.813542	-0.863738	H	0.706446	6.276358	-2.676406	
H	-2.866335	4.423265	-0.333615	C	1.907812	7.614090	-1.459378	
H	-4.327251	4.454572	-1.327051	C	-0.351448	6.710858	-0.833682	
H	-2.905809	2.432151	-4.163442	H	2.948366	8.639614	0.145289	
H	-4.349534	3.274726	-3.593542	C	0.964858	8.077128	0.822174	
C	0.570514	-0.568417	-1.823635	H	-0.926025	7.089693	1.224327	
C	0.912829	0.369873	-3.005544	H	1.448825	8.529156	-1.855176	
C	-0.116716	-1.839378	-2.369062	H	2.822266	7.433019	-2.038747	
C	1.906762	-1.000308	-1.158369	H	-1.055772	5.878599	-0.955624	
H	-0.003789	0.681224	-3.515773	H	-0.841422	7.611158	-1.226053	
H	1.399467	1.275996	-2.623388	H	1.200164	8.219768	1.884701	
C	1.829192	-0.340423	-4.018481	H	0.499448	9.004967	0.466036	
H	-1.076025	-1.594875	-2.834827	C	4.359019	3.278250	0.610436	
H	-0.319304	-2.533197	-1.547780	C	4.595367	1.796543	1.004645	
C	0.795420	-2.544061	-3.396372	C	5.459853	4.124979	1.288531	
H	2.405775	-0.112351	-0.752894	C	4.505699	3.394348	-0.923054	
H	1.706500	-1.672603	-0.314441	H	4.503698	1.673966	2.086333	
C	2.820447	-1.714652	-2.169133	H	3.824850	1.178259	0.526789	
H	2.046795	0.349283	-4.843040	C	5.987828	1.323036	0.559081	
C	1.108639	-1.588176	-4.560307	H	5.397544	4.009976	2.372980	
C	3.139158	-0.755519	-3.328385	H	5.329085	5.187306	1.061162	
H	0.275850	-3.431917	-3.776932	C	6.855405	3.659261	0.822157	
C	2.107320	-2.965613	-2.711141	H	3.718678	2.807341	-1.413642	
H	3.749255	-2.004571	-1.662076	H	4.379671	4.435256	-1.236233	
H	1.736608	-2.094767	-5.303991	C	5.896049	2.911301	-1.375674	
H	0.180260	-1.293872	-5.066345	H	6.104100	0.278486	0.871073	
H	3.658729	0.132932	-2.947338	C	7.061828	2.192535	1.236038	
H	3.810066	-1.240948	-4.048186	C	6.101293	1.441607	-0.968558	
H	1.894958	-3.662608	-1.890097	H	7.614263	4.288777	1.304137	
H	2.754077	-3.491565	-3.424665	C	6.969481	3.789182	-0.706532	
C	-1.003717	-0.901375	0.679742	H	5.966294	3.007364	-2.466580	
C	-2.209764	-1.799914	0.366398	H	8.064928	1.861808	0.927205	
H	-1.191453	-0.373115	1.620636	H	6.980344	2.088489	2.325484	
H	-0.129908	-1.536239	0.868886	H	5.345824	0.808901	-1.452904	
C	-2.386502	-2.888149	1.431889	H	7.084784	1.090653	-1.308477	
H	-3.125255	-1.201831	0.320849	H	6.837327	4.836252	-1.009652	
H	-2.104620	-2.271902	-0.613677	H	7.969941	3.480818	-1.036946	
C	-3.605554	-3.776505	1.172977	C	2.636984	3.825630	2.979140	
H	-1.479039	-3.506012	1.468380	C	3.176611	5.069172	3.702052	
H	-2.475893	-2.414682	2.418922	H	3.219304	2.958644	3.325207	
H	-3.711387	-4.547075	1.943276	H	1.607377	3.643484	3.308775	
H	-4.527760	-3.184634	1.162388	C	3.305800	4.800381	5.207462	
H	-3.524832	-4.280847	0.203399	H	4.157073	5.351372	3.308048	
O	6.525675	1.448540	4.503991	H	2.522080	5.933564	3.541448	
O	4.271448	1.550646	4.525759	H	2.309504	4.577537	5.615966	
C	5.375188	0.900547	4.269210	H	3.903363	3.890716	5.340556	
O	5.304720	-0.298043	3.757170	C	3.919527	5.977130	5.968637	
Cs	2.298740	-0.260425	3.138089	H	3.321313	6.888082	5.845781	
P	2.576581	3.660534	1.123886	H	3.992309	5.769002	7.041543	
Cs	8.256441	-0.675933	3.256968	H	4.929980	6.196024	5.603506	
C	1.971554	5.313332	0.430502					
C	1.607106	5.149903	-1.069439	Cs3_CO3_HCO3				
C	2.930511	6.517115	0.563769	C	0.000570	-1.072223	2.263825	
C	0.653044	5.617201	1.192652	O	0.100420	-0.409627	3.507123	
H	2.501496	4.935671	-1.658407	O	-0.556489	-0.426919	1.342534	
H	0.940229	4.290145	-1.184908	O	0.513075	-2.210959	2.257862	
C	0.940886	6.426573	-1.614998	Cs	1.318194	-2.374787	-0.785616	
H	3.845470	6.327061	-0.007697	H	-0.364986	0.430540	3.390162	
H	3.226946	6.663826	1.604754	Cs	0.893193	2.225169	0.396493	
C	2.254234	7.798103	0.028845	Cs	3.299717	-1.340992	3.575425	
H	-0.027624	4.763272	1.081708	O	3.891864	-1.260193	0.560334	
H	0.847344	5.737443	2.262401	C	3.427304	-0.057733	0.385739	

O	3.447447	0.800022	1.367864	H	-3.010974	2.290388	-2.785667
O	2.900345	0.275348	-0.758288	C	-3.355346	2.560024	-5.551055
				H	-2.830141	0.493532	-5.257522
CsCl				H	-4.272099	0.993691	-4.401473
Cs	0.000000	0.000000	-0.632502	C	-4.217285	2.340614	-6.796441
Cl	0.000000	0.000000	2.832502	H	-3.764940	3.388638	-4.958038
				H	-2.344001	2.867739	-5.849718
D1_Cs				H	-4.268700	3.243117	-7.413981
Pd	-1.383547	0.966677	0.151686	H	-3.812748	1.532929	-7.417055
P	-1.868294	0.273044	-2.200562	H	-5.241684	2.064572	-6.521678
C	-0.440808	-0.579071	-3.117888	C	-2.270440	2.813081	0.214987
C	0.798473	0.308018	-2.822222	C	-2.745166	3.207327	1.504046
C	-0.592056	-0.684933	-4.652715	C	-2.368923	3.767653	-0.807816
C	-0.174369	-1.991996	-2.546959	C	-3.380034	4.441687	1.693534
H	0.631662	1.315967	-3.229807	C	-2.982883	5.015901	-0.612909
H	0.940620	0.391945	-1.741585	H	-1.948531	3.556057	-1.784518
C	2.066132	-0.296595	-3.452086	C	-3.515317	5.343637	0.633684
H	-0.740952	0.308787	-5.086492	H	-3.749799	4.718795	2.678212
H	-1.464979	-1.291553	-4.915465	H	-3.044471	5.723461	-1.437011
C	0.675557	-1.304621	-5.278943	H	-4.007612	6.299834	0.789910
H	-0.077444	-1.925386	-1.462248	C	1.004378	-0.789530	0.515888
H	-1.019022	-2.649976	-2.776511	O	1.569876	0.353892	0.393902
C	1.099051	-2.592772	-3.170044	O	-0.325031	-0.878278	0.430623
H	2.919635	0.355649	-3.223690	O	1.645573	-1.880720	0.698266
C	1.888311	-0.407137	-4.975368	Cs	-0.685586	-3.726548	1.363283
C	2.304814	-1.692714	-2.848925	C	-2.415600	2.262752	2.584970
H	0.531174	-1.376184	-6.364493	C	-2.783644	2.393938	3.931369
C	0.917964	-2.706175	-4.692978	C	-1.614134	1.169661	2.163804
H	1.262013	-3.590337	-2.740997	C	-2.352987	1.455738	4.874125
H	2.791734	-0.827517	-5.436077	H	-3.406016	3.225860	4.253925
H	1.735567	0.589415	-5.410675	C	-1.191974	0.243814	3.122980
H	2.423591	-1.622376	-1.762368	C	-1.551725	0.383861	4.471427
H	3.222490	-2.130004	-3.265335	H	-2.640520	1.563685	5.916791
H	0.067637	-3.361706	-4.923484	H	-0.581157	-0.594852	2.801683
H	1.808156	-3.155790	-5.151915	H	-1.208615	-0.342243	5.205954
C	-3.362951	-0.871523	-1.989520	Cs	1.675056	3.177198	-0.389348
C	-3.108336	-1.835656	-0.802485				
C	-3.756831	-1.720042	-3.221056	D1_Cs_benz			
C	-4.556221	0.042006	-1.595015	Pd	1.259063	1.491323	0.893373
H	-2.271530	-2.492442	-1.045931	P	-0.060692	0.551412	-0.881846
H	-2.812595	-1.255516	0.076184	C	0.942124	0.030398	-2.409584
C	-4.358293	-2.680324	-0.498400	C	2.131783	1.027094	-2.473466
H	-2.937389	-2.392895	-3.491784	C	0.166024	0.106118	-3.745530
H	-3.947369	-1.084786	-4.087129	C	1.531813	-1.391019	-2.255065
C	-5.017420	-2.555949	-2.914197	H	1.756658	2.054364	-2.570742
H	-4.278559	0.638165	-0.717990	H	2.688356	0.953712	-1.535262
H	-4.787265	0.745187	-2.400067	C	3.050517	0.701165	-3.666139
C	-5.808583	-0.801747	-1.296068	H	-0.231259	1.114970	-3.892656
H	-4.140401	-3.353267	0.341838	H	-0.686103	-0.580631	-3.738070
C	-4.733340	-3.507760	-1.739373	C	1.094704	-0.235948	-4.929400
C	-5.523710	-1.751606	-0.121312	H	2.100504	-1.463768	-1.325036
H	-5.280047	-3.138306	-3.806091	H	0.725151	-2.130979	-2.230660
C	-6.182390	-1.619577	-2.545498	C	2.458507	-1.723879	-3.441494
H	-6.634071	-0.128140	-1.034947	H	3.871604	1.428876	-3.689682
H	-5.615304	-4.127171	-1.531728	C	2.252412	0.776423	-4.979036
H	-3.911791	-4.188544	-1.998462	C	3.620766	-0.717862	-3.492274
H	-5.266843	-1.173108	0.775266	H	0.514382	-0.180549	-5.859168
H	-6.418375	-2.341598	0.115586	C	1.658874	-1.656480	-4.753374
H	-6.402255	-0.945202	-3.383142	H	2.854944	-2.738149	-3.300217
H	-7.090323	-2.206009	-2.355116	H	2.905257	0.558831	-5.834340
C	-2.443435	1.587337	-3.397624	H	1.856668	1.790241	-5.122596
C	-3.258551	1.308145	-4.670733	H	4.207240	-0.783767	-2.569795
H	-1.522201	2.119238	-3.669272	H	4.289611	-0.960357	-4.328909

H	0.839515	-2.387430	-4.734858	H	-4.651562	2.407747	0.887093
H	2.303046	-1.913127	-5.604411	H	-5.457939	4.551554	-0.092989
C	-1.252056	-0.816722	-0.348953	Cs	0.966557	-0.117434	4.240747
C	-0.464059	-1.917010	0.403391				
C	-2.060625	-1.491677	-1.479577	D1_Na			
C	-2.231550	-0.171871	0.661976	Pd	-1.531516	0.910132	0.152895
H	0.204362	-2.414032	-0.301322	P	-2.044487	0.205609	-2.182177
H	0.183655	-1.481692	1.169961	C	-0.532232	-0.520338	-3.066413
C	-1.425799	-2.964929	0.995679	C	0.643690	0.411192	-2.663247
H	-1.381943	-1.983323	-2.183331	C	-0.620261	-0.553824	-4.608648
H	-2.629612	-0.751328	-2.044771	C	-0.209189	-1.946589	-2.561568
C	-3.024647	-2.542838	-0.891739	H	0.439985	1.438370	-2.994919
H	-1.652308	0.285802	1.471020	H	0.736726	0.421565	-1.573788
H	-2.800873	0.629183	0.186453	C	1.964896	-0.082513	-3.279538
C	-3.202043	-1.217134	1.235595	H	-0.814719	0.448981	-5.000518
H	-0.844093	-3.729168	1.528544	H	-1.445586	-1.197075	-4.930992
C	-2.221686	-3.623276	-0.145570	C	0.704433	-1.065002	-5.213224
C	-2.400697	-2.297087	1.978852	H	-0.161885	-1.939302	-1.472242
H	-3.588392	-3.003414	-1.712271	H	-1.004102	-2.637145	-2.859875
C	-3.998400	-1.861118	0.086126	C	1.121523	-2.441178	-3.158700
H	-3.889891	-0.719422	1.930462	H	2.770258	0.601581	-2.982883
H	-2.898737	-4.388997	0.254200	C	1.848081	-0.116630	-4.812472
H	-1.535084	-4.126288	-0.839217	C	2.261654	-1.495035	-2.745017
H	-1.847672	-1.845781	2.812546	H	0.606004	-1.085021	-6.305749
H	-3.076659	-3.046823	2.409575	C	1.007037	-2.480430	-4.692190
H	-4.583839	-1.095505	-0.438772	H	1.322889	-3.450031	-2.776258
H	-4.709545	-2.595864	0.484597	H	2.791723	-0.456302	-5.258263
C	-1.101037	1.976373	-1.504443	H	1.651862	0.892294	-5.198236
C	-2.402223	1.824093	-2.301519	H	2.344782	-1.466348	-1.652962
H	-0.387795	2.579652	-2.080627	H	3.217048	-1.859353	-3.144617
H	-1.314393	2.563909	-0.611220	H	0.208208	-3.171271	-4.991937
C	-2.898523	3.187980	-2.797958	H	1.939985	-2.852297	-5.134858
H	-2.281843	1.150087	-3.154104	C	-3.468289	-1.036147	-2.052604
H	-3.177385	1.384810	-1.664624	C	-3.184049	-2.038416	-0.904409
C	-4.298385	3.121144	-3.410901	C	-3.773669	-1.843230	-3.335673
H	-2.903743	3.892520	-1.958314	C	-4.725352	-0.221038	-1.644264
H	-2.184997	3.582823	-3.533814	H	-2.300599	-2.632684	-1.146221
H	-4.620828	4.098736	-3.784203	H	-2.958748	-1.484225	0.011470
H	-4.334461	2.414568	-4.248245	C	-4.383748	-2.976078	-0.680520
H	-5.031377	2.791001	-2.665844	H	-2.902859	-2.442861	-3.616608
C	0.368959	3.114005	1.713437	H	-3.985957	-1.178051	-4.173323
C	-0.491968	4.186658	1.967312	C	-4.983592	-2.772750	-3.107183
C	1.609222	3.012246	2.253515	H	-4.511150	0.334033	-0.722706
C	0.025378	5.186080	2.830653	H	-4.976678	0.514763	-2.412840
C	2.126593	3.970299	3.120261	C	-5.930518	-1.155929	-1.429359
C	1.298029	5.080323	3.395957	H	-4.138337	-3.674049	0.130891
H	-0.596848	6.044481	3.074007	C	-4.669728	-3.762014	-1.971628
H	3.115715	3.905522	3.571709	C	-5.619221	-2.147156	-0.295498
H	1.650208	5.866979	4.060086	H	-5.183602	-3.324184	-4.033966
C	3.094363	-0.999098	0.951068	C	-6.214989	-1.929669	-2.729754
O	2.383420	-1.409586	1.947637	H	-6.803788	-0.548626	-1.161919
O	2.999468	0.253502	0.538212	H	-5.515100	-4.445006	-1.820060
O	3.900475	-1.772342	0.320939	H	-3.799700	-4.376013	-2.238509
Cs	2.400284	-4.320495	0.720411	H	-5.431024	-1.602689	0.638820
C	-1.859383	4.306455	1.408618	H	-6.479602	-2.805527	-0.120831
C	-2.332475	5.512376	0.865859	H	-6.452125	-1.227903	-3.539609
C	-2.721383	3.198498	1.412545	H	-7.089585	-2.578892	-2.597467
C	-3.618852	5.599860	0.330888	C	-2.654316	1.536455	-3.341252
H	-1.676835	6.378062	0.844679	C	-3.437284	1.263270	-4.634770
C	-4.005521	3.281221	0.876468	H	-1.747591	2.101674	-3.590350
H	-2.365714	2.270875	1.842853	H	-3.248633	2.206908	-2.715716
C	-4.460346	4.484311	0.330257	C	-3.590715	2.543501	-5.465012
H	-3.961680	6.538317	-0.095411	H	-2.951469	0.499607	-5.245946

H	-4.434765	0.880533	-4.396344	D2a_Cs				
C	-4.409009	2.324660	-6.739547	Pd	1.880337	2.000750	1.180572	
H	-4.063783	3.319735	-4.849071	C	2.555059	3.862983	1.456962	
H	-2.593912	2.924243	-5.725152	C	1.635468	4.795190	2.011580	
H	-4.503086	3.248524	-7.319158	C	3.871773	4.280181	1.232425	
H	-3.940013	1.571904	-7.383283	C	2.044039	6.097802	2.316686	
H	-5.419814	1.973887	-6.502690	C	4.278857	5.588649	1.542379	
C	-2.077628	2.875994	0.147210	H	4.262308	3.034977	3.425496	
C	-2.361821	3.433749	1.430269	C	3.365386	6.494985	2.082821	
C	-2.060933	3.761424	-0.938160	H	1.339987	6.808340	2.743959	
C	-2.717595	4.781490	1.566559	H	5.306832	5.894651	1.362278	
C	-2.395709	5.117361	-0.797505	H	3.677989	7.507299	2.324079	
H	-1.773139	3.409936	-1.919717	C	2.809972	-0.341373	0.598748	
C	-2.750847	5.623681	0.451971	O	1.548316	-0.152860	0.951640	
H	-2.941290	5.188592	2.549521	O	3.522720	0.752373	0.465456	
H	-2.377700	5.770080	-1.666965	O	3.283847	-1.493845	0.417084	
H	-3.025348	6.668688	0.566017	Cs	0.548133	-2.266958	-1.059602	
C	0.710111	-1.073978	0.782216	C	0.292604	4.229713	2.220922	
O	1.450943	-0.039614	0.664601	C	-0.821011	4.906710	2.730142	
O	-0.592005	-1.015411	0.503181	C	0.197362	2.859120	1.849816	
O	1.157459	-2.217600	1.155080	C	-2.044189	4.242637	2.875622	
Na	-0.898131	-3.122875	1.189533	H	-0.743977	5.953940	3.013936	
C	-2.134752	2.513394	2.556481	C	-1.037543	2.217220	1.997833	
C	-2.360661	2.801184	3.909494	C	-2.154083	2.899820	2.508638	
C	-1.580839	1.264923	2.169763	H	-2.906422	4.774138	3.269210	
C	-2.027633	1.864735	4.892373	H	-1.139967	1.170538	1.713558	
H	-2.791805	3.754620	4.205098	H	-3.105627	2.383519	2.615063	
C	-1.250424	0.343967	3.169596	Cs	1.175269	-0.559728	4.032910	
C	-1.467019	0.639399	4.524303	Cs	6.043468	-0.128757	1.935672	
H	-2.203192	2.093584	5.940003	O	4.767884	2.236953	3.648534	
H	-0.814911	-0.610938	2.892162	C	3.904702	1.424837	4.404327	
H	-1.197243	-0.085818	5.288580	O	4.308277	0.246068	4.549915	
Na	0.970522	2.069599	0.863469	O	2.847034	1.960497	4.811489	
			H	4.594350	3.582243	0.814717		
D2_Cs								
Pd	-1.016551	0.959970	0.769412	D2_Cs_benz				
C	-1.935057	2.735132	0.576755	Pd	2.472320	2.672643	0.171286	
C	-2.558124	3.252345	1.747036	C	1.266751	4.023173	1.042780	
C	-2.000066	3.495296	-0.596681	C	0.179003	4.699017	1.596292	
C	-3.201179	4.494901	1.720411	C	2.476396	4.586854	0.829768	
C	-2.646683	4.741958	-0.621121	C	0.442560	6.050727	1.946679	
H	-1.548373	3.115312	-1.511975	C	2.761858	5.905018	1.160024	
C	-3.243405	5.242029	0.537879	H	2.121850	2.566827	2.937230	
H	-3.675533	4.887078	2.617396	C	1.694409	6.632642	1.736734	
H	-2.685208	5.316648	-1.543918	H	-0.343983	6.640833	2.410892	
H	-3.745105	6.205916	0.522547	H	3.726074	6.382620	0.997380	
C	0.499849	-0.634846	-0.584409	H	1.848597	7.669422	2.027709	
O	0.003290	0.472027	-1.103478	C	3.309969	0.356695	-0.654765	
O	0.103302	-0.892601	0.649839	O	2.033719	0.600102	-0.403327	
O	1.303704	-1.376842	-1.200569	O	4.088064	1.418835	-0.633849	
Cs	1.415278	-3.620177	1.004446	O	3.742410	-0.805953	-0.845945	
C	-2.448951	2.354743	2.908867	Cs	-0.687143	1.464707	-1.513343	
C	-2.971447	2.586817	4.186048	C	-1.151836	4.079100	1.791565	
C	-1.737377	1.155798	2.628106	C	-2.334939	4.809705	1.583785	
C	-2.798660	1.639066	5.200632	C	-1.257214	2.724129	2.161194	
H	-3.517112	3.503708	4.398048	C	-3.585547	4.206867	1.727433	
C	-1.575373	0.223139	3.657435	H	-2.271138	5.851257	1.282513	
C	-2.101371	0.458335	4.937516	C	-2.510045	2.124454	2.302578	
H	-3.207865	1.823426	6.190382	H	-0.357735	2.144654	2.357702	
H	-1.032564	-0.700914	3.466565	C	-3.680134	2.858941	2.083284	
H	-1.966665	-0.279489	5.725394	H	-4.486642	4.788410	1.553615	
Cs	2.028419	2.713562	-0.919117	H	-2.571965	1.079588	2.596381	
			H	-4.652917	2.388935	2.195030		

Cs	1.711606	-1.975699	1.373727	H	-4.128193	0.160913	4.713795
Cs	5.573847	1.141632	2.069494	Na	1.984536	2.347841	1.222945
O	2.783371	2.016064	3.389351	Na	3.413835	-1.835855	1.530654
C	2.272885	0.706938	3.403803	O	2.327769	-1.268098	-0.452091
O	3.129140	-0.171789	3.658462	C	2.176148	-0.087365	0.034251
O	1.053479	0.574217	3.138887	O	2.989985	0.373194	0.922403
				O	1.154455	0.651350	-0.363500
D2_Na							
Pd	-1.031704	0.932492	0.772639	E1_Cs			
C	-1.936846	2.705762	0.575049	Pd	-1.509071	0.120230	1.590238
C	-2.532317	3.246212	1.747416	C	-1.326730	1.743890	0.394101
C	-2.012704	3.440522	-0.612769	C	-1.519117	2.968979	1.069052
C	-3.151817	4.499030	1.711126	C	-0.955279	1.722822	-0.945258
C	-2.636372	4.699799	-0.644820	C	-1.346826	4.172807	0.375078
H	-1.603683	3.032376	-1.536577	C	-0.777296	2.937238	-1.626815
C	-3.198391	5.228734	0.517164	H	-0.760149	0.793671	-1.474330
H	-3.605493	4.912624	2.608720	C	-0.979818	4.154366	-0.971925
H	-2.686231	5.256905	-1.577061	H	-1.489739	5.121963	0.883941
H	-3.681358	6.201613	0.495843	H	-0.479001	2.921354	-2.671352
C	0.547981	-0.626001	-0.618401	H	-0.845950	5.089269	-1.507661
O	0.096236	0.513437	-1.097175	C	0.078974	-1.239704	3.090290
O	0.123548	-0.939546	0.589655	O	0.469975	-0.207661	2.356084
O	1.331970	-1.378620	-1.255455	O	-1.217876	-1.480786	3.025059
C	-2.432316	2.351040	2.909775	O	0.868470	-1.924953	3.768046
C	-2.931528	2.593299	4.193724	Cs	-1.229679	-4.158244	4.521659
C	-1.759821	1.133600	2.620993	C	-1.867710	2.828625	2.485742
C	-2.772362	1.635883	5.201131	C	-2.138591	3.852608	3.404022
H	-3.446958	3.524833	4.415614	C	-1.935890	1.505264	2.950960
C	-1.609403	0.189068	3.638854	C	-2.462035	3.544109	4.726869
C	-2.113486	0.436326	4.925669	H	-2.098021	4.889697	3.084125
H	-3.162324	1.827821	6.196892	C	-2.243985	1.170724	4.256636
H	-1.093947	-0.748019	3.438029	C	-2.513181	2.215126	5.154424
H	-1.989593	-0.307363	5.709134	H	-2.673907	4.345608	5.427730
Na	1.094319	2.474067	-0.843537	H	-2.264748	0.132574	4.565430
Na	1.250512	-2.904251	0.461056	H	-2.762446	1.982113	6.185469
				Cs	2.603905	0.013300	0.216549
D2a_Na							
Pd	-0.596918	0.961938	0.993509	Cl	1.081133	-0.809402	-2.813272
C	-0.944079	2.852656	0.442841	C	-3.453820	0.011624	1.016827
C	-1.911914	3.550472	1.214724	C	-3.833001	-1.252908	0.521029
C	-0.292355	3.522021	-0.597207	C	-4.414725	1.016825	1.145772
C	-2.181815	4.896582	0.947108	C	-5.180622	-1.490188	0.200250
C	-0.569654	4.874807	-0.859636	C	-5.748935	0.771297	0.810582
H	0.434948	2.989390	-1.205306	H	-4.133474	1.994469	1.518230
C	-1.506761	5.559330	-0.084624	C	-6.135538	-0.486975	0.343725
H	-2.919531	5.435348	1.536550	H	-5.466526	-2.464365	-0.186925
H	-0.056009	5.385634	-1.670114	H	-6.483939	1.564517	0.915047
H	-1.720935	6.605128	-0.285551	H	-7.171010	-0.680950	0.080966
C	0.636181	-1.261094	2.642062	C	-2.819982	-2.319625	0.336632
O	0.548887	-0.346096	3.655518	C	-1.579771	-2.025286	-0.258394
O	-0.185447	-1.123833	1.665638	C	-3.058153	-3.635786	0.765128
O	1.502710	-2.144238	2.759379	C	-0.586121	-3.000905	-0.378961
Na	0.094036	-1.604318	-0.599561	H	-1.413621	-1.051827	-0.711918
C	-2.563356	2.714168	2.234522	C	-2.074096	-4.615233	0.629606
C	-3.572166	3.116017	3.114907	H	-4.010128	-3.881125	1.226349
C	-2.095365	1.371717	2.251212	C	-0.828039	-4.297837	0.073491
C	-4.130685	2.198567	4.012006	H	0.344285	-2.736714	-0.872022
H	-3.930557	4.142384	3.106129	H	-2.275113	-5.628902	0.965971
C	-2.675730	0.463856	3.141569	H	-0.064962	-5.063977	-0.024884
H	-0.160027	0.282660	3.426491	E2_Cs			
C	-3.688469	0.876061	4.023451	Pd	-1.542339	-0.008150	-0.090066
H	-4.912766	2.518221	4.694716	C	-1.562787	2.011877	-0.138849
H	-2.342134	-0.570384	3.154799	C	-2.296188	2.617835	0.902007

C	-0.797471	2.787199	-0.998898	H	-2.044235	4.768905	-2.155579
C	-2.264536	4.011867	1.046484	H	-3.556243	5.342142	-0.266343
C	-0.766211	4.177327	-0.843121	C	1.079600	-2.244830	0.313372
H	-0.270159	2.311167	-1.813451	O	1.157204	-2.182020	1.585149
C	-1.501686	4.789160	0.175416	O	-0.070436	-1.927048	-0.303259
H	-2.823402	4.488584	1.847428	O	2.056371	-2.620485	-0.428771
H	-0.185997	4.781576	-1.534928	Cs	0.861638	-2.161596	-3.229933
H	-1.482468	5.869230	0.288718	C	-2.557755	1.245415	1.831694
C	-0.172657	-1.687803	1.370808	C	-3.152672	1.385079	3.095261
O	0.127836	-0.392056	1.299173	C	-1.744859	0.121402	1.576428
O	-1.134918	-2.067375	0.565979	C	-2.912974	0.433274	4.087766
O	0.433152	-2.473934	2.130117	H	-3.781647	2.245511	3.309979
Cs	1.433335	-3.428007	-0.951985	C	-1.454838	-0.796460	2.576896
C	-2.981231	1.676144	1.789134	C	-2.053603	-0.640861	3.833949
C	-3.784656	1.994841	2.892760	H	-3.380636	0.539442	5.062929
C	-2.741907	0.321833	1.493866	H	-0.746430	-1.593677	2.367126
C	-4.324837	0.979828	3.684344	H	-1.852145	-1.368222	4.616513
H	-3.984936	3.034671	3.136154	Cs	1.150902	3.610831	1.620345
C	-3.259688	-0.693360	2.284622	Cs	3.768395	-0.508186	1.081637
H	1.622705	0.140036	0.525548	O	2.601942	1.299749	-1.434653
C	-4.057834	-0.359058	3.387972	C	1.445466	0.951727	-1.089830
H	-4.949651	1.234250	4.535486	O	0.516033	0.578574	-1.933845
H	-3.035763	-1.728310	2.054780	O	1.088471	0.927544	0.186117
H	-4.470153	-1.148090	4.010944	C	-2.549788	-0.595302	-1.195571
Cs	2.679583	1.754388	-2.803678	C	-3.578723	-1.453637	-0.757210
Cs	2.477740	-0.563695	3.468270	C	-2.593317	-0.115817	-2.515765
O	3.301489	-1.432725	0.508218	C	-4.636722	-1.745088	-1.646961
C	3.434492	-0.316064	-0.061778	C	-3.632329	-0.438241	-3.390482
O	4.363028	0.093076	-0.793593	H	-1.792992	0.527561	-2.865000
O	2.404447	0.610569	0.144356	C	-4.678363	-1.247019	-2.945000
Cl	-0.092090	-0.437192	-2.210125	H	-5.424746	-2.408845	-1.301736
C	-3.259697	-0.260762	-1.160724	H	-3.626003	-0.048000	-4.405174
C	-3.822572	-1.514526	-0.876950	H	-5.505969	-1.499571	-3.601679
C	-3.891681	0.573312	-2.097586	C	-3.633823	-2.171752	0.547642
C	-5.005358	-1.940674	-1.481714	C	-2.610653	-3.055156	0.920035
H	-3.321665	-2.169448	-0.173187	C	-4.775450	-2.080757	1.356621
C	-5.096677	0.134011	-2.684254	C	-2.736330	-3.831966	2.070682
C	-5.660173	-1.101838	-2.383079	H	-1.695778	-3.062386	0.334973
H	-5.412756	-2.918510	-1.238685	C	-4.890137	-2.844093	2.519520
H	-5.579839	0.786647	-3.406394	H	-5.573355	-1.399191	1.074346
H	-6.589506	-1.408403	-2.854126	C	-3.872867	-3.731546	2.876086
C	-3.375745	1.876465	-2.610704	H	-1.931102	-4.506443	2.350519
C	-3.952550	3.086933	-2.208337	H	-5.775430	-2.749161	3.142261
C	-2.394798	1.893570	-3.610709	H	-3.963571	-4.333552	3.775958
C	-3.541392	4.292713	-2.775714				
H	-4.716429	3.079461	-1.436804	G_Cs			
C	-1.988406	3.098151	-4.185038	Pd	0.825301	0.801116	0.179311
H	-1.936327	0.958751	-3.911618	C	2.614886	0.304105	-0.585605
C	-2.559856	4.302184	-3.768763	C	2.748239	-0.648192	-1.621244
H	-3.986297	5.225190	-2.441095	C	3.766831	0.782508	0.049922
H	-1.225436	3.096238	-4.959214	C	4.028011	-1.110951	-1.971144
H	-2.241967	5.241207	-4.212712	C	5.038089	0.322469	-0.316112
			H	3.674284	1.503136	0.858358	
F_Cs			C	5.167708	-0.633435	-1.325850	
Pd	-0.872942	0.079609	-0.239722	H	4.128534	-1.819799	-2.787994
C	-1.743453	1.906418	-0.341273	H	5.919955	0.709072	0.188450
C	-2.574589	2.239006	0.751405	H	6.149424	-0.990459	-1.622575
C	-1.546105	2.815910	-1.376431	C	1.557239	-1.152477	-2.347722
C	-3.229245	3.479538	0.767327	C	1.437731	-2.510479	-2.673840
C	-2.197673	4.058622	-1.346969	C	0.500976	-0.276198	-2.692504
H	-0.877816	2.557771	-2.191521	C	0.300562	-3.005885	-3.314799
C	-3.045624	4.383306	-0.283110	H	2.236705	-3.190160	-2.392555
H	-3.871712	3.747459	1.602311	C	-0.645200	-0.783778	-3.317710

C	-0.748920	-2.141185	-3.630574	O	0.788294	0.867143	1.117384
H	0.229402	-4.063794	-3.549910	C	-3.314160	0.327859	-0.609972
H	-1.471583	-0.110791	-3.521223	C	-3.195893	-1.092798	-0.412418
H	-1.645717	-2.518070	-4.113128	C	-3.760599	1.114120	0.486211
C	0.551103	1.179797	-2.353442	C	-3.611284	-1.643493	0.801441
C	-0.521798	1.712025	-1.599783	C	-4.155464	0.529172	1.699091
C	1.561134	2.064903	-2.849403	H	-3.893204	2.179175	0.337080
C	-0.573753	3.091308	-1.296729	C	-4.106331	-0.851165	1.842953
H	-1.421474	1.110871	-1.417265	H	-3.508351	-2.713275	0.948098
C	1.479914	3.417008	-2.520275	H	-4.516467	1.160692	2.503808
C	0.431942	3.933534	-1.741369	H	-4.420692	-1.317597	2.770964
H	2.238335	4.090588	-2.907651	C	-2.612850	-1.990133	-1.443209
H	0.398581	4.997845	-1.527089	C	-1.436877	-1.640978	-2.128274
C	2.680130	1.601567	-3.707359	C	-3.217464	-3.222683	-1.732364
C	2.461257	0.773975	-4.819944	C	-0.886050	-2.499528	-3.075689
C	3.992117	2.009086	-3.422577	H	-0.954634	-0.694727	-1.902638
C	3.527982	0.352255	-5.611767	C	-2.666671	-4.081569	-2.684245
H	1.452220	0.461406	-5.064129	H	-4.137651	-3.497370	-1.225946
C	5.058602	1.589073	-4.214511	C	-1.499580	-3.723209	-3.359883
H	4.175826	2.621288	-2.546303	H	0.026698	-2.215593	-3.590902
C	4.831517	0.754769	-5.310560	H	-3.154176	-5.027327	-2.900573
H	3.340230	-0.287181	-6.469415	H	-1.070032	-4.390540	-4.100698
H	6.068756	1.901170	-3.966565				
H	5.661954	0.420908	-5.925553	G_Cs'			
O	-3.661225	2.532131	-0.621775	Pd	0.835174	0.809021	0.234612
C	-3.795984	1.242773	-0.567064	C	2.619749	0.285380	-0.537701
O	-4.384646	0.686261	0.452734	C	2.750092	-0.649001	-1.590178
Cs	-2.297440	-1.604573	0.409109	C	3.779822	0.754502	0.093142
Cs	-3.097188	2.790686	2.338136	C	4.028941	-1.098195	-1.963248
O	-0.766616	0.887624	1.692342	C	5.049543	0.309745	-0.294780
C	0.059301	0.381271	2.572584	H	3.693846	1.460184	0.915552
O	-0.231673	0.084197	3.742057	C	5.173432	-0.626335	-1.323505
O	1.289884	0.177331	2.083341	H	4.124508	-1.790442	-2.794744
Cs	2.604641	-2.571102	2.221588	H	5.934821	0.692980	0.206434
O	-3.299800	0.487123	-1.513604	H	6.153436	-0.972251	-1.638487
H	-1.461619	3.438482	-0.778174	C	1.564039	-1.152949	-2.325785
				C	1.466483	-2.505979	-2.678540
				C	0.505838	-0.286103	-2.686574
G_Cs_cfl'				C	0.359164	-3.002565	-3.367138
Pd	-1.164682	0.814952	0.461027	C	2.264854	-3.181254	-2.386161
C	-1.229253	2.658062	-0.277326	H	-0.605590	-0.794300	-3.368793
C	-1.987849	3.067322	-1.394305	C	-0.684688	-2.144811	-3.712178
C	-0.536519	3.616508	0.476989	H	0.309533	-4.056804	-3.622262
C	-2.090982	4.452086	-1.653192	H	-1.405888	-0.115656	-3.648350
C	-0.624782	4.978591	0.183461	H	-1.553213	-2.519391	-4.244656
H	0.077805	3.281711	1.307902	C	0.541207	1.168356	-2.349280
C	-1.425448	5.398653	-0.879481	C	-0.499914	1.701004	-1.553741
H	-2.722787	4.790723	-2.468210	C	1.534761	2.055160	-2.865302
H	-0.087060	5.703101	0.789518	C	-0.541420	3.075285	-1.235055
H	-1.534511	6.455062	-1.106178	H	-1.330425	1.059500	-1.276261
C	-2.663297	2.134756	-2.342406	C	1.458099	3.409147	-2.539148
C	-2.689231	2.510899	-3.700759	C	0.440669	3.922120	-1.723502
C	-3.285170	0.911459	-1.988430	H	2.204839	4.083112	-2.946863
C	-3.353285	1.769722	-4.671768	H	0.416555	4.982179	-1.492768
H	-2.154599	3.405510	-3.999319	C	2.645671	1.588648	-3.732333
C	-3.987517	0.196897	-2.974916	C	2.418467	0.766422	-4.846681
C	-4.033240	0.610781	-4.300878	C	3.959589	1.988876	-3.447296
H	-3.340757	2.098758	-5.706297	C	3.481142	0.344902	-5.643964
H	-4.506207	-0.709949	-2.687793	H	1.407802	0.457934	-5.088758
H	-4.582125	0.027221	-5.033152	C	5.021737	1.567826	-4.244411
Cs	3.782132	1.540034	1.463673	H	4.148272	2.593636	-2.566832
O	1.784093	-0.767261	2.294755	C	4.786977	0.741077	-5.344470
C	0.767754	-0.341906	1.714596	H	3.288407	-0.290008	-6.503717

H	6.034043	1.873018	-3.997326				
H	5.613973	0.406895	-5.963789				
O	-0.772436	1.012639	1.685468				
C	-0.009469	0.465842	2.596374				
O	-0.331002	0.211651	3.763391				
O	1.224585	0.173367	2.137720				
Cs	2.545430	-2.566663	2.284968				
H	-1.350509	3.453048	-0.619479				
H_Cs'							
Pd	0.720700	0.392546	0.725400	H	0.738150	0.171479	0.601327
C	2.714465	0.202170	0.545431	C	2.720051	0.059500	0.377391
C	3.323768	-0.494555	-0.526743	C	3.271920	-0.628848	-0.726875
C	3.560663	0.715555	1.546342	C	3.592885	0.563415	1.354389
C	4.719037	-0.668106	-0.561322	C	4.659922	-0.825783	-0.807266
C	4.949031	0.546078	1.505010	C	4.975241	0.365707	1.266025
H	3.125796	1.255272	2.385098	H	3.191732	1.112455	2.202894
C	5.534704	-0.147718	0.443979	C	5.511189	-0.330718	0.181443
H	5.165217	-1.207150	-1.393839	H	5.072430	-1.358564	-1.660276
H	5.570143	0.957932	2.297073	H	5.629998	0.759918	2.038946
H	6.612062	-0.278956	0.396214	H	6.583860	-0.480319	0.099950
C	2.499974	-1.127580	-1.594323	C	2.388368	-1.197454	-1.781388
C	2.689236	-2.492567	-1.874692	C	2.520456	-2.551288	-2.130557
C	1.548756	-0.403137	-2.350386	C	1.416312	-0.414219	-2.447378
C	1.939583	-3.155390	-2.846600	C	1.698276	-3.141188	-3.091973
H	3.437345	-3.038778	-1.305980	H	3.270428	-3.148917	-1.620659
C	0.808890	-1.082749	-3.333226	C	0.589670	-1.021573	-3.404754
C	0.984631	-2.444549	-3.577316	C	0.718278	-2.372750	-3.726604
H	2.100296	-4.213760	-3.030475	H	1.817127	-4.192625	-3.337051
H	0.094456	-0.519209	-3.926120	H	-0.155087	-0.414301	-3.909042
H	0.389827	-2.941036	-4.338695	H	0.064361	-2.818787	-4.470099
C	1.315611	1.061086	-2.161389	C	1.246998	1.043461	-2.174491
C	0.903119	1.545255	-0.900519	C	0.928520	1.477453	-0.874062
C	1.408464	1.936540	-3.274322	C	1.327029	1.989100	-3.224605
C	0.563860	2.905920	-0.788193	C	0.667868	2.832168	-0.627060
H	-1.585669	2.731970	-1.945566	H	-1.412850	1.613842	-0.660069
C	1.042323	3.282151	-3.125446	C	1.036049	3.337000	-2.960120
C	0.612452	3.764879	-1.889883	H	0.699824	3.756184	-1.677001
H	1.128093	3.951416	-3.976154	H	1.108795	4.058456	-3.767859
H	0.331834	4.809486	-1.781412	H	0.486110	4.803783	-1.484533
C	1.930913	1.492648	-4.595121	C	1.756827	1.610918	-4.597450
C	1.231645	1.784525	-5.775891	C	1.017372	2.024012	-5.715505
C	3.151316	0.803887	-4.694024	C	2.929054	0.865901	-4.805458
C	1.727462	1.386855	-7.018784	O	2.912555	0.681086	-8.204328
H	0.284262	2.311836	-5.712711	C	2.591856	0.942720	-7.200506
C	3.649358	0.409359	-5.933776	H	0.838211	2.010124	-7.859964
H	3.706794	0.579737	-3.789099	H	4.253965	-0.038135	-6.235865
C	2.937411	0.695535	-7.102418	C	1.428872	0.549684	-3.948836
H	1.166315	1.614383	-7.920541	C	2.302161	0.053529	-0.007039
H	4.596482	-0.119499	-5.989789	O	-2.225858	1.123102	-0.865916
H	3.324089	0.384355	-8.068223	C	-3.227682	-0.746579	-0.189889
O	-2.840917	3.564314	-0.287769	O	-1.398796	-0.025793	0.905809
C	-3.203111	2.553614	-0.932683	Cs	-1.239680	-3.225545	-0.163108
O	-4.189853	1.799871	-0.756725	H	0.434939	3.168359	0.378761
Cs	-2.615630	-0.912842	-1.239395	I_Cs			
Cs	-3.635762	2.116407	2.424716	Pd	0.359691	1.500249	0.804740
O	-1.390173	0.353862	1.251676	C	3.158547	0.699318	0.622113
C	-1.176839	-0.405244	2.313033	C	3.498309	-0.615141	0.210762
O	-2.112139	-0.787384	3.056390	C	3.720578	1.196570	1.818243
O	0.085704	-0.722681	2.515589	C	4.429730	-1.351601	0.974353
Cs	1.378048	-3.366017	1.976094	C	4.609157	0.444120	2.572293
O	-2.374237	2.167411	-2.004487	H	3.462986	2.190527	2.161127
H	0.221714	3.295519	0.165880	C	4.981173	-0.837882	2.139920
				C	4.738168	-2.335668	0.640377
				C	5.027189	0.857970	3.484860
				C	5.700359	-1.422682	2.705243
				C	2.832285	-1.190867	-0.961375

C	2.840031	-2.584801	-1.180458	H	0.676460	-2.728075	-3.721536
C	2.107350	-0.352422	-1.853544	C	1.989382	1.160276	-1.516901
C	2.160379	-3.159893	-2.243214	C	2.324305	1.624543	-0.188209
H	3.360831	-3.231565	-0.484086	C	1.597157	2.100609	-2.497376
C	1.403250	-0.967995	-2.914275	C	2.037538	2.988667	0.158677
C	1.429949	-2.339693	-3.113818	C	1.337827	3.433445	-2.122064
H	2.176909	-4.236648	-2.381887	C	1.505628	3.863728	-0.816372
H	0.789799	-0.365699	-3.565853	H	1.030963	4.137926	-2.888499
H	0.863865	-2.773730	-3.932675	H	1.320876	4.900370	-0.552623
C	2.006918	1.093134	-1.585861	C	1.517319	1.788584	-3.949327
C	2.271919	1.525392	-0.224928	C	0.380271	2.130451	-4.697004
C	1.605734	2.054971	-2.542397	C	2.605746	1.201182	-4.616031
C	1.920039	2.862696	0.161980	C	0.322760	1.873313	-6.068073
H	-0.526675	1.176990	-2.338193	H	-0.469457	2.581756	-4.193472
C	1.281128	3.365544	-2.123024	C	2.550155	0.946472	-5.983947
C	1.390690	3.753912	-0.802318	H	3.494676	0.943158	-4.049328
H	0.956668	4.079341	-2.872586	C	1.405957	1.277934	-6.716144
H	1.148015	4.770496	-0.507856	H	-0.570449	2.135027	-6.627641
C	1.557262	1.809277	-4.010033	H	3.402032	0.493044	-6.482193
C	0.412550	2.148310	-4.750237	H	1.362087	1.076448	-7.782108
C	2.672560	1.294615	-4.690962	O	-1.458268	0.882256	1.749803
C	0.379845	1.957135	-6.132668	C	-1.106754	-0.266801	2.569428
H	-0.460261	2.533574	-4.230168	O	-1.646665	-1.329618	2.213780
C	2.638992	1.106315	-6.070536	O	-0.302721	0.002729	3.475449
H	3.564077	1.040020	-4.126411	Cs	1.203686	-2.700603	2.926870
C	1.490359	1.434133	-6.797605	H	2.456718	3.431981	1.055050
H	-0.516680	2.214233	-6.689359	H	-2.061031	0.539108	1.073254
H	3.511125	0.709029	-6.581599				
H	1.464203	1.286094	-7.872956	INT1			
O	-2.214336	2.623996	-2.146973	Pd	1.173911	0.245278	-0.668404
C	-2.403621	1.386737	-2.046319	P	-0.355409	-1.250475	-1.554975
O	-3.433334	0.754927	-1.722565	C	-1.949738	-0.316108	-1.973107
Cs	-1.765413	-1.769288	-0.297341	C	-2.673802	-0.059987	-0.623180
Cs	-3.311141	2.877692	0.829871	C	-2.914463	-1.024442	-2.950509
O	-1.392421	0.644327	1.636135	C	-1.589390	1.077246	-2.558317
C	-1.108642	-0.076388	2.735242	H	-2.948865	-1.001740	-0.141068
O	-1.599423	-1.258379	2.804039	H	-1.990341	0.462317	0.057454
O	-0.352696	0.422665	3.637532	C	-3.946848	0.779346	-0.839817
Cs	1.351131	-2.106059	3.636847	H	-3.187862	-2.016076	-2.580563
O	-1.284384	0.573071	-2.296385	H	-2.423412	-1.166154	-3.918532
H	2.299855	3.291998	1.082149	C	-4.187780	-0.177360	-3.152613
			H	-0.913651	1.591917	-1.866914	
			H	-1.052581	0.971005	-3.504151	
I_Cs'							
Pd	0.407460	1.747832	0.867416	C	-2.858857	1.920404	-2.783633
C	3.202822	0.787221	0.656731	H	-4.442061	0.923153	0.128419
C	3.548856	-0.522588	0.233238	C	-4.890483	0.031343	-1.799336
C	3.757623	1.276095	1.858904	C	-3.573228	2.143477	-1.441136
C	4.492855	-1.254118	0.987094	H	-4.858682	-0.707880	-3.839357
C	4.651808	0.524867	2.605462	C	-3.802883	1.186419	-3.752381
H	3.483609	2.260803	2.215617	H	-2.565853	2.886901	-3.212136
C	5.038802	-0.746437	2.156797	H	-5.814823	0.605387	-1.940565
H	4.807823	-2.234175	0.647358	H	-5.173619	-0.938310	-1.369798
H	5.062199	0.930862	3.524777	H	-2.919998	2.693354	-0.754472
H	5.763463	-1.330249	2.715932	H	-4.475902	2.750189	-1.589265
C	2.854901	-1.109922	-0.917968	H	-3.310806	1.042738	-4.722907
C	2.893041	-2.499891	-1.161379	H	-4.703290	1.788017	-3.929969
C	2.051277	-0.289067	-1.753508	C	0.412858	-2.078192	-3.080417
C	2.144454	-3.082259	-2.172183	C	0.603048	-1.016879	-4.188776
H	3.491800	-3.140217	-0.524156	C	-0.344474	-3.292982	-3.662352
C	1.259519	-0.913061	-2.742986	C	1.819287	-2.568175	-2.639991
C	1.304633	-2.280903	-2.957312	H	-0.370053	-0.663139	-4.541465
H	2.188049	-4.155476	-2.330320	H	1.137624	-0.152459	-3.776752
H	0.584538	-0.311367	-3.335054	C	1.377461	-1.606477	-5.380588

H	-1.356226	-3.013317	-3.967132	C	-3.805464	0.880322	-1.567687
H	-0.436457	-4.071444	-2.899312	H	-3.173779	-2.138142	-2.952825
C	0.421082	-3.873489	-4.871291	H	-2.281417	-1.501588	-4.330016
H	2.376254	-1.726659	-2.213684	C	-3.999173	-0.305110	-3.776563
H	1.723787	-3.323207	-1.850257	H	-0.668860	1.352495	-2.503438
C	2.589848	-3.163896	-3.831895	H	-0.780288	0.571012	-4.065996
H	1.491692	-0.830706	-6.147590	C	-2.534835	1.723074	-3.552311
C	0.584839	-2.794327	-5.955675	H	-4.340283	1.166239	-0.651897
C	2.762768	-2.082616	-4.912234	C	-4.754730	0.104581	-2.498750
H	-0.149740	-4.718868	-5.274474	C	-3.288448	2.141285	-2.279275
C	1.808158	-4.354779	-4.412681	H	-4.674913	-0.856437	-4.442194
H	3.574125	-3.500156	-3.483504	C	-3.485241	0.958531	-4.490427
H	1.106857	-3.212680	-6.825396	H	-2.145332	2.614150	-4.060236
H	-0.400007	-2.454648	-6.301066	H	-5.621790	0.725272	-2.758488
H	3.332178	-1.236050	-4.507458	H	-5.136541	-0.787252	-1.984592
H	3.332230	-2.482928	-5.760533	H	-2.614877	2.697362	-1.614564
H	1.701890	-5.141535	-3.654943	H	-4.125332	2.806065	-2.529864
H	2.355798	-4.790581	-5.257863	H	-2.958592	0.680339	-5.412338
C	-0.836790	-2.662894	-0.430152	H	-4.330171	1.596640	-4.780366
C	-2.062251	-3.555042	-0.682134	C	0.502572	-2.431501	-3.179438
H	-0.921087	-2.211683	0.563911	C	0.813232	-1.539368	-4.404470
H	0.064848	-3.286012	-0.385073	C	-0.258872	-3.688728	-3.656687
C	-2.121752	-4.721325	0.311404	C	1.853073	-2.897538	-2.569377
H	-2.981791	-2.968463	-0.589119	H	-0.119180	-1.215617	-4.877375
H	-2.057412	-3.953703	-1.699814	H	1.344909	-0.636633	-4.083049
C	-3.354316	-5.605448	0.107706	C	1.652550	-2.308622	-5.441382
H	-1.210698	-5.326026	0.211365	H	-1.231441	-3.415503	-4.076737
H	-2.115188	-4.324166	1.335087	H	-0.445887	-4.353253	-2.807838
H	-3.378982	-6.431680	0.825395	C	0.570280	-4.453651	-4.710420
H	-4.277174	-5.027305	0.230831	H	2.410854	-2.024821	-2.211366
H	-3.366474	-6.036620	-0.899768	H	1.670670	-3.537265	-1.697212
Cl	2.555672	1.897166	1.682905	C	2.685156	-3.673137	-3.606747
C	2.514654	1.890911	-0.105911	H	1.854165	-1.648714	-6.294249
C	1.774736	2.893911	-0.810641	C	0.860883	-3.540874	-5.914339
C	3.498128	1.115776	-0.770752	C	2.979820	-2.757713	-4.807319
C	2.109748	3.110354	-2.156326	H	-0.000799	-5.330283	-5.040669
C	3.782008	1.365563	-2.123867	C	1.898391	-4.908184	-4.080268
H	4.104114	0.423248	-0.198627	H	3.627156	-3.989431	-3.142066
C	3.109066	2.377068	-2.803699	H	1.432626	-4.090494	-6.672932
H	1.553588	3.864792	-2.703321	H	-0.079602	-3.224464	-6.383654
H	4.546748	0.776699	-2.619692	H	3.554022	-1.881965	-4.478915
H	3.339755	2.583752	-3.843416	H	3.591568	-3.289164	-5.547429
C	0.730203	3.725957	-0.165053	H	1.702445	-5.576903	-3.232306
C	0.725137	5.116524	-0.354031	H	2.488868	-5.474937	-4.811383
C	-0.290453	3.149213	0.609192	C	-0.958296	-2.658919	-0.592207
C	-0.273083	5.909289	0.213784	C	-2.221880	-3.505365	-0.788251
H	1.516372	5.577501	-0.936969	H	-1.040688	-2.055010	0.317774
C	-1.283819	3.941277	1.180364	H	-0.101255	-3.320391	-0.416870
H	-0.306952	2.069969	0.732577	C	-2.454968	-4.440112	0.405224
C	-1.280454	5.325098	0.983019	H	-3.100619	-2.862000	-0.899205
H	-0.259085	6.983769	0.058528	H	-2.166183	-4.099864	-1.704977
H	-2.069101	3.475795	1.768215	C	-3.738401	-5.263265	0.274749
H	-2.058167	5.941162	1.423707	H	-1.592132	-5.110835	0.512214
INT1_Cs							
Pd	0.950999	0.266179	-0.672944	H	-3.882897	-5.923253	1.136331
P	-0.328868	-1.410251	-1.824733	H	-4.616595	-4.611075	0.201113
C	-1.843246	-0.470628	-2.463365	H	-3.715010	-5.887945	-0.625376
C	-2.618840	-0.023162	-1.195239	Cs	2.752448	0.620206	4.190159
C	-2.806275	-1.215984	-3.412096	O	1.675714	-1.242954	1.960010
C	-1.352051	0.819268	-3.168964	O	-0.182926	-0.175401	1.232537
H	-2.995580	-0.899327	-0.660306	C	0.524232	-0.735329	2.207343
H	-1.927046	0.496809	-0.523880	O	0.021670	-0.706872	3.394895
				Cs	-2.891521	-0.100522	2.578812

Cl	3.271798	2.196618	0.848826	C	3.159752	-1.823952	-2.581385	
C	1.941316	2.084492	-0.478104	H	2.216098	0.135561	-5.279780	
C	1.026235	3.210937	-0.489751	C	1.350584	-1.819507	-4.904915	
C	2.390037	1.530827	-1.739913	C	3.401853	-0.891657	-3.781004	
C	0.634132	3.729727	-1.711427	H	0.605711	-3.663045	-4.035384	
C	2.007467	2.174993	-2.957301	C	2.463123	-3.110207	-3.059254	
H	3.295208	0.929664	-1.749116	H	4.116951	-2.074722	-2.107792	
C	1.142224	3.242879	-2.945365	H	1.964666	-2.329441	-5.658007	
H	-0.108229	4.523406	-1.721045	H	0.394549	-1.568271	-5.382114	
H	2.425703	1.812138	-3.892971	H	3.911812	0.021937	-3.449205	
H	0.831466	3.714758	-3.872570	H	4.055305	-1.380289	-4.514907	
C	0.497232	3.774655	0.773841	H	2.306413	-3.789916	-2.211912	
C	0.380535	5.164594	0.942954	H	3.097426	-3.636213	-3.784087	
C	0.091617	2.931882	1.826630	C	-0.632428	-1.079037	0.352409	
C	-0.124613	5.704170	2.127214	C	-1.855223	-1.966166	0.081582	
H	0.708631	5.824452	0.145280	H	-0.768496	-0.524069	1.286355	
C	-0.406803	3.476593	3.011313	H	0.246331	-1.715117	0.519040	
H	0.127877	1.851323	1.690692	C	-2.021750	-3.040236	1.163439	
C	-0.516268	4.862721	3.170920	H	-2.764925	-1.357307	0.052493	
H	-0.200320	6.782152	2.238387	H	-1.784865	-2.452422	-0.895412	
H	-0.714576	2.812269	3.815672	C	-3.258974	-3.914123	0.945035	
H	-0.902218	5.280758	4.096239	H	-1.122419	-3.670173	1.186192	
				H	-2.079187	-2.554665	2.146965	
INT1_Na								
Pd	1.243757	1.891874	0.332854	H	-3.357259	-4.675231	1.725883	
P	-0.024140	0.228413	-0.831615	H	-4.173133	-3.309499	0.950089	
C	-1.553664	1.114441	-1.505738	Na	1.905112	1.844602	5.524630	
C	-2.380552	1.528969	-0.258388	O	1.621550	0.751841	3.571064	
C	-2.455017	0.327378	-2.481451	O	-0.038090	1.528832	2.242697	
C	-1.101526	2.429560	-2.195421	C	0.515074	1.372773	3.417007	
H	-2.716962	0.649033	0.295962	O	-0.093566	1.917076	4.444542	
H	-1.727778	2.097328	0.411998	Na	-1.622430	2.884991	3.060860	
C	-3.602301	2.369603	-0.665246	Cl	3.782964	3.480770	1.800836	
H	-2.792375	-0.608826	-2.029359	C	2.468348	3.603220	0.513766	
H	-1.892540	0.064041	-3.383366	C	1.683583	4.822453	0.516447	
C	-3.677615	1.181295	-2.880590	C	2.780082	2.964876	-0.748253	
H	-0.462484	2.994699	-1.509640	C	1.262831	5.333143	-0.701923	
H	-0.493287	2.213902	-3.076460	C	2.397097	3.610698	-1.965499	
C	-2.317007	3.275879	-2.612707	H	3.618284	2.274642	-0.786043	
H	-4.173830	2.625437	0.236822	C	1.643052	4.758923	-1.941761	
C	-4.486413	1.550718	-1.623553	H	0.604912	6.197235	-0.701502	
C	-3.130484	3.655044	-1.364372	H	2.725124	3.182124	-2.908463	
H	-4.307240	0.600057	-3.565639	H	1.327813	5.232861	-2.866366	
C	-3.201362	2.467531	-3.579073	C	1.290170	5.488743	1.777947	
H	-1.957801	4.185386	-3.110455	C	1.176776	6.887272	1.857573	
H	-5.374734	2.130142	-1.905611	C	0.990939	4.735018	2.927076	
H	-4.839306	0.640101	-1.122400	C	0.758288	7.507701	3.035897	
H	-2.509257	4.247805	-0.679927	H	1.434974	7.492670	0.994420	
H	-3.992399	4.274657	-1.643594	C	0.570939	5.352912	4.104096	
H	-2.634408	2.214729	-4.484276	H	1.065372	3.658001	2.876915	
H	-4.065151	3.066884	-3.894355	C	0.450256	6.745514	4.165243	
C	0.893828	-0.733472	-2.176942	H	0.682514	8.590558	3.073511	
C	1.153345	0.175810	-3.399852	H	0.329216	4.736414	4.965246	
C	0.223864	-2.040417	-2.657674	H	0.126770	7.229723	5.081791	
C	2.268249	-1.103277	-1.554126					
H	0.205669	0.433344	-3.882316	INT1_PBu3				
H	1.616140	1.111887	-3.071116	Pd	2.220457	1.489293	-0.124453	
C	2.052495	-0.535507	-4.427448	P	0.610876	0.036765	-0.883868	
H	-0.760916	-1.833899	-3.087976	C	0.058614	-1.164199	0.436291	
H	0.073564	-2.714442	-1.808862	C	-1.405214	-1.620051	0.438689	
C	1.112528	-2.749009	-3.701878	H	0.292740	-0.693934	1.396344	
H	2.760323	-0.191368	-1.198583	H	0.730748	-2.027629	0.353127	
H	2.121835	-1.748574	-0.679068	C	-1.692543	-2.627972	1.557261	

H	-2.061195	-0.751122	0.568119	C	-1.249640	2.558471	-1.869286
H	-1.672109	-2.064922	-0.525381	H	-2.878108	0.562212	0.469043
C	-3.159248	-3.063019	1.596054	H	-2.002695	2.045793	0.776943
H	-1.048134	-3.507068	1.425304	C	-3.795755	2.301005	-0.417053
H	-1.412002	-2.183904	2.521592	H	-2.771806	-0.574695	-1.800541
H	-3.342663	-3.782936	2.400040	H	-1.880348	0.166046	-3.125859
H	-3.819632	-2.203743	1.758871	C	-3.730852	1.175374	-2.658400
H	-3.455025	-3.533329	0.651466	H	-0.668910	3.154624	-1.164794
Cl	3.152955	1.816137	3.023657	H	-0.608711	2.387654	-2.737696
C	2.813710	2.842756	1.607647	C	-2.504124	3.337072	-2.300556
C	1.723462	3.761781	1.639971	H	-4.403203	2.498630	0.473929
C	3.836664	2.947175	0.633906	C	-4.604592	1.468529	-1.426876
C	1.733360	4.794933	0.694892	C	-3.367335	3.630024	-1.061911
C	3.770584	3.984569	-0.323210	H	-4.294718	0.569896	-3.377772
H	4.727546	2.335560	0.721675	C	-3.305820	2.501254	-3.313293
C	2.739673	4.915892	-0.271251	H	-2.187329	4.279255	-2.763050
H	0.904347	5.494933	0.694811	H	-5.506518	2.014848	-1.728896
H	4.559032	4.067722	-1.063705	H	-4.933276	0.529688	-0.963785
H	2.701309	5.728449	-0.988995	H	-2.798701	4.231412	-0.342150
C	0.592518	3.643987	2.589894	H	-4.253633	4.210710	-1.345468
C	0.064861	4.787433	3.209681	H	-2.695760	2.303274	-4.203752
C	-0.020948	2.404139	2.835070	H	-4.191962	3.056424	-3.644475
C	-1.048544	4.695785	4.045443	C	0.830291	-0.579981	-1.979907
H	0.538124	5.750254	3.044207	C	1.020790	0.326005	-3.221017
C	-1.130731	2.312414	3.671067	C	0.147281	-1.895259	-2.432257
H	0.361935	1.520640	2.337868	C	2.218360	-0.968099	-1.399682
C	-1.651541	3.458467	4.278188	H	0.049373	0.550516	-3.669873
H	-1.440832	5.591251	4.517745	H	1.469622	1.279129	-2.939046
H	-1.597718	1.346290	3.837553	C	1.895607	-0.379959	-4.273012
H	-2.519233	3.387035	4.926776	H	-0.856992	-1.704240	-2.817709
C	-0.934410	0.938058	-1.383012	H	0.051722	-2.574353	-1.581256
H	-1.749950	0.232923	-1.575779	C	0.996519	-2.594363	-3.516839
H	-0.702028	1.431648	-2.334346	H	2.738153	-0.084951	-1.018824
C	0.986988	-1.030735	-2.357352	H	2.084552	-1.640936	-0.544712
H	1.924868	-1.547807	-2.122216	C	3.076524	-1.668389	-2.469898
H	1.223139	-0.330804	-3.168718	H	2.025540	0.295693	-5.126477
C	-0.068841	-2.040495	-2.818484	C	1.185378	-1.665612	-4.728373
H	-0.248520	-2.775012	-2.024870	C	3.268002	-0.724785	-3.670050
H	-1.024589	-1.533005	-2.997776	H	0.473760	-3.507110	-3.826066
C	0.353439	-2.780724	-4.093155	C	2.371877	-2.955221	-2.931398
H	1.314687	-3.280943	-3.916174	H	4.050436	-1.913287	-2.030393
H	0.530999	-2.049062	-4.892302	H	1.776226	-2.173938	-5.500150
C	-0.685493	-3.806299	-4.552365	H	0.213059	-1.418994	-5.173192
H	-0.363119	-4.323080	-5.461918	H	3.782512	0.191315	-3.353842
H	-0.857879	-4.564203	-3.779810	H	3.901272	-1.203585	-4.426811
H	-1.646965	-3.324853	-4.763713	H	2.253662	-3.643643	-2.085295
C	-1.345728	1.981106	-0.339032	H	2.979892	-3.468850	-3.686168
H	-0.496140	2.649964	-0.156712	C	-0.572017	-0.947789	0.633545
H	-1.544508	1.490348	0.620964	C	-1.747283	-1.910745	0.385203
C	-2.570301	2.807367	-0.737149	H	-0.749731	-0.413635	1.573734
H	-3.429176	2.141074	-0.893495	H	0.346355	-1.525014	0.792646
H	-2.380235	3.295168	-1.702651	C	-1.786956	-3.017686	1.445506
C	-2.916014	3.862527	0.317846	H	-2.693951	-1.363664	0.410144
H	-3.127654	3.395543	1.285871	H	-1.684033	-2.366926	-0.604475
H	-2.078325	4.552731	0.468973	C	-2.966855	-3.971468	1.246626
H	-3.791310	4.452647	0.027649	H	-0.844817	-3.580220	1.412645
				H	-1.839729	-2.562425	2.442958
INT2				H	-2.977118	-4.756732	2.008815
Pd	1.392908	1.562924	0.789170	H	-3.920513	-3.435075	1.304596
P	-0.081628	0.356680	-0.608153	H	-2.918125	-4.456808	0.265455
C	-1.647476	1.208873	-1.217958	Cl	2.957366	2.289571	2.470616
C	-2.552429	1.497829	0.010376	C	1.856495	3.054145	-0.438891
C	-2.474693	0.383978	-2.235460	C	1.451127	4.386060	-0.205160

C	2.731306	2.763234	-1.487271	C	2.220823	-2.595972	-5.501165
C	1.854054	5.359194	-1.144463	H	-0.058716	-5.607475	-4.375429
C	3.142497	3.753381	-2.383149	C	1.854445	-4.629075	-4.068331
H	3.107076	1.757443	-1.614959	H	3.486910	-3.216521	-3.851523
C	2.676709	5.056913	-2.224672	H	0.644893	-4.601866	-6.556828
H	1.499785	6.376862	-1.014864	H	-0.922394	-3.965860	-6.048069
H	3.812817	3.495070	-3.197565	H	2.641487	-1.582859	-5.536453
H	2.959608	5.835569	-2.926005	H	2.751331	-3.194930	-6.252045
C	0.667123	4.844826	0.971702	H	2.006998	-5.071995	-3.076060
C	0.944096	6.092657	1.557343	H	2.385922	-5.260114	-4.791797
C	-0.359741	4.075522	1.534052	C	-0.779873	-2.236055	-0.532705
C	0.210995	6.551753	2.651275	C	-1.928843	-3.233628	-0.350452
H	1.757943	6.696815	1.170219	H	-0.783190	-1.519482	0.291405
C	-1.098716	4.529807	2.624365	H	0.188240	-2.739512	-0.445342
H	-0.570006	3.105883	1.107603	C	-1.750393	-4.057476	0.930925
C	-0.818465	5.775559	3.188707	H	-2.885704	-2.704361	-0.292892
H	0.451784	7.515308	3.090339	H	-2.005609	-3.912727	-1.204090
H	-1.894556	3.910466	3.028071	C	-2.905137	-5.032449	1.170049
H	-1.388871	6.134384	4.039855	H	-0.802578	-4.608681	0.875020
				H	-1.657414	-3.376808	1.788062
INT2_Cs				H	-2.757796	-5.611093	2.087519
Pd	0.920848	0.685794	-1.449985	H	-3.857873	-4.497875	1.259850
P	-0.584039	-1.164631	-2.036231	H	-3.000130	-5.740402	0.339029
C	-2.286883	-0.519637	-2.508985	Cs	3.646432	1.215718	2.766230
C	-2.895395	0.104859	-1.223176	O	2.368575	-1.471059	0.047197
C	-3.269873	-1.563307	-3.086083	O	0.956731	0.247556	0.534585
C	-2.119607	0.634907	-3.533934	C	1.692691	-0.842629	0.900487
H	-3.028386	-0.656582	-0.449382	O	1.606928	-1.087802	2.146998
H	-2.205313	0.856010	-0.822439	Cs	-1.067044	0.411624	2.891044
C	-4.258526	0.752858	-1.530739	Cl	1.154268	2.055347	5.153968
H	-3.409052	-2.389096	-2.384418	C	2.213118	2.178342	-1.031745
H	-2.866166	-1.993380	-4.008099	C	1.929983	3.354309	-0.298829
C	-4.630671	-0.903749	-3.386255	C	3.510402	1.988332	-1.533357
H	-1.437420	1.388844	-3.120949	C	2.951635	4.309390	-0.120838
H	-1.668219	0.270666	-4.458308	C	4.517665	2.941128	-1.344949
C	-3.481176	1.279870	-3.854558	H	3.747642	1.071105	-2.069732
H	-4.667463	1.169797	-0.601877	C	4.233624	4.108663	-0.632196
C	-5.216559	-0.315093	-2.089407	H	2.728957	5.228310	0.414915
C	-4.082871	1.872191	-2.570915	H	5.513801	2.769253	-1.744243
H	-5.311841	-1.664650	-3.785866	H	5.001791	4.861299	-0.480104
C	-4.435925	0.215264	-4.424055	C	0.599038	3.614109	0.311444
H	-3.329198	2.075051	-4.594375	C	0.506158	4.182778	1.594732
H	-6.199451	0.129705	-2.289110	C	-0.598215	3.319753	-0.365728
H	-5.366065	-1.111485	-1.349149	C	-0.732086	4.437260	2.187191
H	-3.424269	2.657614	-2.182550	H	1.414029	4.400909	2.148096
H	-5.051262	2.340891	-2.786030	C	-1.837722	3.570327	0.225488
H	-4.025762	-0.202466	-5.352327	H	-0.548337	2.899115	-1.365209
H	-5.401324	0.672893	-4.673244	C	-1.912613	4.131444	1.504326
C	0.161656	-2.284661	-3.364844	H	-0.771565	4.859570	3.186786
C	-0.020616	-1.693122	-4.782259	H	-2.749417	3.336911	-0.314442
C	-0.378554	-3.733146	-3.350557	H	-2.878107	4.327948	1.961050
C	1.685357	-2.324256	-3.067376				
H	-1.080386	-1.651986	-5.048664	INT2_Na			
H	0.363903	-0.665815	-4.809267	Pd	0.882870	0.559544	-0.418832
C	0.717898	-2.554735	-5.825727	P	-0.599221	-1.256379	-1.119946
H	-1.455304	-3.743354	-3.548773	C	-2.215605	-0.450371	-1.643450
H	-0.223649	-4.176111	-2.362344	C	-2.828732	0.154327	-0.349914
C	0.352776	-4.591118	-4.401646	C	-3.251307	-1.365301	-2.332135
H	2.080379	-1.301799	-3.106855	C	-1.891066	0.736362	-2.591971
H	1.872047	-2.675462	-2.049047	H	-3.069896	-0.633261	0.369784
C	2.418566	-3.198175	-4.099559	H	-2.092795	0.810998	0.126639
H	0.563887	-2.112695	-6.817585	C	-4.108335	0.942919	-0.681948
C	0.146560	-3.983739	-5.799680	H	-3.497123	-2.218706	-1.695117

H	-2.835364	-1.767589	-3.262099	C	1.883319	3.133562	0.966051
C	-4.530887	-0.564944	-2.650972	C	3.385112	1.900191	-0.489806
H	-1.158658	1.398697	-2.111525	C	2.927786	4.047817	1.206470
H	-1.435246	0.377072	-3.516232	C	4.408455	2.822888	-0.254922
C	-3.168147	1.527157	-2.931023	H	3.584999	1.037230	-1.124981
H	-4.527034	1.342505	0.250203	C	4.177460	3.896827	0.608297
C	-5.127268	0.000227	-1.348553	H	2.744334	4.896075	1.859630
C	-3.774263	2.098677	-1.639766	H	5.378654	2.694099	-0.726707
H	-5.256309	-1.234571	-3.128095	H	4.963646	4.618378	0.808774
C	-4.185891	0.590846	-3.606633	C	0.569519	3.362713	1.619036
H	-2.905713	2.344937	-3.612621	C	-0.632969	3.245569	0.899273
H	-6.055082	0.543574	-1.566065	C	0.505597	3.727774	2.975577
H	-5.384476	-0.818867	-0.665055	C	-1.863422	3.475810	1.517493
H	-3.063324	2.789825	-1.171307	H	-0.594511	2.973743	-0.150594
H	-4.680097	2.673956	-1.867336	C	-0.725718	3.959527	3.595230
H	-3.770271	0.193611	-4.541227	H	1.422050	3.796905	3.555689
H	-5.093692	1.148971	-3.866851	C	-1.916782	3.833832	2.870725
C	0.163884	-2.363167	-2.438133	H	-2.781582	3.383865	0.946061
C	0.233252	-1.622575	-3.794106	H	-0.754104	4.232177	4.646137
C	-0.538967	-3.725071	-2.641290	H	-2.873160	4.019330	3.350279
C	1.619940	-2.633326	-1.965020				
H	-0.776098	-1.434529	-4.171520	INT2_PBu3			
H	0.721428	-0.648301	-3.662940	Pd	1.922043	1.889964	0.167612
C	0.999322	-2.465827	-4.830877	P	0.322761	0.500289	-0.741281
H	-1.576075	-3.579021	-2.959117	C	-0.419215	-0.544597	0.594918
H	-0.562096	-4.275723	-1.696267	C	-1.710800	-1.304565	0.260991
C	0.217145	-4.564622	-3.690984	H	-0.590033	0.115516	1.451566
H	2.143468	-1.680522	-1.817230	H	0.373273	-1.238210	0.900816
H	1.615428	-3.146947	-0.996735	C	-2.174192	-2.179016	1.431631
C	2.376550	-3.486576	-2.999407	H	-2.504158	-0.591242	0.012180
H	1.028260	-1.916155	-5.779158	H	-1.571202	-1.931779	-0.624530
C	0.266175	-3.804854	-5.028034	C	-3.479598	-2.917332	1.127367
C	2.431826	-2.727279	-4.336017	H	-1.385687	-2.902737	1.675015
H	-0.309575	-5.516917	-3.825585	H	-2.301730	-1.550217	2.322333
C	1.649536	-4.828476	-3.194844	H	-3.793561	-3.536348	1.973517
H	3.393803	-3.665696	-2.631619	H	-4.288850	-2.211463	0.909746
H	0.782125	-4.408569	-5.784678	H	-3.367401	-3.572347	0.256160
H	-0.751757	-3.624469	-5.396455	Cl	3.845280	3.019470	1.105521
H	2.965415	-1.776958	-4.206835	C	1.116442	3.446865	-0.748564
H	2.986424	-3.311966	-5.080140	C	0.513863	4.470495	0.005382
H	1.623706	-5.384449	-2.249169	C	1.246146	3.560036	-2.134377
H	2.192075	-5.447416	-3.920042	C	0.036937	5.600152	-0.686386
C	-0.933738	-2.365675	0.329423	C	0.762625	4.691830	-2.798194
C	-2.166991	-3.275546	0.397685	H	1.724039	2.769007	-2.703112
H	-0.910035	-1.693790	1.192238	C	0.150221	5.712235	-2.070623
H	-0.023606	-2.971125	0.418798	H	-0.447293	6.388395	-0.117405
C	-2.139263	-4.157579	1.651414	H	0.865447	4.767625	-3.876589
H	-3.080413	-2.672452	0.414281	H	-0.239189	6.590161	-2.576357
H	-2.237057	-3.912447	-0.488975	C	0.360456	4.418078	1.483188
C	-3.376080	-5.050729	1.771198	C	0.742193	5.521318	2.261840
H	-1.233391	-4.777741	1.635741	C	-0.179755	3.297869	2.134883
H	-2.056653	-3.516686	2.539715	C	0.607272	5.498973	3.650075
H	-3.335510	-5.672601	2.671013	H	1.170402	6.391174	1.773336
H	-4.291444	-4.450093	1.819948	C	-0.318346	3.274766	3.522207
H	-3.463747	-5.718066	0.906458	H	-0.511530	2.448965	1.550980
Na	3.186439	1.148594	3.855833	C	0.079382	4.373601	4.286736
O	2.558917	-0.238953	2.086460	H	0.920934	6.358648	4.234628
O	0.400068	0.232355	1.543250	H	-0.745048	2.399936	4.003986
C	1.381368	0.039943	2.436887	H	-0.024469	4.354781	5.367270
O	1.013143	0.199444	3.663174	C	-1.068357	1.162555	-1.747781
Na	-1.092767	0.867627	3.139067	H	-1.634344	0.315618	-2.149314
Cl	3.574625	3.270826	5.302175	H	-0.602796	1.672970	-2.596530
C	2.127123	2.047829	0.104133	C	1.236882	-0.631405	-1.882814

H	2.123275	-0.964514	-1.330950	C	-3.238183	-3.407113	0.523302
H	1.605694	0.013981	-2.689282	C	-3.087897	-1.767209	2.295068
C	0.491676	-1.838273	-2.465790	C	-3.310229	-4.426079	1.474653
H	0.209869	-2.523374	-1.658640	H	-3.288867	-3.651935	-0.531957
H	-0.439030	-1.516369	-2.947963	C	-3.154173	-2.788021	3.244838
C	1.348840	-2.595873	-3.486834	H	-2.978884	-0.739062	2.617143
H	2.285654	-2.908881	-3.008049	C	-3.262385	-4.121134	2.839575
H	1.630402	-1.911384	-4.297407	H	-3.409959	-5.457693	1.150212
C	0.629184	-3.816301	-4.064870	H	-3.110406	-2.531777	4.298654
H	1.256649	-4.340868	-4.792094	H	-3.313867	-4.915803	3.577946
H	0.365000	-4.528202	-3.274933				
H	-0.297413	-3.523239	-4.570968				
C	-1.992969	2.133169	-1.005860	INT3_Cs_cf2			
H	-1.393859	2.902614	-0.516536	Pd	-0.396843	-0.460728	0.871972
H	-2.538512	1.606932	-0.213204	C	-0.054403	1.472794	0.498516
C	-2.986763	2.820324	-1.947631	C	-1.023140	2.396099	0.978582
H	-3.630739	2.067767	-2.420913	C	1.024532	1.962847	-0.243805
H	-2.425505	3.304903	-2.756786	C	-0.890568	3.762857	0.712307
C	-3.839252	3.863486	-1.222395	C	1.152120	3.334753	-0.513011
H	-4.413082	3.408026	-0.407484	H	1.767217	1.269876	-0.633967
H	-3.205277	4.644437	-0.787742	C	0.196337	4.232751	-0.032901
H	-4.547914	4.345439	-1.903143	H	-1.637790	4.467692	1.069733
			H	1.993214	3.699087	-1.098483	
			H	0.292212	5.295126	-0.240482	
			C	0.594671	-2.752612	0.231079	
INT3_Cs			O	1.178899	-1.605038	-0.069309	
Pd	0.122972	1.082353	1.640548	O	-0.422815	-2.652988	1.061010
C	-1.097546	2.563698	1.056438	O	0.976280	-3.843814	-0.261904
C	-2.245995	2.782895	1.865863	C	-2.132611	1.751092	1.699899
C	-0.944062	3.338636	-0.096654	C	-3.241250	2.398065	2.257635
C	-3.194060	3.747824	1.510124	C	-2.010941	0.334166	1.768011
C	-1.895934	4.306944	-0.451975	C	-4.245594	1.656890	2.890101
H	-0.079402	3.184723	-0.739634	H	-3.332812	3.480362	2.197729
C	-3.020369	4.510249	0.349995	C	-3.035041	-0.385777	2.394363
H	-4.072280	3.910219	2.131250	C	-4.144751	0.265673	2.956568
H	-1.759372	4.898207	-1.354856	H	-5.104515	2.164163	3.321241
H	-3.758940	5.259351	0.076986	C	-2.982948	-1.472975	2.434521
C	1.999487	-0.419795	0.719253	H	-4.929178	-0.313743	3.438526
O	1.614492	0.673042	0.091301	Cl	-0.295227	-0.303388	-3.373116
O	1.518761	-0.561647	1.938583	C	-1.737644	-0.846634	-2.502705
O	2.732303	-1.290938	0.178728	C	-1.722634	-2.136915	-1.978551
Cs	0.745248	-3.462700	1.809376	C	-2.852196	-0.000868	-2.383676
C	-2.296185	1.911422	3.050725	C	-2.857659	-2.627097	-1.335572
C	-3.324899	1.852609	3.998038	H	-0.831460	-2.748118	-2.048048
C	-1.163127	1.060005	3.167793	C	-3.982235	-0.532825	-1.739088
C	-3.234199	0.973059	5.083167	C	-3.993962	-1.827005	-1.223698
H	-4.202140	2.487674	3.896321	H	-2.837269	-3.624719	-0.911015
C	-1.083570	0.201920	4.269420	H	-4.854121	0.104057	-1.628939
C	-2.109703	0.157087	5.226275	H	-4.881048	-2.200220	-0.722235
H	-4.036487	0.930868	5.814838	C	-2.897969	1.397187	-2.884013
H	-0.226564	-0.460515	4.373883	C	-3.944317	1.800610	-3.727376
H	-2.034917	-0.520888	6.073568	C	-1.947662	2.346045	-2.476789
Cs	2.194624	-0.172820	-2.754066	C	-4.034252	3.122041	-4.165853
Cl	-1.009850	-2.193496	-1.462805	C	-4.681907	1.069988	-4.046060
C	-2.203264	-0.910631	-1.173956	H	-2.042937	3.667288	-2.912296
C	-3.059553	-0.953565	-0.061391	C	-1.151865	2.056801	-1.801563
C	-2.200381	0.156645	-2.070517	C	-3.082247	4.059429	-3.759380
C	-3.901399	0.158365	0.123208	H	-4.846063	3.417660	-4.823838
C	-3.052602	1.237441	-1.855424	H	-1.306380	4.388219	-2.572849
H	-1.527030	0.144536	-2.919655	H	-3.152841	5.089249	-4.096980
C	-3.901548	1.239173	-0.750336	Cs	2.741013	-2.519349	-2.518318
H	-4.562329	0.159635	0.983243	Cs	0.158509	-2.350970	4.057069
H	-3.035166	2.079746	-2.537839				
H	-4.541420	2.090920	-0.555599				
C	-3.114436	-2.065095	0.922227				

INT3_Cs_cf3

Pd	0.101717	1.288939	1.739442	O	0.396642	-0.501499	1.314380
C	-1.064847	2.887030	1.460647	O	1.186222	-0.005524	3.379431
C	-2.194164	2.999949	2.317648	O	2.596907	-0.393902	1.668649
C	-0.909529	3.826371	0.435877	C	-3.076406	2.937675	1.629713
C	-3.146348	4.003435	2.104491	C	-4.115995	3.865107	1.775050
C	-1.858010	4.841583	0.234835	C	-3.320569	1.533197	1.713980
H	-0.052939	3.758864	-0.231816	C	-5.436979	3.437471	1.923300
C	-2.981304	4.921448	1.060870	H	-3.903009	4.930262	1.734990
H	-4.021610	4.075600	2.746349	C	-4.661322	1.144370	1.826926
H	-1.723829	5.559978	-0.570804	C	-5.710934	2.070662	1.920224
H	-3.724232	5.697820	0.899268	H	-6.239903	4.163258	2.018721
C	1.909703	0.007862	0.429292	H	-4.922459	0.095650	1.861732
O	1.522957	1.223199	0.095609	H	-6.735728	1.716718	2.004419
O	1.470631	-0.417569	1.596897	Cl	-0.703758	0.592712	-2.750265
O	2.606039	-0.709906	-0.337450	C	-2.269133	-0.132141	-2.358439
Cs	1.855249	-3.397333	1.110681	C	-2.295531	-1.510575	-2.149049
C	-2.225191	1.976430	3.374005	C	-3.417452	0.666746	-2.233965
C	-3.181770	1.865823	4.388359	C	-3.494024	-2.131603	-1.805446
C	-1.148037	1.052413	3.290761	H	-1.385971	-2.090448	-2.249939
C	-3.088841	0.838609	5.333551	C	-4.604108	0.007311	-1.862948
H	-4.004426	2.575318	4.447458	C	-4.651211	-1.367005	-1.652877
C	-1.075899	0.033918	4.245317	H	-3.515950	-3.205353	-1.651908
C	-2.036726	-0.076270	5.262421	H	-5.504554	0.602481	-1.755211
H	-3.833736	0.756065	6.120636	H	-5.586339	-1.840489	-1.373355
H	-0.269697	-0.695920	4.197992	C	-3.447573	2.134719	-2.453012
H	-1.963882	-0.877187	5.995012	C	-4.063698	2.956008	-1.497978
Cs	0.666470	0.729924	-2.737351	C	-2.919972	2.722861	-3.613804
C	-3.409112	-0.256826	-2.505139	C	-4.122997	4.336717	-1.683675
C	-3.245819	0.354561	-1.250321	H	-4.464689	2.514926	-0.594405
C	-3.412656	0.509139	-3.672116	C	-2.988541	4.102233	-3.801645
C	-3.106827	1.751442	-1.191050	H	-2.467505	2.098064	-4.375779
C	-3.254992	1.898023	-3.604495	C	-3.584345	4.915343	-2.833443
H	-3.544786	0.022219	-4.633830	H	-4.582154	4.953660	-0.918269
C	-3.104772	2.515151	-2.359569	H	-2.579532	4.542073	-4.706378
H	-2.963770	2.233232	-0.231796	H	-3.628836	5.990794	-2.977317
H	-3.253512	2.491425	-4.514011	Cs	2.120696	-1.310308	-1.163701
H	-2.975442	3.590420	-2.287305	Cs	3.381929	2.101794	3.427563
C	-3.259335	-0.425353	0.013685	P	-2.556690	-1.831185	2.580745
C	-2.483985	-1.571453	0.255097	C	-1.374114	-3.311448	2.361899
C	-4.082289	0.007955	1.069070	C	-0.865437	-3.223743	0.897289
C	-2.539024	-2.266907	1.461515	C	-1.997441	-4.716540	2.546247
C	-4.142825	-0.665923	2.283168	C	-0.165832	-3.171778	3.317394
H	-4.679690	0.900199	0.915565	H	-1.703182	-3.346257	0.201103
C	-3.372896	-1.810658	2.479962	H	-0.425280	-2.237794	0.746966
H	-1.924728	-3.148101	1.604497	C	0.184638	-4.313963	0.618937
H	-4.768529	-0.286272	3.081493	H	-2.824346	-4.856241	1.843089
H	-3.400973	-2.336430	3.427636	H	-2.402381	-4.843307	3.553216
H	-3.543314	-1.331247	-2.566251	C	-0.941773	-5.812334	2.278788
Cl	-1.322462	-2.161714	-0.951736	H	0.275197	-2.177916	3.225686
				H	-0.498329	-3.287553	4.353326

INT3_Cs_P

Pd	-1.619098	0.367569	1.646997	H	0.523322	-4.224467	-0.423228
C	-0.838750	2.181365	1.101568	C	-0.438868	-5.702727	0.829547
C	-1.697778	3.296839	1.269976	C	1.376703	-4.125253	1.576348
C	0.465317	2.412932	0.648173	H	-1.409351	-6.792911	2.434064
C	-1.238036	4.596201	1.012379	C	0.248105	-5.645530	3.239930
C	0.919762	3.713683	0.381021	H	1.726359	-4.130214	3.714564
H	1.135672	1.569485	0.518166	H	0.298421	-6.490302	0.625308
C	0.070644	4.807446	0.571493	H	-1.272186	-5.847748	0.129679
H	-1.901290	5.448485	1.137599	H	1.821906	-3.132026	1.448600
H	1.934167	3.870601	0.017782	H	2.153646	-4.872598	1.366277
H	0.418985	5.816324	0.365807	H	-0.089993	-5.745027	4.279589
C	1.404522	-0.294578	2.154475	H	0.987010	-6.437806	3.061844

C	-2.985603	-1.597838	4.421173	C	0.466089	-1.263493	-2.880116
C	-1.842400	-0.782944	5.084716	C	-1.292800	0.439505	-2.911873
C	-3.207449	-2.901436	5.222060	C	-0.464352	-2.241878	-2.536545
C	-4.261345	-0.722975	4.522252	H	1.515581	-1.510904	-2.989133
H	-0.890878	-1.310891	5.014623	C	-2.204825	-0.575104	-2.570109
H	-1.712241	0.154919	4.535511	C	-1.807910	-1.895254	-2.384881
C	-2.170445	-0.484368	6.559152	H	-0.136194	-3.265152	-2.385220
H	-2.309246	-3.522182	5.192133	H	-3.245264	-0.299410	-2.440089
H	-4.019234	-3.486988	4.783278	H	-2.541604	-2.648057	-2.116665
C	-3.542758	-2.582741	6.692817	C	-1.790318	1.835104	-3.028287
H	-4.096226	0.215805	3.991085	C	-2.591808	2.357805	-1.997785
H	-5.114113	-1.214792	4.046047	C	-1.509697	2.643819	-4.141302
C	-4.607880	-0.422638	5.992933	C	-3.082097	3.662616	-2.070775
H	-1.333026	0.071194	6.999924	H	-2.798940	1.751181	-1.126161
C	-2.376318	-1.803135	7.324864	C	-1.999624	3.949144	-4.211647
C	-3.452671	0.360162	6.639136	H	-0.913947	2.248841	-4.956796
H	-3.692557	-3.526639	7.231815	C	-2.783256	4.465609	-3.175279
C	-4.827264	-1.739341	6.756657	H	-3.694522	4.044212	-1.259266
H	-5.524653	0.179588	6.019385	H	-1.774908	4.560541	-5.080689
H	-2.588582	-1.597551	8.381985	H	-3.161565	5.482045	-3.232271
H	-1.460072	-2.406486	7.289074	P	-2.738266	-1.846159	2.760521
H	-3.306692	1.314057	6.116356	C	-1.931596	-3.499336	2.314822
H	-3.691085	0.594309	7.684817	C	-1.920916	-3.563975	0.761954
H	-5.663820	-2.296110	6.314775	C	-2.671197	-4.753700	2.833981
H	-5.091972	-1.531237	7.801294	C	-0.464132	-3.526307	2.807907
C	-4.084203	-2.458444	1.703099	H	-2.948204	-3.536069	0.377218
C	-5.110315	-3.401996	2.343485	H	-1.396757	-2.692946	0.363348
H	-3.673152	-2.938512	0.809964	C	-1.220780	-4.846501	0.278484
H	-4.607578	-1.582572	1.317646	H	-3.693368	-4.770360	2.444708
C	-6.140762	-3.876388	1.310669	H	-2.735452	-4.746568	3.925760
H	-4.623667	-4.274277	2.786889	C	-1.947664	-6.032892	2.362538
H	-5.637679	-2.898150	3.159181	H	0.058970	-2.643251	2.435095
C	-7.203046	-4.797575	1.913871	H	-0.433774	-3.510020	3.901613
H	-6.624536	-3.001487	0.855958	C	0.241164	-4.803920	2.316418
H	-5.618987	-4.395570	0.495244	H	-1.236282	-4.861774	-0.818377
H	-7.923064	-5.129012	1.158758	C	-1.953307	-6.082637	0.825172
H	-6.744230	-5.690069	2.354306	C	0.234524	-4.839585	0.778553
H	-7.761007	-4.287238	2.707113	H	-2.481929	-6.902764	2.763470
INT3c_Cs							
Pd	-1.772743	-0.269944	1.380374	H	1.275958	-4.795051	2.681105
C	-3.526130	3.325800	3.810718	H	-1.461894	-6.999519	0.476173
C	-2.941679	2.668719	2.712152	H	-2.985639	-6.104592	0.453332
C	-2.744205	4.023259	4.732567	H	0.759467	-3.962129	0.382489
C	-1.543880	2.727252	2.579669	H	0.762529	-5.731820	0.418640
C	-1.356341	4.082787	4.576346	H	-0.479384	-6.019198	3.968116
H	-3.219868	4.513877	5.577062	H	0.010067	-6.956291	2.552509
C	-0.755048	3.429657	3.495973	C	-2.489358	-1.360724	4.561955
H	-1.072285	2.233652	1.737006	C	-1.077511	-0.742386	4.725799
H	-0.750030	4.630197	5.292627	C	-2.654473	-2.515212	5.576281
H	0.321637	3.472939	3.335783	C	-3.514081	-0.240501	4.882094
C	-3.803724	1.986257	1.705087	H	-0.311154	-1.480918	4.477227
C	-4.971896	2.661285	1.292706	H	-0.983400	0.091027	4.020757
C	-3.508873	0.720243	1.144499	C	-0.868417	-0.240049	6.165958
C	-5.845294	2.116118	0.355154	H	-1.918622	-3.300032	5.379518
H	-5.180483	3.644170	1.706348	H	-3.643066	-2.970823	5.484209
C	-4.413197	0.182646	0.211367	C	-2.458355	-1.987169	7.011864
C	-5.564891	0.861649	-0.188737	H	-3.389434	0.581437	4.173352
H	-6.730941	2.666567	0.051497	H	-4.537423	-0.609160	4.775870
H	-4.208455	-0.794578	-0.216437	C	-3.313300	0.272992	6.320361
H	-6.233203	0.416215	-0.921186	H	0.145057	0.172308	6.256720
Cl	1.303676	1.235604	-3.462720	C	-1.039334	-1.408600	7.151576
C	0.047209	0.052230	-3.070221	H	-1.899335	0.856387	6.472266
				H	-2.588196	-2.820899	7.712309

C	-3.499234	-0.892353	7.308700	C	-2.029281	-0.929687	-1.148127
H	-4.057565	1.053821	6.517508	C	-2.959457	-0.939518	-0.095214
H	-0.872929	-1.060353	8.178583	C	-1.967192	0.109906	-2.075341
H	-0.294337	-2.188776	6.947572	C	-3.815019	0.174218	-0.006927
H	-1.765513	1.699198	5.788529	C	-2.837021	1.190970	-1.957730
H	-1.756163	1.234674	7.492790	H	-1.232919	0.075999	-2.872199
H	-4.512291	-1.305315	7.220681	C	-3.760279	1.224448	-0.914570
H	-3.383416	-0.534376	8.339348	H	-4.536546	0.198874	0.802457
C	-4.561068	-2.097989	2.511441	H	-2.776828	2.009130	-2.666770
C	-5.427012	-2.890267	3.502084	H	-4.416469	2.077717	-0.792853
H	-4.639373	-2.545839	1.514033	C	-3.096229	-2.019774	0.914736
H	-4.972823	-1.092468	2.402248	C	-3.180327	-3.373136	0.546678
C	-6.845311	-3.086686	2.952801	C	-3.214632	-1.682592	2.274073
H	-4.994307	-3.867214	3.728127	C	-3.363309	-4.362905	1.512760
H	-5.492366	-2.356047	4.454844	H	-3.121737	-3.649554	-0.500087
C	-7.756756	-3.829461	3.931951	C	-3.397859	-2.674399	3.239034
H	-7.277580	-2.106432	2.712477	H	-3.136738	-0.646190	2.579404
H	-6.790246	-3.638703	2.005150	C	-3.471010	-4.018149	2.863858
H	-8.762402	-3.962067	3.520624	H	-3.436739	-5.402700	1.208206
H	-7.356512	-4.822642	4.165032	H	-3.474932	-2.386803	4.282616
H	-7.850598	-3.280452	4.875679	H	-3.618853	-4.789480	3.613773
C	0.528465	0.150423	0.343881				
O	-0.523444	0.918719	0.129582				
O	0.292119	-0.882021	1.131883				
O	1.657618	0.405642	-0.121901				
Cs	0.851587	3.708345	-0.505137				
Cs	2.171643	0.386163	3.346974				
Cs	4.576702	1.016202	-0.719897				
O	3.706237	3.688841	0.534147				
C	3.434501	3.089164	1.657501				
O	4.269044	2.217465	2.145269				
O	2.307006	3.328587	2.268091				
H	-4.601843	3.273997	3.950420				
INT4_Cs							
Pd	0.122001	1.114023	1.535915	Pd	-1.501888	0.138929	1.576918
C	-1.159292	2.568834	1.047885	C	-1.359657	1.761905	0.372331
C	-2.281668	2.733731	1.901997	C	-1.549202	2.986727	1.048404
C	-1.059159	3.372979	-0.089018	C	-1.049061	1.751618	-0.982661
C	-3.271069	3.673898	1.597414	C	-1.425653	4.191614	0.346800
C	-2.049193	4.321845	-0.387813	C	-0.924909	2.963833	-1.676919
H	-0.214411	3.252222	-0.763980	H	-0.896433	0.819549	-1.518822
C	-3.155104	4.468297	0.451680	C	-1.115989	4.177804	-1.014072
H	-4.133307	3.795529	2.249280	H	-1.566615	5.139123	0.859143
H	-1.958500	4.938853	-1.278725	H	-0.681406	2.953784	-2.735516
H	-3.923981	5.200226	0.219390	H	-1.021492	5.113814	-1.556005
C	1.973792	-0.373060	0.448795	C	0.086625	-1.216386	3.062129
O	1.494239	0.701869	-0.159096	O	0.482023	-0.201003	2.312152
O	1.647348	-0.506664	1.705546	O	-1.217189	-1.451260	2.998961
O	2.668902	-1.217579	-0.189545	O	0.860087	-1.898684	3.758682
Na	0.213953	-3.085049	2.406619	Cs	-1.252161	-4.127402	4.485035
C	-2.251007	1.842646	3.071236	C	-1.861620	2.845828	2.473334
C	-3.237928	1.722523	4.055684	C	-2.121794	3.869783	3.394887
C	-1.076947	1.041473	3.130151	C	-1.913335	1.523053	2.942163
C	-3.066672	0.828585	5.119633	C	-2.418726	3.561955	4.723961
H	-4.146040	2.318145	3.997408	H	-2.093007	4.906598	3.072902
C	-0.913718	0.174517	4.214389	C	-2.197359	1.189203	4.253510
C	-1.901154	0.065140	5.206645	C	-2.455598	2.233491	5.154202
H	-3.838080	0.736504	5.879154	H	-2.621389	4.363599	5.427396
H	-0.015230	-0.435134	4.288831	H	-2.208228	0.151216	4.563148
H	-1.761017	-0.619360	6.039971	H	-2.685460	2.000832	6.189838
Na	1.838482	-0.327445	-2.133071	C	-3.454281	0.014223	1.019276
Cl	-0.817556	-2.212590	-1.318276	C	-3.831421	-1.243354	0.501781
				C	-4.421536	1.010174	1.171066
				C	-5.179088	-1.480525	0.179966
				C	-5.755907	0.764830	0.837439
				H	-4.143768	1.982203	1.560709
				C	-6.138388	-0.485330	0.345974
				H	-5.462471	-2.448094	-0.225230
				H	-6.494538	1.551819	0.961841
				H	-7.173769	-0.679172	0.082755
				C	-2.817963	-2.307125	0.305645
				C	-1.559863	-1.995325	-0.240301
				C	-3.063516	-3.634894	0.690748
				C	-0.555245	-2.960355	-0.342596

H	-1.392915	-1.005310	-0.656001	H	0.549243	4.031879	-4.373487
C	-2.071335	-4.607063	0.562122				
H	-4.027191	-3.895809	1.117443	INT5_Na			
C	-0.806687	-4.270607	0.063525	Pd	-0.442958	1.509775	2.036964
H	0.411327	-2.688162	-0.754587	C	-1.331397	3.187830	1.425156
H	-2.278604	-5.629335	0.866282	C	-2.650819	3.404177	1.904761
H	-0.033732	-5.028087	-0.019837	C	-0.780792	4.096844	0.520807
			C	-3.379360	4.517910	1.472017	
INT5_Cs				C	-1.516814	5.211091	0.092004
Pd	-0.371856	1.352752	2.244358	H	0.211398	3.916842	0.120776
C	-1.354348	2.964157	1.591516	C	-2.812385	5.421509	0.567895
C	-2.645571	3.181229	2.150861	H	-4.392909	4.682032	1.830078
C	-0.924246	3.815065	0.568641	H	-1.082793	5.902636	-0.625950
C	-3.439688	4.245360	1.706543	H	-3.384519	6.281955	0.231957
C	-1.729622	4.869943	0.114821	C	1.470191	-1.001664	2.454165
H	0.029505	3.622040	0.090094	O	2.544492	-0.137370	2.501287
C	-2.982524	5.091689	0.690733	O	0.318416	-0.524809	2.717399
H	-4.428839	4.404271	2.129762	O	1.737832	-2.173711	2.124217
H	-1.383940	5.504271	-0.698444	C	-3.131749	2.341619	2.799911
H	-3.609521	5.907467	0.341160	C	-4.411000	2.246315	3.357832
C	1.587015	-1.064807	2.633904	C	-2.171771	1.319056	3.028027
O	2.623492	-0.192300	2.418315	C	-4.754618	1.142373	4.144928
O	0.458835	-0.568571	2.982059	H	-5.149313	3.022968	3.172656
O	1.827672	-2.278107	2.478519	C	-2.531162	0.224520	3.819581
Cs	-1.242211	-1.889043	0.653277	H	2.191292	0.768070	2.391671
C	-3.049133	2.145364	3.115367	C	-3.817450	0.133404	4.376196
C	-4.281406	2.071234	3.777018	H	-5.750649	1.071446	4.573081
C	-2.070295	1.128452	3.294041	H	-1.810371	-0.569705	3.993727
C	-4.563469	0.991013	4.620417	H	-4.084263	-0.725621	4.987271
H	-5.028850	2.848714	3.634916	O	1.018841	-0.190336	-0.228604
C	-2.374230	0.057282	4.141869	C	1.746135	0.845237	-0.015563
H	2.220529	0.677236	2.116841	O	2.903754	0.967722	-0.567809
C	-3.611777	-0.015703	4.800968	O	1.372796	1.780505	0.837527
H	-5.520825	0.937734	5.131959	Cl	-4.237615	0.059583	-4.179759
H	-1.637705	-0.730408	4.280532	C	-4.155346	0.023604	-2.414157
H	-3.830129	-0.856885	5.455502	C	-5.011760	-0.856507	-1.750590
Cs	3.172734	4.219037	0.525019	C	-3.230153	0.823121	-1.725819
Cs	3.527755	-1.681785	-0.292541	C	-4.959481	-0.953153	-0.360085
O	0.895575	0.068645	-0.249529	H	-5.706873	-1.460174	-2.323026
C	1.642764	1.074708	-0.005477	C	-3.199807	0.696857	-0.325525
O	2.598224	1.452239	-0.761755	C	-4.048321	-0.173790	0.356747
O	1.462362	1.758048	1.144518	H	-5.633166	-1.631319	0.154351
Cl	-3.737588	-0.380502	-4.285774	H	-2.499706	1.309718	0.230248
C	-4.015816	0.053933	-2.594337	H	-3.995965	-0.224968	1.439622
C	-4.966232	-0.681020	-1.883925	C	-2.293065	1.775859	-2.378189
C	-3.267925	1.079196	-1.997180	C	-0.916564	1.662177	-2.138220
C	-5.190221	-0.391635	-0.536580	C	-2.758075	2.828400	-3.180277
H	-5.516944	-1.471558	-2.381314	C	-0.020951	2.572898	-2.699898
C	-3.516672	1.345684	-0.639688	H	-0.536816	0.864915	-1.509338
C	-4.463251	0.625175	0.088473	C	-1.862527	3.743079	-3.733955
H	-5.929996	-0.962439	0.016287	H	-3.823008	2.936863	-3.357831
H	-2.943841	2.126603	-0.156536	C	-0.490434	3.616063	-3.499229
H	-4.619809	0.859065	1.136853	H	1.041585	2.461637	-2.503226
C	-2.219344	1.866662	-2.701291	H	-2.236836	4.558035	-4.346308
C	-0.891697	1.781233	-2.262413	H	0.204206	4.328132	-3.935096
C	-2.538682	2.738322	-3.752187	Na	3.049108	-1.361763	0.206870
C	0.105132	2.552866	-2.864736	Na	3.219661	3.016513	0.395600
H	-0.616025	1.111101	-1.453908	Na	-0.732762	-1.220302	0.751519
C	-1.544820	3.515658	-4.347702				
H	-3.567025	2.814684	-4.092264	J_Cs			
C	-0.221086	3.425202	-3.905263	Pd	0.067337	1.677962	-1.197140
H	1.123805	2.455397	-2.498830	C	-0.456382	3.626919	-1.164770
H	-1.804290	4.193990	-5.155375	C	-0.851041	4.154706	-2.419802

C	-0.383705	4.470017	-0.056166	O	0.371899	-1.977961	1.448751
C	-1.142605	5.524616	-2.524606	Na	1.861789	-2.280199	-0.244567
C	-0.679358	5.834836	-0.178227	H	0.319949	0.179285	3.543465
H	-0.089737	4.075028	0.907408	Na	1.052879	1.534846	0.373423
C	-1.057196	6.363487	-1.412743	Na	2.973974	-0.785846	3.142791
H	-1.437106	5.940861	-3.484184	O	3.560320	-1.287110	0.988856
H	-0.613185	6.477891	0.695615	C	3.019661	-0.159685	0.631836
H	-1.287547	7.420688	-1.511202	O	2.959288	0.826515	1.478939
C	1.494638	-0.981210	-2.125672	O	2.453978	-0.051567	-0.533106
O	2.059283	-0.175321	-3.070578	NaCl			
O	0.547482	-0.504536	-1.404786	Na	0.000000	0.000000	-0.281002
O	1.945327	-2.142330	-2.033589	Cl	0.000000	0.000000	2.281002
Cs	2.095058	-1.443779	1.153166	P_Cs			
C	-0.902431	3.202601	-3.543129	Pd	0.144324	-0.167284	-0.280195
C	-1.311906	3.532093	-4.845888	C	-2.788205	1.869173	-0.242146
C	-0.507042	1.883029	-3.223043	C	-2.340678	1.828702	1.099562
C	-1.347346	2.550678	-5.838394	C	-3.191380	3.099460	-0.791193
H	-1.612872	4.547726	-5.092061	C	-2.336974	3.033548	1.828116
C	-0.565144	0.914716	-4.227925	C	-3.185929	4.280425	-0.050066
H	1.914900	0.774879	-2.779081	H	-3.546013	3.114225	-1.817428
C	-0.979974	1.238050	-5.527034	C	-2.757154	4.244680	1.278485
H	-1.668999	2.807022	-6.844345	H	-1.984852	3.007694	2.854799
H	-0.280428	-0.107827	-4.003876	H	-3.522026	5.209626	-0.501192
H	-1.019244	0.467916	-6.294524	H	-2.745840	5.148803	1.881200
Cs	2.924493	4.265134	-3.901080	O	1.180799	-2.932427	-0.256027
Cs	5.082186	-0.832462	-2.528352	C	1.961417	-2.534227	0.671992
O	3.376045	0.834383	-0.518217	O	0.089990	-2.200324	-0.572039
C	3.309927	1.769669	-1.376007	Cs	1.014505	-2.239985	-3.549972
O	4.327680	2.355654	-1.876428	C	-1.926038	0.597782	1.834331
O	2.109673	2.142979	-1.884980	C	-2.567914	0.387433	3.072980
C	0.365861	1.680097	0.894883	C	-0.924034	-0.304124	1.406448
C	-0.818541	1.398828	1.616875	C	-2.243653	-0.685754	3.894056
C	1.517678	2.008920	1.616426	H	-3.365027	1.063595	3.366871
C	-0.821676	1.416314	3.021468	C	-0.599297	-1.376366	2.262583
C	1.511348	2.048216	3.018461	C	-1.242418	-1.569158	3.486512
H	2.438815	2.199960	1.077314	H	-2.771060	-0.833215	4.832559
C	0.341600	1.741750	3.722340	H	0.198249	-2.045995	1.954077
H	-1.730520	1.194041	3.575632	H	-0.964251	-2.410440	4.118682
H	2.417360	2.311573	3.561110	Cs	0.837906	4.886966	-0.215736
H	0.332091	1.764552	4.809006	Cs	3.860655	-0.340551	-0.045011
C	-2.003026	1.128926	0.784231	O	1.728645	2.681616	-2.267065
C	-3.262833	0.760574	1.281286	C	1.240607	1.709852	-1.644372
C	-1.824851	1.264759	-0.613412	O	1.435980	0.454051	-1.976619
C	-4.334600	0.535273	0.417052	O	0.487391	1.881012	-0.564923
H	-3.409358	0.645871	2.351968	C	-2.879959	0.684888	-1.142155
C	-2.901711	1.042582	-1.471000	C	-3.629832	-0.474277	-0.840556
C	-4.154299	0.676349	-0.959322	C	-2.242275	0.772988	-2.391083
H	-5.304084	0.252260	0.817568	C	-3.673213	-1.516351	-1.782189
H	-2.771215	1.146975	-2.541015	C	-2.330869	-0.250149	-3.331512
H	-4.983875	0.503945	-1.640306	H	-1.649348	1.655772	-2.603539
Na2CO3							
C	-0.002928	1.170122	-0.126183	C	-3.039315	-1.412957	-3.018708
O	-0.027509	-0.124903	-0.421949	H	-4.254535	-2.403022	-1.548566
O	1.137281	1.758027	-0.006909	H	-1.841763	-0.143541	-4.296126
O	-1.120098	1.792603	0.029526	H	-3.112858	-2.225067	-3.736425
Na	-2.258265	-0.068408	-0.406686	C	-4.414912	-0.628291	0.410100
Na	2.201441	-0.132856	-0.494871	C	-4.321842	-1.810779	1.157742
Na3_CO3_HCO3							
C	0.133386	-0.858361	1.944380	C	-5.299855	0.371629	0.841078
O	0.579795	-0.716646	3.279076	H	-5.081661	-1.985899	2.312373
O	-0.416265	0.154376	1.449614	C	-3.620797	-2.578686	0.847374
				C	-6.061314	0.196438	1.995400

H	-5.391671	1.286487	0.265862	H	-1.546293	-5.318255	-1.265569
C	-5.954823	-0.982762	2.736418	H	-0.029038	-4.474724	-1.469410
H	-4.982170	-2.901195	2.888075	C	0.503523	-6.868602	-0.229181
H	-6.744133	0.979409	2.312944	H	0.588853	-5.026807	0.904101
H	-6.545647	-1.116685	3.637752	H	-0.923552	-5.902104	1.079424
P_nBu_2Ad				H	0.951753	-7.486859	0.555310
P	-2.491016	-2.260782	-1.110149	H	-0.228091	-7.484921	-0.764131
C	-4.157453	-3.177238	-1.195309	H	1.294535	-6.604148	-0.940160
C	-4.811978	-2.938336	0.194180	PBu3			
C	-4.120842	-4.702886	-1.441769	P	-3.741948	1.672971	0.154567
C	-5.068016	-2.523457	-2.262309	C	-5.328543	2.418377	-0.501374
H	-4.195763	-3.387601	0.982747	C	-3.170425	0.671291	-1.313403
H	-4.856846	-1.862141	0.398343	C	-4.344491	0.352206	1.347948
C	-6.229664	-3.538038	0.250155	C	-4.821893	-0.999304	0.800928
H	-3.521016	-5.188474	-0.666137	H	-5.144533	0.825561	1.932502
H	-3.651844	-4.927642	-2.404264	H	-3.525316	0.180556	2.056326
C	-5.545178	-5.295549	-1.405597	C	-5.357452	-1.921239	1.902421
H	-5.107269	-1.438084	-2.106002	H	-5.601460	-0.855238	0.046497
H	-4.656108	-2.691002	-3.261916	H	-3.993325	-1.504198	0.289900
C	-6.490274	-3.113382	-2.209254	C	-5.807415	-3.282490	1.366025
H	-6.654992	-3.355703	1.244758	H	-4.580875	-2.062966	2.665936
C	-6.161757	-5.051740	-0.017396	H	-6.197576	-1.427425	2.408826
C	-7.105875	-2.866539	-0.821488	H	-6.188578	-3.924411	2.166839
H	-5.484290	-6.374019	-1.597844	H	-6.603694	-3.168499	0.621563
C	-6.417620	-4.626205	-2.481594	H	-4.976521	-3.808685	0.882469
H	-7.104050	-2.627869	-2.977965	H	-5.012438	3.087161	-1.313340
H	-7.167129	-5.488973	0.032178	H	-5.703445	3.076296	0.293073
H	-5.555496	-5.543891	0.753873	H	-3.926099	-0.064476	-1.609103
H	-7.176937	-1.788705	-0.627961	H	-3.068632	1.374534	-2.149483
H	-8.125421	-3.270845	-0.783916	C	-1.828213	-0.025255	-1.057656
H	-5.993335	-4.808578	-3.477399	H	-1.067964	0.726535	-0.808162
H	-7.425112	-5.061301	-2.474896	H	-1.908452	-0.678039	-0.177983
C	-1.696547	-2.132570	-2.829329	C	-1.350755	-0.857482	-2.252519
C	-2.337142	-0.925781	-3.570149	H	-1.270796	-0.207504	-3.134051
C	-1.775314	-3.370267	-3.750150	H	-2.114294	-1.608716	-2.494498
C	-0.205976	-1.768934	-2.586552	C	-0.009744	-1.549522	-1.997527
H	-3.396955	-1.111307	-3.761186	H	0.311268	-2.135814	-2.864575
H	-2.280306	-0.035646	-2.931916	H	0.775701	-0.817054	-1.779479
C	-1.621944	-0.659892	-4.909087	H	-0.074976	-2.228866	-1.139962
H	-2.821751	-3.615679	-3.958105	C	-6.461903	1.510898	-0.991348
H	-1.333874	-4.242662	-3.262755	H	-6.845527	0.917428	-0.153059
C	-1.045430	-3.099454	-5.081545	H	-6.081354	0.794927	-1.730387
H	-0.146412	-0.877084	-1.949232	C	-7.621521	2.300633	-1.610347
H	0.306434	-2.575200	-2.055160	H	-7.996208	3.025960	-0.875625
C	0.518161	-1.507700	-3.920712	H	-7.244786	2.890186	-2.456773
H	-2.109907	0.185277	-5.410324	C	-8.768762	1.401701	-2.077431
C	-1.713096	-1.912737	-5.798688	H	-9.179926	0.823458	-1.242233
C	-0.144908	-0.324668	-4.645574	H	-9.585357	1.986450	-2.513203
H	-1.109027	-3.995279	-5.711730	H	-8.426264	0.688660	-2.835945
C	0.431432	-2.767683	-4.801287	Pd_2P			
H	1.569779	-1.273709	-3.713581	P	-2.313381	1.992747	0.497330
H	-1.220293	-1.726431	-6.761440	Pd	-2.568111	-0.212428	-0.212931
H	-2.763806	-2.147121	-6.012608	P	-2.531921	-2.339345	-1.167115
H	-0.067707	0.582753	-4.033067	C	-0.575472	2.566380	0.010702
H	0.372912	-0.121811	-5.591793	C	0.449226	1.467336	0.403917
H	0.917133	-3.612559	-4.296327	C	-0.099111	3.911888	0.598155
H	0.966662	-2.603648	-5.745172	C	-0.574701	2.646683	-1.540590
C	-1.408160	-3.453552	-0.138212	H	0.489013	1.349296	1.489202
C	-0.794809	-4.732733	-0.730637	H	0.114442	0.507652	-0.007830
H	-2.026912	-3.722718	0.727596	C	1.855147	1.817939	-0.117786
H	-0.599389	-2.839578	0.275201	H	-0.054491	3.848597	1.690455

H	-0.798938	4.713471	0.351375	H	-7.206862	-1.690505	-0.769687	
C	1.303356	4.261975	0.056575	H	-8.200963	-3.138639	-0.962134	
H	-0.897642	1.679821	-1.945061	H	-6.052907	-4.722954	-3.618006	
H	-1.289178	3.396219	-1.891572	H	-7.514937	-4.939525	-2.651476	
C	0.826163	3.002493	-2.068298	C	-1.682860	-2.200703	-2.852197	
H	2.552430	1.029775	0.192215	C	-2.280543	-0.992543	-3.624135	
C	2.301005	3.167204	0.473796	C	-1.743423	-3.444599	-3.764534	
C	1.827019	1.912334	-1.651735	C	-0.200558	-1.850583	-2.547927	
H	1.614293	5.226068	0.477299	H	-3.332854	-1.169228	-3.858279	
C	1.259183	4.357734	-1.479474	H	-2.243704	-0.107432	-2.977568	
H	0.784592	3.069884	-3.162586	C	-1.506484	-0.742666	-4.931729	
H	3.308711	3.419950	0.120395	H	-2.784330	-3.673762	-4.015649	
H	2.348347	3.100546	1.568338	H	-1.335821	-4.321721	-3.256660	
H	1.533959	0.946981	-2.082975	C	-0.952978	-3.189233	-5.064676	
H	2.827057	2.149089	-2.036922	H	-0.173603	-0.957336	-1.912149	
H	0.556057	5.142193	-1.787610	H	0.281882	-2.657150	-1.989092	
H	2.246956	4.638223	-1.866426	C	0.580323	-1.606022	-3.850843	
C	-2.668010	2.250215	2.340031	H	-1.965344	0.104583	-5.456230	
C	-3.976243	1.462630	2.626448	C	-1.574815	-1.999696	-5.817521	
C	-2.881425	3.709012	2.801430	C	-0.038506	-0.420249	-4.609358	
C	-1.538511	1.613516	3.182495	H	-1.000312	-4.088961	-5.690344	
H	-4.803739	1.881010	2.040243	C	0.515225	-2.871707	-4.725375	
H	-3.848066	0.423635	2.299562	H	1.624647	-1.381824	-3.600058	
C	-4.329005	1.512374	4.123995	H	-1.039050	-1.826878	-6.759550	
H	-3.711525	4.155087	2.245747	H	-2.618406	-2.222516	-6.074178	
H	-1.991906	4.313091	2.600418	H	0.022583	0.490191	-4.000030	
C	-3.214358	3.753626	4.307713	H	0.520806	-0.228712	-5.534000	
H	-1.376254	0.578702	2.855505	H	0.970058	-3.717961	-4.194720	
H	-0.601595	2.155863	3.025659	H	1.089764	-2.721568	-5.648126	
C	-1.887819	1.652958	4.681423	C	-1.504317	-3.525852	-0.145146	
H	-5.258842	0.953956	4.287733	C	-0.907962	-4.824249	-0.709502	
C	-4.516359	2.974836	4.563800	H	-2.150358	-3.762022	0.709171	
C	-3.188531	0.872123	4.933783	H	-0.695581	-2.915163	0.269160	
H	-3.343660	4.800254	4.609416	C	-0.311024	-5.698767	0.399312	
C	-2.069454	3.118317	5.115878	H	-1.659483	-5.402976	-1.252360	
H	-1.066292	1.198133	5.248309	H	-0.121458	-4.589979	-1.434293	
H	-4.779038	3.017954	5.628369	C	0.333718	-6.977179	-0.141295	
H	-5.343609	3.432471	4.006382	H	0.432621	-5.116237	0.959230	
H	-3.060857	-0.177002	4.638257	H	-1.101219	-5.957249	1.116810	
H	-3.432478	0.881017	6.003667	H	0.749181	-7.589444	0.665508	
H	-1.138042	3.675693	4.952770	H	-0.398356	-7.587754	-0.682055	
H	-2.293343	3.169406	6.188836	H	1.147363	-6.743212	-0.837101	
C	-4.228952	-3.172866	-1.277163	C	-3.516612	3.134277	-0.370975	
C	-4.905016	-2.922246	0.098764	C	-3.320392	4.654950	-0.464249	
C	-4.227129	-4.695812	-1.536832	H	-4.477364	2.919117	0.112561	
C	-5.087506	-2.478488	-2.360191	H	-3.609984	2.724257	-1.381828	
H	-4.321129	-3.393850	0.898669	C	-4.555494	5.346576	-1.054081	
H	-4.911684	-1.844911	0.302990	H	-3.104824	5.087705	0.515856	
C	-6.340410	-3.477762	0.114067	H	-2.455886	4.884462	-1.095664	
H	-3.661588	-5.205129	-0.750830	C	-4.369272	6.858409	-1.201402	
H	-3.741655	-4.925740	-2.489920	H	-4.785099	4.903597	-2.032217	
C	-5.670365	-5.242442	-1.540532	H	-5.422914	5.140660	-0.412888	
H	-5.089362	-1.394713	-2.188505	H	-5.262977	7.334744	-1.617079	
H	-4.655487	-2.650707	-3.350568	H	-4.161655	7.324470	-0.231466	
C	-6.527719	-3.023767	-2.346453	H	-3.527926	7.087924	-1.865066	
H	-6.783021	-3.290154	1.099995					
C	-6.313211	-4.990699	-0.165603	Pd_2PBu3				
C	-7.168013	-2.768467	-0.971635	Pd	1.151056	0.044433	-0.226195	
H	-5.638015	-6.320285	-1.741523	P	-0.407918	-1.298291	-1.298692	
C	-6.494734	-4.536020	-2.630793	C	-1.920674	-0.378330	-1.865598	
H	-7.106659	-2.512988	-3.125562	C	0.231119	-2.071610	-2.859575	
H	-7.332611	-5.396358	-0.146022	C	-1.071987	-2.731801	-0.304506	
H	-5.742391	-5.507903	0.616103	C	-1.570493	-3.973182	-1.054347	

H	-1.872421	-2.312423	0.318490	H	-1.826167	3.878488	2.603846
H	-0.273316	-3.020296	0.386910	H	-0.842589	3.970893	4.070460
C	-2.156041	-5.025207	-0.105315	C	5.307589	2.697312	0.091788
H	-2.327745	-3.698199	-1.795367	H	5.803865	2.221229	0.945304
H	-0.742165	-4.422222	-1.615352	H	4.913263	3.654974	0.453373
C	-2.634720	-6.279596	-0.840020	C	6.348835	2.964707	-1.001270
H	-1.399146	-5.298246	0.641641	H	6.737747	2.006056	-1.369227
H	-2.991172	-4.581030	0.452207	H	5.856512	3.444592	-1.857354
H	-3.052626	-7.016313	-0.146506	C	7.506486	3.839126	-0.513786
H	-3.410421	-6.032387	-1.573670	H	8.030546	3.366119	0.324438
H	-1.809651	-6.757992	-1.379873	H	8.238072	4.015920	-1.308733
H	-1.542915	0.408077	-2.531249	H	7.144398	4.814440	-0.169328
H	-2.302722	0.139631	-0.977814	Pd_P			
H	-0.514143	-2.746665	-3.293324	P	-2.175491	2.070337	0.451186
H	0.372139	-1.248081	-3.569798	Pd	-2.260396	-0.025215	-0.314858
C	1.560129	-2.803868	-2.644384	C	-0.525290	2.893912	0.011451
H	2.283228	-2.102017	-2.208281	C	0.636352	1.902891	0.290671
H	1.429363	-3.604102	-1.903605	C	-0.222826	4.224219	0.739074
C	2.127984	-3.402256	-3.934752	C	-0.547763	3.138480	-1.521719
H	2.255162	-2.601854	-4.675749	H	0.695678	1.668422	1.356159
H	1.397062	-4.101970	-4.361427	H	0.427755	0.960228	-0.229973
C	3.462073	-4.119441	-3.715712	C	1.981200	2.489617	-0.178983
H	3.851515	-4.537751	-4.649407	H	-0.164500	4.055611	1.818664
H	4.216073	-3.431715	-3.316265	H	-1.021494	4.950350	0.570266
H	3.352795	-4.942273	-3.000091	C	1.118107	4.808269	0.249761
C	-3.053408	-1.149884	-2.550088	H	-0.744350	2.186494	-2.031480
H	-3.474429	-1.884870	-1.854137	H	-1.356396	3.820938	-1.794811
H	-2.663612	-1.715580	-3.405287	C	0.791232	3.731882	-1.998179
C	-4.175960	-0.223882	-3.033532	H	2.777690	1.770821	0.049514
H	-4.564565	0.346307	-2.179516	C	2.251357	3.814261	0.556566
H	-3.757779	0.514467	-3.730367	C	1.930789	2.745738	-1.694029
C	-5.318891	-0.984344	-3.710052	H	1.302831	5.753699	0.774413
H	-5.772143	-1.706652	-3.021707	C	1.049229	5.061537	-1.266376
H	-6.107495	-0.304927	-4.048992	H	0.732765	3.910281	-3.078903
H	-4.958282	-1.540643	-4.582703	P	2.720761	1.467599	0.717156
C	4.164125	1.805759	-0.403387	C	3.215403	4.231126	0.238766
C	2.068927	3.162523	1.094398	H	2.314095	3.638968	1.638142
C	3.476989	0.893922	2.324316	H	1.766253	1.803105	-2.231033
C	4.035230	1.943579	3.293488	H	2.887897	3.155472	-2.040986
H	4.259380	0.177017	2.044164	H	0.248672	5.777468	-1.492600
H	2.701693	0.308433	2.829988	C	1.989326	5.506248	-1.616347
C	4.659481	1.302844	4.538491	C	-2.531287	2.161732	2.318106
H	4.785734	2.566916	2.797163	C	-3.734671	1.215846	2.582423
H	3.232673	2.621530	3.607493	C	-2.910312	3.558331	2.864874
C	5.201838	2.339024	5.525832	C	-1.319033	1.616462	3.107350
H	3.908799	0.674507	5.035641	H	-4.617494	1.568282	2.034904
H	5.467773	0.627450	4.228390	H	-3.496930	0.218206	2.193875
H	5.645985	1.861402	6.405041	C	-4.056599	1.142502	4.086972
H	5.972505	2.961798	5.057673	H	-3.804313	3.923582	2.351496
H	4.404377	3.005321	5.873720	H	-2.111218	4.281947	2.684967
H	3.719107	2.231843	-1.311614	C	-3.208057	3.483474	4.377247
H	4.553441	0.822942	-0.694206	H	-1.050148	0.624836	2.722696
H	2.837675	3.774534	1.577537	H	-0.451806	2.267428	2.965947
H	1.848643	3.627547	0.126145	C	-1.636754	1.537951	4.611698
C	0.799569	3.116835	1.952299	H	-4.910743	0.469898	4.232485
H	0.045760	2.507261	1.436629	C	-4.403619	2.545639	4.614024
H	1.009464	2.602687	2.899810	C	-2.832122	0.598844	4.842596
C	0.229717	4.506485	2.251701	H	-3.450528	4.491168	4.736375
H	0.017433	5.019464	1.304227	C	-1.976255	2.947897	5.127512
H	0.993650	5.108155	2.761924	H	-0.755439	1.153338	5.139318
C	-1.039057	4.452400	3.105833	H	-4.641324	2.498503	5.684286
H	-1.431517	5.454545	3.306136	H	-5.292798	2.932631	4.100340
				H	-2.589706	-0.411506	4.489388

H	-3.052217	0.523855	5.915019	H	3.861253	-1.640261	-1.863938
H	-1.120921	3.618646	4.974939	H	1.728125	-1.775305	-5.435093
H	-2.176812	2.918243	6.205851	H	0.129491	-1.092982	-5.121099
C	-3.518043	3.127844	-0.321607	H	3.577397	0.518949	-3.084369
C	-3.503316	4.664516	-0.300252	H	3.780586	-0.811956	-4.228363
H	-4.438771	2.765720	0.151384	H	2.123755	-3.420412	-2.079556
H	-3.577055	2.788161	-1.360100	H	2.909599	-3.142911	-3.637267
C	-4.818571	5.244569	-0.835335	C	-0.885818	-0.936189	0.662286
H	-3.332938	5.047856	0.708261	C	-2.044605	-1.896169	0.355884
H	-2.679638	5.042776	-0.913855	H	-1.070534	-0.451023	1.626745
C	-4.815314	6.774672	-0.866757	H	0.035234	-1.516168	0.801783
H	-5.003058	4.852598	-1.844185	C	-2.100868	-3.046569	1.368357
H	-5.648761	4.888028	-0.211162	H	-2.996888	-1.356857	0.382174
H	-5.763831	7.170742	-1.243355	H	-1.957290	-2.311058	-0.651363
H	-4.654277	7.187421	0.135644	C	-3.272521	-3.998649	1.117996
H	-4.014580	7.152981	-1.512277	H	-1.155336	-3.604399	1.329421
				H	-2.171047	-2.631127	2.382802
Pd_P2_Na2CO3							
Pd	1.035685	2.059754	0.432080	H	-4.229690	-3.469125	1.182905
P	-0.368539	0.446827	-0.487739	H	-3.208620	-4.445429	0.119408
C	-1.957193	1.265305	-1.105984	O	6.249651	1.453049	4.753439
C	-2.800242	1.581199	0.159629	O	3.996399	1.503329	4.673151
C	-2.813982	0.461836	-2.108421	C	5.106833	0.871204	4.518102
C	-1.589336	2.630005	-1.749231	O	5.112465	-0.378015	4.103928
H	-3.088007	0.660484	0.674428	Na	2.126420	-0.475617	3.174489
H	-2.188738	2.165439	0.859587	P	2.553866	3.694544	1.140388
C	-4.071770	2.364370	-0.215750	Na	7.328679	-0.320798	3.981425
H	-3.092895	-0.509088	-1.690946	C	2.030991	5.340401	0.369656
H	-2.239319	0.267056	-3.019883	C	1.635918	5.105074	-1.113491
C	-4.086988	1.254285	-2.473385	C	3.056240	6.494190	0.421482
H	-0.988865	3.203252	-1.034169	C	0.741704	5.763493	1.125172
H	-0.969108	2.484461	-2.636587	H	2.507733	4.799885	-1.696860
C	-2.854584	3.416260	-2.134573	H	0.917412	4.279723	-1.164601
H	-4.652394	2.552697	0.695600	C	1.036393	6.381096	-1.731429
C	-4.909340	1.528480	-1.201165	H	3.954131	6.220414	-0.142624
C	-3.682915	3.699987	-0.871221	H	3.370130	6.688855	1.450127
H	-4.683120	0.660416	-3.176997	C	2.446317	7.774737	-0.188385
C	-3.691568	2.590244	-3.127466	H	0.013019	4.944011	1.074942
H	-2.552412	4.362743	-2.600133	H	0.957602	5.938304	2.182942
H	-5.831680	2.064120	-1.458743	C	0.144481	7.042510	0.513573
H	-5.205442	0.580992	-0.732839	H	0.779945	6.180087	-2.779238
H	-3.098909	4.308371	-0.168602	C	2.072006	7.517886	-1.659081
H	-4.583539	4.272445	-1.126850	C	-0.228177	6.784782	-0.955897
H	-3.114482	2.403855	-4.042267	H	3.187377	8.581571	-0.131355
H	-4.590733	3.147604	-3.419074	C	1.184287	8.175159	0.596908
C	0.585390	-0.429342	-1.873412	H	-0.752338	7.321635	1.080512
C	0.816974	0.560836	-3.039599	H	1.663005	8.431702	-2.108791
C	-0.029644	-1.732104	-2.430705	H	2.967625	7.246760	-2.232715
C	1.973526	-0.780060	-1.268414	H	-0.978958	5.986192	-1.018515
H	-0.136996	0.815801	-3.510718	H	-0.673785	7.685144	-1.397854
H	1.248058	1.490337	-2.647454	H	1.440161	8.372071	1.645888
C	1.745006	-0.054000	-4.102587	H	0.765362	9.102584	0.186103
H	-1.021142	-1.544968	-2.853529	C	4.319220	3.201376	0.664077
H	-0.151239	-2.460030	-1.622718	C	4.479249	1.730767	1.134408
C	0.890985	-2.341422	-3.510228	C	5.456958	4.023182	1.310777
H	2.424865	0.131621	-0.862104	C	4.480694	3.233043	-0.872834
H	1.854926	-1.477975	-0.429650	H	4.366189	1.668752	2.219915
C	2.896534	-1.403139	-2.329900	H	3.679769	1.127310	0.688611
H	1.883226	0.671402	-4.913610	C	5.850405	1.167470	0.725117
C	1.093829	-1.334338	-4.655878	H	5.382770	3.956482	2.399479
C	3.105621	-0.393250	-3.471336	H	5.379300	5.080013	1.037878
H	0.421607	-3.253497	-3.898706	C	6.831498	3.469571	0.877340
C	2.254232	-2.686210	-2.884928	H	3.668833	2.660200	-1.338563

H	4.406404	4.261554	-1.239380	C	-4.231508	-0.358769	-3.141134
C	5.848552	2.660162	-1.288493	H	-4.592559	0.360509	-2.394122
H	5.920128	0.133436	1.084305	H	-3.854729	0.236716	-3.983063
C	6.963174	2.016112	1.365045	C	-5.390572	-1.241471	-3.609704
C	5.977772	1.204752	-0.806299	H	-5.801084	-1.825265	-2.778144
H	7.617137	4.085193	1.333300	H	-6.204181	-0.643178	-4.032154
C	6.960075	3.516822	-0.655118	H	-5.060679	-1.948512	-4.379246
H	5.929815	2.697118	-2.382216				
H	7.949835	1.615552	1.092618	Q_Cs			
H	6.868668	1.979872	2.457258	C	-2.768237	0.812055	-0.326713
H	5.194967	0.586609	-1.264600	C	-1.640809	0.789027	0.531741
H	6.944258	0.789515	-1.120802	C	-0.619177	1.722836	0.227581
H	6.881672	4.552778	-1.010193	C	-0.675429	2.612572	-0.847886
H	7.945874	3.143380	-0.960874	C	-1.789335	2.604597	-1.687453
C	2.598354	3.936059	2.986595	C	-2.820582	1.710455	-1.413266
C	3.215042	5.172890	3.658224	C	-3.995265	-0.020344	-0.155961
H	3.102856	3.040502	3.373548	C	-4.019412	-1.419280	-0.298032
H	1.553534	3.843819	3.304746	C	-5.245308	-2.096603	-0.214050
C	3.306412	4.974055	5.177011	C	-6.439959	-1.419098	0.016508
H	4.216332	5.371641	3.266650	C	-6.419975	-0.032086	0.169215
H	2.621754	6.069679	3.445487	C	-5.209473	0.650415	0.072146
H	2.293991	4.828254	5.579375	H	0.267550	1.737221	0.854048
H	3.848851	4.041286	5.370924	H	0.147213	3.302228	-1.024746
C	3.977586	6.150092	5.889206	H	-1.858268	3.280482	-2.535252
H	3.432533	7.085144	5.713305	H	-3.697905	1.693624	-2.055161
H	4.025727	5.991049	6.971683	H	-5.248101	-3.177588	-0.317464
H	5.002685	6.293956	5.528185	H	-7.374001	-1.969098	0.082079
				H	-7.338899	0.515043	0.358421
Pd_PBu3				H	-5.188592	1.730852	0.181451
Pd	1.092978	0.361746	-0.577916	C	-2.300336	-2.944102	0.664993
P	-0.372513	-1.064708	-1.414383	C	-1.242711	-3.845673	0.511389
C	-1.933212	-0.273609	-2.050254	C	-0.652917	-4.046557	-0.741430
C	0.221245	-2.038107	-2.879589	C	-1.114559	-3.332910	-1.851356
C	-0.959324	-2.366644	-0.208521	C	-2.184902	-2.442251	-1.710052
C	-1.455006	-3.709876	-0.760672	C	-2.791971	-2.253304	-0.466241
H	-1.743366	-1.883270	0.388273	C	-2.939326	-2.636709	1.975460
H	-0.125523	-2.542239	0.478072	C	-3.827797	-3.542174	2.568655
C	-1.982173	-4.629900	0.346349	C	-4.577303	-3.172834	3.688372
H	-2.244235	-3.557521	-1.503408	C	-4.446373	-1.879326	4.198335
H	-0.635904	-4.217775	-1.283328	C	-3.529545	-0.984251	3.629687
C	-2.447105	-5.987000	-0.187219	C	-2.734745	-1.353566	2.530346
H	-1.196008	-4.777287	1.098624	H	-0.871742	-4.378852	1.382169
H	-2.812234	-4.131286	0.864080	H	0.165844	-4.752876	-0.848869
H	-2.820967	-6.627523	0.617990	H	-0.657727	-3.481845	-2.825745
H	-3.252769	-5.8666841	-0.920399	H	-2.565046	-1.905206	-2.574392
H	-1.625715	-6.517016	-0.682502	H	-3.960221	-4.526222	2.124399
H	-1.603513	0.395518	-2.854670	H	-5.274088	-3.875592	4.136429
H	-2.287908	0.378315	-1.243974	H	-5.052482	-1.566489	5.046297
H	-0.537652	-2.770750	-3.174519	H	-3.411843	0.007767	4.060085
H	0.318034	-1.323298	-3.705048	Pd	-1.045496	-0.384601	2.088929
C	1.563768	-2.730802	-2.626977	C	-1.287688	0.762056	6.060781
H	2.307235	-1.970716	-2.353200	O	-1.992871	1.461722	5.292540
H	1.480659	-3.399503	-1.759748	O	-1.789953	-0.509058	6.388963
C	2.058045	-3.532273	-3.835168	O	-0.175892	1.021455	6.575478
H	2.135722	-2.863064	-4.702331	Cs	1.024025	-1.922850	6.497946
H	1.307649	-4.289491	-4.098429	Cs	1.880396	-0.976660	-0.451510
C	3.407098	-4.209322	-3.582660	Cs	0.540919	2.752237	3.961806
H	3.743349	-4.773837	-4.458251	O	2.379786	-0.780678	3.835758
H	4.179366	-3.469221	-3.344392	C	1.281019	-0.673513	3.236687
H	3.345211	-4.905868	-2.738825	O	0.224962	-1.390635	3.549797
C	-3.076124	-1.168896	-2.541027	O	1.090282	0.189966	2.251961
H	-3.459761	-1.767709	-1.706889	H	-2.556958	-0.651041	5.813235
H	-2.708620	-1.878312	-3.292573				

R_Cs				C	0.258066	4.810815	1.350156
Pd	-0.109482	1.472795	-2.256834	H	-1.669382	5.236524	2.210306
C	-1.490578	4.938669	-0.326793	H	2.050652	4.110168	0.351853
C	-1.608481	5.176786	-1.716434	H	0.630839	5.820315	1.503440
C	-1.821246	5.967989	0.570750	C	1.160063	-0.465423	1.780633
C	-2.077972	6.435094	-2.138938	O	0.456100	-0.564043	0.667844
C	-2.280628	7.207246	0.132625	O	0.616177	0.049814	2.820056
H	-1.720614	5.775328	1.634524	O	2.368494	-0.910666	1.779472
C	-2.414157	7.439798	-1.236435	C	-2.916565	2.741056	1.739133
H	-2.186747	6.612299	-3.203997	C	-3.979735	3.539897	2.182407
H	-2.539035	7.977275	0.852990	C	-3.155416	1.417638	1.295945
H	-2.782294	8.394139	-1.600696	C	-5.288357	3.057518	2.132042
C	1.775174	-0.835866	-2.044511	H	-3.792819	4.551682	2.534027
O	2.169564	-0.865090	-3.285442	C	-4.473790	0.980754	1.186715
O	1.567511	0.342393	-1.470332	C	-5.538314	1.788813	1.602798
O	1.648072	-1.898520	-1.353966	H	-6.111009	3.681372	2.470902
Cs	3.406426	-0.510533	0.935047	H	-4.687921	0.006398	0.764415
C	-1.208036	4.204026	-2.765299	H	-6.559082	1.422692	1.522438
C	-0.407229	4.652710	-3.814085	Cl	-0.222109	0.600553	-2.240837
C	-1.734101	2.857432	-2.796335	C	-2.095993	0.149634	-1.252610
C	-0.076863	3.827751	-4.908852	C	-2.174567	-1.254380	-1.291226
H	-0.031618	5.671595	-3.782717	C	-3.170457	0.961131	-1.716277
C	-1.385924	2.029574	-3.920662	C	-3.337827	-1.887287	-1.721074
H	3.481087	0.030371	-3.298246	H	-1.304805	-1.826082	-1.003296
C	-0.552736	2.529860	-4.960462	C	-4.306551	0.268206	-2.172350
H	0.551703	4.216557	-5.704580	C	-4.412358	-1.122741	-2.177048
H	-1.970441	1.132565	-4.110270	H	-3.382451	-2.972947	-1.729758
H	-0.329565	1.890010	-5.809199	H	-5.140709	0.851725	-2.547505
Cs	2.989213	3.296505	-2.049925	H	-5.313015	-1.597548	-2.552988
Cs	3.915656	-3.353222	-3.003565	C	-3.207385	2.443421	-1.657842
O	5.004476	-0.800742	-1.687131	C	-4.444577	3.105435	-1.517860
C	4.947678	0.408234	-2.049836	C	-2.053188	3.242645	-1.712750
O	5.439026	1.404365	-1.456537	C	-4.525614	4.493184	-1.466538
O	4.250331	0.691995	-3.213866	H	-5.351429	2.526906	-1.392105
C	-0.991552	3.670479	0.274984	C	-2.133639	4.633802	-1.657660
C	-1.715045	2.463401	0.177137	H	-1.087171	2.770028	-1.788105
C	0.150646	3.714935	1.091044	C	-3.367699	5.271905	-1.543571
C	-1.299041	1.353860	0.930977	H	-5.495726	4.967145	-1.344635
C	0.567634	2.598716	1.816535	H	-1.217934	5.216811	-1.690297
H	0.700322	4.648731	1.168693	H	-3.428539	6.355598	-1.497966
C	-0.171795	1.415397	1.747815	Cs	2.366542	-1.816344	-1.321692
H	-1.872672	0.434839	0.863152	Cs	2.219140	-1.002183	5.149334
H	1.452300	2.660274	2.443971	P	-2.448016	-1.962344	2.343677
H	0.126011	0.543978	2.323652	C	-1.271774	-3.468651	2.361811
C	-2.968770	2.363992	-0.617784	C	-0.684023	-3.552528	0.927844
C	-4.162036	2.034524	0.038586	C	-1.898713	-4.844522	2.686362
C	-2.972048	2.532905	-2.017006	C	-0.106344	-3.212069	3.342960
C	-5.355554	1.877603	-0.666066	H	-1.489960	-3.755519	0.212008
H	-4.146022	1.902190	1.116411	H	-0.236601	-2.588412	0.675153
C	-4.178788	2.373439	-2.713054	C	0.374578	-4.665606	0.828877
C	-5.362451	2.047783	-2.050485	H	-2.691489	-5.071063	1.967129
H	-6.269592	1.625232	-0.137346	H	-2.350547	-4.845722	3.681914
H	-4.180390	2.506273	-3.790787	C	-0.829973	-5.957786	2.605039
H	-6.283260	1.929851	-2.613877	H	0.321245	-2.231323	3.131743
				H	-0.484555	-3.196409	4.369607
TS_CCI_frmC1_Cs				C	0.958335	-4.318427	3.236473
Pd	-1.468605	0.350907	0.894561	H	0.760914	-4.699103	-0.199148
C	-0.699298	2.212839	0.945478	C	-0.259595	-6.021449	1.177831
C	-1.532786	3.184688	1.541221	C	1.521300	-4.353922	1.806768
C	0.581301	2.550447	0.521798	H	-1.301705	-6.915635	2.857728
C	-1.034958	4.477771	1.758476	C	0.312999	-5.667278	3.592898
C	1.059377	3.853634	0.716602	H	1.772579	-4.108166	3.943932
H	1.199887	1.813010	0.027894	H	0.487532	-6.822623	1.105831

H	-1.058967	-6.257047	0.463442	H	-0.419125	3.088757	-0.763523
H	1.963156	-3.376406	1.580557	H	-0.446219	2.473130	-2.400801
H	2.307710	-5.116105	1.726306	C	-2.261018	3.494796	-1.832192
H	-0.073351	-5.638312	4.620360	H	-4.122938	2.568490	0.935385
H	1.059698	-6.470640	3.549298	C	-4.444524	1.694820	-1.025977
C	-2.927633	-1.499034	4.129457	C	-3.073648	3.749956	-0.552618
C	-1.806490	-0.607472	4.718623	H	-4.266663	0.944698	-3.054426
C	-3.190802	-2.675016	5.098839	C	-3.147574	2.796073	-2.878210
C	-4.200004	-0.617230	4.057209	H	-1.891074	4.446885	-2.232687
H	-0.877565	-1.171948	4.783859	H	-5.326274	2.309323	-1.247368
H	-1.603433	0.221539	4.037845	H	-4.807787	0.740603	-0.623058
C	-2.188634	-0.089208	6.116045	H	-2.455588	4.269887	0.187860
H	-2.297285	-3.297490	5.197462	H	-3.934918	4.394229	-0.771591
H	-3.986884	-3.317805	4.715744	H	-2.579746	2.629552	-3.802727
C	-3.581885	-2.144495	6.494482	H	-4.005301	3.430966	-3.133665
H	-4.011062	0.231136	3.401697	C	0.904515	-0.547238	-1.884443
H	-5.037264	-1.171198	3.624422	C	1.133536	0.498979	-2.999612
C	-4.599948	-0.103508	5.452036	C	0.208697	-1.787339	-2.489096
H	-1.363193	0.522005	6.504879	C	2.293469	-0.995347	-1.352575
C	-2.437127	-1.282821	7.055867	H	0.174943	0.813819	-3.421151
C	-3.463637	0.763771	6.017819	H	1.617913	1.386985	-2.583147
H	-3.759896	-2.999469	7.159014	C	1.992898	-0.094502	-4.130919
C	-4.860350	-1.295066	6.388604	H	-0.786986	-1.530811	-2.861187
H	-5.511233	0.499480	5.353028	H	0.082327	-2.555036	-1.719898
H	-2.691314	-0.927456	8.062960	C	1.057341	-2.372598	-3.637826
H	-1.523556	-1.886345	7.145662	H	2.805827	-0.133125	-0.911977
H	-3.290140	1.624532	5.359335	H	2.168015	-1.735436	-0.552851
H	-3.738084	1.156569	7.005605	C	3.145384	-1.596567	-2.485712
H	-5.685546	-1.905867	6.000260	H	2.135400	0.672017	-4.902502
H	-5.160075	-0.939451	7.382957	C	1.263189	-1.309305	-4.730800
C	-3.989187	-2.681424	1.564182	C	3.358388	-0.531760	-3.575040
C	-4.995844	-3.584800	2.293021	H	0.529929	-3.237679	-4.057866
H	-3.608497	-3.209300	0.683841	C	2.423987	-2.814571	-3.087208
H	-4.534609	-1.828858	1.154048	H	4.114058	-1.904371	-2.073483
C	-6.042645	-4.138440	1.318192	H	1.846367	-1.730806	-5.559068
H	-4.499433	-4.420634	2.791630	H	0.293920	-0.998979	-5.141638
H	-5.510362	-3.022694	3.078892	H	3.887195	0.333140	-3.156085
C	-7.096624	-5.005834	2.009624	H	3.982653	-0.935992	-4.381855
H	-6.530731	-3.302555	0.799475	H	2.289513	-3.589402	-2.321805
H	-5.533817	-4.723974	0.540527	H	3.030390	-3.253200	-3.889654
H	-7.828248	-5.396456	1.294923	C	-0.593380	-1.196911	0.609584
H	-6.632092	-5.861010	2.513848	C	-1.824752	-2.032789	0.226863
H	-7.642543	-4.432457	2.767473	H	-0.736103	-0.793961	1.617129
H	2.410087	1.679997	-2.869009	H	0.284178	-1.851036	0.683531
Cs	4.292690	1.530232	1.729123	C	-1.947753	-3.282758	1.107131
O	3.081127	0.989787	-2.759695	H	-2.734296	-1.433362	0.337327
C	3.849417	1.380159	-1.648229	H	-1.785968	-2.339464	-0.821045
O	4.655154	0.503985	-1.255386	C	-3.189430	-4.114272	0.777760
O	3.611922	2.519811	-1.181784	H	-1.046517	-3.897950	0.983804
TS1							
Pd	1.495735	1.549358	0.831975	H	-4.104433	-3.528616	0.921409
P	0.010622	0.248947	-0.413562	H	-3.171748	-4.449906	-0.265298
C	-1.515351	1.229159	-0.950284	Cl	3.122721	3.084634	1.911469
C	-2.341990	1.508904	0.333841	C	2.534198	3.314397	0.031226
C	-2.422131	0.550244	-2.001488	C	1.715523	4.430671	-0.260570
C	-1.053466	2.600716	-1.503231	C	3.472404	2.826155	-0.895718
H	-2.694429	0.573901	0.777997	C	1.764536	4.905521	-1.584562
H	-1.703525	1.998867	1.077395	C	3.489635	3.334506	-2.189601
C	-3.554762	2.402694	0.011871	H	4.153281	2.037512	-0.600156
H	-2.768551	-0.422837	-1.645675	C	2.618406	4.369247	-2.544439
H	-1.861587	0.375943	-2.924745	H	1.088741	5.708854	-1.860246
C	-3.636259	1.450645	-2.312996	H	4.182237	2.920100	-2.915708

H	2.617076	4.766840	-3.553733	H	4.006769	-1.512109	-4.526876
C	0.807152	5.092931	0.707278	H	2.144356	-3.887111	-2.274061
C	0.657172	6.490803	0.668078	H	2.937578	-3.737118	-3.845776
C	0.051325	4.376441	1.649976	C	-0.603305	-1.088032	0.404582
C	-0.223489	7.144361	1.528817	C	-1.867797	-1.923460	0.169543
H	1.249787	7.071164	-0.031801	H	-0.685635	-0.520909	1.337250
C	-0.827443	5.028243	2.512752	H	0.253004	-1.756529	0.554668
H	0.139547	3.292324	1.684073	C	-2.089682	-2.925610	1.308927
C	-0.972670	6.416112	2.455262	H	-2.747093	-1.274854	0.100745
H	-0.317999	8.224983	1.479965	H	-1.814764	-2.464446	-0.779911
H	-1.408840	4.446926	3.222485	C	-3.371004	-3.744707	1.138544
H	-1.659095	6.924084	3.125721	H	-1.223946	-3.598183	1.370269
				H	-2.121774	-2.382404	2.263415
				H	-3.507218	-4.453715	1.961540
TS1_Cs				Pd	1.363575	1.816232	0.357038
P	0.025864	0.191704	-0.788735	H	-4.252064	-3.093142	1.107922
C	-1.461991	1.176860	-1.406533	H	-3.350541	-4.316608	0.203984
C	-2.242946	1.597477	-0.132227	Cs	3.253022	2.323259	5.068738
C	-2.421888	0.462450	-2.381480	O	2.238725	0.339883	2.830703
C	-0.950213	2.480061	-2.076067	O	0.316412	1.368064	2.227635
H	-2.630155	0.711179	0.378459	C	1.083843	0.780733	3.151341
H	-1.553889	2.098825	0.556178	O	0.610793	0.729636	4.343838
C	-3.419755	2.519095	-0.492982	Cs	-2.345253	1.340063	3.722418
H	-2.800810	-0.466247	-1.945225	Cl	3.927033	3.925064	1.945943
H	-1.890032	0.192399	-3.299808	C	2.289772	3.594219	0.382585
C	-3.602700	1.392696	-2.734144	C	1.483573	4.775798	0.328299
H	-0.268569	2.995655	-1.393218	C	2.887690	3.065336	-0.805890
H	-0.375447	2.249983	-2.975076	C	1.228084	5.317967	-0.928794
C	-2.123823	3.402524	-2.444421	C	2.637744	3.700759	-2.052002
H	-3.960204	2.784703	0.424984	H	3.715878	2.367907	-0.729644
C	-4.366153	1.775200	-1.452735	C	1.804814	4.800901	-2.110633
C	-2.886091	3.793500	-1.167856	H	0.523045	6.141635	-1.005167
H	-4.276319	0.864118	-3.419751	H	3.136579	3.334391	-2.945507
C	-3.071101	2.669370	-3.410682	H	1.589185	5.279670	-3.060855
H	-1.722948	4.302892	-2.925965	C	0.881485	5.358749	1.548981
H	-5.225388	2.409927	-1.703690	C	0.707871	6.748712	1.662600
H	-4.760246	0.873567	-0.965868	C	0.478010	4.542564	2.623109
H	-2.216410	4.328512	-0.482240	C	0.146064	7.312566	2.808769
H	-3.715672	4.470137	-1.409939	H	1.040258	7.394595	0.855602
H	-2.537781	2.410494	-4.334280	C	-0.076301	5.111994	3.770316
H	-3.907506	3.322070	-3.691892	H	0.570797	3.461759	2.541250
C	0.889774	-0.770006	-2.160345	C	-0.246407	6.496945	3.872265
C	1.189761	0.158489	-3.360422	H	0.028038	8.390329	2.875562
C	0.150892	-2.027621	-2.669650	H	-0.377575	4.468906	4.594019
C	2.245952	-1.221437	-1.551370	H	-0.676316	6.933822	4.768981
H	0.254387	0.474799	-3.832074	TS1_Na			
H	1.702583	1.062072	-3.013114	Pd	1.296804	1.745193	0.486987
C	2.048935	-0.571419	-4.409388	P	-0.011330	0.154432	-0.743747
H	-0.823266	-1.758849	-3.089931	C	-1.483608	1.168196	-1.348516
H	-0.031284	-2.714501	-1.837523	C	-2.263580	1.571571	-0.067177
C	1.000937	-2.752413	-3.734847	C	-2.441405	0.478944	-2.343056
H	2.784158	-0.343718	-1.175734	C	-0.961165	2.481206	-1.990192
H	2.072695	-1.881135	-0.692443	H	-2.643038	0.686218	0.450525
C	3.096309	-1.959109	-2.601301	H	-1.571097	2.074438	0.617283
H	2.242312	0.112350	-5.244986	C	-3.437718	2.501175	-0.416225
C	1.282057	-1.806487	-4.915285	H	-2.827015	-0.455321	-1.927607
C	3.380778	-1.010414	-3.778196	H	-1.904889	0.224909	-3.263325
H	0.448069	-3.631219	-4.088770	C	-3.615687	1.422082	-2.681868
C	2.333385	-3.196819	-3.106080	H	-0.280682	2.981928	-1.295056
H	4.040980	-2.268967	-2.138139	H	-0.385464	2.267797	-2.892290
H	1.868002	-2.327954	-5.682662	C	-2.128881	3.417578	-2.344261
H	0.338827	-1.496046	-5.382926	H	-3.979021	2.749132	0.505899
H	3.936138	-0.132068	-3.425171	C	-4.382367	1.780234	-1.395253

C	-2.897117	3.786704	-1.064790	H	3.324686	2.990981	-2.718666
H	-4.288562	0.910530	-3.380822	H	1.843503	4.964147	-3.053972
C	-3.074900	2.709190	-3.330126	C	0.881764	5.388238	1.490279
H	-1.720687	4.325221	-2.805736	C	0.534437	6.748474	1.422369
H	-5.238418	2.423097	-1.635743	C	0.623979	4.701487	2.689817
H	-4.781670	0.870119	-0.929472	C	-0.067586	7.391820	2.504355
H	-2.230207	4.308427	-0.365915	H	0.759767	7.319181	0.527559
H	-3.723190	4.469895	-1.299658	C	0.037251	5.347392	3.776648
H	-2.538451	2.466501	-4.256316	H	0.887303	3.656019	2.767638
H	-3.906161	3.372313	-3.601458	C	-0.320074	6.696794	3.688935
C	0.889923	-0.748548	-2.132605	H	-0.323672	8.444251	2.425669
C	1.186063	0.209842	-3.308315	H	-0.131294	4.793049	4.696033
C	0.168876	-2.002260	-2.676570	H	-0.776407	7.201555	4.535009
C	2.246878	-1.196021	-1.522478				
H	0.250065	0.523731	-3.780012				
H	1.684782	1.110750	-2.936494	Pd	1.798189	1.498565	0.946820
C	2.062065	-0.486504	-4.366627	P	0.317155	0.136530	-0.174995
H	-0.802681	-1.731599	-3.102036	C	-0.471129	-1.318325	0.680381
H	-0.016996	-2.709003	-1.862385	C	-1.803685	-1.845179	0.132701
C	1.036083	-2.694429	-3.748810	H	-0.599537	-1.021545	1.726771
H	2.773115	-0.320184	-1.126606	H	0.287145	-2.111635	0.682222
H	2.075601	-1.875087	-0.678230	C	-2.311837	-3.060687	0.917056
C	3.113042	-1.901390	-2.581862	H	-2.558365	-1.051210	0.178644
H	2.252915	0.218390	-5.184983	H	-1.706780	-2.115244	-0.923640
C	1.314535	-1.719376	-4.905804	C	-3.655959	-3.575914	0.397543
C	3.394524	-0.923606	-3.735513	H	-1.562869	-3.861911	0.865519
H	0.496143	-3.571538	-4.125779	H	-2.402318	-2.793115	1.978097
C	2.368321	-3.136679	-3.118227	H	-4.000999	-4.442584	0.970337
H	4.057868	-2.210050	-2.118370	H	-4.427067	-2.800325	0.466092
H	1.912913	-2.216038	-5.679873	H	-3.582070	-3.876991	-0.653552
H	0.371016	-1.410488	-5.373766	Cl	3.335402	3.488596	1.317895
H	3.937527	-0.046942	-3.359494	C	2.116589	3.349525	-0.197218
H	4.031455	-1.401241	-4.490528	C	0.993784	4.214631	-0.223870
H	2.180393	-3.846091	-2.302270	C	2.751885	2.934906	-1.385452
H	2.984565	-3.654661	-3.863768	C	0.449560	4.484236	-1.493920
C	-0.657570	-1.189556	0.368629	C	2.173665	3.225928	-2.614209
C	-1.931081	-1.987430	0.057657	H	3.666923	2.358636	-1.322891
H	-0.740136	-0.699462	1.343768	C	1.005305	3.994745	-2.672494
H	0.189615	-1.879710	0.468172	H	-0.451146	5.087297	-1.541529
C	-2.133885	-3.130510	1.059362	H	2.639432	2.857417	-3.523100
H	-2.806200	-1.330436	0.095688	H	0.543562	4.225282	-3.626568
H	-1.903987	-2.400613	-0.954966	C	0.361669	4.819505	0.972957
C	-3.421884	-3.917030	0.805937	C	-0.150952	6.127177	0.894674
H	-1.270607	-3.807593	1.012008	C	0.216186	4.129759	2.188906
H	-2.144268	-2.719072	2.077644	C	-0.796481	6.715083	1.981350
H	-3.544270	-4.730384	1.528370	H	-0.026082	6.694857	-0.021697
H	-4.300987	-3.266986	0.881579	C	-0.425919	4.717037	3.276985
H	-3.422177	-4.357942	-0.197398	H	0.582267	3.108316	2.267552
Na	2.992066	2.498409	4.441746	C	-0.939024	6.012274	3.179403
O	2.252901	0.642578	3.316889	H	-1.180535	7.726932	1.893237
O	0.261304	1.123225	2.352074	H	-0.534710	4.155276	4.200074
C	1.103013	1.182982	3.372978	H	-1.440952	6.468987	4.026832
O	0.714878	1.860265	4.414585	C	-1.086730	1.134626	-0.853197
Na	-1.350889	2.212353	3.484171	H	-1.754568	0.504531	-1.449827
Cl	3.851875	3.836224	2.203437	H	-0.618554	1.854795	-1.533364
C	2.272711	3.492755	0.519059	C	1.126069	-0.541739	-1.701144
C	1.523730	4.699473	0.350066	H	2.004636	-1.101318	-1.359746
C	2.924790	2.865623	-0.587528	H	1.512923	0.346520	-2.215126
C	1.356902	5.152215	-0.958852	C	0.302033	-1.395879	-2.670494
C	2.777751	3.425086	-1.886519	H	0.005640	-2.330988	-2.181584
H	3.730678	2.160045	-0.411309	H	-0.625335	-0.876648	-2.941203
C	1.986027	4.541712	-2.064357	C	1.079972	-1.727238	-3.949691
H	0.681557	5.982662	-1.141334	H	2.013855	-2.238413	-3.681139

H	1.373562	-0.791304	-4.443024	H	-3.962127	-3.579333	-0.469470	
C	0.276718	-2.594892	-4.921261	H	-2.335185	-3.615838	-1.158356	
H	0.850389	-2.819996	-5.826014	H	-3.242852	-0.918048	2.087199	
H	-0.004464	-3.547169	-4.457552	H	-4.495634	-1.996507	1.457159	
H	-0.646809	-2.090471	-5.227171	H	-4.886460	-0.199482	-1.838687	
C	-1.863992	1.882141	0.233505	H	-5.475100	-1.565035	-0.886187	
H	-1.152861	2.398927	0.882821	C	-0.965062	2.314877	-2.091687	
H	-2.400851	1.167794	0.871712	C	-1.963472	2.155103	-3.247546	
C	-2.851831	2.907224	-0.331669	H	-0.086480	2.855652	-2.455669	
H	-3.615975	2.394216	-0.930754	H	-1.400950	2.963004	-1.329733	
H	-2.313897	3.570191	-1.020514	C	-2.191216	3.495353	-3.957671	
C	-3.516018	3.743070	0.765326	H	-1.620824	1.418576	-3.977909	
H	-4.062269	3.105232	1.469963	H	-2.924560	1.792024	-2.870487	
H	-2.766650	4.303063	1.334390	C	-3.224955	3.395920	-5.081522	
H	-4.227742	4.461842	0.346045	H	-2.512788	4.243425	-3.221096	
				H	-1.235850	3.854481	-4.362724	
				H	-3.370204	4.360335	-5.578487	
TS2_Cs								
Pd	0.462585	1.370600	1.003557	H	-2.910304	2.671437	-5.841103	
P	-0.258871	0.860726	-1.163794	H	-4.196449	3.068782	-4.694098	
C	1.074629	0.174698	-2.300135	C	0.095361	3.324001	0.808966	
C	2.270012	1.161642	-2.207014	C	-0.667940	3.891058	1.860483	
C	0.675517	0.036575	-3.786704	C	0.701868	4.177449	-0.122328	
C	1.532790	-1.198032	-1.765848	C	-0.839752	5.283060	1.927878	
H	1.966483	2.147073	-2.584195	C	0.546350	5.565887	-0.031541	
H	2.614870	1.285024	-1.174012	H	1.313636	3.764252	-0.917873	
C	3.455423	0.645401	-3.043563	C	-0.237490	6.119192	0.986377	
H	0.391253	1.013224	-4.188838	H	-1.423276	5.712538	2.738430	
H	-0.183926	-0.630378	-3.902316	H	1.036269	6.212239	-0.755210	
C	1.868913	-0.505225	-4.603401	H	-0.364897	7.195711	1.054807	
H	1.768337	-1.091328	-0.703753	C	1.884044	-0.400728	2.829402	
H	0.719046	-1.925651	-1.848921	O	1.967639	0.812080	3.364867	
C	2.738967	-1.708226	-2.577151	O	1.239235	-0.540194	1.697031	
H	4.276351	1.366797	-2.957774	O	2.413920	-1.389837	3.400937	
C	3.040796	0.487331	-4.514694	Cs	3.558710	-2.793141	0.927763	
C	3.905887	-0.710175	-2.472705	C	-1.210672	2.949075	2.859657	
H	1.553623	-0.617941	-5.647993	C	-2.446935	3.162326	3.490037	
C	2.310590	-1.869408	-4.046262	C	-0.494940	1.741133	3.080395	
H	3.046333	-2.689670	-2.191887	C	-3.002609	2.185098	4.315923	
H	3.886379	0.124464	-5.113275	H	-2.998402	4.078702	3.296054	
H	2.741792	1.458224	-4.930840	C	-1.094572	0.764378	3.894208	
H	4.217535	-0.573486	-1.430171	H	0.861587	1.424559	3.074417	
H	4.768430	-1.090921	-3.036087	C	-2.329824	0.975171	4.511664	
H	1.487554	-2.592370	-4.119811	H	-3.964925	2.359089	4.789040	
H	3.144355	-2.263808	-4.640428	H	-0.570837	-0.173098	4.062772	
C	-1.706224	-0.319730	-0.846366	H	-2.764336	0.206005	5.144670	
C	-1.315820	-1.418028	0.178218	Cs	3.433862	3.708567	2.757081	
C	-2.261981	-1.025105	-2.105570	Cs	5.149010	-0.202451	4.233406	
C	-2.815689	0.552557	-0.193791	O	4.941239	-0.146630	1.021027	
H	-0.538680	-2.062948	-0.239268	C	4.899794	1.150498	1.116377	
H	-0.891601	-0.968032	1.075931	O	5.655717	1.759981	1.986005	
C	-2.540291	-2.277966	0.543655	O	4.088017	1.846106	0.373784	
H	-1.493757	-1.679078	-2.532020					
H	-2.535825	-0.304922	-2.877650	TS2_Cs'				
C	-3.498064	-1.871990	-1.734979	Pd	-0.062994	1.298439	1.022951	
H	-2.414569	1.026458	0.708681	P	-0.854305	0.812283	-1.125966	
H	-3.128642	1.354229	-0.867822	C	0.480362	-0.093747	-2.114136	
C	-4.038981	-0.309564	0.160924	C	1.797975	0.675102	-1.816501	
H	-2.223324	-3.041672	1.264952	C	0.259395	-0.103468	-3.643811	
C	-3.094842	-2.955410	-0.720455	C	0.645952	-1.549892	-1.621118	
C	-3.625925	-1.389849	1.173778	H	1.709821	1.717475	-2.147946	
H	-3.884455	-2.342276	-2.647432	H	1.969743	0.693039	-0.736673	
C	-4.582883	-0.970178	-1.118409	C	2.986254	0.000896	-2.523684	
H	-4.807775	0.337780	0.600276	H	0.171525	0.918877	-4.023677	

H	-0.668032	-0.628662	-3.894780	H	-0.026831	6.302554	-0.498434
C	1.451037	-0.789193	-4.346709	H	-0.730239	7.128292	1.744572
H	0.800650	-1.530389	-0.540849	C	1.965249	-0.516090	1.910299
H	-0.260944	-2.123651	-1.837685	O	2.244189	0.639811	2.474342
C	1.839621	-2.220470	-2.324622	O	0.769102	-0.658294	1.355353
H	3.897707	0.567337	-2.297648	O	2.778981	-1.473334	1.900725
C	2.743187	-0.011151	-4.042743	Cs	0.606846	-3.703506	1.782245
C	3.125509	-1.440053	-2.001365	C	-0.839442	2.765609	3.434629
H	1.264034	-0.789302	-5.427408	C	-1.684175	2.943240	4.541755
C	1.595745	-2.235450	-3.842925	C	-0.137711	1.542146	3.270280
H	1.931555	-3.250176	-1.955422	C	-1.854111	1.924069	5.477949
H	3.591792	-0.477638	-4.558539	H	-2.241796	3.869235	4.651598
H	2.660977	1.016735	-4.418605	C	-0.359194	0.518743	4.207635
H	3.288521	-1.431711	-0.916639	H	1.070633	1.265941	2.725473
H	3.991451	-1.928070	-2.466700	C	-1.195451	0.701982	5.309382
H	0.686930	-2.807261	-4.071481	H	-2.512908	2.076280	6.328316
H	2.428786	-2.729576	-4.358667	H	0.160819	-0.426380	4.079635
C	-2.415946	-0.207569	-0.836063	H	-1.334835	-0.097232	6.032416
C	-2.168002	-1.242950	0.291062				
C	-2.942992	-0.958498	-2.081205				
C	-3.498710	0.782068	-0.325305	TS2_Na			
H	-1.404895	-1.954448	-0.026467	Pd	0.358360	1.405468	1.002411
H	-1.779059	-0.735005	1.177457	P	-0.292018	0.886798	-1.195823
C	-3.464304	-1.998351	0.632208	C	1.053965	0.205060	-2.319498
H	-2.195527	-1.678313	-2.428178	C	2.252552	1.184944	-2.195125
H	-3.129988	-0.268065	-2.904810	C	0.666196	0.098731	-3.812118
C	-4.247701	-1.704862	-1.732230	C	1.505867	-1.182331	-1.814840
H	-3.122456	1.299664	0.565024	H	1.956973	2.183408	-2.540533
H	-3.712807	1.547339	-1.075893	H	2.554956	1.267755	-1.146725
C	-4.798538	0.026803	0.008138	C	3.443375	0.687249	-3.037163
H	-3.248952	-2.725246	1.425742	H	0.385033	1.083532	-4.196070
C	-3.974317	-2.731919	-0.619993	H	-0.193854	-0.564121	-3.943239
C	-4.526676	-0.999949	1.119615	C	1.863233	-0.428246	-4.631166
H	-4.607653	-2.218898	-2.631480	H	1.731045	-1.115858	-0.746539
C	-5.307015	-0.696202	-1.252615	H	0.691693	-1.905049	-1.924114
H	-5.548169	0.751711	0.346959	C	2.718601	-1.678738	-2.625807
H	-4.891008	-3.287887	-0.386857	H	4.265976	1.405330	-2.936265
H	-3.227716	-3.462249	-0.958251	C	3.030466	0.566692	-4.513223
H	-4.174754	-0.489781	2.025065	C	3.888380	-0.685997	-2.507226
H	-5.452044	-1.528020	1.381778	H	1.554958	-0.516452	-5.679902
H	-5.518538	0.033285	-2.044794	C	2.298967	-1.806444	-4.101441
H	-6.247613	-1.216642	-1.033436	H	3.022243	-2.660461	-2.240376
C	-1.348777	2.253385	-2.189238	H	3.881106	0.223603	-5.115081
C	-2.283115	2.110853	-3.400490	H	2.729079	1.546366	-4.905971
H	-0.396037	2.676838	-2.526565	H	4.211443	-0.573832	-1.467509
H	-1.766925	2.991473	-1.501310	H	4.744729	-1.054244	-3.086765
C	-2.323280	3.411367	-4.212318	H	1.474819	-2.524827	-4.198541
H	-1.973439	1.292603	-4.054736	H	3.135262	-2.188920	-4.699299
H	-3.298151	1.874952	-3.067335	C	-1.717007	-0.315430	-0.874368
C	-3.283539	3.330210	-5.400916	C	-1.302321	-1.388655	0.168647
H	-2.614990	4.239756	-3.553635	C	-2.246458	-1.047394	-2.129473
H	-1.310731	3.643559	-4.567869	C	-2.853429	0.534625	-0.237986
H	-3.292893	4.263996	-5.971829	H	-0.498292	-2.012939	-0.227559
H	-2.995805	2.522651	-6.083427	H	-0.912150	-0.911393	1.069259
H	-4.308040	3.131977	-5.066388	C	-2.504724	-2.279331	0.534019
C	-0.383178	3.285408	1.070680	H	-1.458919	-1.681939	-2.549357
C	-0.710293	3.771647	2.363583	H	-2.537168	-0.338813	-2.906673
C	-0.124337	4.223169	0.064585	C	-3.458946	-1.925766	-1.756007
C	-0.851255	5.148855	2.588667	H	-2.472108	1.027458	0.663213
C	-0.242386	5.598358	0.301072	H	-3.182854	1.321085	-0.921774
H	0.193642	3.896233	-0.917517	C	-4.055135	-0.357335	0.118344
C	-0.629063	6.062927	1.558943	H	-2.171931	-3.025562	1.265857
H	-1.105626	5.507821	3.582566	C	-3.029230	-2.985501	-0.727234
H				C	-3.619186	-1.414224	1.146165

H	-3.825939	-2.417207	-2.665037	H	2.690241	0.912887	-0.973371
C	-4.572440	-1.048178	-1.156024	C	3.622671	0.237856	-2.815343
H	-4.844196	0.273651	0.544907	H	0.728114	1.130702	-4.172486
H	-3.878956	-3.631977	-0.474380	H	-0.088566	-0.424135	-3.988547
H	-2.247682	-3.627765	-1.152796	C	2.002429	-0.564424	-4.555273
H	-3.255797	-0.922388	2.057233	H	1.552280	-1.303158	-0.728163
H	-4.473187	-2.041914	1.430266	H	0.425447	-1.903691	-1.964583
H	-4.894057	-0.295182	-1.886921	C	2.499501	-1.991571	-2.558020
H	-5.448228	-1.665445	-0.920618	H	4.542745	0.807339	-2.636559
C	-1.007884	2.334910	-2.122105	C	3.302304	0.224251	-4.319701
C	-2.007875	2.161413	-3.274682	C	3.798162	-1.204681	-2.308797
H	-0.135748	2.885959	-2.486954	H	1.757909	-0.564756	-5.624484
H	-1.449304	2.976066	-1.356827	C	2.181376	-2.009851	-4.061948
C	-2.275043	3.502105	-3.969939	H	2.614888	-3.019370	-2.190042
H	-1.649201	1.440743	-4.013160	H	4.126988	-0.235595	-4.878616
H	-2.956618	1.768947	-2.896536	H	3.192344	1.251253	-4.690632
C	-3.314057	3.385257	-5.087197	H	4.033154	-1.199462	-1.237603
H	-2.611666	4.234011	-3.223969	H	4.636716	-1.687225	-2.826881
H	-1.332530	3.890422	-4.377895	H	1.265774	-2.586836	-4.245421
H	-3.489212	4.350349	-5.572881	H	2.990966	-2.499119	-4.618087
H	-2.985633	2.677349	-5.856406	C	-1.683214	0.009222	-0.835737
H	-4.273158	3.027960	-4.695661	C	-1.347737	-0.975171	0.313252
C	0.072694	3.366982	0.815288	C	-2.254708	-0.805347	-2.020622
C	-0.656913	3.965992	1.870073	C	-2.767273	0.988784	-0.311072
C	0.709654	4.182504	-0.125086	H	-0.587277	-1.678743	-0.028972
C	-0.788398	5.361252	1.919743	H	-0.924822	-0.425316	1.156914
C	0.597477	5.576296	-0.048554	C	-2.602357	-1.747292	0.755860
H	1.299161	3.740734	-0.921386	H	-1.507249	-1.515989	-2.384866
C	-0.166772	6.164533	0.962889	H	-2.511244	-0.154198	-2.857062
H	-1.354440	5.818679	2.727013	C	-3.516365	-1.573919	-1.571628
H	1.102827	6.198156	-0.782454	H	-2.365732	1.554932	0.533762
H	-0.263785	7.244788	1.015380	H	-3.041912	1.711639	-1.084249
C	2.044293	-0.204718	2.815194	C	-4.024027	0.212973	0.123210
O	1.977829	0.996910	3.370586	H	-2.326487	-2.433950	1.566663
O	1.315300	-0.470818	1.771651	C	-3.158010	-2.546465	-0.435062
O	2.852073	-1.066880	3.277068	C	-3.661263	-0.754827	1.261739
C	-1.206336	3.040223	2.874811	H	-3.906519	-2.134049	-2.429971
C	-2.401987	3.282393	3.566507	C	-4.579168	-0.576800	-1.076201
C	-0.529594	1.800803	3.032626	H	-4.774481	0.932152	0.472950
C	-2.953500	2.300182	4.390357	H	-4.046430	-3.113844	-0.130583
H	-2.926517	4.223590	3.425307	H	-2.411064	-3.272666	-0.782039
C	-1.127653	0.816803	3.837311	H	-3.272853	-0.195736	2.121574
H	0.849508	1.517972	3.055327	H	-4.555426	-1.295206	1.597860
C	-2.323416	1.058270	4.518256	H	-4.854187	0.112226	-1.884833
H	-3.883598	2.496009	4.916016	H	-5.489689	-1.114988	-0.784432
H	-0.635748	-0.146288	3.947275	C	-0.757909	2.413138	-2.372542
H	-2.759488	0.288089	5.148389	C	-1.734651	2.178384	-3.535258
O	5.545375	-0.722021	1.785406	H	0.161444	2.871645	-2.756128
C	5.046713	0.462843	1.611304	H	-1.196702	3.157863	-1.709230
O	5.264409	1.397223	2.492275	C	-1.858194	3.437807	-4.402193
O	4.234310	0.686295	0.619322	H	-1.432459	1.341339	-4.167745
Na	3.486772	-1.524219	1.026980	H	-2.725072	1.928880	-3.142216
Na	4.904042	-0.335878	4.016827	C	-2.876497	3.272318	-5.532307
Na	3.280619	2.380911	1.871256	H	-2.141278	4.287536	-3.767249
				H	-0.873838	3.683276	-4.822465

TS2a_Cs

Pd	0.618917	1.693349	0.893774	H	-2.599045	2.442982	-6.192703
P	-0.161891	1.057426	-1.248163	H	-3.874708	3.058620	-5.133895
C	1.143057	0.132085	-2.273544	C	-0.360535	3.425597	0.819177
C	2.470016	0.905377	-2.043694	C	-1.134336	3.636147	1.990058
C	0.845022	0.112666	-3.790997	C	-0.202995	4.485057	-0.080357
C	1.339043	-1.325554	-1.795170	C	-1.817755	4.849550	2.164662
H	2.359456	1.947934	-2.369150	C	-0.874965	5.698494	0.110576

H	0.450024	4.377718	-0.940677	H	-1.866241	-3.532452	1.155942
C	-1.701568	5.872248	1.222247	C	-2.840967	-3.286123	-0.754245
H	-2.414600	5.010289	3.058597	C	-3.322549	-1.919894	1.296807
H	-0.743359	6.507082	-0.603729	H	-3.744463	-2.536019	-2.577400
H	-2.227750	6.810646	1.371925	C	-4.418446	-1.338537	-0.897324
C	2.547898	-0.054559	1.956314	H	-4.587418	-0.195585	0.943883
O	2.475125	1.006961	2.746321	H	-3.671434	-3.962041	-0.513671
O	1.664000	-0.154971	0.973369	H	-2.084848	-3.876223	-1.287316
O	3.408556	-0.948591	2.128253	H	-2.916957	-1.497641	2.225548
Cs	1.430237	-3.278697	1.689076	H	-4.150516	-2.584970	1.573513
C	-1.165339	2.546474	2.999110	H	-4.785509	-0.517333	-1.526212
C	-2.318208	2.341841	3.777151	H	-5.275634	-1.988480	-0.680334
C	-0.067981	1.637816	3.107195	C	-0.923996	2.240340	-1.450086
C	-2.420973	1.264256	4.655803	C	-1.873872	2.345385	-2.649538
H	-3.164651	3.012587	3.659828	H	-0.095681	2.944194	-1.558459
C	-0.220029	0.546226	3.982506	H	-1.444433	2.569017	-0.550242
H	1.283099	1.515528	2.802730	C	-2.727676	3.616274	-2.558885
C	-1.365502	0.356762	4.759067	H	-1.306467	2.364154	-3.585512
H	-3.325517	1.126784	5.241564	H	-2.540128	1.480844	-2.711264
H	0.601832	-0.159281	4.072454	C	-3.657197	3.793322	-3.760947
H	-1.434847	-0.490858	5.436038	H	-3.319739	3.580151	-1.634468
				H	-2.067389	4.488447	-2.463934
TS3_Cs							
Pd	1.053451	0.871561	1.081066	H	-3.085698	3.865217	-4.693200
P	-0.128304	0.651019	-0.923998	H	-4.340243	2.941482	-3.856611
C	1.055612	0.172466	-2.319404	C	1.006191	2.875647	0.887202
C	2.092440	1.323372	-2.413104	C	-0.113600	3.592423	1.375756
C	0.449122	-0.032319	-3.728307	C	2.132427	3.478977	0.337773
C	1.795446	-1.120203	-1.905080	C	-0.122844	4.990750	1.192374
H	1.591160	2.244890	-2.728771	C	2.075681	4.880233	0.189587
H	2.533829	1.520990	-1.435138	H	3.404517	2.707549	0.195321
C	3.195987	0.982263	-3.429463	C	0.955004	5.630693	0.580134
H	-0.059490	0.877071	-4.056571	H	-0.969160	5.569468	1.555984
H	-0.288947	-0.833998	-3.730037	H	2.931902	5.416304	-0.227583
C	1.561334	-0.384322	-4.740195	H	0.930889	6.710209	0.438568
H	2.207856	-0.976259	-0.903096	C	1.809525	-0.452175	3.228711
H	1.094369	-1.959920	-1.847797	O	2.152795	0.798267	2.983377
C	2.910175	-1.457478	-2.911457	O	1.360544	-1.120047	2.189384
H	3.909607	1.814369	-3.460392	O	1.927553	-0.964205	4.370738
C	2.575079	0.768888	-4.818783	Cs	-0.415817	-2.932061	4.045773
C	3.920656	-0.298710	-2.986426	C	-1.266976	2.947598	2.055254
H	1.099107	-0.540077	-5.722747	C	-2.586710	3.303702	1.725765
C	2.277640	-1.673842	-4.297959	C	-1.077638	1.962831	3.045124
H	3.417594	-2.374440	-2.585476	C	-3.678144	2.681501	2.334218
H	3.355791	0.537406	-5.554762	H	-2.754268	4.056395	0.960993
H	2.074368	1.686444	-5.153311	C	-2.169019	1.342498	3.655559
H	4.395773	-0.124026	-2.014994	H	-0.067419	1.694384	3.336661
H	4.720353	-0.547036	-3.695961	C	-3.474795	1.690626	3.297408
H	1.562840	-2.506127	-4.258303	H	-4.687230	2.961921	2.046044
H	3.050192	-1.944297	-5.028643	H	-1.998883	0.590596	4.421361
C	-1.545016	-0.599241	-0.703411	H	-4.322144	1.199556	3.766505
C	-1.065575	-1.766691	0.196056	Cs	2.839341	3.675330	3.805707
C	-2.137505	-1.219833	-1.989228	Cs	4.463173	-0.996549	1.195486
C	-2.659464	0.161513	0.060504	O	4.328209	2.037513	0.117142
H	-0.283163	-2.338152	-0.315237	C	5.276669	2.303255	1.061275
H	-0.607956	-1.370349	1.104522	O	6.251879	1.489261	1.112703
C	-2.239404	-2.705427	0.536767	O	5.108893	3.306619	1.821000
H	-1.377470	-1.827651	-2.487277	TS3_Cs'			
H	-2.452732	-0.450367	-2.697930	Pd	1.062739	0.121915	1.581755
C	-3.333000	-2.132773	-1.644136	P	-0.400715	-0.345113	-0.133257
H	-2.248857	0.594247	0.974929	C	0.664995	-0.882217	-1.606371
H	-3.042034	0.989227	-0.541848	C	1.880908	0.086379	-1.632256

C	-0.044490	-0.796574	-2.977464	C	2.069852	1.686323	2.815880
C	1.202756	-2.316646	-1.397892	C	0.764680	4.082173	3.358937
H	1.539018	1.119590	-1.767607	C	2.714999	2.650957	3.595495
H	2.403166	0.039357	-0.673031	H	2.886563	0.683681	2.442782
C	2.851834	-0.292457	-2.764829	C	2.052002	3.861764	3.847780
H	-0.392302	0.224715	-3.159333	H	0.249092	5.009548	3.595315
H	-0.921486	-1.450256	-3.002244	H	3.719451	2.486142	3.977902
C	0.932980	-1.195507	-4.104828	H	2.539696	4.633168	4.437642
H	1.706537	-2.352631	-0.428754	C	3.591813	-1.315417	1.620648
H	0.375181	-3.033147	-1.395081	O	3.915864	-0.119086	2.043440
C	2.180268	-2.694999	-2.525770	O	2.305907	-1.625200	1.477370
H	3.691428	0.413028	-2.756827	O	4.465681	-2.182071	1.349201
C	2.123545	-0.221890	-4.117753	Cs	2.629643	-4.677930	1.484730
C	3.370298	-1.720795	-2.521234	C	-1.311480	3.332400	2.163863
H	0.399935	-1.141697	-5.061859	C	-1.686954	4.500944	1.484524
C	1.447130	-2.627570	-3.876162	C	-2.296764	2.374447	2.446165
H	2.539567	-3.717629	-2.351422	C	-3.008690	4.694982	1.080699
H	2.811593	-0.480927	-4.932258	H	-0.932582	5.248353	1.256995
H	1.771489	0.800956	-4.302865	C	-3.617391	2.564288	2.041005
H	3.888882	-1.774012	-1.555830	H	-2.011110	1.480319	2.988035
H	4.089957	-1.999818	-3.301445	C	-3.977799	3.725296	1.352515
H	0.608536	-3.335986	-3.884448	H	-3.280924	5.599690	0.545224
H	2.123149	-2.915333	-4.691207	H	-4.363979	1.808350	2.265880
C	-1.660485	-1.645098	0.379778	H	-5.004228	3.874830	1.032078
C	-0.947968	-2.742089	1.210855				
C	-2.420860	-2.314256	-0.787700	TS3a_Cs			
C	-2.672930	-0.946661	1.322928	Pd	-1.419650	0.220677	0.898930
H	-0.211564	-3.257216	0.592749	C	-0.593825	2.053439	0.799576
H	-0.402162	-2.270880	2.034910	C	-1.341061	3.104107	1.368836
C	-1.967676	-3.761295	1.749234	C	0.681061	2.257751	0.291544
H	-1.719113	-2.832734	-1.447787	C	-0.758659	4.377159	1.435880
H	-2.936094	-1.562900	-1.390750	C	1.253772	3.536066	0.360458
C	-3.443320	-3.328657	-0.237146	H	1.175757	1.395136	-0.134243
H	-2.125799	-0.500339	2.159124	C	0.531457	4.588545	0.936566
H	-3.192169	-0.133901	0.810075	H	-1.313823	5.208989	1.861995
C	-3.703478	-1.958800	1.853797	H	2.253232	3.709590	-0.030156
H	-1.429577	-4.528814	2.319774	H	0.971518	5.580362	0.988910
C	-2.709720	-4.414784	0.569787	C	0.751214	-0.864552	1.920802
C	-2.979062	-3.047398	2.662148	O	0.403406	-0.932357	0.649357
H	-3.971065	-3.787921	-1.081506	O	-0.173569	-0.402123	2.731061
C	-4.450831	-2.601598	0.671531	O	1.904631	-1.178463	2.313905
H	-4.414893	-1.428429	2.498254	C	-2.685720	2.703238	1.792718
H	-3.427307	-5.157684	0.939678	C	-3.680941	3.529776	2.325778
H	-1.997838	-4.945313	-0.075824	C	-2.958444	1.333675	1.571296
H	-2.460736	-2.597199	3.518103	C	-4.936064	3.000278	2.633039
H	-3.702995	-3.768180	3.062284	H	-3.485406	4.586851	2.487657
H	-4.985389	-1.832125	0.100280	C	-4.211443	0.811407	1.872736
H	-5.202272	-3.309605	1.042530	C	-5.203024	1.647025	2.406206
C	-1.306143	1.162094	-0.724334	H	-5.709727	3.645072	3.040243
C	-2.548787	1.078292	-1.621959	H	-4.432599	-0.232612	1.665924
H	-0.527326	1.754677	-1.219135	H	-6.185387	1.242025	2.635645
H	-1.556506	1.713136	0.181560	Cl	-0.7711891	0.036696	-2.361138
C	-2.933469	2.465384	-2.151087	C	-2.441082	-0.183403	-0.935836
H	-2.395789	0.402099	-2.467154	C	-2.532383	-1.575310	-0.694051
H	-3.391356	0.672935	-1.051883	C	-3.596087	0.555425	-1.334327
C	-4.234151	2.448105	-2.956175	C	-3.745161	-2.249939	-0.867840
H	-3.029756	3.155596	-1.305171	H	-1.629770	-2.120122	-0.436076
H	-2.114443	2.849491	-2.773788	C	-4.770075	-0.178342	-1.549522
H	-4.482498	3.444382	-3.335959	C	-4.863665	-1.556226	-1.322965
H	-4.159689	1.771230	-3.814893	H	-3.792259	-3.320007	-0.683036
H	-5.072437	2.107699	-2.337641	H	-5.654387	0.353649	-1.887371
C	0.792894	1.929064	2.340666	H	-5.801335	-2.072304	-1.503456
C	0.086989	3.105380	2.596247	C	-3.627308	2.033989	-1.414717

C	-4.824556	2.727331	-1.146313	P	-2.463515	-1.967978	2.302097
C	-2.486063	2.798924	-1.709169	C	-1.296550	-3.482141	2.314482
C	-4.883824	4.116518	-1.194376	C	-0.784628	-3.611649	0.855049
H	-5.706216	2.174702	-0.842976	C	-1.935559	-4.838651	2.697259
C	-2.545734	4.191248	-1.756289	C	-0.083280	-3.229795	3.241529
H	-1.549335	2.293193	-1.892560	H	-1.630107	-3.817443	0.186383
C	-3.742880	4.861265	-1.506009	H	-0.339145	-2.662309	0.550584
H	-5.819215	4.620548	-0.967365	C	0.246512	-4.746732	0.730028
H	-1.643111	4.753711	-1.978482	H	-2.767345	-5.064186	2.023076
H	-3.786048	5.946231	-1.538364	H	-2.337267	-4.810349	3.713563
Cs	2.617362	-1.118852	-1.375981	C	-0.896166	-5.976866	2.587538
Cs	1.681795	1.503152	4.233941	H	0.365233	-2.260648	3.015020
				H	-0.415379	-3.197161	4.283800
TS3a_Cs_P							
Pd	-1.613074	0.272246	0.736749	C	0.950945	-4.361682	3.103211
C	-0.820874	2.126991	0.791715	H	0.584056	-4.808944	-0.314207
C	-1.635259	3.106383	1.407466	C	-0.398717	-6.081346	1.135732
C	0.479690	2.439408	0.402402	C	1.443109	-4.438893	1.647947
C	-1.105993	4.381157	1.663446	H	-1.376965	-6.918632	2.881569
C	0.993938	3.720808	0.648343	C	0.299314	-5.693082	3.512834
H	1.082397	1.679550	-0.079603	H	1.799341	-4.145974	3.765656
C	0.205542	4.686880	1.288015	H	0.325967	-6.900888	1.043271
H	-1.722521	5.143883	2.133178	H	-1.237919	-6.312020	0.466477
H	2.009768	3.964491	0.345212	H	1.893369	-3.477667	1.372858
H	0.606364	5.678808	1.479025	H	2.209047	-5.219596	1.546192
C	1.097724	-0.585418	1.380937	H	-0.035678	-5.640975	4.557230
O	0.264440	-0.642041	0.345897	C	1.026882	-6.512907	3.447279
O	0.653949	-0.152924	2.501629	C	-2.852359	-1.440940	4.090740
O	2.298417	-0.980225	1.196678	C	-1.699324	-0.539528	4.601290
C	-3.021459	2.677726	1.627123	C	-3.078580	-2.589450	5.101110
C	-4.065777	3.490184	2.091089	C	-4.120410	-0.550600	4.053628
C	-3.281019	1.351850	1.201817	H	-0.756222	-1.086322	4.617352
C	-5.378800	3.017605	2.082289	C	-1.563651	0.278169	3.888456
H	-3.861748	4.503824	2.428037	H	-2.015989	0.009753	6.005699
C	-4.606199	0.924174	1.138261	H	-2.184685	-3.213717	5.175278
C	-5.652035	1.744031	1.576096	H	-3.894010	-3.235954	4.769573
H	-6.187145	3.651427	2.436659	C	-3.405333	-2.021940	6.497830
H	-4.839824	-0.054489	0.736098	H	-3.955566	0.277729	3.366774
H	-6.677340	1.384785	1.529423	C	-4.980393	-1.108204	3.674024
Cl	-0.487653	0.563821	-2.473463	C	-4.453405	0.001639	5.451201
C	-2.297663	0.062769	-1.386445	H	-1.172716	0.620259	6.356801
C	-2.339136	-1.343756	-1.389465	C	-2.229485	-1.158666	6.984517
C	-3.414277	0.839190	-1.808961	C	-3.286555	0.872276	5.945194
C	-3.506431	-2.015395	-1.744390	H	-3.559669	-2.858354	7.191044
H	-1.442159	-1.884107	-1.125053	C	-4.680551	-1.164274	6.428018
C	-4.551194	0.105395	-2.195253	H	-5.363295	0.610488	5.378191
C	-4.619870	-1.287414	-2.164610	H	-2.433263	-0.774226	7.992314
H	-3.524637	-3.101506	-1.722334	H	-1.317802	-1.766920	7.046738
H	-5.419784	0.655065	-2.541110	H	-3.135963	1.716083	5.259232
H	-5.525974	-1.792333	-2.483930	H	-3.512917	1.289870	6.934950
C	-3.484754	2.321107	-1.773914	H	-5.527182	-1.776886	6.092213
C	-4.736020	2.964033	-1.667554	C	-4.933245	-0.781708	7.425536
C	-2.344938	3.142064	-1.817308	C	-4.049677	-2.700367	1.626377
C	-4.843853	4.350767	-1.647165	C	-5.031706	-3.562929	2.434302
H	-5.636852	2.374781	-1.549435	H	-3.718159	-3.263280	0.747197
C	-2.452219	4.532385	-1.792945	H	-4.604941	-1.855170	1.214505
H	-1.368772	2.686985	-1.862552	C	-6.137534	-4.128068	1.534332
C	-3.699606	5.150128	-1.717962	H	-4.524008	-4.391458	2.933846
H	-5.825104	4.808217	-1.555438	H	-5.495589	-2.966996	3.226690
H	-1.547168	5.132523	-1.823571	C	-7.171643	-4.946252	2.310934
H	-3.781487	6.233136	-1.698913	H	-6.635292	-3.300632	1.010962
Cs	2.034178	-1.941012	-1.720074	H	-5.681083	-4.751475	0.753607
Cs	1.104554	2.031497	4.417870	H	-7.948323	-5.345272	1.650435
				H	-6.699394	-5.793176	2.821754

H	-7.663990	-4.333214	3.074362	H	1.833661	4.219509	-0.220659
				H	0.226708	5.953482	0.526187
TS3a_Na				C	0.152987	-1.840131	1.999539
Pd	-1.543688	0.243251	0.994803	O	0.699221	-0.773235	1.432518
C	-0.630241	2.050355	1.061235	O	-1.137716	-1.746783	2.212424
C	-1.440569	3.133914	1.466504	O	0.836879	-2.853537	2.284578
C	0.700005	2.254516	0.711342	Cs	2.473850	-2.305133	-0.519656
C	-0.885373	4.417589	1.528960	C	-2.830909	2.633226	1.867643
C	1.245786	3.546104	0.779991	C	-3.923138	3.371249	2.341423
H	1.330346	1.425688	0.409470	C	-2.881026	1.219212	1.877269
C	0.453000	4.622531	1.186418	C	-5.067179	2.713581	2.798800
H	-1.501280	5.261224	1.828247	H	-3.893930	4.458037	2.334592
H	2.286814	3.705142	0.510926	C	-4.028486	0.570653	2.328374
H	0.875086	5.622230	1.230696	H	3.644976	2.705108	0.186610
C	1.082727	-0.794988	1.684197	C	-5.123527	1.316048	2.786498
O	0.153952	-1.112625	0.802590	H	-5.915628	3.289272	3.158153
O	0.767533	-0.476461	2.877643	H	-4.083581	-0.513941	2.301190
O	2.311748	-0.769012	1.265934	H	-6.019271	0.806383	3.132968
Na	2.748005	0.609335	3.065718	Cs	1.757403	1.737707	-3.233435
C	-2.827283	2.763507	1.755496	Cs	2.339062	0.890136	3.389224
C	-3.856757	3.609417	2.180968	O	4.312215	-0.119534	0.962680
C	-3.095147	1.394786	1.544124	C	3.936381	0.817294	0.232068
C	-5.136123	3.094030	2.399907	O	3.508153	0.801941	-0.951007
H	-3.667035	4.668008	2.336661	O	3.967481	2.082162	0.852751
C	-4.368247	0.881599	1.765029	Cl	-0.615528	-0.585790	-1.720212
C	-5.393236	1.735752	2.196250	C	-2.538918	-0.417509	-0.547393
H	-5.935136	3.753857	2.725435	C	-2.860475	-1.726336	-0.188330
H	-4.580747	-0.166305	1.569407	C	-3.477496	0.480342	-1.080119
H	-6.391840	1.340468	2.362613	C	-4.190454	-2.138979	-0.244968
Na	1.576764	-1.033717	-0.927228	H	-2.092908	-2.378781	0.202021
Cl	-0.664020	0.027181	-2.146112	C	-4.807409	0.009995	-1.128372
C	-2.447382	-0.253753	-0.878508	C	-5.173411	-1.268146	-0.720408
C	-2.525668	-1.633507	-0.626040	H	-4.443563	-3.147430	0.069911
C	-3.558600	0.515077	-1.320515	H	-5.561961	0.690602	-1.511365
C	-3.759147	-2.284639	-0.749838	H	-6.209054	-1.585216	-0.789016
H	-1.624592	-2.178950	-0.373601	C	-3.242333	1.886539	-1.492439
C	-4.747199	-0.211345	-1.490478	C	-4.087691	2.886209	-0.982351
C	-4.863575	-1.575979	-1.209922	C	-2.265852	2.255910	-2.428103
H	-3.823369	-3.347297	-0.536941	C	-3.944286	4.215403	-1.373662
H	-5.624161	0.319426	-1.843744	H	-4.834945	2.619083	-0.244674
H	-5.814648	-2.075176	-1.362998	C	-2.129576	3.585572	-2.830112
C	-3.567985	1.993586	-1.448097	H	-1.628396	1.486169	-2.842511
C	-4.776655	2.696431	-1.270138	C	-2.962916	4.573068	-2.299633
C	-2.405718	2.750274	-1.671492	H	-4.594684	4.973180	-0.946621
C	-4.823111	4.084767	-1.335118	H	-1.377039	3.853176	-3.567429
H	-5.682568	2.160017	-1.016617	H	-2.849239	5.608589	-2.606820
C	-2.453058	4.141921	-1.735965				
H	-1.456815	2.248484	-1.778127	TS3c_Cs			
C	-3.659622	4.820128	-1.573388	Pd	-1.946938	-0.461256	0.289002
H	-5.768494	4.594876	-1.175214	C	-1.766569	3.280530	3.229296
H	-1.533047	4.695370	-1.898604	C	-1.971538	2.715806	1.956354
H	-3.693451	5.904765	-1.616031	C	-0.627830	4.035664	3.512272
			C	-0.997610	2.935899	0.973837	
TS3b_Cs			C	0.321776	4.270490	2.512964	
Pd	-1.204511	0.282536	1.283000	H	-0.490678	4.451088	4.506624
C	-0.687723	2.177145	0.849879	C	0.124476	3.719626	1.244070
C	-1.590627	3.174370	1.297910	H	-1.139125	2.517306	-0.009759
C	0.540844	2.560878	0.308402	H	1.199698	4.875759	2.718865
C	-1.256977	4.528338	1.171147	H	0.842986	3.916667	0.454333
C	0.872744	3.921276	0.194623	C	-3.257780	2.036727	1.628026
H	1.255590	1.807546	-0.011112	C	-4.430200	2.704939	2.043681
C	-0.028215	4.901457	0.619591	C	-3.401539	0.840691	0.894032
H	-1.951490	5.296138	1.502303	C	-5.703459	2.241417	1.730468

H	-4.323379	3.634012	2.595327	C	-3.229516	-1.506987	6.527999
C	-4.687859	0.408291	0.546380	H	-4.583534	-0.092030	3.111301
C	-5.834796	1.088359	0.956594	H	-5.152098	-1.602895	3.815847
H	-6.579257	2.789655	2.063754	C	-4.811181	-0.039711	5.261863
H	-4.806503	-0.479229	-0.066832	H	-1.723130	1.488170	5.651719
H	-6.815144	0.718108	0.670427	C	-2.274123	-0.316026	6.726655
Cl	-0.112970	0.008733	-3.156567	C	-3.859813	1.151730	5.455320
C	-2.396450	-0.039673	-1.695568	H	-3.123035	-2.209910	7.363199
C	-2.769545	-1.369293	-1.972423	C	-4.680107	-1.006062	6.449022
C	-3.139743	1.062933	-2.173756	H	-5.843763	0.321946	5.185629
C	-4.016660	-1.625087	-2.562443	H	-2.511476	0.207641	7.661115
H	-2.079813	-2.176607	-1.758015	H	-1.239432	-0.674211	6.808130
C	-4.371494	0.762633	-2.766123	H	-3.982734	1.847547	4.620021
C	-4.815594	-0.555068	-2.950754	H	-4.112721	1.694584	6.374854
H	-4.321044	-2.649248	-2.754243	H	-5.363886	-1.855096	6.321988
H	-5.002879	1.588880	-3.079578	H	-4.958427	-0.501497	7.382667
H	-5.773639	-0.732586	-3.428866	C	-4.137912	-2.801480	1.657751
C	-2.769357	2.486634	-1.974842	C	-4.845720	-3.946738	2.393628
C	-3.681717	3.351102	-1.349482	H	-3.920098	-3.094453	0.625473
C	-1.540662	2.999968	-2.417265	H	-4.814007	-1.946849	1.577416
C	-3.361982	4.692810	-1.148777	C	-6.301353	-4.094425	1.936319
H	-4.622568	2.956712	-0.981439	H	-4.317953	-4.888300	2.212031
C	-1.230562	4.347079	-2.227027	H	-4.825288	-3.786233	3.477000
H	-0.840185	2.328591	-2.900168	C	-7.020736	-5.258112	2.621158
C	-2.135204	5.196318	-1.586356	H	-6.835498	-3.156402	2.138765
H	-4.068486	5.342210	-0.640391	H	-6.324537	-4.231442	0.847025
H	-0.275797	4.731691	-2.575046	H	-8.060116	-5.338724	2.287553
H	-1.885880	6.241184	-1.426670	H	-6.524235	-6.210403	2.403557
P	-2.560937	-2.069631	2.312552	H	-7.026951	-5.128934	3.709401
C	-1.342162	-3.519863	2.488726	C	0.608767	-0.868625	0.209426
C	-1.255012	-4.171020	1.080920	O	0.088311	0.218618	0.753656
C	-1.654028	-4.668459	3.485007	O	-0.259893	-1.689924	-0.290713
C	0.024655	-2.905594	2.880731	O	1.843780	-1.065210	0.224215
H	-2.204131	-4.672452	0.856911	Cs	2.543127	1.632690	-1.354842
H	-1.079108	-3.406419	0.328450	Cs	1.825878	0.633273	3.335632
C	-0.117065	-5.207750	1.032404	Cs	4.572839	-2.347386	0.652138
H	-2.609728	-5.136351	3.241635	O	5.127197	0.688404	0.219927
H	-1.725620	-4.307015	4.507841	C	4.594785	1.006452	1.355764
C	-0.534040	-5.735580	3.437377	O	4.749890	0.233768	2.386719
H	0.270877	-2.084784	2.208492	O	3.870338	2.076391	1.458062
H	-0.037999	-2.497481	3.897238	H	-2.505192	3.127532	4.006593
C	1.135337	-3.966828	2.825355				
H	-0.057007	-5.612128	0.014344				
C	-0.421849	-6.336840	2.027914	TS3b_Na			
C	1.217443	-4.529611	1.395183	Pd	-1.312978	0.731714	1.713183
H	-0.783911	-6.522923	4.159103	C	-1.306337	2.727158	1.496806
C	0.810736	-5.092366	3.820622	C	-2.514027	3.403579	1.790323
H	2.088076	-3.493861	3.097292	C	-0.164285	3.464788	1.191317
H	0.370751	-7.095911	2.004799	C	-2.562177	4.799905	1.733984
H	-1.359554	-6.836235	1.753073	C	-0.221549	4.865050	1.123857
H	1.420631	-3.712496	0.694530	H	0.792522	2.971708	1.037747
H	2.038121	-5.255730	1.323116	C	-1.421535	5.527556	1.385459
H	0.761212	-4.688594	4.840240	H	-3.486912	5.324262	1.960037
H	1.605004	-5.849605	3.809242	H	0.673636	5.431494	0.881482
C	-2.998571	-1.302293	4.004463	H	-1.466098	6.611520	1.334407
C	-2.046712	-0.104526	4.233979	C	0.586248	-1.067110	1.931638
C	-2.861813	-2.242468	5.223813	O	0.830279	0.197523	1.596500
C	-4.454765	-0.771392	3.954890	O	-0.626547	-1.363427	2.231394
H	-1.017096	-0.473041	4.307047	O	1.550066	-1.903892	1.930719
H	-2.089502	0.572622	3.382022	C	-3.602734	2.505458	2.185319
C	-2.409555	0.641450	5.531682	C	-4.911115	2.876380	2.516330
H	-1.829243	-2.588680	5.309293	C	-3.213607	1.148321	2.263364
H	-3.499110	-3.123923	5.107100	C	-5.820529	1.911414	2.957515
			H	-5.219222	3.916334	2.444612	

C	-4.115008	0.199206	2.732006	C	-2.062042	0.090342	-1.403858
H	4.619025	-0.011109	-3.098012	C	-1.877018	-1.297211	-1.466340
C	-5.419983	0.579969	3.080748	C	-3.188856	0.739534	-1.960688
H	-6.835341	2.201088	3.214587	C	-2.911544	-2.108508	-1.948223
H	-3.825593	-0.844468	2.804256	H	-0.932631	-1.725993	-1.159914
H	-6.122563	-0.168795	3.437142	C	-4.200530	-0.125015	-2.419337
O	3.138833	-0.623414	-0.548385	C	-4.082209	-1.516411	-2.413643
C	3.453269	-0.004722	-1.612987	H	-2.776630	-3.185542	-1.973836
O	2.913482	1.032389	-2.060048	H	-5.131233	0.307354	-2.767810
O	4.483146	-0.567323	-2.315739	H	-4.899276	-2.125524	-2.786139
Cl	-0.424226	-1.027630	-1.154976	C	-3.368730	2.208887	-2.008173
C	-2.414347	-0.224672	-0.215646	C	-4.436327	2.797694	-2.712613
C	-2.998323	-1.398385	0.234603	C	-2.482162	3.066883	-1.337574
C	-3.036069	0.730786	-1.017744	C	-4.625188	4.178127	-2.714967
C	-4.358494	-1.579010	-0.011324	H	-5.127426	2.185479	-3.280339
H	-2.412940	-2.105310	0.807141	C	-2.673175	4.446293	-1.333726
C	-4.416899	0.511110	-1.214637	H	-1.644222	2.646446	-0.806960
C	-5.073040	-0.615846	-0.727430	C	-3.749102	5.013639	-2.017845
H	-4.848917	-2.472477	0.363134	H	-5.459262	4.601083	-3.267292
H	-4.961774	1.253316	-1.790671	H	-1.977440	5.074541	-0.784709
H	-6.130874	-0.751782	-0.926419	H	-3.900007	6.089045	-2.016491
C	-2.417641	1.956501	-1.582637	P	-2.450281	-1.949745	2.348870
C	-3.002134	3.201359	-1.306476	C	-1.360941	-3.517179	2.367065
C	-1.300670	1.913633	-2.431902	C	-0.871696	-3.687717	0.904222
C	-2.464285	4.374864	-1.831572	C	-2.066813	-4.830291	2.778476
H	-3.862275	3.244856	-0.648777	C	-0.122099	-3.311860	3.267749
C	-0.763103	3.089836	-2.958974	H	-1.731149	-3.834986	0.239753
H	-0.864224	0.957064	-2.688905	H	-0.361068	-2.776672	0.588656
C	-1.339987	4.325452	-2.657179	C	0.084271	-4.886303	0.775199
H	-2.917319	5.328887	-1.582725	H	-2.914610	-5.021549	2.114550
H	0.100073	3.035639	-3.616405	H	-2.456537	-4.761228	3.797908
H	-0.920415	5.239829	-3.065822	C	-1.090945	-6.022721	2.673084
Na	1.165404	1.019001	-0.549074	H	0.366114	-2.372489	3.003585
Na	1.855226	-2.493028	-0.240980	H	-0.426087	-3.235027	4.315810
Na	3.134868	-0.180778	1.693758	C	0.849283	-4.499451	3.130575
				H	0.401289	-4.973859	-0.271914
				C	-0.629216	-6.175041	1.213797
TS3c_Na							
Pd	-1.537510	0.148135	0.721605	C	1.311817	-4.639680	1.669573
C	-0.745689	1.950902	1.200103	H	-1.615086	-6.932174	2.992226
C	-1.620862	2.794303	1.917427	C	0.133919	-5.787252	3.574194
C	0.564441	2.337750	0.949682	H	1.718923	-4.321658	3.778323
C	-1.127147	3.993010	2.452530	H	0.044916	-7.035784	1.117663
C	1.042097	3.549127	1.467724	H	-1.493512	-6.365552	0.564672
H	1.208824	1.719527	0.341477	H	1.825633	-3.727178	1.342558
C	0.201766	4.362975	2.234615	H	2.023497	-5.470658	1.577234
H	-1.786021	4.650513	3.013683	H	-0.180026	-5.698399	4.622231
H	2.066110	3.842105	1.254712	H	0.816405	-6.644667	3.511588
H	0.574333	5.298390	2.642300	C	-2.797114	-1.333380	4.108202
C	1.409067	-0.719322	1.295293	C	-1.598402	-0.448692	4.540285
O	0.459211	-0.704633	0.398267	C	-3.032376	-2.433259	5.169216
O	1.206706	-0.484070	2.526927	C	-4.046857	-0.414018	4.068339
O	2.614199	-1.006412	0.858086	H	-0.672690	-1.026901	4.553135
C	-3.017788	2.356792	1.890515	H	-1.457668	0.345042	3.800084
C	-4.114802	3.060623	2.404544	C	-1.852235	0.168395	5.927708
C	-3.230625	1.161657	1.164047	H	-2.163267	-3.091945	5.239174
C	-5.413756	2.611874	2.158771	H	-3.885479	-3.057037	4.887674
H	-3.958264	3.971224	2.976438	C	-3.289909	-1.797503	6.551352
C	-4.528886	0.764866	0.862565	H	-3.896987	0.381090	3.341565
C	-5.621662	1.480939	1.365150	H	-4.930558	-0.973970	3.753617
H	-6.260941	3.159957	2.560423	C	-4.310350	0.210127	5.450958
H	-4.703652	-0.093707	0.226451	H	-0.979063	0.769108	6.212710
H	-6.632061	1.151714	1.138093	C	-2.070909	-0.951928	6.960873
Cl	-0.151852	1.035585	-2.447486	C	-3.100727	1.064044	5.865785

H	-3.445925	-2.599454	7.283775	O	1.490145	1.498063	0.797604
C	-4.539844	-0.902522	6.486367	C	-2.604377	0.121897	0.232745
H	-5.202634	0.844335	5.378799	C	-3.085681	-1.222233	0.264371
H	-2.229981	-0.520881	7.957638	C	-3.159767	0.971455	-0.753104
H	-1.177472	-1.587203	7.021430	C	-3.998509	-1.638734	-0.722178
H	-2.949058	1.871044	5.138381	C	-4.065856	0.531264	-1.714946
H	-3.283483	1.531270	6.842234	H	-2.866391	2.008194	-0.785833
H	-5.416730	-1.501518	6.208244	C	-4.478513	-0.797098	-1.721501
H	-4.744156	-0.468214	7.473524	H	-4.351123	-2.664959	-0.674560
C	-4.069253	-2.574827	1.664138	H	-4.433337	1.233740	-2.457895
C	-5.081414	-3.400149	2.475630	H	-5.176439	-1.168259	-2.465795
H	-3.779832	-3.129358	0.763626	C	-2.876175	-2.267066	1.319074
H	-4.582690	-1.685158	1.297888	C	-1.814383	-3.177416	1.302257
C	-6.218037	-3.908215	1.580029	C	-3.883546	-2.425888	2.284307
H	-4.609627	-4.252284	2.969065	C	-1.736412	-4.189683	2.260795
H	-5.511369	-2.786912	3.273523	H	-1.026521	-3.046078	0.574959
C	-7.280283	-4.687029	2.358973	C	-3.804272	-3.432991	3.245453
H	-6.683779	-3.054970	1.068989	H	-4.722244	-1.736142	2.289111
H	-5.795880	-4.544021	0.790211	C	-2.723325	-4.317883	3.240292
H	-8.079119	-5.044924	1.701486	H	-0.895501	-4.877521	2.241820
H	-6.841451	-5.558788	2.857564	H	-4.586125	-3.528268	3.993541
H	-7.738424	-4.059910	3.132085	H	-2.655793	-5.103433	3.987495
H	3.294533	4.178120	-1.644493				
O	3.176977	3.297660	-2.031747				
C	3.600107	2.403364	-1.083593	TS4_Cs'			
O	3.496112	1.184823	-1.401902	Pd	-1.058037	0.454412	-0.765094
O	4.043716	2.857468	0.004156	C	-1.063730	2.378473	-0.363072
Na	4.134443	0.687621	0.819485	C	-1.910128	3.141165	-1.183179
Na	1.865949	-0.387746	-1.368567	C	-0.296436	2.931313	0.650523
Na	3.126043	-1.520316	3.100482	C	-1.971645	4.525854	-0.957461
			C	-0.376406	4.316219	0.858268	
			H	0.330787	2.296054	1.265941	
TS4_Cs			C	-1.206145	5.105814	0.054655	
Pd	-0.547656	0.810219	0.540530	H	-2.622921	5.145160	-1.567128
C	-1.087227	2.749939	0.351680	H	0.204555	4.771691	1.655120
C	-2.097664	3.196375	1.234714	H	-1.263783	6.176423	0.224950
C	-0.567191	3.629030	-0.599290	C	-2.637246	2.386531	-2.207671
C	-2.567563	4.516456	1.153661	C	-3.179418	2.967330	-3.357520
C	-1.045529	4.945234	-0.678904	C	-2.661825	0.965489	-2.051169
H	0.186443	3.267871	-1.292981	C	-3.701078	2.177039	-4.380718
C	-2.041038	5.388700	0.199912	H	-3.146092	4.046497	-3.474440
H	-3.346016	4.861992	1.829105	C	-3.123513	0.184646	-3.124633
H	-0.648638	5.620760	-1.433295	C	-3.644386	0.784776	-4.269250
H	-2.411701	6.407788	0.134601	H	-4.117184	2.641032	-5.269121
C	0.950385	-1.652462	1.488848	H	-3.113445	-0.894166	-3.054678
O	0.924767	-1.215301	2.683557	H	-4.014214	0.157312	-5.074837
O	0.091843	-1.186838	0.577435	Cs	3.110724	2.746984	-1.691755
O	1.781339	-2.539778	1.072365	O	2.715773	0.186344	0.203693
Cs	1.418757	-1.912732	-2.015029	C	1.484487	0.192503	-0.031984
C	-2.523629	2.190549	2.211472	O	0.557051	-0.100857	0.838237
C	-3.150889	2.478210	3.428590	O	1.031671	0.548752	-1.239425
C	-2.072294	0.860746	1.956314	C	-3.150193	0.255410	-0.399637
C	-3.247657	1.505949	4.426164	C	-3.483617	-1.126091	-0.298919
H	-3.503481	3.487456	3.623322	C	-3.897807	1.173482	0.363948
C	-2.048143	-0.060953	3.013448	C	-4.573551	-1.517586	0.487567
C	-2.646630	0.258209	4.232628	C	-4.963340	0.760371	1.156860
H	-3.733833	1.740927	5.368501	H	-3.662602	2.228568	0.310521
H	-1.519331	-0.991757	2.883407	C	-5.317936	-0.589142	1.213084
H	-2.640094	-0.474470	5.034890	H	-4.813546	-2.575132	0.549458
Cs	2.658169	4.316215	1.233490	H	-5.521454	1.497693	1.726124
Cs	3.824215	-0.254364	2.025006	H	-6.153432	-0.916575	1.823288
O	3.170039	1.623882	-0.670919	C	-2.696718	-2.174216	-1.001938
C	1.939584	1.391105	-0.448438	C	-1.302878	-2.273330	-0.839734
O	1.081811	1.055370	-1.352917	C	-3.335272	-3.073387	-1.871420

C	-0.563555	-3.198624	-1.583537				
H	-0.783034	-1.696023	-0.071000				
C	-2.597298	-4.007769	-2.597277				
H	-4.411203	-3.009246	-2.001750				
C	-1.206065	-4.063014	-2.469057				
H	0.512220	-3.251315	-1.447545				
H	-3.107705	-4.685984	-3.274274				
H	-0.633077	-4.783064	-3.044524				
TS4a_Cs				TS5_Cs			
Pd	-0.577329	0.173737	-0.305554	Pd	-0.961439	0.203084	-0.445279
C	-2.054395	1.691967	-0.241491	C	0.916174	-0.028752	-1.128072
C	-2.527673	1.828151	1.101090	C	1.251365	-0.916350	-2.179103
C	-2.098707	2.825111	-1.080586	C	1.961473	0.552767	-0.394429
C	-3.151369	3.023376	1.493427	C	2.597983	-1.219156	-2.440479
C	-2.684586	4.014448	-0.659206	C	3.302598	0.258109	-0.671197
H	-1.700332	2.755502	-2.085752	H	1.729224	1.229853	0.424059
C	-3.248823	4.106206	0.622657	C	3.623680	-0.639183	-1.692667
H	-3.517650	3.122325	2.511133	H	2.836843	-1.890221	-3.261558
H	-2.717214	4.866460	-1.332639	H	4.091502	0.725079	-0.086491
H	-3.732654	5.023408	0.944852	H	4.660737	-0.871452	-1.917268
C	1.455876	-2.234326	-0.277946	C	0.185805	-1.521840	-3.020390
O	1.686539	-2.455432	0.963314	C	0.126141	-2.903925	-3.248158
O	0.231283	-1.878963	-0.674244	C	-0.805991	-0.690707	-3.584254
O	2.372581	-2.351367	-1.170726	C	-0.912672	-3.463758	-3.995536
Cs	0.948780	-1.572594	-3.712374	C	-0.912672	-3.463758	-3.995536
C	-2.152271	0.765668	2.038659	C	-0.2627020	-0.612240	-4.714813
C	-2.572267	0.667879	3.374161	H	-2.727238	-3.068055	-5.097424
C	-1.218372	-0.166556	1.546312	C	-0.733721	0.780261	-3.336750
C	-2.056206	-0.332141	4.196738	C	-1.551304	1.297696	-2.301761
H	-3.305540	1.364663	3.769361	C	0.208026	1.590641	-3.996921
C	-0.670288	-1.145171	2.368404	C	-1.420742	2.662817	-1.963127
C	-1.103447	-1.226885	3.698977	H	-2.684732	0.789632	-2.170688
H	-2.396057	-0.411830	5.225736	C	0.316399	2.937709	-3.609593
H	0.098771	-1.809803	1.965306	C	-0.489040	3.476707	-2.605415
H	-0.697607	-1.998856	4.349684	H	1.043647	3.567337	-4.114844
Cs	0.996313	3.685289	1.429361	C	-0.386929	4.525152	-2.338136
Cs	4.125958	-0.505150	0.601308	C	1.143166	1.049188	-5.016914
O	2.796852	1.604807	-1.654044	H	0.686980	0.317460	-6.124271
C	1.684535	1.213480	-1.215867	C	2.523885	1.259734	-4.877595
O	0.662830	0.949775	-1.995496	C	1.585156	-0.193321	-7.060470
O	1.473260	1.037073	0.074035	H	-0.377057	0.151974	-6.250561
C	-2.497192	0.148765	-1.254817	C	2.890394	1.800157	-4.010602
C	-3.677282	-0.556586	-0.910966	H	3.423813	0.750456	-5.813646
C	-2.210460	0.299953	-2.635549	C	2.957714	0.019723	-6.908456
C	-4.494518	-1.066234	-1.938336	H	1.212445	-0.754409	-7.912525
C	-3.024537	-0.221573	-3.630879	C	4.489161	0.915919	-5.682001
H	-1.313236	0.839784	-2.913899	H	3.656842	-0.380752	-7.636529
C	-4.186769	-0.917892	-3.285833	O	3.677760	-2.315340	-0.818479
H	-5.396438	-1.597129	-1.646996	Cs	-4.563947	2.194847	-1.186486
H	-2.751956	-0.081258	-4.673876	C	4.801931	0.967443	-1.456785
H	-4.840154	-1.330117	-4.048516	O	-5.781664	0.309074	-0.949333
C	-4.197411	-0.791730	0.466386	Cs	-3.967760	-0.630892	-0.717691
C	-3.761048	-1.880606	1.230420	Cs	0.935450	-0.630892	1.411202
C	-5.235859	0.009512	0.956640	O	-3.983916	-0.717691	1.225310
C	-4.343859	-2.156002	2.465495	H	-2.094828	0.308513	-2.283147
H	-2.951906	-2.498433	0.856908				
C	-5.814939	-0.259413	2.197652				
H	-5.582766	0.848851	0.361414				
C	-5.371968	-1.345562	2.952983				
H	-3.989566	-2.998338	3.051324				
H	-6.615932	0.373500	2.569116				
H	-5.822384	-1.558992	3.918022				
TS5_Cs'				Pd	0.754850	0.300503	0.485099
				C	2.569795	0.322087	-0.338759
				C	2.881537	-0.506469	-1.439633
				C	3.595705	1.000251	0.328338
				C	4.225525	-0.695456	-1.794530
				C	4.932690	0.809010	-0.040802

H	3.358140	1.669243	1.152626	H	0.466710	-2.873545	-4.050404
C	5.246379	-0.045880	-1.099347	C	1.568368	1.132527	-1.922080
H	4.463936	-1.324236	-2.647939	C	1.552164	1.628875	-0.585981
H	5.722252	1.330658	0.493257	C	1.499820	2.040361	-3.011056
H	6.280259	-0.187716	-1.399445	C	1.516667	3.028348	-0.379041
C	1.794655	-1.144132	-2.227914	H	-0.867678	1.831736	-2.686830
C	1.829403	-2.502107	-2.570654	C	1.380977	3.413990	-2.757687
C	0.681675	-0.367364	-2.620128	C	1.396422	3.905677	-1.446913
C	0.767835	-3.093132	-3.260435	H	1.334519	4.100152	-3.597201
H	2.682907	-3.101810	-2.268050	H	1.329825	4.976174	-1.271350
C	-0.387372	-0.969100	-3.287999	C	1.611052	1.611050	-4.433841
C	-0.349871	-2.329276	-3.607008	C	0.617056	1.956515	-5.360535
H	0.807884	-4.148366	-3.513867	C	2.728612	0.889919	-4.881941
H	-1.245472	-0.365444	-3.566791	C	0.730638	1.580794	-6.700361
H	-1.183994	-2.785960	-4.130891	H	-0.260353	2.497299	-5.019378
C	0.682477	1.089502	-2.291105	C	2.845215	0.518451	-6.219617
C	-0.012159	1.513491	-1.124791	H	3.502677	0.619046	-4.171002
C	1.470126	1.993012	-3.026196	C	1.844393	0.859839	-7.134227
C	0.120855	2.862210	-0.707911	H	-0.052710	1.849220	-7.403141
H	-1.069461	0.962754	-0.785801	H	3.718278	-0.036368	-6.550602
C	1.561333	3.321393	-2.578832	H	1.933851	0.566970	-8.175993
C	0.897332	3.760451	-1.431292	O	-2.379379	3.232840	-1.821435
H	2.174714	4.017072	-3.144068	C	-2.702867	2.071319	-2.165633
H	0.991469	4.794757	-1.115013	O	-3.789826	1.466686	-2.050491
C	2.289385	1.554308	-4.185918	Cs	-2.752819	-1.432358	-1.435344
C	1.717539	0.911168	-5.293420	Cs	-2.220733	2.983142	1.240943
C	3.675090	1.772474	-4.172476	O	-1.509703	0.054170	0.961769
C	2.512965	0.494172	-6.359748	C	-1.298897	-1.019338	1.694293
H	0.646684	0.741710	-5.317547	O	-2.154414	-1.948348	1.784775
C	4.471777	1.353749	-5.238259	O	-0.118742	-1.098322	2.266605
H	4.128336	2.243839	-3.306217	Cs	0.436975	-3.948740	1.433461
C	3.892983	0.712226	-6.334896	O	-1.674504	1.296879	-2.750647
H	2.054892	0.001011	-7.211908	H	1.568109	3.414862	0.635024
H	5.544311	1.520697	-5.207212				
H	4.511948	0.383349	-7.164171				
O	-2.331836	0.470346	-0.385333	TS6_Cs'			
C	-2.212790	-0.191758	0.733755	Pd	1.044665	0.168167	0.998389
O	-3.113712	-0.970229	1.146219	C	3.004103	0.463127	0.546987
O	-1.089652	-0.069830	1.435162	C	3.639453	-0.461400	-0.315872
Cs	-1.158778	-3.328096	0.458656	C	3.779317	1.191234	1.467172
H	-0.421854	3.191099	0.173872	C	5.020920	-0.682458	-0.186257
			C	5.148216	0.955319	1.586603	
			H	3.303383	1.939479	2.093661	
			C	5.770474	0.011243	0.761669	
TS6_Cs			H	5.512152	-1.383560	-0.855020	
Pd	0.729599	0.425615	0.829435	H	5.731442	1.510645	2.315900
C	2.735609	0.610410	0.520108	H	6.839085	-0.163973	0.840967
C	3.362337	-0.415102	-0.243893	C	2.845859	-1.160149	-1.347577
C	3.516601	1.294846	1.480858	C	3.093484	-2.511444	-1.644951
C	4.699821	-0.760137	0.014574	C	1.828353	-0.471921	-2.063240
C	4.836900	0.936355	1.727958	C	2.343341	-3.194279	-2.600652
H	3.069219	2.110675	2.041634	H	3.867265	-3.035924	-1.092581
C	5.434098	-0.101716	0.997285	C	1.068514	-1.183215	-3.007171
H	5.174239	-1.533831	-0.583294	C	1.314005	-2.527969	-3.275976
H	5.408182	1.463492	2.487791	H	2.546971	-4.241374	-2.804689
H	6.470077	-0.373168	1.176721	H	0.277451	-0.666901	-3.538962
C	2.594756	-1.077210	-1.311811	H	0.707285	-3.053108	-4.007699
C	2.749988	-2.453198	-1.564762	C	1.593158	0.973324	-1.826137
C	1.685170	-0.328480	-2.114281	C	1.567060	1.442797	-0.491855
C	2.000227	-3.103636	-2.541188	C	1.413482	1.896539	-2.887709
H	3.446198	-3.021309	-0.954039	C	1.381800	2.811076	-0.226392
C	0.933511	-1.006705	-3.091862	C	1.165096	3.243463	-2.590480
C	1.073941	-2.375776	-3.299662	C	1.146898	3.699573	-1.271105
H	2.125003	-4.170803	-2.701558	H	1.039893	3.945104	-3.409167
H	0.216338	-0.446675	-3.680268				

H	0.975732	4.752049	-1.063260	H	-1.009549	-1.690834	3.353733
C	1.550244	1.517799	-4.321127	C	-2.537057	1.127712	-0.065614
C	0.549084	1.854216	-5.243734	C	-3.857053	1.008107	0.424950
C	2.701481	0.863241	-4.787980	C	-2.339644	1.921376	-1.245515
C	0.686181	1.532497	-6.595295	C	-4.954234	1.619613	-0.166851
H	-0.346802	2.357591	-4.892564	H	-4.018760	0.454265	1.342000
C	2.841403	0.545630	-6.137048	C	-3.464085	2.547789	-1.810159
H	3.485348	0.603373	-4.083941	C	-4.752547	2.409337	-1.292021
C	1.831980	0.875363	-7.046302	H	-5.943485	1.497943	0.264478
H	-0.103463	1.793141	-7.293847	H	-3.353708	3.160820	-2.694480
H	3.740399	0.042732	-6.481150	H	-5.580416	2.918648	-1.777363
H	1.939976	0.623904	-8.097035				
O	-2.203722	0.842622	1.523284				
C	-1.889980	-0.500931	1.542807	TSM_Cs			
O	-2.765426	-1.321649	1.224436	Pd	-0.186393	1.504257	-1.219528
O	-0.692909	-0.755677	1.905730	C	-0.620576	3.480806	-1.328948
Cs	-0.536745	-3.470009	0.304533	C	-0.915648	3.916634	-2.640126
H	1.415391	3.169876	0.797195	C	-0.564634	4.396260	-0.277861
H	-3.129186	0.889629	1.240502	C	-1.085905	5.290614	-2.874854
			C	-0.738994	5.763683	-0.530610	
			H	-0.374143	4.057712	0.734055	
			C	-0.989521	6.210278	-1.830314	
TSL_Cs			H	-1.288997	5.639325	-3.883326	
Pd	0.043484	1.839311	-1.186568	H	-0.677284	6.473557	0.289434
C	-0.181058	3.713417	-0.491587	H	-1.117136	7.270039	-2.029023
C	-0.614530	4.585119	-1.523164	C	1.732620	-0.226202	-1.975224
C	0.044181	4.245271	0.782274	O	1.888976	1.090311	-2.301759
C	-0.760290	5.957233	-1.276243	O	0.610560	-0.502395	-1.379500
C	-0.118061	5.616871	1.029006	O	2.619045	-1.054117	-2.234687
H	0.327422	3.581826	1.594599	Cs	3.577641	-1.370900	0.816517
C	-0.506055	6.474826	-0.004079	C	-1.081692	2.888685	-3.691676
H	-1.092471	6.621819	-2.069808	C	-1.975926	3.065444	-4.757887
H	0.049202	6.010823	2.029139	C	-0.430888	1.641879	-3.519241
H	-0.631008	7.537367	0.184381	C	-2.236857	2.016839	-5.641673
C	1.412383	0.179538	-2.857350	H	-2.506483	4.005813	-4.874044
O	1.880378	1.408975	-2.773234	O	-0.731581	0.595970	-4.404386
O	0.388802	-0.102927	-2.088399	H	0.831022	1.446402	-2.962651
O	1.926847	-0.690404	-3.612027	Cs	1.826722	-2.431026	-0.704999
Cs	1.826722	-2.431026	-0.704999	C	-1.622815	0.773153	-5.464792
C	-0.913856	3.942700	-2.822880	H	-2.939058	2.164794	-6.456943
C	-0.959950	4.615971	-4.054037	H	-0.249380	-0.368753	-4.264922
C	-1.111557	2.542818	-2.816698	H	-1.842549	-0.045321	-6.144061
C	-1.215731	3.917602	-5.234914	Cs	3.297311	4.080266	-0.957684
H	-0.776327	5.686358	-4.092441	Cs	4.906330	0.554864	-3.660414
C	-1.339890	1.839905	-3.998577	O	5.757833	0.154342	-0.645399
H	2.924544	1.641781	-1.538367	C	5.331246	1.363312	-0.449989
C	-1.395045	2.528038	-5.211524	O	5.671372	2.315482	-1.269321
H	-1.260880	4.454381	-6.178071	O	4.524510	1.622028	0.548472
H	-1.463732	0.762807	-3.963341	C	0.122294	1.529255	0.774228
H	-1.575260	1.987206	-6.136704	C	-1.043895	1.463324	1.558592
Cs	3.695341	4.056496	1.395853	C	1.386027	1.604599	1.342211
Cs	4.794082	0.449605	-3.730507	C	-0.923867	1.502020	2.953724
O	4.005484	-0.276435	-0.743450	C	1.487576	1.651429	2.743932
C	4.029907	0.819579	-0.119948	H	2.304088	1.621779	0.752108
O	4.460019	1.057042	1.034062	C	0.340313	1.603735	3.540531
O	3.529269	1.933195	-0.793926	H	-1.809631	1.455377	3.580973
C	-0.119430	0.982637	0.658658	H	2.470079	1.724205	3.202392
C	-1.452852	0.522006	0.779021	H	0.429133	1.642120	4.622163
C	0.848097	0.538548	1.569276	C	-2.280818	1.349898	0.780104
C	-1.739069	-0.473343	1.736096	C	-3.579412	1.193414	1.280455
C	0.532231	-0.397922	2.563245	C	-2.098850	1.371340	-0.616650
H	1.873684	0.892444	1.491345	C	-4.658789	1.065357	0.403956
C	-0.759457	-0.928101	2.621252	H	-3.746540	1.163914	2.353359
H	-2.727451	-0.918619	1.794818	C	-3.160688	1.246326	-1.499905
H	1.293884	-0.731313	3.265390	C	-4.452940	1.086662	-0.976882

H	-5.662439	0.946219	0.800289	C	-1.690355	3.306011	0.414256
H	-3.001791	1.275145	-2.571263	C	-2.515201	3.121922	-0.696902
H	-5.294545	0.986255	-1.655987	C	-3.145629	1.894142	-0.866866
				C	-3.925599	-0.335332	-0.262729
				C	-3.661567	-1.722061	-0.385588
TSN_Cs				C	-4.650873	-2.562375	-0.930392
Pd	0.091411	1.174554	-1.979806	C	-5.920268	-2.108153	-1.270813
C	-1.175964	4.882225	-0.247862	C	-6.231291	-0.770774	-1.036206
C	-1.371439	5.013989	-1.640451	C	-5.244996	0.082900	-0.555298
C	-1.799269	5.790723	0.628059	H	-0.774344	2.368872	2.096758
C	-2.272607	6.017332	-2.067522	H	-1.211722	4.263898	0.601831
C	-2.649735	6.794057	0.176922	H	-2.680563	3.922319	-1.412312
H	-1.623548	5.671599	1.692904	H	-3.798994	1.761302	-1.723623
C	-2.906925	6.889690	-1.189842	H	-4.413332	-3.616751	-1.036417
H	-2.479504	6.102069	-3.128660	H	-6.658851	-2.794309	-1.673701
H	-3.123017	7.469343	0.883170	H	-7.227820	-0.387517	-1.234051
H	-3.595705	7.636052	-1.574087	H	-5.496014	1.125309	-0.393876
C	0.627158	-1.878226	-2.108868	C	-2.446575	-2.795616	1.524991
O	1.123611	-1.419080	-3.295446	C	-1.490762	-3.705505	1.988590
O	0.229702	-1.008101	-1.254688	C	-0.560681	-4.277089	1.119325
O	0.615058	-3.118703	-1.926639	Cs	2.289066	-1.689474	0.973705
Cs	2.289066	-1.689474	0.973705	C	-0.580132	-3.945427	-0.235440
C	-0.689561	4.277733	-2.756700	C	-1.553788	-3.066230	-0.719313
C	-0.238496	5.128487	-3.795824	C	-2.485765	-2.479567	0.143020
C	-0.615192	2.863584	-2.963154	C	-3.347006	-2.058182	2.464269
C	0.175175	4.661916	-5.040083	C	-4.741929	-2.149331	2.384287
H	-0.230496	6.198518	-3.610434	C	-5.549598	-1.282390	3.120327
C	-0.367414	2.435655	-4.303079	C	-4.974625	-0.297519	3.934184
H	1.621150	-0.522748	-3.079593	C	-3.590163	-0.226576	4.045722
C	0.056256	3.295576	-5.310234	C	-2.758535	-1.114282	3.337001
H	0.530802	5.356544	-5.795089	H	-1.463166	-3.936319	3.048712
H	-0.471738	1.380349	-4.537279	H	0.181138	-4.972321	1.501313
H	0.299825	2.900142	-6.293043	H	0.142209	-4.383019	-0.918231
Cs	3.102372	3.650935	-2.025372	H	-1.606434	-2.842933	-1.781769
Cs	3.470381	-3.435104	-3.388937	H	-5.198926	-2.869686	1.715014
O	3.679494	-0.914789	-1.716637	H	-6.630323	-1.362683	3.043271
C	3.136234	0.234203	-1.584793	H	-5.610324	0.389810	4.485980
O	3.309945	0.982410	-0.564513	H	-3.086942	0.476180	4.703599
O	2.321980	0.668925	-2.567636	Pd	-0.954258	-0.410259	2.074808
C	-0.431956	3.786242	0.426419	C	-0.214685	-0.459485	5.492872
C	-0.970226	2.485046	0.393173	O	-0.713032	0.672912	5.117360
C	0.647172	4.071322	1.276579	O	-0.866978	-1.573856	5.238367
C	-0.456499	1.517232	1.271478	O	0.931797	-0.527720	6.083176
C	1.175299	3.089605	2.115996	Cs	1.624385	-3.295178	4.857379
H	1.048288	5.081147	1.297907	Cs	0.553712	0.275512	-2.037220
C	0.599926	1.815751	2.132798	Cs	1.986083	1.460093	3.912668
H	-0.894032	0.523877	1.262067	O	2.680502	-1.180303	1.164112
H	2.008561	3.324420	2.771493	C	1.509508	-0.947567	1.532516
H	0.975653	1.059473	2.816540	O	0.902047	-1.543320	2.517726
C	-2.118501	2.155821	-0.510055	O	0.769507	-0.005029	0.943396
C	-3.419252	2.082726	-0.003015	H	-1.751540	-1.282828	3.919051
C	-1.847609	1.808357	-1.861624				
C	-4.483135	1.683436	-0.815906	TS4a_Cs'			
H	-3.594202	2.334315	1.040421	Pd	-0.634597	0.591141	-0.348083
C	-2.934069	1.383100	-2.655727	C	-2.258049	1.914283	-0.175486
C	-4.229598	1.323382	-2.143959	C	-2.636878	1.981143	1.190075
H	-5.492518	1.646397	-0.417310	C	-2.530618	2.970881	-1.044228
H	-2.756714	1.119541	-3.694999	C	-3.337599	3.113701	1.627442
H	-5.046427	0.999363	-2.784173	C	-3.220530	4.093797	-0.580111
				H	-2.235935	2.909931	-2.085032
				C	-3.639945	4.155302	0.751352
TSP_Cs				H	-3.621387	3.192039	2.672451
C	-2.976629	0.800048	0.026065	H	-3.440902	4.907704	-1.263948
C	-2.028925	0.949354	1.072549	H	-4.188891	5.020311	1.110440

C	-2.151041	0.912481	2.075514	O	0.514859	1.917884	-0.577384
C	-2.517802	0.723506	3.413036	C	-2.878217	0.680367	-1.092306
C	-1.200508	0.052077	1.492372	C	-3.627277	-0.475865	-0.772758
C	-1.938654	-0.308038	4.155386	C	-2.161949	0.714591	-2.299970
H	-3.261456	1.365379	3.875054	C	-3.594266	-1.564905	-1.659885
C	-0.612436	-0.966573	2.234074	C	-2.150257	-0.370321	-3.174050
C	-0.989619	-1.151249	3.572299	H	-1.582870	1.602041	-2.529779
H	-2.234741	-0.457595	5.189406	C	-2.863832	-1.523508	-2.845318
H	0.137154	-1.611157	1.783355	H	-4.182083	-2.446206	-1.422579
H	-0.544485	-1.953736	4.154554	H	-1.575987	-0.317981	-4.093595
Cs	2.167871	2.281917	2.148958	H	-2.866852	-2.378839	-3.514142
O	2.905120	1.058351	-1.607568	C	-4.462418	-0.587373	0.449727
C	1.723903	0.896969	-1.276813	C	-4.425602	-1.760669	1.217877
O	0.677812	1.255712	-1.978522	C	-5.325334	0.445790	0.847843
O	1.397839	0.331282	-0.095185	C	-5.214190	-1.894414	2.358635
C	-2.475404	0.195716	-1.328393	H	-3.742380	-2.555434	0.937203
C	-3.578808	-0.592147	-0.948320	C	-6.112464	0.314305	1.990575
C	-2.166005	0.345941	-2.693644	H	-5.379857	1.353486	0.257616
C	-4.296321	-1.254165	-1.964049	C	-6.058969	-0.855509	2.752533
C	-2.893106	-0.321326	-3.675349	H	-5.157230	-2.804419	2.948361
H	-1.323595	0.962559	-2.983818	H	-6.774833	1.124166	2.282463
C	-3.964978	-1.136169	-3.309723	H	-6.670305	-0.955200	3.644463
H	-5.144802	-1.863171	-1.666940	TSP_Cs'			
H	-2.616626	-0.201916	-4.718650	C	-2.817748	0.892212	0.145914
H	-4.544563	-1.661633	-4.062176	C	-2.142819	1.145989	1.357002
C	-4.131812	-0.753872	0.427768	C	-1.228827	2.219032	1.396433
C	-3.769497	-1.839939	1.231831	C	-0.939545	3.008629	0.281814
C	-5.129636	0.121427	0.873961	C	-1.578082	2.726620	-0.926782
C	-4.379758	-2.037129	2.469480	C	-2.505149	1.689491	-0.978451
H	-2.999269	-2.521985	0.887905	C	-3.913194	-0.099852	-0.094246
C	-5.738473	-0.072499	2.113865	C	-3.741143	-1.498277	-0.112451
H	-5.419226	0.959366	0.247907	C	-4.784730	-2.312610	-0.576287
C	-5.365473	-1.153640	2.913802	C	-6.007968	-1.778406	-0.972761
H	-4.081679	-2.877311	3.088832	C	-6.203270	-0.398992	-0.905141
H	-6.506501	0.617249	2.451505	C	-5.159090	0.422337	-0.486852
H	-5.838497	-1.306328	3.879363	H	-0.715605	2.447225	2.333260
P_Cs'				H	-0.228876	3.826826	0.360727
Pd	0.113471	-0.083143	-0.386080	H	-1.366534	3.312963	-1.815928
C	-2.815051	1.887375	-0.219353	H	-3.013117	1.475664	-1.914697
C	-2.359693	1.861258	1.119872	H	-4.627229	-3.386377	-0.609256
C	-3.236948	3.107033	-0.772015	H	-6.801242	-2.433174	-1.319978
C	-2.379926	3.057582	1.856108	H	-7.154706	0.038108	-1.192612
C	-3.250437	4.286413	-0.026594	H	-5.295262	1.499412	-0.468878
H	-3.589514	3.115737	-1.799071	C	-2.480660	-2.570349	1.757315
C	-2.825044	4.259137	1.303313	C	-1.346956	-3.218773	2.260614
H	-2.025992	3.037309	2.882501	C	-0.264881	-3.504237	1.425735
H	-3.599755	5.210971	-0.476776	C	-0.304033	-3.128029	0.080213
H	-2.833152	5.164021	1.904311	C	-1.420467	-2.452395	-0.421363
C	-1.907668	0.623029	1.811903	C	-2.513088	-2.170295	0.404929
C	-2.509724	0.314444	3.045109	C	-3.639108	-2.234293	2.634506
C	-0.916676	-0.239499	1.302779	C	-4.846972	-2.930612	2.538448
C	-2.162841	-0.827968	3.761540	C	-5.955327	-2.526894	3.286267
H	-3.299439	0.960494	3.415952	C	-5.870063	-1.431286	4.150304
C	-0.575186	-1.386788	2.034742	C	-4.655753	-0.761500	4.283445
C	-1.195118	-1.692505	3.250294	C	-3.522793	-1.156799	3.541434
H	-2.657743	-1.049353	4.702301	H	-1.306575	-3.485154	3.312072
H	0.201334	-2.055337	1.661115	H	0.604283	-4.018139	1.825314
H	-0.914604	-2.591024	3.793601	H	0.530300	-3.358363	-0.576452
Cs	0.776900	4.966859	-0.246928	H	-1.452582	-2.147204	-1.463175
O	1.686391	2.753700	-2.301087	H	-4.929888	-3.777299	1.865968
C	1.223901	1.762149	-1.709554	H	-6.890530	-3.070889	3.191818
O	1.342394	0.520377	-2.078929	H	-6.738112	-1.118430	4.722592

H	-4.565951	0.057954	4.990833	C	-2.177925	6.079524	-1.963220				
Pd	-1.928061	0.294333	3.144269	C	-2.525975	6.640658	0.350328				
C	-0.086875	-0.998384	4.618260	H	-1.509231	5.359299	1.744667				
O	0.349701	-0.238215	3.674805	C	-2.786290	6.876316	-0.998842				
O	-1.401476	-0.731205	4.999457	H	-2.386132	6.271120	-3.010277				
O	0.530339	-1.892302	5.205122	H	-2.980647	7.255164	1.121266				
Cs	1.796545	0.016142	1.039209	H	-3.457551	7.673821	-1.302727				
H	-2.410759	-1.184446	4.313634	C	-0.655639	4.360004	-2.821654				
Q_Cs'											
C	-2.508269	0.692509	0.060017	C	0.235205	4.900040	-5.060850				
C	-1.605560	0.368393	1.093430	H	-0.091628	6.321894	-3.495353				
C	-0.240529	0.641466	0.910130	C	-0.429751	2.647640	-4.534944				
C	0.219049	1.257853	-0.260434	H	2.573020	-2.089380	-0.791081				
C	-0.685359	1.624979	-1.260802	C	0.046424	3.575652	-5.458648				
C	-2.042715	1.336276	-1.096625	H	0.627381	5.641793	-5.749969				
C	-3.930324	0.259612	0.159303	H	-0.592968	1.625062	-4.862000				
C	-4.216550	-1.102201	-0.060720	H	0.272777	3.262268	-6.474213				
C	-5.525563	-1.565554	0.096300	Cs	3.366881	3.511080	-2.250671				
C	-6.551111	-0.688509	0.456035	O	0.828507	-0.882641	-1.504005				
C	-6.271642	0.665243	0.654027	C	2.018560	-0.474040	-1.590551				
C	-4.964555	1.134465	0.505010	O	2.395873	0.629924	-2.065995				
H	0.470367	0.397875	1.694170	O	3.014045	-1.293260	-1.123033				
H	1.280403	1.458566	-0.382802	C	-0.349371	3.584961	0.267912				
H	-0.336943	2.114317	-2.165689	C	-0.929901	2.307316	0.159235				
H	-2.751893	1.585980	-1.881756	C	0.825643	3.754942	1.012833				
H	-5.737569	-2.618577	-0.063275	C	-0.338448	1.232169	0.841076				
H	-7.564481	-1.059986	0.575380	C	1.429794	2.668777	1.648667				
H	-7.066525	1.352244	0.929175	H	1.256145	4.749076	1.098750				
H	-4.737430	2.182958	0.676575	C	0.834784	1.406208	1.574386				
C	-2.461192	-2.838246	0.473398	H	-0.786736	0.248281	0.757041				
C	-1.389258	-3.637986	0.049073	H	2.345424	2.811216	2.215090				
C	-0.943321	-3.610587	-1.271672	H	1.287672	0.557774	2.078365				
C	-1.582826	-2.786982	-2.199740	C	-2.144345	2.094640	-0.696512				
C	-2.654680	-1.994707	-1.791598	C	-3.423457	2.012516	-0.140081				
C	-3.102883	-2.008826	-0.464584	C	-1.955244	1.869283	-2.087052				
C	-2.946498	-2.947047	1.876685	C	-4.532224	1.728325	-0.942272				
C	-3.455931	-4.202243	2.260413	H	-3.546653	2.164892	0.929140				
C	-3.966467	-4.430878	3.535968	C	-3.078884	1.569008	-2.875451				
C	-3.969688	-3.387017	4.461206	C	-4.353370	1.499149	-2.309444				
C	-3.452283	-2.143500	4.092055	H	-5.524144	1.681172	-0.503150				
C	-2.926733	-1.887517	2.807804	H	-2.954255	1.410460	-3.942864				
H	-0.898844	-4.280321	0.774864	H	-5.209645	1.271690	-2.938931				
H	-0.103835	-4.229712	-1.574012	R_Cs'							
H	-1.248984	-2.759547	-3.232701	Pd	-0.344090	1.380451	-2.258922				
H	-3.153165	-1.345543	-2.505147	C	-1.454750	4.805601	-0.390136				
H	-3.459271	-5.004756	1.527300	C	-1.580236	5.065094	-1.777240				
H	-4.360719	-5.407777	3.800226	C	-1.694441	5.848454	0.520301				
H	-4.367150	-3.536073	5.461719	C	-1.962737	6.357825	-2.181739				
H	-3.451621	-1.346732	4.836825	C	-2.070753	7.121372	0.099356				
Pd	-2.242256	-0.008811	2.929983	H	-1.589036	5.640247	1.580660				
C	-2.141367	2.224769	4.733022	C	-2.209345	7.376033	-1.265268				
O	-2.227556	3.276039	5.370226	H	-2.077089	6.552341	-3.243234				
O	-2.636874	1.045079	5.296393	H	-2.261006	7.901434	0.830056				
O	-1.653353	2.023167	3.572374	H	-2.513019	8.357961	-1.615231				
Cs	-1.593052	4.481948	1.699802	C	-1.270815	4.074160	-2.840575				
H	-3.054691	1.273003	6.140139	C	-0.453766	4.459711	-3.902648				
TSN_Cs'											
Pd	-0.004371	1.242200	-2.275130	C	-1.893705	2.770322	-2.863413				
C	-1.096962	4.752154	-0.267424	C	-0.191558	3.605595	-4.991463				
C	-1.303839	5.017971	-1.637966	H	-0.010603	5.451572	-3.884251				
C	-1.693379	5.581713	0.697882	C	-1.600574	1.904125	-3.971755				
				H	1.586283	1.491442	-3.529390				

C	-0.745043	2.337255	-5.022205	H	2.265752	1.623016	0.650852
H	0.451152	3.945034	-5.797984	C	0.403389	1.508902	3.508651
H	-2.230868	1.034074	-4.135025	H	-1.744205	1.363214	3.598976
H	-0.569061	1.674956	-5.864710	H	2.522575	1.643843	3.129630
Cs	3.128285	4.302916	-1.757476	H	0.518510	1.519568	4.588333
O	1.482249	0.318099	-1.618833	C	-2.282708	1.325358	0.805523
C	2.561235	0.890763	-1.991280	C	-3.571667	1.184729	1.334731
O	3.641882	0.953619	-1.393217	C	-2.133207	1.368571	-0.595605
O	2.512837	1.560587	-3.218195	C	-4.675387	1.097146	0.483968
C	-1.016998	3.502303	0.183953	H	-3.712798	1.138867	2.410850
C	-1.792519	2.328691	0.062375	C	-3.221688	1.288469	-1.451968
C	0.144443	3.468202	0.972435	C	-4.503757	1.145682	-0.900665
C	-1.384455	1.164526	0.735902	H	-5.671108	0.990458	0.903450
C	0.551528	2.300291	1.616714	H	-3.088156	1.338831	-2.525835
H	0.723545	4.380370	1.086686	H	-5.364156	1.079158	-1.560196
C	-0.219085	1.142405	1.500087				
H	-1.997577	0.272980	0.649784	J_Cs'			
H	1.459427	2.298454	2.212063	Pd	-0.125952	1.627813	-1.229843
H	0.084009	0.227741	1.999558	C	-0.594886	3.582298	-1.249474
C	-3.089647	2.328941	-0.669195	C	-0.862951	4.109760	-2.536420
C	-4.275802	2.075482	0.030320	C	-0.591625	4.407695	-0.128680
C	-3.135811	2.529993	-2.061186	C	-1.085064	5.488222	-2.660489
C	-5.503461	2.028100	-0.631481	C	-0.819403	5.782983	-0.274688
H	-4.228432	1.914871	1.103318	H	-0.411086	3.990443	0.854575
C	-4.373140	2.481039	-2.715770	C	-1.062613	6.319594	-1.539064
C	-5.551554	2.232098	-2.010751	H	-1.277699	5.918113	-3.639200
H	-6.413622	1.832396	-0.072953	H	-0.810027	6.425811	0.600944
H	-4.404491	2.637436	-3.789930	H	-1.240322	7.384742	-1.654578
H	-6.500427	2.197395	-2.537479	C	1.787161	-0.612412	-1.779346
				O	2.247600	0.258448	-2.770443
TSM_Cs'				O	0.563775	-0.484004	-1.434382
Pd	-0.235239	1.468169	-1.244116	O	2.626779	-1.400387	-1.334724
C	-0.609675	3.445227	-1.372044	C	-0.887037	3.143962	-3.650543
C	-0.957647	3.878802	-2.671050	C	-1.219045	3.452500	-4.974702
C	-0.469788	4.359580	-0.331117	C	-0.579753	1.812408	-3.280980
C	-1.122511	5.254696	-2.895398	C	-1.251686	2.441466	-5.941103
C	-0.639578	5.727595	-0.576963	H	-1.461112	4.471622	-5.264737
H	-0.227303	4.019484	0.668183	C	-0.631952	0.815494	-4.257385
C	-0.963112	6.173686	-1.858968	H	1.480913	0.716763	-3.159706
H	-1.367732	5.607609	-3.892846	C	-0.961916	1.123638	-5.586898
H	-0.517989	6.438115	0.235693	H	-1.511852	2.685833	-6.967093
H	-1.091471	7.234351	-2.052718	H	-0.423825	-0.217258	-3.983610
C	1.754786	-0.201048	-1.988096	H	-1.000395	0.337785	-6.336986
O	1.802836	1.128645	-2.377366	Cs	5.170907	0.460478	-1.453764
O	0.634951	-0.551872	-1.448511	C	0.301281	1.530486	0.804507
O	2.752844	-0.909622	-2.161795	C	-0.822732	1.267882	1.614785
C	-1.149057	2.857375	-3.723047	C	1.554446	1.654688	1.398430
C	-1.982606	3.067546	-4.830999	C	-0.681167	1.132472	3.001863
C	-0.548418	1.589976	-3.521166	C	1.699555	1.521778	2.787415
C	-2.229955	2.029439	-5.731580	H	2.432210	1.867259	0.790267
H	-2.474205	4.025245	-4.975231	C	0.581981	1.260020	3.584766
C	-0.837079	0.556735	-4.422782	H	-1.543909	0.930086	3.631307
H	0.785945	1.385030	-2.984312	H	2.680162	1.625033	3.245671
C	-1.663106	0.767646	-5.530310	H	0.693125	1.157320	4.660341
H	-2.883696	2.201639	-6.581845	C	-2.080176	1.170780	0.863860
H	-0.398959	-0.425613	-4.259586	C	-3.347804	0.893121	1.396095
H	-1.872352	-0.040909	-6.225067	C	-1.988119	1.368950	-0.529427
Cs	4.869598	1.356548	-2.817701	C	-4.471228	0.831366	0.570755
C	0.117216	1.491942	0.744978	H	-3.453553	0.723238	2.463640
C	-1.027640	1.412820	1.558484	C	-3.093541	1.323778	-1.364482
C	1.389348	1.567063	1.291927	C	-4.348150	1.044696	-0.802636
C	-0.874541	1.422171	2.950348	H	-5.444523	0.618078	1.002092
C	1.532143	1.579022	2.687674	H	-2.990779	1.497427	-2.427461

H	-5.221944	1.001531	-1.446000	C	1.451166	-0.700131	-4.338924
				H	0.858383	-1.473227	-0.530944
TSL_Cs'							
Pd	0.089313	2.178729	-1.530815	C	1.915026	-2.120020	-2.322429
C	-0.234517	3.943314	-0.626264	H	3.849950	0.754307	-2.299684
C	-0.870088	4.848493	-1.507941	C	2.710035	0.132614	-4.039903
C	0.120587	4.373299	0.652374	C	3.170202	-1.287204	-2.011589
C	-1.141657	6.158697	-1.096718	H	1.258781	-0.706215	-5.418461
C	-0.162588	5.684842	1.060051	C	1.659598	-2.140375	-3.839387
H	0.609068	3.692504	1.340148	H	2.051190	-3.145014	-1.954523
C	-0.792474	6.575278	0.189522	H	3.575233	-0.294711	-4.561781
H	-1.631985	6.852073	-1.774536	H	2.581227	1.157181	-4.411208
H	0.105980	6.005220	2.063348	H	3.351974	-1.279729	-0.929453
H	-1.014496	7.589016	0.509506	H	4.049918	-1.735056	-2.490190
C	1.321393	-0.525503	-2.520061	H	0.773700	-2.748652	-4.062707
O	2.360576	-0.179471	-1.670004	H	2.508391	-2.598837	-4.361744
O	0.425842	0.361235	-2.724054	C	-2.435584	-0.301184	-0.844269
O	1.362751	-1.670543	-2.987593	C	-2.168165	-1.383180	0.235169
C	-1.185822	4.324305	-2.855621	C	-2.950430	-1.008290	-2.120643
C	-1.388112	5.119216	-3.993609	C	-3.534587	0.645039	-0.286605
C	-1.199546	2.922554	-3.016807	H	-1.396039	-2.073797	-0.108572
C	-1.616203	4.526502	-5.237031	H	-1.791350	-0.913482	1.146525
H	-1.347768	6.201500	-3.913678	C	-3.452802	-2.174400	0.541371
C	-1.394085	2.324886	-4.260683	H	-2.193020	-1.704819	-2.494765
H	2.135459	0.691402	-1.297464	H	-3.146244	-0.289149	-2.916586
C	-1.603083	3.133348	-5.379614	C	-4.244863	-1.787001	-1.805331
H	-1.786783	5.155804	-6.105414	H	-3.164956	1.125525	0.627352
H	-1.381083	1.243900	-4.341495	H	-3.760850	1.441813	-0.999830
H	-1.756707	2.683801	-6.356203	C	-4.821639	-0.145471	0.012629
Cs	1.933787	-3.071558	-0.225008	H	-3.221213	-2.932516	1.300081
C	0.250942	1.231780	0.264156	C	-3.954368	-2.859082	-0.741433
C	-1.019943	0.646953	0.484724	C	-4.530921	-1.218389	1.075273
C	1.309854	0.948760	1.132301	H	-4.597911	-2.264327	-2.727236
C	-1.131684	-0.321767	1.504608	C	-5.318660	-0.817028	-1.280427
C	1.160470	0.042904	2.188585	H	-5.582191	0.551148	0.384744
H	2.273177	1.431895	0.985935	H	-4.862018	-3.438627	-0.531709
C	-0.059768	-0.617832	2.348704	H	-3.198466	-3.562811	-1.113421
H	-2.055628	-0.867358	1.658419	H	-4.186972	-0.744465	2.003243
H	1.989945	-0.160289	2.861629	H	-5.447036	-1.773333	1.312842
H	-0.187110	-1.355760	3.135783	H	-5.541051	-0.055414	-2.038701
C	-2.229630	1.096578	-0.300551	H	-6.251281	-1.361224	-1.086618
C	-3.491206	0.727525	0.218794	C	-1.425044	2.233845	-2.121956
C	-2.239811	1.948278	-1.456822	C	-2.373077	2.107440	-3.323935
C	-4.701489	1.140751	-0.320935	H	-0.480870	2.663704	-2.471163
H	-3.526747	0.123624	1.115847	H	-1.831301	2.962480	-1.416529
C	-3.472047	2.375219	-1.974092	C	-2.437435	3.426434	-4.104049
C	-4.692914	1.982423	-1.424360	H	-2.057533	1.309505	-4.000661
H	-5.633781	0.822897	0.135648	H	-3.381441	1.849690	-2.986895
H	-3.507641	3.029376	-2.833079	C	-3.405440	3.360518	-5.287218
H	-5.616585	2.342768	-1.867149	H	-2.735094	4.234597	-3.423348
				H	-1.430909	3.680895	-4.461450
TS2_Na'							
Pd	-0.136655	1.238658	1.081551	H	-3.431119	4.307533	-5.835349
P	-0.902868	0.773298	-1.094896	H	-3.111974	2.573505	-5.990902
C	0.465397	-0.053651	-2.099818	H	-4.424737	3.140828	-4.950374
C	1.750731	0.768514	-1.804575	C	-0.251562	3.245286	1.046833
C	0.235283	-0.068004	-3.627893	C	-0.539118	3.823682	2.310604
C	0.699678	-1.499757	-1.610868	C	0.117602	4.097020	0.001105
H	1.619167	1.807926	-2.129674	C	-0.534322	5.217058	2.467840
H	1.927287	0.790908	-0.723955	C	0.145823	5.486611	0.171768
C	2.962875	0.149554	-2.522189	H	0.410418	3.690423	-0.958120
H	0.101388	0.951206	-4.002620	C	-0.202785	6.050300	1.399800
H	-0.670666	-0.630558	-3.874815	H	-0.761142	5.648475	3.439313
				H	0.445293	6.123569	-0.656352

H	-0.190830	7.128065	1.532861	C	-4.889732	-0.752052	-1.700578				
C	1.804675	-0.643111	2.126688	H	-5.181685	0.721713	-0.134279				
O	2.126256	0.509324	2.645551	H	-4.527911	-3.330437	-0.776840				
O	0.621488	-0.771764	1.543760	H	-2.846169	-3.527711	-1.281527				
O	2.574354	-1.647479	2.176939	H	-3.886796	-0.500364	1.615736				
C	-0.782873	2.884151	3.418693	H	-5.143590	-1.542221	0.938692				
C	-1.595213	3.190314	4.520512	H	-5.064870	-0.033155	-2.511213				
C	-0.227489	1.584373	3.287346	H	-5.842314	-1.262327	-1.510546				
C	-1.880875	2.219957	5.480628	C	-0.898901	2.166540	-2.499406				
H	-2.038289	4.178437	4.607747	C	-1.770223	2.018377	-3.756523				
C	-0.571438	0.613378	4.242865	H	0.062660	2.612066	-2.783018				
H	0.996707	1.199171	2.799734	H	-1.368884	2.895804	-1.835641				
C	-1.377643	0.922805	5.339199	C	-1.777160	3.315613	-4.574679				
H	-2.512955	2.469416	6.328192	H	-1.428523	1.199085	-4.392841				
H	-0.176876	-0.392559	4.130836	H	-2.799343	1.778976	-3.471915				
H	-1.613977	0.162802	6.078787	C	-2.683379	3.229451	-5.804590				
Na	0.894359	-3.034197	1.531623	H	-2.099073	4.146433	-3.933075				
				H	-0.750073	3.548515	-4.885545				
C1_Na'											
Pd	0.194307	1.288539	0.973834	H	-2.669377	4.161346	-6.378637				
P	-0.431412	0.742141	-1.392881	H	-2.364739	2.420224	-6.471357				
C	0.920370	-0.174846	-2.352573	H	-3.721230	3.030068	-5.514848				
C	2.231611	0.587877	-2.015600	C	-0.173399	3.273939	1.044772				
C	0.755596	-0.193735	-3.888847	C	-0.493205	3.793028	2.330609				
C	1.066492	-1.630210	-1.852653	C	-0.040942	4.178628	-0.011282				
C	2.157527	1.628485	-2.355782	C	-0.777817	5.153692	2.494283				
H	2.370671	0.617790	-0.930944	C	-0.305049	5.546118	0.162446				
C	3.442248	-0.092300	-2.679319	H	0.282430	3.838037	-0.986028				
H	0.684185	0.827952	-4.273570	C	-0.700164	6.029799	1.408613				
H	-0.165384	-0.715196	-4.169276	H	-1.034250	5.540509	3.477283				
C	1.966359	-0.886520	-4.549443	H	-0.201315	6.225034	-0.680149				
H	1.179370	-1.616599	-0.768556	C	-0.919746	7.085016	1.544327				
H	0.165637	-2.203476	-2.090907	C	2.366201	-0.838046	1.546685				
C	2.281492	-2.310500	-2.509072	O	3.027050	0.333642	1.725447				
H	4.348224	0.471034	-2.425298	O	1.107642	-0.789804	1.286576				
C	3.249627	-0.110198	-4.205730	O	3.019729	-1.897111	1.641383				
C	3.561223	-1.534069	-2.154123	C	-0.396713	2.810495	3.417939				
H	1.816866	-0.891537	-5.635981	C	-0.701553	3.037949	4.765103				
C	2.086879	-2.331336	-4.034654	C	0.085061	1.545723	2.996183				
H	2.356390	-3.337830	-2.129906	C	-0.526942	2.019099	5.706002				
H	4.114652	-0.579749	-4.690476	H	-1.078022	4.005604	5.087634				
H	3.181472	0.916264	-4.588098	C	0.245838	0.536565	3.948913				
H	3.704291	-1.532047	-1.066748	H	2.353914	1.048974	1.692590				
H	4.435644	-2.025924	-2.598642	C	-0.052456	0.770934	5.299929				
H	1.183234	-2.899505	-4.290501	H	-0.763283	2.200664	6.750819				
H	2.933945	-2.833188	-4.518839	H	0.595998	-0.444691	3.642811				
C	-2.008944	-0.277424	-1.179218	H	0.084023	-0.022577	6.030804				
C	-1.816124	-1.295862	-0.025283	Na	1.056403	-3.111931	1.457582				
C	-2.496118	-1.044612	-2.429856	TS3_Na'							
C	-3.107232	0.725401	-0.726547	Pd	1.075616	0.116516	1.579862				
H	-1.045892	-2.020320	-0.296335	P	-0.399115	-0.335590	-0.141781				
H	-1.465891	-0.775580	0.872313	C	0.656147	-0.857194	-1.627677				
C	-3.130643	-2.037276	0.276858	C	1.862478	0.122208	-1.667105				
H	-1.743207	-1.777107	-2.737730	C	-0.073716	-0.776888	-2.988963				
H	-2.641587	-0.364434	-3.270489	C	1.211931	-2.285321	-1.430832				
C	-3.819743	-1.775443	-2.122549	H	1.511185	1.153795	-1.787345				
H	-2.764133	1.256709	0.169431	H	2.400032	0.072571	-0.714942				
H	-3.286987	1.479524	-1.497147	C	2.818822	-0.240036	-2.817686				
C	-4.424860	-0.013838	-0.432213	H	-0.435307	0.240744	-3.163161				
H	-2.951554	-2.753913	1.088546	H	-0.943253	-1.440359	-3.002100				
C	-3.598254	-2.785604	-0.983530	C	0.891008	-1.162065	-4.131250				
C	-4.205150	-1.023832	0.705337	H	1.728070	-2.319889	-0.469061				
H	-4.148891	-2.302591	-3.026196	H	0.394987	-3.012577	-1.410752				

C	2.177159	-2.651776	-2.573303	O	2.352403	-1.671492	1.572307
H	3.650846	0.474098	-2.820304	O	4.446440	-2.359635	1.896385
C	2.068579	-0.173176	-4.158758	C	-1.280300	3.333611	2.117543
C	3.355729	-1.664061	-2.591887	C	-1.643909	4.493247	1.417348
H	0.343239	-1.112369	-5.079967	C	-2.273448	2.388169	2.414533
C	1.422964	-2.589295	-3.912697	C	-2.962989	4.690240	1.006424
H	2.550379	-3.669882	-2.403995	H	-0.883314	5.231227	1.180163
H	2.747832	-0.419718	-4.984214	C	-3.591387	2.581256	2.001968
H	1.700396	0.845579	-4.334024	H	-1.996524	1.500973	2.972228
H	3.900669	-1.713014	-1.640403	C	-3.940275	3.732896	1.292236
H	4.061330	-1.933373	-3.387633	H	-3.226873	5.587612	0.454779
H	0.591808	-3.306090	-3.910403	H	-4.344598	1.835338	2.237608
H	2.090503	-2.869398	-4.737050	H	-4.964496	3.884822	0.966041
C	-1.640931	-1.649036	0.381469	Na	2.882032	-3.862046	1.285131
C	-0.916013	-2.745934	1.204433				
C	-2.409727	-2.317621	-0.780483	C2_Na'			
C	-2.646868	-0.954209	1.335113	Pd	1.438660	0.375845	1.434397
H	-0.179516	-3.263229	0.586556	P	0.112906	-0.420987	-0.377849
H	-0.366097	-2.275177	2.026269	C	0.756890	-2.022150	-1.153510
C	-1.931909	-3.766650	1.749945	C	2.295544	-1.840757	-1.282568
H	-1.712544	-2.834321	-1.446956	C	0.193212	-2.360906	-2.552876
H	-2.931492	-1.566350	-1.377683	C	0.496775	-3.212857	-0.205263
C	-3.425751	-3.334477	-0.223034	H	2.520880	-0.994228	-1.941802
H	-2.093384	-0.509119	2.168091	H	2.714059	-1.613108	-0.298001
H	-3.171246	-0.141231	0.827898	C	2.949600	-3.116108	-1.846090
C	-3.671494	-1.968736	1.872218	H	0.411457	-1.547860	-3.251712
H	-1.388394	-4.534113	2.314779	H	-0.893603	-2.476792	-2.515603
C	-2.683487	-4.420057	0.576245	C	0.838775	-3.656454	-3.088047
C	-2.937872	-3.056914	2.672259	H	0.874458	-2.952725	0.786880
H	-3.959394	-3.793197	-1.063964	H	-0.577791	-3.394436	-0.112956
C	-4.427154	-2.610318	0.694565	C	1.166875	-4.491883	-0.740645
H	-4.378536	-1.440524	2.523215	H	4.029707	-2.948634	-1.935973
H	-3.396694	-5.164237	0.951833	C	2.356099	-3.445540	-3.226430
H	-1.977127	-4.949183	-0.076340	C	2.684977	-4.284445	-0.881910
H	-2.414279	-2.607231	3.525243	H	0.405644	-3.884576	-4.069512
H	-3.656568	-3.780554	3.076613	C	0.566089	-4.821635	-2.119509
H	-4.967315	-1.840517	0.128957	H	0.967597	-5.315878	-0.043378
H	-5.174611	-3.320058	1.070150	H	2.827830	-4.348234	-3.634713
C	-1.317640	1.164505	-0.730741	H	2.558443	-2.627326	-3.929135
C	-2.572018	1.067166	-1.611255	H	3.141489	-4.068745	0.091368
H	-0.547104	1.753958	-1.241855	H	3.153089	-5.202066	-1.260063
H	-1.558476	1.724141	0.171650	H	-0.514546	-4.989627	-2.026885
C	-2.945575	2.439986	-2.183552	H	1.005640	-5.746800	-2.512675
H	-2.438530	0.361794	-2.435392	C	-1.667930	-0.572348	0.225444
H	-3.411896	0.691524	-1.017277	C	-1.667590	-1.296782	1.599809
C	-4.263720	2.414111	-2.959416	C	-2.647181	-1.299789	-0.722392
H	-3.012331	3.163136	-1.362892	C	-2.171791	0.872733	0.483140
H	-2.134040	2.785966	-2.837652	H	-1.299447	-2.320862	1.501865
H	-4.502297	3.398377	-3.375000	H	-0.981572	-0.772638	2.276154
H	-4.220707	1.700934	-3.790460	C	-3.086512	-1.322765	2.198067
H	-5.094000	2.115685	-2.309258	H	-2.320340	-2.332042	-0.883606
C	0.819643	1.923621	2.339585	H	-2.671823	-0.812467	-1.700068
C	0.112586	3.104768	2.565559	C	-4.065253	-1.307611	-0.116176
C	2.073772	1.665925	2.855142	H	-1.490087	1.371105	1.176470
C	0.784466	4.083797	3.330600	H	-2.169567	1.462047	-0.436270
C	2.711558	2.634018	3.637178	C	-3.592874	0.855533	1.071666
H	2.896241	0.604146	2.597553	H	-3.054727	-1.856256	3.156250
C	2.057920	3.856900	3.851727	C	-4.040079	-2.049013	1.232030
H	0.272426	5.018588	3.543613	C	-3.578936	0.116521	2.419808
H	3.699609	2.458562	4.055227	H	-4.741389	-1.823242	-0.809117
H	2.539768	4.631043	4.442597	C	-4.544562	0.139280	0.097762
C	3.593278	-1.420588	1.970171	H	-3.917593	1.892116	1.216152
O	3.911353	-0.246281	2.424347	H	-5.049841	-2.089072	1.659538

H	-3.709510	-3.085306	1.083735	C	-4.419268	3.403793	0.182875
H	-2.917587	0.636257	3.124763	C	-5.012269	1.060000	-1.199956
H	-4.584130	0.108880	2.860236	H	-3.149924	0.316503	-0.409084
H	-4.571172	0.672146	-0.861401	C	-5.597542	3.308621	-0.557901
H	-5.566533	0.140542	0.497694	H	-4.188509	4.332103	0.695793
C	0.148687	0.787530	-1.792097	C	-5.902362	2.136663	-1.253784
C	-0.948722	0.848507	-2.863778	H	-5.238072	0.140830	-1.734407
H	1.120310	0.610197	-2.268288	H	-6.275641	4.156505	-0.598205
H	0.229771	1.765043	-1.318939	H	-6.819168	2.064027	-1.831351
C	-0.515667	1.717510	-4.050594	Cs	-1.944805	-3.036882	-3.444674
H	-1.212515	-0.146236	-3.231262				
H	-1.861793	1.269915	-2.430481				
C	-1.640803	1.934537	-5.063759	INT3_Cs_benz			
H	-0.160813	2.686773	-3.678278	Pd	2.834207	1.600727	1.376067
H	0.345945	1.247220	-4.542838	C	2.732415	3.466159	2.087760
H	-1.305228	2.537553	-5.913488	C	2.260190	4.687956	2.558826
H	-2.007928	0.978943	-5.455017	C	3.961202	2.976010	2.347978
H	-2.489319	2.450619	-4.600427	C	3.196343	5.417991	3.339337
C	1.094960	2.310899	1.819170	C	4.896931	3.665433	3.105828
C	0.438506	3.540080	1.848308	H	2.919829	6.395258	3.727856
C	2.015163	1.911246	2.721968	H	5.891956	3.291780	3.340709
C	0.819063	4.377384	2.924928	H	5.160007	5.520694	4.197702
C	2.412964	2.729784	3.775553	C	2.020591	-0.678623	0.424027
H	3.442566	0.370285	2.717956	O	3.265858	-0.484061	0.799571
C	1.785491	3.989064	3.856450	O	1.255244	0.391214	0.428708
H	0.345686	5.351778	3.018389	O	1.580591	-1.822377	0.117346
H	3.150527	2.435568	4.519166	Cs	3.618126	-3.201480	2.133460
H	2.047773	4.670986	4.661785	C	0.886911	5.169214	2.306427
C	3.492787	-1.532630	2.759100	C	0.220093	4.808086	1.121536
O	4.079463	-0.338011	2.989716	C	0.189710	5.947573	3.246585
O	2.373947	-1.556882	2.117994	C	-1.092489	5.212127	0.883981
O	4.060200	-2.559294	3.192484	H	0.748032	4.198900	0.394751
C	-0.616777	3.955815	0.892690	C	-1.125725	6.348689	3.011741
C	-1.900294	4.288286	1.351923	H	0.674448	6.215442	4.180545
C	-0.365846	4.005463	-0.485570	C	-1.774133	5.984160	1.829565
C	-2.915386	4.622111	0.454722	H	-1.585653	4.923815	-0.040201
H	-2.105305	4.252811	2.417789	H	-1.648853	6.939492	3.758304
C	-1.378105	4.342190	-1.385047	H	-2.798515	6.295139	1.648046
H	0.634915	3.788647	-0.845546	Cs	-1.411069	-1.097524	0.715658
C	-2.660311	4.640907	-0.918494	C	3.177477	1.420667	5.532091
H	-3.907457	4.859795	0.827370	C	2.626862	0.203888	5.133074
H	-1.165673	4.376737	-2.449142	C	2.421613	2.587980	5.439875
H	-3.450604	4.895303	-1.618138	C	1.318035	0.168922	4.655179
Na	2.128012	-3.758955	2.896335	H	3.209386	-0.709089	5.177439
			C	1.114661	2.529951	4.970728	
			H	2.857300	3.545611	5.698810	
D1_Cs_benz_noP			C	0.517927	1.319448	4.575587	
Pd	0.042802	0.186569	0.009456	C	-0.884216	1.337709	4.085940
C	-1.163143	1.574680	0.777251	C	-1.258510	2.271998	3.105966
C	-2.258997	2.398497	1.026515	C	-1.864923	0.481011	4.613517
C	-0.001479	1.609305	1.462680	C	-2.578243	2.340187	2.655221
C	-2.064516	3.306679	2.102713	H	-0.511328	2.934985	2.686877
C	0.214000	2.492372	2.512802	C	-3.183907	0.549182	4.161670
C	-0.867249	3.351642	2.819122	H	-1.596205	-0.230272	5.386978
H	-2.873192	3.970299	2.397846	C	-3.545586	1.477409	3.179104
H	1.136219	2.547955	3.088445	H	-2.841729	3.070615	1.897000
H	-0.771783	4.061336	3.638235	H	-3.931250	-0.116465	4.583352
C	0.718982	-1.831762	-1.477506	H	-4.572733	1.530078	2.830521
O	1.543348	-1.322134	-0.589680	H	4.201874	1.453776	5.887875
O	-0.414931	-1.181743	-1.627796	H	0.527062	3.438188	4.892597
Cs	3.029162	-3.910231	0.048643	Cl	0.713210	-1.398206	4.081439
C	-3.517105	2.327580	0.251889				
C	-3.837310	1.154805	-0.457723				

TS3f_Cs_benz

Pd	2.646157	1.576762	2.170768
C	1.920009	3.436834	2.611223
C	1.227908	4.645802	2.598234
C	2.997160	3.202496	3.361545
C	1.741386	5.605211	3.509301
C	3.519242	4.096688	4.281089
C	2.842197	5.336414	4.328707
H	1.242214	6.566256	3.600952
H	4.377149	3.901151	4.918223
H	3.185515	6.105562	5.016641
C	3.249671	-0.284819	0.423131
O	3.965000	-0.086073	1.512235
O	2.260560	0.563633	0.242823
O	3.478599	-1.232712	-0.369639
Cs	4.115675	-3.244306	1.891016
C	0.043157	4.907923	1.757209
C	-0.825323	3.853648	1.429274
C	-0.256378	6.193254	1.276361
C	-1.958901	4.077333	0.650868
H	-0.617531	2.871111	1.837541
C	-1.388200	6.417160	0.491779
H	0.412245	7.018192	1.502954
C	-2.244792	5.360382	0.174443
H	-2.634846	3.255164	0.431575
H	-1.598767	7.417297	0.124063
H	-3.128305	5.535227	-0.432364
Cs	-0.617607	-0.106619	-0.018914
C	3.790640	0.161243	5.858705
C	3.375262	-0.080251	4.552173
C	2.952312	0.849962	6.742170
C	2.143527	0.420038	4.126698
H	4.012595	-0.575077	3.832522
C	1.706463	1.284222	6.299687
H	3.258262	1.030931	7.767468
C	1.240333	1.063555	4.986079
C	-0.078968	1.640198	4.617908
C	-0.331540	2.986955	4.932088
C	-1.113206	0.887134	4.039745
C	-1.575350	3.561805	4.679813
H	0.468359	3.590273	5.346712
C	-2.359619	1.465114	3.787438
H	-0.939198	-0.154776	3.805385
C	-2.597738	2.802866	4.107999
H	-1.738753	4.609399	4.914068
H	-3.149926	0.861780	3.348675
H	-3.565038	3.251827	3.903908
H	4.766728	-0.191998	6.179567
H	1.044736	1.810088	6.981889
Cl	1.177731	-1.208326	2.895858