

Methane CH activation by Palladium Complexes with Chelating bis(NHC) Ligands – a DFT Study

*Dominik Munz, Dirk Meyer, Thomas Strassner**

Physikalische Organische Chemie, Technische Universität Dresden, Bergstrasse 66, 01069

Dresden, Germany

E-mail address: thomas.strassner@chemie.tu-dresden.de

*Corresponding author: Tel.: +49 351 46338571; fax: +49 351 46339679

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Solvent Treatment

Solvent Radius:

The solvent's molecular radius R_{solv} and numerical density was derived as follows by experimental data:

$$R_{\text{solv}} = \sqrt[3]{\frac{3M\Delta}{N_A 4\pi\rho}} = 2.479 \text{ \AA}$$

$$M = 114.02 \text{ g}\cdot\text{mol}^{-1}$$

$$N_A = 6.022\cdot 10^{23} \text{ mol}^{-1}$$

$$\Delta = 0.5$$

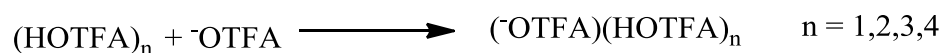
$$\rho = 1.489 \text{ g}\cdot\text{cm}^{-3}$$

M Molecular weight, N_A Avogadro's constant, ρ density of HOTFA at 298 K, Δ estimated packing density.

For the trifluoroacetic acid the experimentally derived radius of 2.479 Å has been used in the calculations. To guarantee consistency we used the same radius for acetic acid but tested the effect with the experimentally derived value for acetic acid (2.247 Å), which only lead to a not significant deviation ($< 0.1 \text{ kcal mol}^{-1}$).

Explicit solvation of anions:

The anions have been solvated by a cluster of HOTFA molecules according to:



A similar procedure has e.g. also been used in:

Ahlquist, M.; Periana, R. A.; Goddard, W. A. *Chem. Commun.* **2009**, 2373.

The electronic energy converged nicely within 3-4 steps as shown in the following two Figures S1 and S2.

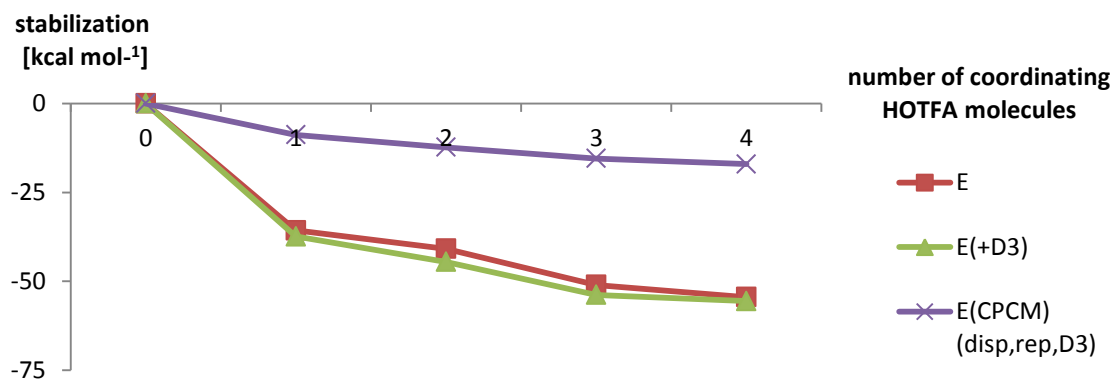


Figure S1. Convergence of stabilization energy of HOTFA coordinated OTFA^- .

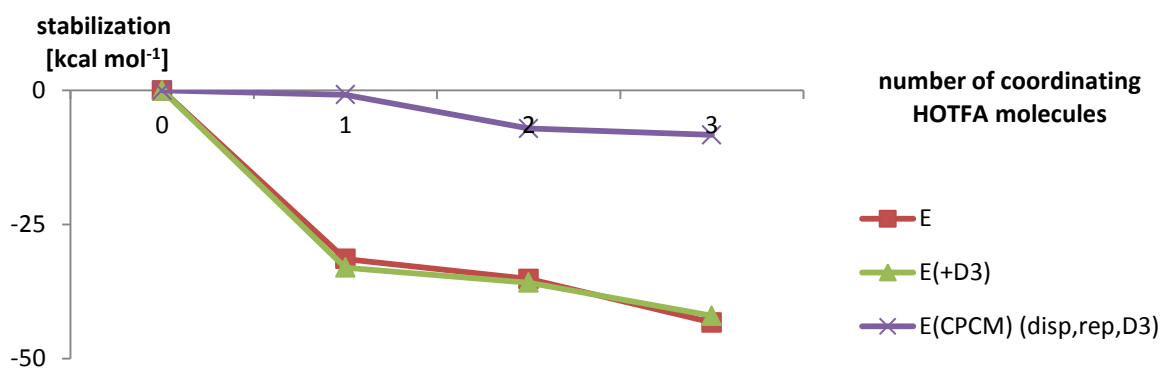


Figure S2. Convergence of stabilization energy of HOTFA coordinated Br^- .

Comparison of Functionals

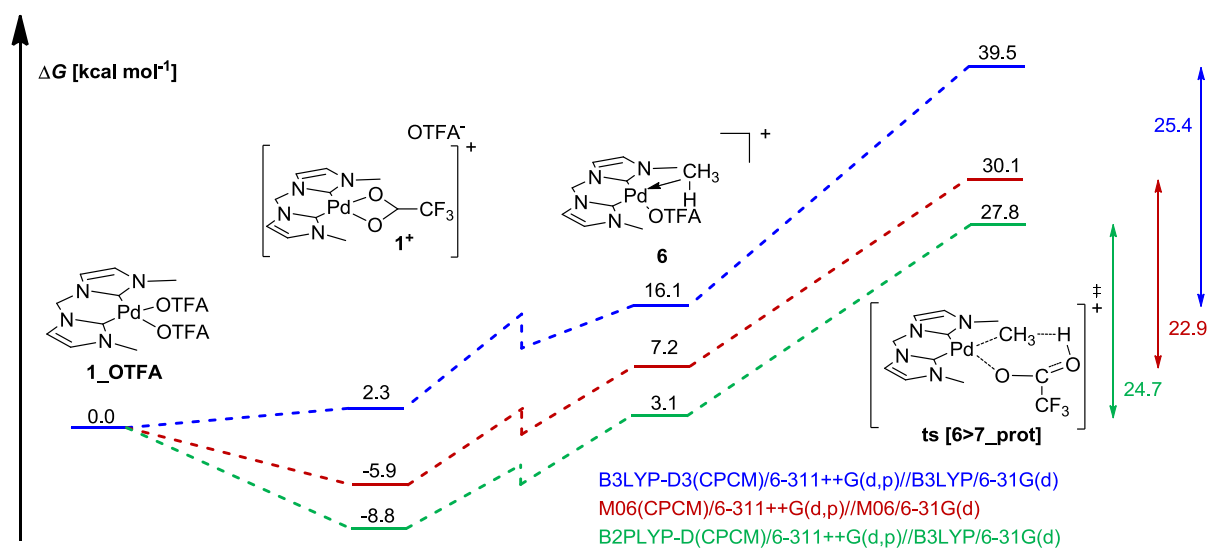


Figure S3. Comparison of functionals for rate determining transition state.

The B3LYP functional has been compared to the M06 functional and to the B2PLYP-D (single points on the B3LYP geometry) functional to test for dispersion interactions (Figure S3). The calculations have been performed with Gaussian09, Rev.B01. The three different functionals calculate similar energies for the transition state of CH activation (25.4 vs. 22.9 vs. 24.6 kcal mol⁻¹). However, the energy for the formation of the methane σ -complex, which is associated with a charge separation, shows a higher deviation (+2.3 vs. -5.9 vs. -8.8 kcal mol⁻¹). We conclude that B3LYP overestimates and M06 and B2PLYP-D underestimate the energy for this process. In any case the differences between the functionals do not affect the conclusions drawn.

Full Gaussian citation (reference 97)

Frisch, M. J. Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian03; Rev. E.01; Wallingford CT, 2004.

Additional Pathways

Regarding Figure 5, $\text{Pd}^{\text{II}-0}$

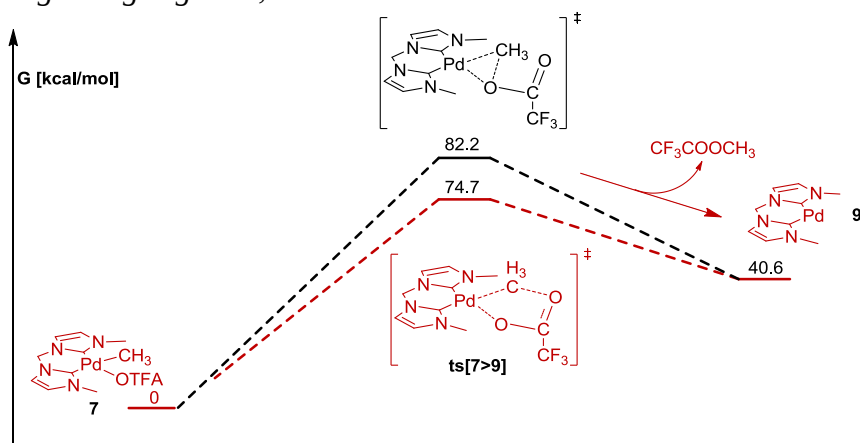


Figure S4. Another reductive elimination transition state from Pd^{II} to Pd^0 .

Regarding Figure 5, $\text{Pd}^{\text{IV}-\text{II}}$

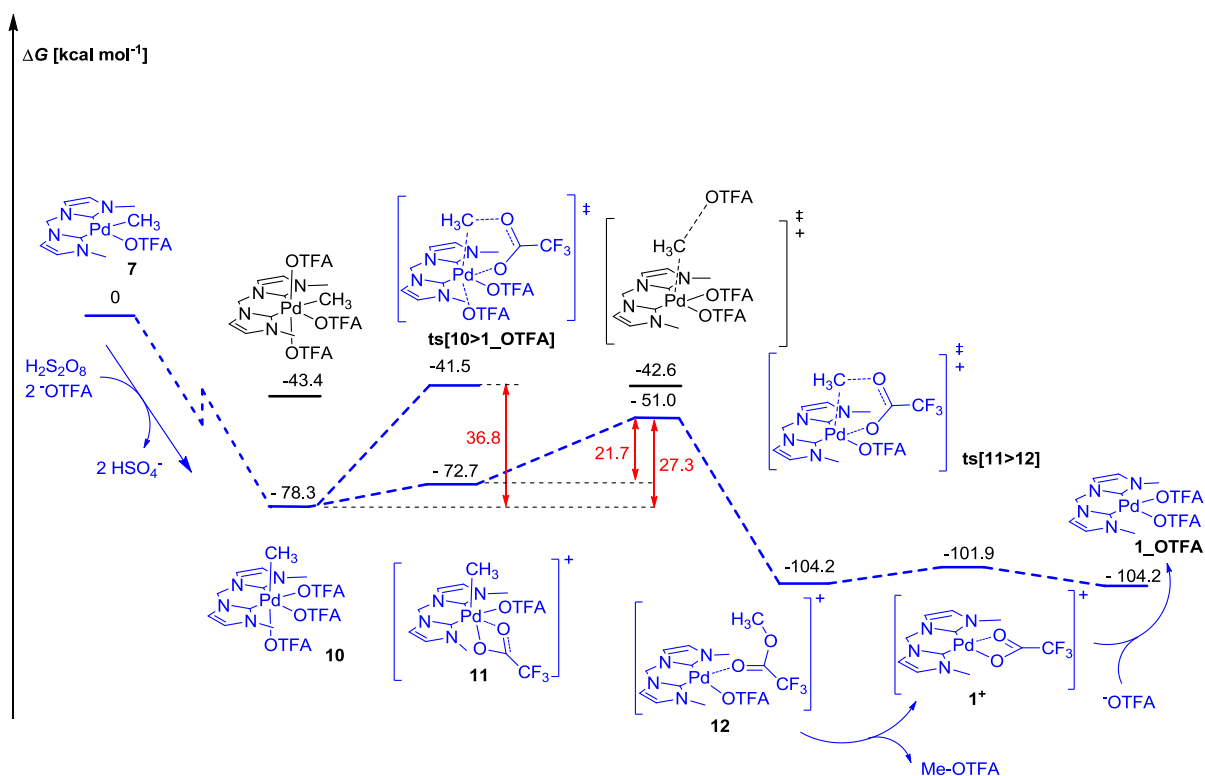


Figure S5. Isomers and other transition states for the Pd^{IV} to Pd^{II} reductive elimination.

Electronic Energies of Mechanism

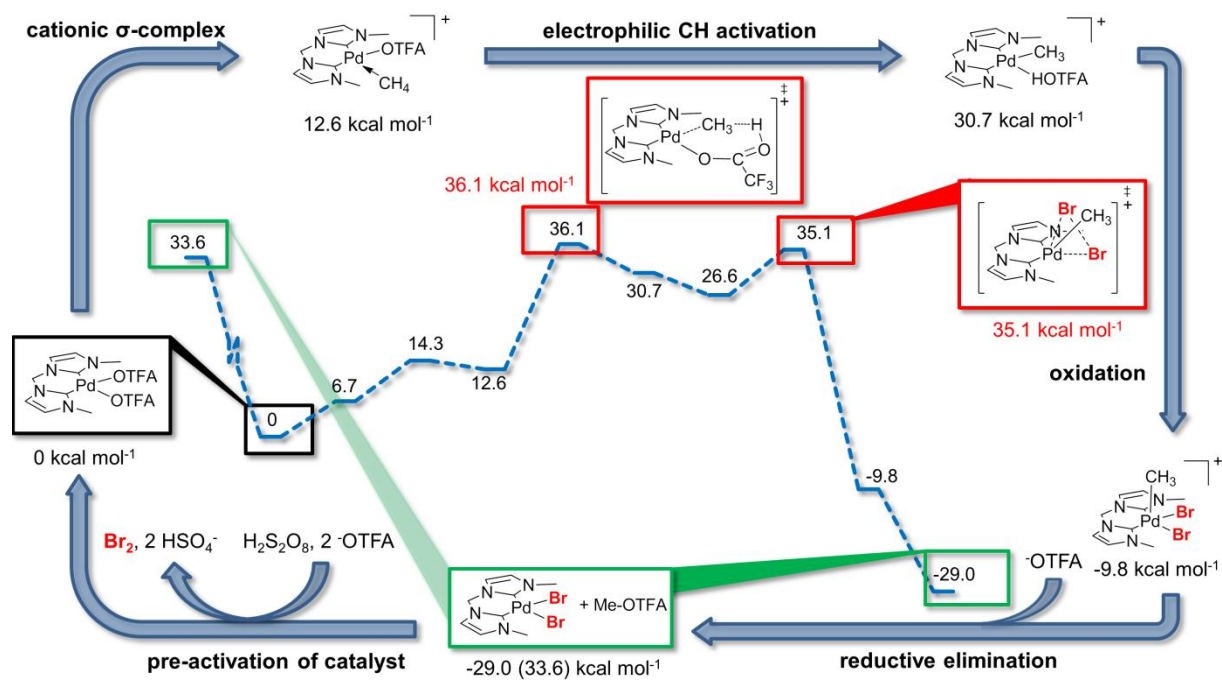


Figure S6. ΔE values of most favorable calculated mechanism. ΔE includes solvent and dispersion corrections [$E_{\text{solv}+\text{D3}}$ ($G_{\text{disp,rep,cav}}$)]. Values are given on the triple- ζ level of theory 6-311++G(d,p) in [kcal mol⁻¹].

Energies of Optimized Molecular Structures

Given are the non-zero-point vibrational energy corrected electronic energy (E), the non-zero-point vibrational energy corrected electronic energy including the D3 correction ($E+D3$), the thermal enthalpy (H) and the Gibbs Free Energy (G) on the double- ζ level of theory (6-31G(d)). The solvent corrected energies [$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)] and Gibbs Free Energies [$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)] are given on the triple- ζ level of theory (6-311++G(d,p)) including dispersion, repulsion and cavity energies. All values are given in Hartree.

Name	E	E(+D3)	H	G	$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)	$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)
methane	-40.5176631	-40.51957626	-40.468641	-40.489773	-40.5342662	-40.50637606
methane (solv. HOAc)	-40.5176631	-40.51957626	-40.468641	-40.489773	-40.5299322	-40.50204206
TFA	-526.7759289	-526.7841215	-526.7296	-526.768357	-526.973147	-526.9655747
4TFA	-2107.167446	-2107.2176001	-2106.976475	-2107.07779	-2107.89982	-2107.810161
3TFA	-1580.371818	-1580.4065572	-1580.228605	-1580.31136	-1580.9273	-1580.866844
OTFA_minus_HOTFA5	-2633.484621	-2633.543934	-2633.258358	-2633.38586	-2634.45251	-2634.353749
Br2	-5142.796235	-5142.799003	-5142.791811	-5142.81969	-5148.27874	-5148.302196
HOTFA3_Br_minus	-4151.905093	-4151.937844	-4151.762368	-4151.86055	-4155.26641	-4155.263360
HOTFA3	-1580.371818	-1580.406557	-1580.228605	-1580.31136	-1580.9273	-1580.896110
MeOTFA	-566.0840521	-566.0962377	-566.00774	-566.050922	-566.280761	-566.2476305
H2S2O8	-1399.09126	-1399.11349	-1399.024	-1399.073	-1399.389	-1399.371293
HSO4_HOTFA4_minus	-2280.124611	-2280.172694	-2279.948542	-2280.04809	-2280.88591	-2280.809386
HBr	-2572.001914	-2572.002599	-2571.992721	-2572.01527	-2574.74819	-2574.761545
HOAc_Tetramer	-916.37321	-916.4163998	-916.096623	-916.177335	-916.718443	-916.5225678
HOAc	-229.0776098	-229.0846099	-228.439472	-229.042925	-229.174664	-229.1399793
OAc_minus_pentamer	-1144.9432	-1144.994096	-1144.61	-1144.71	-1145.43429	-1145.203452
MeBr	-2611.315402	-2611.31972	-2611.273877	-2611.30179	-2614.07242	-2614.058807

Scheme 4	E	E(+D3)	H	G	$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)	$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)
1_Br	-5838.81642	-5838.890999	-5838.584773	-5838.65009	-5844.54258	-5844.376252
1_OTFA	-1748.334565	-1748.429834	-1748.036499	-1748.12767	-1748.93729	-1748.730394

Scheme 5	E	E(+D3)	H	G	$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)	$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)
2	-4666.277311	-4666.383018	-4665.978565	-4666.06941	-4669.57952	-4669.371617
ts[2>3]	-4666.260687	-4666.372153	-4665.963789	-4666.05067	-4669.57257	-4669.362551
3	-3270.941834	-3270.954459	-3270.906349	-3270.94638	-3273.83454	-3273.839088
4	-1395.367138	-1395.443202	-1395.105625	-1395.17353	-1395.77855	-1395.584947
5	-3970.650213	-3970.679537	-3970.582999	-3970.63587	-3973.73734	-3973.722992
ts[5>3]	-3970.620737	-3970.649944	-3970.552735	-3970.60745	-3973.71942	-3973.706139

Figure 1	E	E(+D3)	H	G	$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)	$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)
1_plus	-1221.934478	-1222.007568	-1221.671438	-1221.74365	-1222.37395	-1222.18312
1_plus_vac	-1221.904918	-1221.98113	-1221.642394	-1221.71607	-1222.36185	-1222.172996
6	-1262.432387	-1262.518709	-1262.11908	-1262.2012	-1262.89873	-1262.667539

Figure 2	E	E(+D3)	H	G	$E_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)	$G_{\text{solv}+D3}$ ($G_{\text{disp,rep,cav}}$)
ts[6>7_prot]	-1262.398383	-1262.484404	-1262.089904	-1262.16735	-1262.86129	-1262.63026
7_prot	-1262.415606	-1262.499944	-1262.102011	-1262.18081	-1262.86992	-1262.635127

7	-1262.01726	-1262.101595	-1261.7172	-1261.79542	-1262.44452	-1262.222681
ts[6>7]	-1788.78222	-1788.886308	-1788.439	-1788.53689	-1789.40588	-1789.160543
ts[6>8]	-1788.74788	-1788.857641	-1788.40357	-1788.49973	-1789.37686	-1789.128701
8	-1788.76022	-1788.87036	-1788.41397	-1788.50879	-1789.38595	-1789.134521

Figure 5	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
ts[7>9]	-1261.906752	-1261.98912	-1261.609729	-1261.69058	-1262.31987	-1262.103694
9	-695.8637895	-695.921535	-695.640828	-695.697306	-696.076768	-695.910284
10	-2314.366435	-2314.499531	-2313.99165	-2314.10245	-2315.18479	-2314.920801
ts[10>1_OTFA]	-2314.312964	-2314.443145	-2313.940724	-2314.05384	-2315.12127	-2314.862146
11	-1787.962515	-1788.070422	-1787.623307	-1787.7149	-1788.61588	-1788.368269
ts[11>12]	-1787.93237	-1788.039028	-1787.595124	-1787.68759	-1788.57854	-1788.333759
12	-1788.035147	-1788.13663	-1787.693804	-1787.7864	-1788.66742	-1788.418678

Figure 7	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
13	-6364.727011	-6364.81729	-6364.458568	-6364.54448	-6370.65388	-6370.471349
ts[13>14]	-6364.698612	-6364.794354	-6364.430911	-6364.51267	-6370.63565	-6370.449713
14	-6364.720286	-6364.818772	-6364.451342	-6364.5328	-6370.6588	-6370.471314
15	-6891.119492	-6891.246997	-6890.81514	-6890.91457	-6897.22388	-6897.018948
ts[14>16]	-6405.187788	-6405.30148	-6404.8731	-6404.958	-6411.1564	-6410.926616
16	-6405.25276	-6405.365507	-6404.9318	-6405.017	-6411.2169	-6410.981175

Figure 9	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
9	-695.8637895	-695.921535	-695.640828	-695.697306	-696.076768	-695.910284
ts[9>17]	-736.35347	-736.4194607	-736.08461	-736.14698	-736.589818	-736.3833331
17	-736.37752	-736.4446665	-736.10657	-736.16704	-736.616869	-736.4063895

Figure 10	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
18	-735.6081652	-735.6742947	-735.343525	-735.403852	-735.880227	-735.6759133
19	-5878.425257	-5878.50617	-5878.154292	-5878.22739	-5884.18211	-5883.984241
ts[19>20]	-5878.40763	-5878.49296	-5878.137353	-5878.20687	-5884.16855	-5883.967791
20	-5878.450884	-5878.538728	-5878.178617	-5878.24783	-5884.24012	-5884.037069
ts[20>23]	-5878.439204	-5878.525914	-5878.16844	-5878.23784	-5884.21422	-5884.012853
23	-5878.504478	-5878.58648	-5878.231409	-5878.30403	-5884.26826	-5884.067812
21	-2134.72662	-2134.831143	-2134.392219	-2134.48191	-2135.29095	-2135.046243
ts[21>22]	-2134.6986056	-2134.807057	-2134.366979	-2134.45618	-2135.27657	-2135.034143
22	-2134.8207999	-2134.937466	-2134.48476	-2134.56747	-2135.42421	-2135.17088

Figure 12	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
1_OAc	-1152.907208	-1152.998705	-1152.567142	-1152.64799	-1153.3052	-1153.045976
24	-924.2410776	-924.3130119	-923.957002	-924.023671	-924.572188	-924.3547817
25	-964.7288131	-964.8130193	-964.394433	-964.470431	-965.085638	-964.8272561
ts[25>26_prot]	-964.7014778	-964.7860327	-964.371794	-964.443169	-965.060667	-964.8023581
26_prot	-964.7249227	-964.808224	-964.389965	-964.463967	-965.076773	-964.8158175

Figure 13	E	E(+D3)	H	G	E _{solv+D3} (G _{disp,rep,cav})	G _{solv+D3} (G _{disp,rep,cav})
ts[7>27]	-735.577837	-735.6455673	-735.314632	-735.373397	-735.852191	-735.6477513
27	-735.6177901	-735.6874516	-735.351497	-735.411523	-735.896301	-735.6900334
ts[18>28]	-1261.970568	-1262.056362	-1261.672529	-1261.75124	-1262.39846	-1262.179132
28	-1262.028902	-1262.11567	-1261.72766	-1261.80622	-1262.45277	-1262.230081

XYZ coordinates

In alphabetical order.

10

C	1.33223	1.20908	-1.33945
N	2.17247	0.79103	-2.31864
C	3.12398	1.76760	-2.58850
C	2.84962	2.79911	-1.75137
N	1.74853	2.43688	-0.98658
C	2.05058	-0.48587	-3.01523
N	1.86407	-1.59093	-2.09342
C	1.01098	-1.58159	-1.03766
N	1.21482	-2.73549	-0.38542
C	2.19188	-3.47464	-1.02747
C	2.61052	-2.76392	-2.10164
Pd	-0.07949	0.04112	-0.51962
C	-1.18861	0.10144	-2.30576
C	0.68441	-3.10360	0.93160
C	1.15006	3.32393	0.02642
O	-1.57872	-1.11584	0.32804
C	-2.11608	-2.16708	-0.18217
O	-1.78725	-2.83707	-1.15477
C	-3.32209	-2.66017	0.66768
F	-4.03878	-1.66881	1.20118
F	-4.14184	-3.42335	-0.07315
F	-2.84488	-3.43014	1.68063
H	3.34066	3.75076	-1.62183
H	3.89812	1.63667	-3.32815
H	3.34503	-2.98042	-2.86096
H	2.50511	-4.43720	-0.65576
H	0.44088	4.00195	-0.45275
H	0.62157	2.72743	0.76567
H	1.96052	3.88162	0.49902
H	1.34002	-3.87345	1.34157
H	0.72464	-2.22827	1.57704
H	-0.32797	-3.48923	0.84302
H	1.22082	-0.44276	-3.72414
H	2.97550	-0.65563	-3.56673
H	-1.60530	-0.89705	-2.41312
H	-0.55071	0.39097	-3.13905
H	-1.90349	0.88752	-2.06805
C	2.36759	-0.20156	1.58174
O	3.01097	-1.05985	0.97428
O	1.21069	0.29587	1.32425
O	-1.28093	1.70054	-0.09647
C	-2.31409	1.87636	0.68214
O	-2.70988	1.31284	1.67679
C	3.08800	0.41233	2.82448
C	-3.12450	3.08017	0.11168
F	-4.13310	3.43689	0.91130
F	-3.64550	2.75740	-1.09872
F	-2.33821	4.17079	-0.07194
F	2.64816	1.64234	3.15676
F	2.89943	-0.38781	3.89824
F	4.41540	0.49865	2.60897

11

C	-2.74410	-3.32571	1.02925
N	-2.47915	-2.22697	0.22136

C	-1.23494	-1.75247	0.46478
N	-0.71422	-2.52991	1.43118
C	-1.62929	-3.51335	1.78121
C	-3.39873	-1.59887	-0.71298
N	-3.45091	-0.15619	-0.49371
C	-4.62205	0.58636	-0.44714
C	-4.24130	1.87744	-0.28019
N	-2.85582	1.90119	-0.22695
C	-2.36176	0.65260	-0.36024
Pd	-0.44548	-0.09143	-0.34716
O	0.50514	1.73084	-0.85754
C	0.81964	1.98474	0.35970
C	1.69712	3.22100	0.62125
F	0.85820	4.29060	0.67518
C	-2.09287	3.14565	-0.01980
C	0.59497	-2.36923	2.09482
O	1.33103	-1.14151	-0.48196
C	2.52875	-0.66336	-0.26278
O	2.87841	0.42126	0.15279
C	-0.62796	-0.80021	-2.29708
O	0.33043	1.34016	1.31743
C	3.58479	-1.75879	-0.59181
F	3.45346	-2.17813	-1.86179
F	4.82200	-1.31097	-0.40959
F	3.39555	-2.83132	0.22001
F	2.33187	3.12416	1.78487
F	2.57142	3.42248	-0.35988
H	-1.40776	-4.24964	2.53833
H	-3.67861	-3.86411	0.99364
H	-5.60009	0.13961	-0.53863
H	-4.82863	2.77778	-0.18770
H	1.37867	-2.82225	1.48956
H	0.79996	-1.30759	2.23231
H	0.53209	-2.85640	3.06851
H	-1.61801	3.12525	0.96090
H	-1.33952	3.24557	-0.79797
H	-2.79381	3.97850	-0.07226
H	-3.09357	-1.81177	-1.73976
H	-4.39537	-2.00784	-0.54816
H	-0.52143	-1.88181	-2.26631
H	0.23954	-0.30494	-2.72911
H	-1.56672	-0.44359	-2.71595

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C	-4.48077	-1.42272	0.70467
N	-3.43959	-0.50633	0.77423
C	-2.30397	-1.01563	0.22595
N	-2.64059	-2.25146	-0.20067
C	-3.97118	-2.52252	0.09449
C	-3.50018	0.83844	1.33459
N	-2.93559	1.79303	0.39038
C	-1.73389	1.59578	-0.21062
N	-1.54275	2.66309	-1.01036
C	-2.61463	3.53933	-0.89608
C	-3.49666	2.99596	-0.01891
Pd	-0.58668	0.02945	0.17266

O	0.99769	1.37594	0.23569	H	0.21715	2.26289	-2.35418
C	2.25053	1.09778	0.25140	H	0.20156	4.01687	-2.02519
C	3.11040	2.38276	0.40504	C	2.24745	-1.25470	-0.52416
F	2.76432	3.29334	-0.53698	O	2.34680	-0.51921	-1.49010
C	-0.38590	2.90044	-1.88841	C	3.28126	-2.38317	-0.28339
C	-1.74531	-3.19175	-0.88220	F	2.70145	-3.49636	0.18595
O	0.62684	-1.66154	0.82000	F	4.17393	-1.95013	0.64267
C	1.68718	-2.07024	0.33173	F	3.94524	-2.67817	-1.39939
C	1.88937	-2.25216	-1.18796				
F	3.15347	-2.18728	-1.56166	14			
O	2.63789	-2.64886	1.00401	C	1.74406	0.12497	-0.99898
F	1.39823	-3.47507	-1.50552	N	1.64935	1.12475	-1.91428
F	1.16600	-1.34342	-1.87222	C	2.83506	1.22738	-2.62767
O	2.82124	0.01101	0.17523	C	3.66177	0.27665	-2.12670
F	4.41136	2.12821	0.27890	N	2.98054	-0.39005	-1.11721
F	2.89322	2.93818	1.61193	C	0.46665	1.95662	-2.11939
C	2.59039	-2.55961	2.45245	N	0.04417	2.54700	-0.85462
H	-2.65576	4.46245	-1.45301	C	-0.29840	3.87086	-0.60744
H	-4.44870	3.35056	0.34445	C	-0.74439	3.90767	0.67547
H	-5.46825	-1.21643	1.08769	N	-0.66879	2.61514	1.18274
H	-4.43370	-3.46280	-0.16283	C	-0.18470	1.79123	0.24136
H	0.44773	3.30021	-1.31280	Pd	0.14996	-0.24606	0.17071
H	-0.08609	1.95770	-2.34527	Br	0.36008	-2.71967	-0.03680
H	-0.69182	3.60115	-2.66648	C	-1.05124	2.23999	2.55410
H	-2.34808	-3.85720	-1.50215	C	3.62364	-1.44686	-0.31506
H	-1.05700	-2.63678	-1.51593	Br	1.62774	-0.08743	2.13386
H	-1.18358	-3.77768	-0.15208	O	-1.93259	-0.53017	0.91381
H	-2.94124	0.87270	2.27339	C	-2.32647	-0.51674	-0.27972
H	-4.54199	1.09838	1.52255	O	-1.50327	-0.32984	-1.23673
H	3.47388	-3.09464	2.79391	C	-3.82325	-0.65911	-0.61728
H	1.67731	-3.02649	2.82553	F	-4.32416	0.58065	-0.79022
H	2.63323	-1.50749	2.73895	F	-3.98353	-1.35168	-1.74487
				F	-4.47375	-1.25635	0.37676
13				H	-1.10655	4.73150	1.27114
C	3.16926	3.11560	0.42550	H	-0.20771	4.64702	-1.35176
C	2.39598	3.67807	-0.53777	H	2.97124	1.94236	-3.42431
N	1.27224	2.86871	-0.65057	H	4.67222	0.00908	-2.39408
C	1.35384	1.82485	0.20861	H	-1.43118	1.21949	2.54826
N	2.50716	1.98172	0.88348	H	-0.18350	2.31190	3.21201
Pd	0.00338	0.37357	0.24841	H	-1.83576	2.92110	2.88688
Br	-3.49620	-2.10656	-0.28334	H	2.86165	-2.12484	0.06187
C	0.15548	3.02576	-1.57409	H	4.30765	-1.98903	-0.96968
N	-1.10177	2.89158	-0.84444	H	4.17017	-0.98932	0.51128
C	-1.33795	1.85437	0.00164	H	-0.34523	1.34819	-2.52383
N	-2.54956	2.10215	0.54179	H	0.72185	2.75284	-2.81760
C	-3.08140	3.27629	0.02158				
C	-2.16820	3.78061	-0.84730	15			
C	-3.22241	1.27144	1.54549	C	3.47074	-2.61455	0.90699
C	3.04003	1.08608	1.91979	N	2.13122	-2.25812	0.87525
O	1.37746	-1.17308	0.45054	C	1.91177	-1.30471	-0.07041
Br	-1.17326	-1.99255	0.12012	N	3.11693	-1.05024	-0.61775
H	-4.05040	3.64717	0.31837	C	4.08379	-1.85771	-0.03574
H	-2.18630	4.67016	-1.45801	C	1.10889	-2.73972	1.79945
H	2.54178	4.56107	-1.14050	N	0.47663	-1.60737	2.45823
H	4.12160	3.42012	0.83126	C	0.40038	-1.37981	3.82762
H	-2.48061	0.63790	2.03184	C	-0.15845	-0.15259	3.97045
H	-3.68476	1.92020	2.29202	N	-0.39628	0.34766	2.69776
H	-3.98243	0.64657	1.07153	C	-0.02902	-0.55529	1.77349
H	2.22549	0.49070	2.32783	Pd	0.08035	-0.40598	-0.29048
H	3.78794	0.41780	1.48818	O	1.20837	1.33697	0.09330
H	3.48818	1.69325	2.70844	C	-0.98366	1.66938	2.45576

C	3.45759	0.00413	-1.58512	H	-3.39326	-2.68590	1.90986
H	5.11548	-1.81525	-0.34714	H	2.16052	2.71772	0.40067
H	3.85221	-3.37247	1.57308	H	1.45621	3.66748	1.73909
H	0.72974	-2.10451	4.55556	H	1.31421	1.89039	1.74594
H	-0.41264	0.40907	4.85572	H	-2.44660	1.53806	-2.40674
H	2.62991	0.12160	-2.28281	H	-3.68012	2.41495	-1.47637
H	3.62629	0.94081	-1.05268	H	-1.24401	-0.44576	-2.85366
H	4.35931	-0.30780	-2.11531	H	1.91871	-2.02454	0.27280
H	-1.15643	1.80324	1.39143	H	0.54644	-0.52592	-2.74331
H	-1.93600	1.73541	2.98530				
H	-0.29146	2.43759	2.80935	17			
H	0.35897	-3.30654	1.24510	N	-2.73751	-0.05354	0.55538
H	1.59031	-3.36191	2.55365	C	-1.51483	0.03649	-0.03427
C	0.84095	2.54583	-0.22628	N	-1.46501	1.33807	-0.45935
O	-0.17348	2.97496	-0.72467	C	-2.62592	2.03696	-0.14497
C	1.95264	3.53858	0.23984	C	-3.42934	1.15227	0.49700
F	3.18314	3.17046	-0.18947	C	-0.32003	1.84371	-1.20117
F	1.72127	4.77686	-0.19681	N	0.91946	1.67510	-0.46119
F	1.99260	3.57151	1.59510	C	1.78188	2.68676	-0.05140
O	-1.79495	0.46288	-0.47342	C	2.78294	2.07020	0.62395
C	-2.78114	0.10805	0.28136	N	2.49677	0.70788	0.61235
O	-2.80350	-0.60641	1.27340	C	1.34271	0.43632	-0.05486
C	-4.09032	0.83592	-0.13960	H	-4.41844	1.27290	0.91202
F	-4.19361	1.01504	-1.46125	H	-2.77995	3.07220	-0.40974
F	-5.16887	0.15552	0.27770	H	1.62018	3.72832	-0.28472
F	-4.11523	2.05329	0.45522	H	3.66159	2.47348	1.10407
Br	-0.98794	-2.62716	-0.77372	H	-0.24266	1.29804	-2.14435
Br	0.22132	-0.14838	-2.81382	H	-0.47060	2.90599	-1.40310
				Pd	0.10096	-1.27742	-0.29606
16				C	3.31087	-0.30171	1.27986
C	-2.30356	-0.35596	-0.20505	H	4.33268	-0.28144	0.88772
N	-3.17707	0.55878	-0.70417	H	3.33402	-0.11340	2.35828
C	-4.48377	0.18708	-0.42008	H	2.86226	-1.27450	1.08534
C	-4.40040	-0.97801	0.26469	C	-3.24394	-1.26733	1.18496
N	-3.05642	-1.29763	0.40074	H	-3.25935	-1.15655	2.27439
C	-2.79974	1.77684	-1.40258	H	-4.25686	-1.47580	0.82669
N	-1.77050	2.49203	-0.66578	H	-2.57303	-2.08137	0.90567
C	-0.65712	1.90146	-0.16255	C	1.61680	-2.67419	-0.68333
N	0.05706	2.89251	0.40705	H	2.54196	-2.18771	-1.02089
C	-0.60621	4.10275	0.25359	H	-0.84315	-2.56733	-0.46931
C	-1.75938	3.85802	-0.41620	H	1.83627	-3.25385	0.22566
Pd	-0.32015	-0.12427	-0.34205	H	1.30778	-3.38693	-1.45396
C	-0.34472	0.03067	-2.46730				
C	1.34192	2.77952	1.11646	18			
C	-2.63339	-2.49582	1.15026	C	-1.57369	-0.08829	-0.03742
Br	0.05307	-2.61505	-0.77176	N	-2.77755	-0.23296	0.56273
O	1.84217	0.25877	-0.54300	C	-3.52481	0.93786	0.49006
C	2.81285	-0.41040	-0.17126	H	-4.51659	1.01790	0.90827
O	2.82808	-1.60481	0.31993	N	-1.57695	1.20092	-0.48123
Br	-0.07587	-0.30308	2.26707	C	-2.76490	1.85051	-0.16692
C	4.21741	0.22539	-0.31861	H	-2.96559	2.87601	-0.43738
F	5.16751	-0.54526	0.19314	C	1.27221	0.42072	-0.02139
F	4.45309	0.42894	-1.62034	N	0.79301	1.62086	-0.45806
F	4.22464	1.41364	0.31194	C	1.60862	2.66099	-0.02829
H	-0.25833	1.08544	-2.72587	H	1.41088	3.69358	-0.27126
H	-5.17177	-1.60856	0.67824	N	2.38513	0.71648	0.68570
H	-5.33390	0.77541	-0.72858	C	2.60935	2.08954	0.68481
H	-2.55580	4.51496	-0.72994	H	3.45432	2.52922	1.19176
H	-0.20114	5.02290	0.64502	C	-0.44723	1.75904	-1.21389
H	-2.55247	-3.34410	0.47052	C	-3.24764	-1.46160	1.20223
H	-1.67771	-2.29786	1.62969	H	-2.42465	-2.17645	1.22626

H	-3.56788	-1.24891	2.22525
H	-4.08306	-1.88609	0.63870
C	3.25217	-0.23310	1.38862
H	2.71919	-1.17334	1.50788
H	4.17066	-0.39764	0.81946
H	3.49755	0.17436	2.37170
H	-0.34247	1.24293	-2.17040
H	-0.62703	2.81898	-1.39405
Pd	0.22975	-1.23128	-0.32725
C	1.89973	-2.31750	-0.79857
H	2.14416	-2.96704	0.05055
H	1.49954	-2.91694	-1.63286
H	2.79417	-1.79380	-1.13983

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C	1.21457	3.51151	-0.42211
N	1.27305	2.14495	-0.66720
C	0.39855	1.45652	0.11910
N	-0.20482	2.41013	0.86354
C	0.27317	3.67640	0.54109
C	2.19312	1.45211	-1.56170
N	2.97183	0.47079	-0.81515
C	4.35178	0.45728	-0.64806
C	4.61662	-0.55148	0.21784
N	3.39757	-1.12359	0.56996
C	2.38053	-0.50265	-0.06695
Pd	0.38082	-0.67057	-0.02005
Br	-2.05753	-1.39195	-0.17530
Br	-3.71721	0.30074	-0.17619
C	3.27371	-2.21303	1.54166
C	-1.19413	2.16133	1.91232
C	0.57470	-2.76300	-0.34219
H	-0.09377	4.57049	1.02157
H	1.82135	4.23060	-0.95095
H	5.00816	1.14419	-1.15978
H	5.55272	-0.91177	0.61578
H	-1.33322	1.08556	2.00957
H	-0.83303	2.56797	2.86062
H	-2.14631	2.62844	1.65061
H	2.22055	-2.35248	1.77574
H	3.68556	-3.13644	1.12651
H	3.81771	-1.94503	2.45054
H	1.62909	0.94576	-2.34748
H	2.87250	2.17648	-2.01114
H	1.60110	-3.00158	-0.62550
H	0.31030	-3.30827	0.56957
H	-0.07362	-3.08144	-1.16524

1_Br

N	-2.52492	1.31944	0.72829
C	-1.38074	1.06809	0.05105
N	-1.19155	2.17488	-0.72500
C	-2.20467	3.10696	-0.53704
C	-3.04533	2.55949	0.37592
C	0.00011	2.31721	-1.54893
N	1.19180	2.17472	-0.72507
C	2.20507	3.10665	-0.53723
C	3.04575	2.55908	0.37565
N	2.52520	1.31910	0.72809
C	1.38092	1.06790	0.05098
H	-3.96432	2.93284	0.80032

H	-2.24884	4.04066	-1.07599
H	2.24930	4.04034	-1.07619
H	3.96483	2.93230	0.79995
H	0.00003	1.54269	-2.31885
H	0.00017	3.30430	-2.01311
Pd	-0.00003	-0.41995	0.01206
C	-3.11029	0.45090	1.75269
H	-2.71620	0.71775	2.73816
H	-4.19473	0.58211	1.74311
H	-2.86158	-0.58281	1.50607
C	3.11061	0.45052	1.75242
H	4.19516	0.58067	1.74188
H	2.71759	0.71824	2.73809
H	2.86076	-0.58308	1.50651
Br	1.81858	-2.14226	-0.25848
Br	-1.81895	-2.14192	-0.25872

1_OAc

C	1.37567	-0.99383	0.15692
N	1.19168	-2.02328	-0.71379
C	2.27754	-2.89019	-0.70467
C	3.14646	-2.38993	0.20882
N	2.57191	-1.23813	0.73510
C	-0.00039	-2.10236	-1.54519
N	-1.19235	-2.02305	-0.71365
C	-1.37599	-0.99358	0.15709
N	-2.57226	-1.23754	0.73533
C	-3.14716	-2.38919	0.20910
C	-2.27845	-2.88965	-0.70449
Pd	-0.00001	0.44870	0.35394
C	-3.19504	-0.39378	1.75289
C	3.19518	-0.39434	1.75231
O	-2.44312	1.18568	-1.41118
C	-2.28178	2.02643	-0.52062
O	-1.43786	1.94853	0.46929
C	-3.10831	3.31354	-0.50174
H	-3.51679	3.49874	0.49715
H	-2.45836	4.16191	-0.74466
H	-3.91527	3.25802	-1.23574
H	4.11369	-2.74470	0.52920
H	2.33884	-3.75692	-1.34427
H	-2.34005	-3.75633	-1.34413
H	-4.11444	-2.74370	0.52956
H	4.22648	-0.17994	1.45926
H	2.63536	0.53962	1.80664
H	3.18735	-0.90397	2.72108
H	-2.63562	0.54047	1.80649
H	-4.22671	-0.17999	1.46071
H	-3.18611	-0.90315	2.72180
H	-0.00036	-1.27215	-2.25570
H	-0.00051	-3.05309	-2.08026
O	1.43787	1.94843	0.46918
C	2.28252	2.02593	-0.52014
O	2.44462	1.18478	-1.41018
C	3.10900	3.31306	-0.50114
H	2.45900	4.16150	-0.74366
H	3.51768	3.49799	0.49773
H	3.91585	3.25773	-1.23527

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1_OTFA.log	Energy: -1097095.6745925		
C	1.36963	1.63691	-0.16329

N	1.19207	2.64821	0.72794
C	2.29143	3.49700	0.74581
C	3.16029	3.00223	-0.17094
N	2.57251	1.87238	-0.72888
C	-0.00056	2.72652	1.55986
N	-1.19292	2.64802	0.72756
C	-1.36996	1.63664	-0.16367
N	-2.57273	1.87176	-0.72966
C	-3.16096	3.00149	-0.17193
C	-2.29252	3.49652	0.74507
Pd	-0.00002	0.19461	-0.37119
C	-3.21442	1.03035	-1.74130
C	3.21480	1.03110	-1.74026
O	-2.44359	-0.60560	1.42530
C	-2.31989	-1.33550	0.44570
O	-1.45917	-1.29115	-0.50763
C	-3.39143	-2.43468	0.21455
F	-4.35866	-1.93748	-0.61138
F	-2.90054	-3.53981	-0.36604
F	-3.99200	-2.79542	1.35729
H	4.13415	3.35006	-0.47831
H	2.35723	4.35397	1.39786
H	-2.35877	4.35345	1.39712
H	-4.13482	3.34906	-0.47960
H	4.02980	0.46161	-1.28816
H	2.47820	0.33029	-2.12863
H	3.59750	1.66510	-2.54437
H	-2.47719	0.33063	-2.13041
H	-4.02865	0.45967	-1.28927
H	-3.59813	1.66443	-2.54485
H	-0.00064	1.89760	2.27210
H	-0.00072	3.67732	2.09430
O	1.45926	-1.29094	-0.50752
C	2.32032	-1.33523	0.44553
O	2.44428	-0.60532	1.42508
C	3.39188	-2.43431	0.21405
F	2.90095	-3.53946	-0.36646
F	4.35885	-1.93698	-0.61213
F	3.99277	-2.79503	1.35662

1_plus_vac

C	4.58732	-0.95888	-0.11139
C	4.34007	0.19828	-0.77861
N	2.96203	0.36643	-0.76105
C	2.35675	-0.65668	-0.10551
N	3.36038	-1.46314	0.30200
Pd	0.34968	-0.78129	0.10097
C	2.20065	1.45229	-1.37110
N	1.22217	1.96616	-0.42191
C	0.37165	1.17256	0.27286
N	-0.38588	1.98798	1.02737
C	-0.03212	3.30939	0.78102
C	0.97715	3.30192	-0.12530
C	-1.47203	1.59947	1.93913
C	3.19133	-2.70800	1.05778
H	-0.52726	4.12986	1.27705
H	1.53062	4.10876	-0.58015
H	5.00947	0.89732	-1.25611
H	5.51778	-1.45967	0.10850
H	-1.39390	0.53662	2.15628
H	-1.37951	2.18019	2.85872

H	-2.43560	1.79533	1.46387
H	3.89631	-2.72575	1.89159
H	2.17510	-2.74507	1.45364
H	3.36536	-3.57033	0.40889
H	1.68848	1.08966	-2.26619
H	2.88352	2.25722	-1.64271
O	-1.64588	-1.02810	0.25255
C	-2.41440	-0.35530	-0.56145
O	-2.08091	0.50481	-1.35844
C	-3.91297	-0.67868	-0.33858
F	-4.32125	-0.01080	0.76987
F	-4.12232	-1.98612	-0.13948
F	-4.65338	-0.27293	-1.36918

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C	-2.63137	-3.23385	-0.33124
C	-3.44729	-2.34720	0.29362
N	-2.69363	-1.19527	0.48081
C	-1.43658	-1.36025	-0.00492
N	-1.40250	-2.61200	-0.50876
Pd	0.01247	-0.00004	0.04428
C	-3.12053	0.00010	1.19449
N	-2.69353	1.19543	0.48080
C	-1.43646	1.36031	-0.00492
N	-1.40227	2.61204	-0.50878
C	-2.63110	3.23399	-0.33130
C	-3.44709	2.34741	0.29357
C	-0.26245	3.23661	-1.19660
C	-0.26275	-3.23661	-1.19665
H	-2.81380	4.24311	-0.66728
H	-4.47104	2.43469	0.62288
H	-4.47123	-2.43439	0.62296
H	-2.81416	-4.24296	-0.66719
H	0.65332	2.71385	-0.92476
H	-0.41467	3.19103	-2.27820
H	-0.19135	4.27857	-0.87883
H	-0.41467	-3.19036	-2.27826
H	0.65316	-2.71437	-0.92428
H	-0.19216	-4.27878	-0.87946
H	-2.69732	0.00009	2.20333
H	-4.20889	0.00015	1.26083
O	1.87108	1.10319	0.10803
C	2.49561	-0.00015	0.12720
O	1.87102	-1.10343	0.10801
C	4.03230	-0.00008	0.22121
F	4.38771	0.00179	1.51580
F	4.53402	1.08904	-0.36904
F	4.53405	-1.09083	-0.36593

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C	-1.26528	1.28457	-0.09149
N	-0.93607	2.43013	0.56788
C	-1.86224	3.43333	0.31491
C	-2.77841	2.89058	-0.52470
N	-2.39283	1.57965	-0.77288
C	0.28386	2.58238	1.34934
N	1.44526	2.16654	0.57373
C	2.57220	2.94134	0.33463
C	3.35773	2.20984	-0.49401
N	2.69729	1.01522	-0.74910
C	1.52299	0.97555	-0.08386

Pd	-0.04172	-0.39680	0.02487	H	-0.62330	2.29409	-2.23873
Br	-1.99791	-1.92040	0.08187	H	0.89101	2.10834	-1.31076
C	3.25721	-0.00640	-1.64908	H	3.62854	-0.89259	-3.06749
C	-3.14781	0.70688	-1.68690	H	4.63945	2.14634	1.94303
Br	1.50397	-2.33489	0.04537				
H	4.31919	2.43236	-0.93060	22			
H	2.71158	3.92037	0.76689	C	2.34393	3.40018	0.84941
H	-1.78951	4.41939	0.74739	N	2.12102	2.23530	0.12720
H	-3.66179	3.31784	-0.97378	C	0.90918	1.71958	0.42698
H	2.45213	-0.59740	-2.07797	N	0.36309	2.53423	1.34854
H	3.80614	0.50799	-2.44009	C	1.23358	3.58349	1.60852
H	3.92257	-0.66775	-1.09239	C	3.04313	1.60094	-0.79366
H	-3.96873	0.22809	-1.15112	N	3.14410	0.17014	-0.52555
H	-3.53336	1.32533	-2.49973	C	4.34029	-0.52833	-0.58573
H	-2.49103	-0.06284	-2.08360	C	4.01721	-1.83859	-0.46545
H	0.21745	1.99829	2.26836	N	2.63900	-1.92334	-0.33934
H	0.39980	3.63388	1.61115	C	2.09471	-0.68845	-0.36517
H	-0.17353	-1.68720	2.33538	Pd	0.16691	-0.02126	-0.25289
C	-0.05667	-0.62615	2.14938	O	-1.63199	1.09268	-0.40921
H	-0.91856	-0.03431	2.44317	S	-3.09478	0.80310	-0.75849
H	0.91739	-0.23827	2.43293	O	-2.89458	0.04149	-2.19898
				C	1.96446	-3.23140	-0.21247
21				C	-0.92739	2.38011	2.05347
C	-4.58150	1.43974	-0.16074	C	0.30485	0.45216	-2.28701
N	-3.56627	0.54637	-0.48305	O	-3.71999	-0.17467	0.15756
C	-2.34346	1.14422	-0.39255	O	-3.81371	2.04657	-0.96189
N	-2.60217	2.41628	-0.01130	O	-0.78539	-1.91665	-0.45703
C	-3.97239	2.61528	0.12812	S	-1.05248	-2.19751	1.05869
C	-3.72051	-0.87265	-0.77314	O	-2.61050	-2.25234	1.23779
N	-3.00334	-1.68335	0.20339	O	-0.49727	-0.94688	1.72806
C	-1.67739	-1.48816	0.46226	O	-0.52255	-3.45868	1.53141
N	-1.38802	-2.41977	1.40028	H	0.98696	4.35851	2.31776
C	-2.50325	-3.18939	1.71382	H	3.24984	3.97915	0.75705
C	-3.53075	-2.72232	0.96097	H	5.29372	-0.03808	-0.70911
Pd	-0.68115	0.10500	-0.61027	H	4.63970	-2.71964	-0.44894
O	2.00666	0.19571	1.94373	H	-1.71751	2.86447	1.47967
S	2.74429	1.30387	1.39499	H	-1.14700	1.32129	2.17307
O	3.19619	0.95509	-0.20429	H	-0.82033	2.84861	3.03275
O	3.70074	-0.40905	-0.27053	H	1.03895	-3.21802	-0.78150
S	2.66400	-1.33950	-1.20516	H	2.64249	-3.98530	-0.61309
O	3.31378	-2.62493	-1.17395	H	1.74135	-3.44079	0.83329
C	-0.07003	-2.61859	2.00486	H	2.71891	1.76464	-1.82476
C	-1.60899	3.45713	0.26471	H	4.02983	2.04398	-0.65909
C	0.09636	1.57466	-1.84280	H	0.15199	1.52711	-2.34867
O	1.29094	-1.14044	-0.78397	H	1.24998	0.10560	-2.69928
O	2.78416	-0.63600	-2.63998	H	-0.55351	-0.11447	-2.64406
O	2.23733	2.64888	1.23364	H	-3.77422	-0.23109	-2.52687
O	4.17098	1.30595	2.12852	H	-3.05917	-1.44213	0.82052
H	-2.46836	-3.98628	2.44085				
H	-4.56249	-3.03293	0.89790	23			
H	-5.62511	1.16602	-0.17639	C	-3.86053	-0.81763	-0.61777
H	-4.38355	3.56914	0.42013	N	-2.61476	-0.22248	-0.77448
H	0.42674	-3.48236	1.55347	C	-1.69425	-0.81225	0.03579
H	0.52967	-1.72458	1.84595	N	-2.36288	-1.76809	0.71012
H	-0.18814	-2.78812	3.07774	C	-3.69465	-1.79260	0.31008
H	-1.59387	4.18906	-0.54706	C	-2.29179	0.94047	-1.59025
H	-1.86929	3.95479	1.20181	N	-1.70323	1.97718	-0.74785
H	-0.62935	2.99385	0.36000	C	-2.14866	3.28187	-0.58140
H	-3.33266	-1.07709	-1.77333	C	-1.34430	3.83447	0.36152
H	-4.78069	-1.12460	-0.73692	N	-0.43945	2.85390	0.75596
H	0.52544	1.00926	-2.67894	C	-0.64917	1.70930	0.06893

Pd	0.18987	-0.16104	0.04485
Br	1.00989	-2.48908	-0.20603
C	0.56881	3.05774	1.80007
C	-1.81903	-2.67875	1.72568
Br	2.61775	0.90262	-0.21035
C	3.99607	-0.52941	-0.33227
H	-4.39801	-2.49907	0.72300
H	-4.73021	-0.50729	-1.17599
H	-2.97261	3.69596	-1.14207
H	-1.33605	4.82605	0.78744
H	-1.69485	-3.67547	1.29816
H	-0.84814	-2.31193	2.04883
H	-2.51259	-2.71100	2.56909
H	0.09137	3.49675	2.67907
H	0.99909	2.09364	2.06677
H	1.35613	3.72472	1.43935
H	-1.58306	0.65621	-2.37111
H	-3.20506	1.32295	-2.04577
H	3.44149	-1.46504	-0.38211
H	4.60138	-0.43962	0.56659
H	4.55707	-0.31578	-1.23914

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C	1.98898	-3.23634	0.39160
C	2.83212	-2.34429	-0.18720
N	2.08238	-1.19646	-0.41339
C	0.80039	-1.36690	0.00327
N	0.74891	-2.62073	0.50234
Pd	-0.64844	-0.00002	-0.11217
C	2.53861	0.00005	-1.10589
N	2.08234	1.19653	-0.41339
C	0.80033	1.36693	0.00327
N	0.74881	2.62075	0.50234
C	1.98885	3.23641	0.39160
C	2.83203	2.34440	-0.18720
C	-0.42498	3.24990	1.12294
C	-0.42485	-3.24992	1.12294
H	2.15910	4.24483	0.73600
H	3.87282	2.42508	-0.46057
H	3.87291	-2.42493	-0.46057
H	2.15927	-4.24475	0.73600
H	-1.32228	2.71464	0.81504
H	-0.32594	3.22311	2.21150
H	-0.48642	4.28661	0.78567
H	-0.32584	-3.22310	2.21150
H	-1.32218	-2.71472	0.81500
H	-0.48623	-4.28665	0.78570
H	2.15819	0.00004	-2.13163
H	3.62887	0.00007	-1.12681
O	-2.46972	1.09656	-0.25932
C	-3.13022	-0.00007	-0.31097
O	-2.46968	-1.09666	-0.25933
C	-4.61991	-0.00007	-0.46124
H	-4.86935	0.00130	-1.52930
H	-5.04737	0.89826	-0.01014
H	-5.04719	-0.89958	-0.01236

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C	4.02958	-0.18178	-0.09604
C	3.55965	0.77280	-0.93864
N	2.17501	0.68861	-0.88006

C	1.77842	-0.29167	-0.02506
N	2.92484	-0.81519	0.46289
Pd	-0.20164	-0.67613	0.24219
C	1.21205	1.53696	-1.57630
N	0.25901	2.07985	-0.61614
C	-0.42786	1.28384	0.24078
N	-1.22495	2.10106	0.95349
C	-1.04340	3.41606	0.53949
C	-0.11190	3.40808	-0.44816
C	-2.11943	1.69110	2.04570
C	3.01764	-1.89692	1.44635
H	-1.59178	4.23251	0.98322
H	0.29940	4.20831	-1.04372
H	4.07733	1.48389	-1.56386
H	5.04038	-0.46055	0.15919
H	-2.98396	2.35743	2.05222
H	-2.44202	0.66746	1.85622
H	-1.59441	1.76420	3.00187
H	3.82886	-1.67685	2.14315
H	2.08028	-1.95330	1.99946
H	3.21267	-2.85037	0.94833
H	0.67493	0.95038	-2.32599
H	1.74199	2.35869	-2.05771
C	-0.08997	-3.34572	-0.14051
H	-0.39002	-2.74697	-1.00931
H	0.08583	-2.76000	0.78554
O	-2.22767	-0.95880	0.43600
C	-2.75626	-1.04202	-0.77009
O	-2.09172	-0.92769	-1.80250
C	-4.24986	-1.30497	-0.77748
H	-4.77745	-0.51440	-0.23349
H	-4.46625	-2.24797	-0.26444
H	-4.61371	-1.35323	-1.80474
H	0.82777	-3.89032	-0.37085
H	-0.90838	-4.02967	0.09468

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C	3.64579	-1.62436	0.51669
C	3.80444	-0.51774	-0.24894
N	2.52398	-0.08776	-0.57616
C	1.57613	-0.90047	-0.02644
N	2.27780	-1.84037	0.64914
Pd	-0.36295	-0.49557	-0.21893
C	2.18373	1.11615	-1.32183
N	1.35001	1.99899	-0.51629
C	0.19212	1.56214	0.05534
N	-0.29542	2.65591	0.68505
C	0.53696	3.75666	0.50861
C	1.58171	3.34356	-0.25159
C	-1.51522	2.68430	1.49031
C	1.71551	-2.93490	1.44157
H	0.31482	4.72269	0.93554
H	2.44008	3.87844	-0.62840
H	4.69447	-0.01252	-0.59083
H	4.37402	-2.27197	0.97983
H	-2.07524	1.77211	1.29538
H	-1.26555	2.74799	2.55339
H	-2.12067	3.54887	1.20686
H	2.26529	-3.01182	2.38230
H	0.67111	-2.71288	1.64836
H	1.79056	-3.87817	0.89429

H	1.64867	0.83804	-2.23245
H	3.10399	1.63678	-1.58761
C	-0.72326	-2.48710	-0.76332
H	0.15868	-2.92938	-1.23365
H	-2.51250	-2.01255	0.54727
O	-2.47257	0.05925	-0.47765
C	-3.48874	-0.56160	-0.14262
O	-3.44930	-1.72450	0.48760
C	-4.87628	-0.06535	-0.41715
H	-5.35741	-0.73191	-1.14184
H	-4.84110	0.94690	-0.81917
H	-5.47471	-0.09675	0.49844
H	-1.01007	-3.16101	0.05786
H	-1.52581	-2.46958	-1.51002

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C	-1.80628	-2.59102	-1.54275
C	-2.87340	-2.03752	-0.93723
N	-2.47778	-1.64428	0.35672
C	-1.03630	-1.70943	0.43249
N	-0.71990	-2.53972	-0.67781
Pd	-0.08096	0.20150	0.13580
C	-3.19811	-0.63100	1.05970
N	-3.03524	0.70909	0.45742
C	-1.82448	1.16506	0.04725
N	-2.06635	2.44017	-0.36585
C	-3.40762	2.76722	-0.21248
C	-4.02156	1.67399	0.31001
C	-1.04627	3.33414	-0.91069
C	0.62717	-2.89937	-1.09233
H	-3.80338	3.73130	-0.49404
H	-5.05131	1.50377	0.58628
H	-3.89542	-1.93762	-1.26941
H	-1.72750	-3.06425	-2.51028
H	-0.06682	2.87156	-0.77234
H	-1.22227	3.50478	-1.97766
H	-1.07343	4.29070	-0.38044
H	1.26211	-3.04244	-0.21874
H	0.57844	-3.83661	-1.65541
H	1.08633	-2.11844	-1.70953
H	-2.85694	-0.59418	2.09688
H	-4.26584	-0.86638	1.05046
O	2.12184	1.65625	-0.20583
C	2.60424	0.53960	0.03496
O	1.96741	-0.53959	0.27101
C	4.14176	0.37310	0.05384
F	4.53485	-0.49472	-0.90700
F	4.78554	1.53157	-0.15568
F	4.55761	-0.12023	1.24071
C	-0.46047	-2.13912	1.77946
H	0.62904	-2.06925	1.77406
H	-0.82014	-1.48409	2.57761
H	-0.76194	-3.17147	2.00535

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C	1.51927	-0.06360	0.07300
N	2.82657	-0.34660	-0.15355
C	3.60030	0.80677	-0.13908
H	4.66636	0.79116	-0.30794
N	1.48672	1.29028	0.22146
C	2.75760	1.84187	0.10225

H	2.94732	2.90015	0.20091
C	-1.52091	0.36941	0.52735
N	-0.93189	1.56861	0.07828
C	-1.39710	1.84701	-1.20786
H	-0.98440	2.65034	-1.79900
N	-2.51243	0.08822	-0.41856
C	-2.38227	0.96935	-1.49560
H	-3.00853	0.88403	-2.37039
C	0.29798	2.07057	0.62482
C	3.35943	-1.68355	-0.41116
H	2.56670	-2.40866	-0.22427
H	3.69296	-1.76599	-1.44944
H	4.19868	-1.88254	0.26024
C	-3.71732	-0.71128	-0.18661
H	-3.49571	-1.54958	0.47480
H	-4.51402	-0.10224	0.25578
H	-4.06158	-1.10928	-1.14342
H	0.22916	2.07894	1.71507
H	0.44256	3.09686	0.28198
Pd	-0.16153	-1.21496	-0.01078
C	-1.80208	0.17481	2.00537
H	-2.58721	0.86838	2.33606
H	-2.13073	-0.84493	2.21818
H	-0.90349	0.34984	2.59925

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C	3.49708	3.06109	0.45300
N	3.01524	1.85691	-0.04262
C	1.72003	1.65803	0.32282
N	1.39384	2.73987	1.06129
C	2.46931	3.61714	1.14377
C	3.74103	0.87908	-0.84604
N	3.60159	-0.44346	-0.25374
C	4.62648	-1.28840	0.15418
C	4.02373	-2.35697	0.73125
N	2.65049	-2.14471	0.67750
C	2.38954	-0.97455	0.06114
Pd	0.72143	-0.00988	-0.32585
O	-1.14625	1.26794	-0.75659
S	-2.48760	1.38640	-1.30769
O	-2.52721	0.42854	-2.58113
C	1.67732	-3.09440	1.23349
C	0.09376	2.98728	1.69378
Br	-0.25620	-2.01860	-1.38136
O	-3.61131	0.68859	-0.28180
O	-3.08713	2.67286	-1.55904
O	-3.22803	-0.68318	0.02765
S	-2.86030	-0.79022	1.68032
O	-4.27366	-0.39965	2.33593
O	-1.94803	0.26764	2.04046
O	-2.58980	-2.20155	1.81592
H	2.40879	4.54643	1.68905
H	4.50219	3.40977	0.27205
H	5.66849	-1.06119	-0.00924
H	4.44207	-3.24692	1.17523
H	-0.48249	3.69823	1.09597
H	-0.45139	2.04898	1.77387
H	0.26070	3.39761	2.69199
H	1.60708	-3.96915	0.58417
H	2.01230	-3.38707	2.23134
H	0.70130	-2.61918	1.28607

H	3.34269	0.86900	-1.86343
H	4.79716	1.14763	-0.86999
H	-3.34970	0.58277	-3.09306
H	-4.87773	-1.17019	2.29818

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O	-1.31174	1.27228	-0.88168
S	-1.22541	0.17233	0.04684
O	-1.26883	0.34498	1.48616
O	0.06996	-0.80390	-0.34372
Br	1.73344	-0.00692	0.00294
O	-2.31680	-0.93258	-0.40845
H	-2.44471	-1.56123	0.32918

4

C	1.13800	1.36083	-0.01575
N	2.38370	1.19417	0.49865
C	3.15498	2.33177	0.29681
C	2.36130	3.21172	-0.36477
N	1.12847	2.59964	-0.55118
C	2.78422	0.00017	1.22976
N	2.38387	-1.19388	0.49862
C	3.15518	-2.33153	0.29719
C	2.36167	-3.21157	-0.36446
N	1.12891	-2.59949	-0.55133
C	1.13832	-1.36059	-0.01612
Pd	-0.31005	-0.00004	0.04582
O	-2.10825	1.19717	0.11890
S	-3.05375	-0.00017	0.15594
O	-4.15417	0.00028	-0.78547
C	0.01397	-3.22118	-1.28102
C	0.01330	3.22133	-1.28054
O	-2.10836	-1.19748	0.11835
O	-3.66087	-0.00075	1.65630
H	2.56197	-4.21048	-0.72027
H	4.17347	-2.41510	0.64443
H	4.17337	2.41539	0.64377
H	2.56154	4.21054	-0.72083
H	-0.91054	-2.69947	-1.03950
H	0.20476	-3.17047	-2.35625
H	-0.06842	-4.26461	-0.97059
H	-0.06833	4.26502	-0.97077
H	0.20331	3.16980	-2.35587
H	-0.91128	2.70020	-1.03806
H	2.32227	0.00005	2.22124
H	3.86916	0.00027	1.33758
H	-4.63593	0.00075	1.58804

5

O	1.49480	-0.89396	1.48535
S	1.91009	-0.94346	0.09764
O	1.77881	0.61713	-0.60028
O	3.26979	-1.28591	-0.27803
O	0.90381	-1.77374	-0.78157
O	0.39447	0.87040	-0.92533
S	-0.28558	2.06679	0.09130
O	-0.09647	3.36371	-0.53524
O	0.15804	1.83423	1.45154
O	-1.76253	1.59442	-0.19004
Br	-2.09009	-1.47075	0.01349
H	-0.08230	-1.67433	-0.46522

H	-1.88258	0.56720	-0.04120
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6

C	4.61071	-0.40108	-0.20314
C	4.17869	0.62811	-0.97577
N	2.79322	0.61673	-0.89207
C	2.36089	-0.39178	-0.08969
N	3.48381	-1.00720	0.34056
Pd	0.37645	-0.69321	0.20389
C	1.86791	1.55965	-1.51583
N	0.95776	2.08470	-0.50728
C	0.24873	1.27386	0.31485
N	-0.50690	2.08045	1.08250
C	-0.28305	3.40681	0.72863
C	0.63566	3.41488	-0.27007
C	-1.41359	1.67281	2.16746
C	3.53585	-2.15381	1.25195
H	-0.79647	4.21872	1.22011
H	1.07040	4.22849	-0.82978
H	4.72347	1.34760	-1.56753
H	5.60912	-0.74938	0.01257
H	-2.35189	2.22048	2.06244
H	-1.61618	0.60828	2.07412
H	-0.95311	1.90142	3.13184
H	4.37082	-2.02222	1.94285
H	2.60813	-2.19626	1.82216
H	3.66992	-3.08162	0.68952
H	1.29223	1.05634	-2.29662
H	2.43596	2.38299	-1.94848
C	0.25716	-3.32485	-0.23918
H	0.27824	-2.65457	-1.11080
H	0.44599	-2.82857	0.73297
O	-1.65325	-0.89503	0.42621
C	-2.31961	-0.43507	-0.59418
O	-1.86825	0.04956	-1.62063
C	-3.84749	-0.48364	-0.34656
F	-4.15485	0.44391	0.59507
F	-4.23719	-1.68336	0.10888
F	-4.53155	-0.19911	-1.45369
H	1.03222	-4.08273	-0.37143
H	-0.73756	-3.76861	-0.17649

7

C	4.62165	-0.48266	-0.00566
C	4.24401	0.58924	-0.74395
N	2.85640	0.54391	-0.81039
C	2.35522	-0.52909	-0.12154
N	3.45945	-1.14966	0.37001
Pd	0.39224	-0.77853	0.10598
C	1.98651	1.52742	-1.44043
N	1.08376	2.12645	-0.46741
C	0.26787	1.34516	0.29584
N	-0.48607	2.23261	0.98491
C	-0.16031	3.54318	0.64909
C	0.83386	3.48058	-0.27264
C	-1.52214	1.85721	1.94706
C	3.44371	-2.32344	1.23767
H	-0.65881	4.39269	1.09027
H	1.36338	4.25939	-0.79994
H	4.82660	1.35555	-1.23171
H	5.60149	-0.82936	0.28423

H	-1.67495	0.78067	1.87703
H	-1.21394	2.13643	2.95960
H	-2.45820	2.36096	1.69350
H	2.40544	-2.58067	1.43779
H	3.94281	-3.16404	0.74651
H	3.95573	-2.09313	2.17691
H	1.39514	1.03570	-2.21621
H	2.60478	2.30893	-1.88521
O	-1.70137	-1.00465	0.36461
C	-2.40762	-0.49252	-0.57597
O	-2.05560	0.05587	-1.61714
C	-3.92455	-0.53594	-0.24592
F	-4.68830	-0.29202	-1.32222
F	-4.31333	-1.71560	0.27412
F	-4.21363	0.42477	0.67849
C	0.46070	-2.81912	-0.26136
H	-0.33941	-2.99964	-0.98634
H	1.40219	-3.21047	-0.66084
H	0.20963	-3.33793	0.67297

8

C	-4.00254	-0.68653	-1.68222
C	-3.89646	-1.82298	-0.95257
N	-2.54996	-1.95647	-0.63789
C	-1.83488	-0.91277	-1.13573
N	-2.72752	-0.14382	-1.79171
Pd	0.12708	-0.70140	-0.73979
C	-1.96070	-2.96420	0.23805
N	-1.38179	-2.34401	1.41261
C	-0.45125	-1.34881	1.31408
N	-0.27226	-0.93807	2.58659
C	-1.08139	-1.64936	3.46411
C	-1.79450	-2.53506	2.72757
C	0.51230	0.22733	3.00390
C	-2.47541	1.16517	-2.39911
H	-1.07485	-1.45923	4.52622
H	-2.51834	-3.28288	3.01299
H	-4.63773	-2.54405	-0.64562
H	-4.86114	-0.21136	-2.13016
H	1.03105	-0.01089	3.93631
H	1.24045	0.47295	2.22831
H	-0.16638	1.07093	3.15838
H	-2.92193	1.18962	-3.39627
H	-2.91127	1.94361	-1.76820
H	-1.40356	1.32709	-2.46215
H	-1.18985	-3.50643	-0.31371
H	-2.74448	-3.65749	0.54462
O	2.21743	-0.80054	-0.58292
O	-0.04581	1.43814	-0.34722
C	0.60192	-0.30482	-2.73658
H	1.51609	-0.86534	-2.92378
H	0.28291	-2.16161	-1.20045
H	-0.19388	-0.58579	-3.42786
H	0.79349	0.76950	-2.73378
C	2.99677	-0.03466	0.09537
O	2.76563	0.77875	0.97757
C	4.47258	-0.26548	-0.34327
F	4.63220	0.00494	-1.65720
F	5.32346	0.51189	0.34124
F	4.83956	-1.55125	-0.14407
C	-0.99945	1.85609	0.38735

C	-1.03534	3.39838	0.56334
O	-1.91566	1.23194	0.93189
F	-1.18047	3.72683	1.86230
F	-2.11363	3.89284	-0.10467
F	0.04910	4.02945	0.09548

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N	-2.71522	0.09730	0.53874
C	-1.61670	-0.09069	-0.25877
N	-1.22564	1.21298	-0.53469
C	-2.03761	2.14878	0.09568
C	-2.98317	1.44632	0.76592
C	0.00015	1.50613	-1.27002
N	1.22557	1.21284	-0.53413
C	2.03800	2.14857	0.09566
C	2.98369	1.44606	0.76570
N	2.71527	0.09706	0.53897
C	1.61654	-0.09083	-0.25818
H	-3.81297	1.78340	1.36918
H	-1.88876	3.21427	0.00005
H	1.88906	3.21408	0.00025
H	3.81371	1.78310	1.36866
H	0.00028	0.89703	-2.17354
H	0.00027	2.56744	-1.53243
Pd	-0.00028	-1.37602	-0.41332
C	3.50472	-0.99420	1.08340
H	4.55842	-0.88345	0.80250
H	3.42601	-1.02523	2.17575
H	3.10773	-1.92220	0.66920
C	-3.50409	-0.99390	1.08407
H	-3.42286	-1.02598	2.17620
H	-4.55836	-0.88217	0.80572
H	-3.10869	-1.92182	0.66815

br2

Br	0.00000	0.00000	1.16726
Br	0.00000	0.00000	-1.16726

Br_HOTFA3_minus

C	-3.17637	-2.20216	-0.33550
O	-3.15263	-2.67323	-1.44772
C	-4.26165	-2.61081	0.68986
F	-4.93548	-1.53634	1.14606
F	-5.14858	-3.45108	0.13659
F	-3.70903	-3.23166	1.75324
O	-2.36142	-1.32518	0.21658
H	-1.63598	-1.03069	-0.42321
Br	0.04453	-0.16502	-1.52981
H	1.74807	-1.01077	-0.45269
O	2.42429	-1.44446	0.16265
C	3.64886	-1.36080	-0.31863
O	4.03191	-0.86434	-1.35123
C	4.63569	-2.03066	0.66821
F	4.35487	-3.34206	0.81828
F	5.89739	-1.92699	0.22562
F	4.57344	-1.45541	1.88596
O	0.27209	2.64744	-0.04344
C	-0.68014	3.54058	-0.22762
O	-1.68354	3.46045	-0.89560
C	-0.34094	4.82559	0.56616
F	-0.14141	4.55972	1.87238

F	0.78191	5.40185	0.08771
F	-1.33537	5.72045	0.47319
H	0.09113	1.79489	-0.55685

H2SO4

S	0.17797	-0.03761	0.00000
O	0.89155	-0.07437	1.25990
O	0.89155	-0.07444	-1.25989
O	-0.98300	-1.16940	0.00003
H	-1.85387	-0.72923	0.00002
O	-0.87850	1.22724	-0.00004
H	-0.36646	2.05871	-0.00004

HBr

H	0.00000	0.00000	-1.39433
Br	0.00000	0.00000	0.03984

HOAc_Tetramer

C	3.51992	-0.32523	-0.76560
O	3.32055	-1.40759	-0.03749
O	2.89483	0.72628	-0.66141
C	4.62669	-0.50721	-1.77832
H	2.55684	-1.29034	0.60766
O	1.36240	-1.21668	1.76643
C	0.20691	-1.36418	1.38108
O	-0.04208	-1.75058	0.13905
C	-0.97621	-1.12833	2.29467
H	5.54142	-0.83965	-1.27732
H	4.80552	0.42920	-2.30750
H	-0.62153	-0.95308	3.31072
H	-1.53518	-0.25427	1.94559
H	-1.65813	-1.98425	2.27398
H	4.34484	-1.28909	-2.49186
H	1.70927	1.60336	0.15072
O	1.17532	2.38142	0.49145
C	-0.11185	2.21375	0.27637
O	-0.58459	1.18203	-0.20353
C	-0.93691	3.41390	0.67419
H	-0.69800	3.70853	1.70064
H	-2.00143	3.19276	0.58354
H	-0.68319	4.26015	0.02652
H	-2.15257	0.81003	-0.63994
O	-3.10556	0.65455	-0.91187
C	-3.43218	-0.62847	-0.85071
O	-2.67889	-1.52603	-0.48446
C	-4.85242	-0.88568	-1.29082
H	-5.10760	-1.93334	-1.13013
H	-4.95410	-0.64034	-2.35375
H	-5.54137	-0.23713	-0.74078
H	-1.00434	-1.66118	-0.08859

HOAc

C	-1.39759	-0.10988	0.00001
C	0.09248	0.12562	-0.00002
O	0.77873	-1.04661	-0.00001
H	1.72376	-0.80283	0.00009
O	0.64566	1.20201	-0.00000
H	-1.68532	-0.69193	-0.88185
H	-1.91757	0.84830	-0.00037
H	-1.68535	-0.69117	0.88228

HOTFA_Tetramer

C	3.88833	-0.52611	-0.15853
O	3.65058	-0.99068	1.04005
O	3.27965	0.33411	-0.77175
C	5.11168	-1.22733	-0.79246
H	2.83790	-0.56844	1.45437
O	1.48162	0.07429	2.20777
C	0.38848	-0.36758	1.89683
O	0.22249	-1.37560	1.08166
C	-0.89304	0.28190	2.47992
F	6.18800	-1.08291	-0.00319
F	5.38097	-0.70440	-1.98955
F	-0.59664	1.12911	3.45742
F	-1.53951	0.95907	1.50058
F	-1.72273	-0.66404	2.94524
F	4.86006	-2.53860	-0.93764
H	2.04425	1.44875	-0.62762
O	1.40346	2.22156	-0.61325
C	0.18367	1.83522	-0.86815
O	-0.18341	0.69108	-1.09117
C	-0.79988	3.02692	-0.84391
F	-0.75329	3.64074	0.34594
F	-2.04853	2.59218	-1.05680
F	-0.48027	3.90969	-1.79996
H	-1.76642	0.10034	-1.26579
O	-2.67112	-0.29145	-1.44001
C	-2.94089	-1.30854	-0.66449
O	-2.24072	-1.81218	0.19913
C	-4.35513	-1.86298	-0.95057
F	-4.57114	-2.97486	-0.24730
F	-4.49031	-2.13935	-2.25604
F	-5.27441	-0.94540	-0.60812
H	-0.72546	-1.52966	0.79252

HOTFA

C	0.60092	-0.00077	-0.00002
C	-0.93417	0.15989	-0.00002
O	-1.52074	-1.04594	0.00001
H	-2.48575	-0.89500	0.00006
O	-1.49785	1.22234	0.00001
F	0.99668	-0.67968	1.09022
F	1.18823	1.19614	-0.00012
F	0.99664	-0.67989	-1.09010

HSO4_HOTFA3

C	-6.61456	0.48184	0.48763
F	-6.36848	0.65937	1.80062
C	-5.47259	-0.29979	-0.20563
O	-5.69817	-1.29675	-0.85145
O	-4.32429	0.30224	0.02184
F	-6.76593	1.70189	-0.07083
F	-7.78031	-0.17136	0.37005
O	-2.26489	-0.84792	-1.15998
S	-0.87297	-0.78921	-0.66888
O	0.12787	-1.13590	-1.72649
O	-0.79893	-1.97906	0.43021
O	-0.53173	0.47315	0.04694
O	2.61642	-1.44765	-1.13508
C	2.77416	-1.91708	0.07269
C	4.26836	-2.06144	0.43230
F	4.44006	-2.10920	1.75759

O	1.92277	-2.28741	0.86363
F	5.01419	-1.06564	-0.06315
F	4.73236	-3.22392	-0.08920
O	1.45588	2.09812	-0.42319
C	2.57214	1.81976	0.21139
C	3.60888	2.94168	-0.03273
F	4.78309	2.64113	0.53733
O	2.83389	0.86633	0.91086
F	3.81975	3.13590	-1.34913
F	3.17827	4.10928	0.49148
H	0.15631	-2.10468	0.67003
H	1.62006	-1.33740	-1.36285
H	-3.55323	-0.17589	-0.42655
H	0.73851	1.39749	-0.25332

MeBr

C	0.00000	0.00000	-1.53981
H	0.00000	1.03650	-1.87328
H	0.89763	-0.51825	-1.87328
H	-0.89763	-0.51825	-1.87328
Br	0.00000	0.00000	0.42453

MeOTFA

C	0.99499	-0.09005	-0.00007
C	-0.46852	0.40410	0.00000
O	-0.77914	1.56819	-0.00001
O	-1.29381	-0.64384	0.00010
C	-2.70019	-0.32215	0.00021
H	-3.21510	-1.28195	0.00022
H	-2.95403	0.25585	0.89202
H	-2.95416	0.25590	-0.89154
F	1.23649	-0.84008	-1.08993
F	1.83225	0.94900	-0.00039
F	1.23672	-0.83960	1.09007

methane

C	0.00000	0.00000	0.00000
H	0.36452	-1.03107	-0.00000
H	0.36454	0.51553	0.89293
H	0.36454	0.51553	-0.89293
H	-1.09361	0.00001	0.00000

OAc_minus_pentamer

C	-2.08865	4.07573	1.37163
H	-1.13218	4.59659	1.24331
C	-1.84608	2.57459	1.32907
O	-1.58144	2.16773	0.08935
H	-2.52076	4.35428	2.33492
H	-2.74612	4.38753	0.55385
O	-1.88145	1.86491	2.31650
O	-1.03938	-0.42144	-0.20765
C	0.09971	-0.97803	-0.20786
C	0.17729	-2.47973	-0.43239
H	-0.78063	-2.96136	-0.22508
O	1.19014	-0.34493	-0.05804
H	0.43595	-2.65663	-1.48539
H	0.97696	-2.90944	0.17738
O	1.51298	2.29170	-0.00000
C	1.59625	2.87339	-1.19456
C	1.68609	4.38574	-1.06176
H	2.38979	4.66778	-0.27216

O	1.58773	2.29705	-2.26619
H	0.70035	4.77581	-0.78143
H	1.98664	4.82520	-2.01508
O	3.69148	-1.12914	-0.01676
C	4.02763	-2.26897	0.57305
C	5.53731	-2.45051	0.60226
H	5.78746	-3.40270	1.07340
O	3.25153	-3.08702	1.03870
H	5.93806	-2.42107	-0.41697
H	6.00212	-1.62736	1.15616
O	-3.50832	-1.21716	-0.60917
C	-3.88766	-2.47322	-0.41306
C	-5.38577	-2.63459	-0.61669
H	-5.66555	-3.68290	-0.49847
O	-3.15509	-3.39972	-0.10792
H	-5.92736	-2.02165	0.11242
H	-5.67099	-2.27998	-1.61310
H	-1.33133	1.18902	0.07211
H	1.34637	1.29910	-0.09379
H	2.68664	-0.97352	-0.01170
H	-2.51745	-1.08110	-0.43904

OAc_minus

C	-1.35442	-0.05536	-0.00004
C	0.22052	0.00188	-0.00019
O	0.69581	1.16637	0.00011
O	0.80894	-1.10858	0.00006
H	-1.75046	0.47206	0.88052
H	-1.73359	-1.08571	-0.00008
H	-1.75062	0.47220	-0.88045

OTFA_minus_pentamer

C	0.85245	4.48227	-0.54322
F	0.07523	4.66656	0.54022
C	1.00602	2.98784	-0.90885
O	1.09319	2.26090	0.19055
F	0.32375	5.16900	-1.56337
F	2.06680	5.01170	-0.26995
O	1.07040	2.62406	-2.05866
O	1.28890	-0.38073	-0.11441
C	0.29579	-1.11918	0.10014
C	0.58405	-2.64536	0.11020
F	1.77770	-2.91153	0.67551
O	-0.89662	-0.77059	0.27489
F	-0.35123	-3.32635	0.79707
F	0.60942	-3.11583	-1.14887
O	-1.92031	1.67128	-0.15827
C	-2.25160	2.37794	0.90909
C	-2.94805	3.69065	0.48261
F	-4.26025	3.44961	0.25694
O	-2.11366	2.08846	2.07292
F	-2.42978	4.21017	-0.64336
F	-2.86000	4.61022	1.45227
O	-3.11652	-2.23728	0.54776
C	-3.30912	-3.08504	-0.44579
C	-4.65991	-3.81290	-0.25822
F	-4.86017	-4.70478	-1.23752
O	-2.58933	-3.31086	-1.38975
F	-4.69469	-4.46911	0.91898
F	-5.68492	-2.93726	-0.27296
O	3.83496	-1.07465	-0.55551

C	4.56564	-1.26834	0.52701
C	6.00993	-1.64107	0.11942
F	6.79870	-1.73876	1.19821
O	4.23212	-1.19232	1.68541
F	6.03170	-2.82728	-0.52257
F	6.54046	-0.71657	-0.70481
H	1.16074	1.27960	-0.02464
H	-1.49017	0.80185	0.10287
H	-2.23368	-1.76908	0.43661
H	2.88242	-0.86741	-0.31084

7

OTFA_minus

C	-0.51308	0.01320	0.00001
C	1.06601	0.00988	-0.00002
O	1.53208	-1.14809	-0.00001
O	1.59066	1.14056	-0.00001
F	-1.03195	-0.63120	-1.08803
F	-1.08046	1.25004	-0.00213
F	-1.03199	-0.62753	1.09018

ts11_12

C	2.46773	3.50195	0.66127
N	1.45181	2.81946	0.00318
C	1.29160	1.57708	0.52329
N	2.19251	1.47926	1.52078
C	2.93438	2.65097	1.61039
C	0.59275	3.32903	-1.05303
N	-0.81029	3.12450	-0.70335
C	-1.30645	1.93390	-0.26403
N	-2.61478	2.15854	-0.02122
C	-2.94005	3.47485	-0.31627
C	-1.80725	4.08950	-0.74281
Pd	-0.14261	0.28405	-0.06464
O	-1.65869	-1.04510	-0.60504
C	-2.01184	-1.61510	0.50314
C	-3.07596	-2.71877	0.30799
F	-4.24637	-2.12362	-0.03349
C	-3.58566	1.18251	0.50297
C	2.36872	0.33342	2.43020
O	1.15851	-1.35176	0.19111
C	2.06174	-1.40421	-0.69270
C	3.21651	-2.40207	-0.39459
F	3.84067	-2.76847	-1.51146
O	2.15099	-0.71669	-1.72819
F	4.10855	-1.77326	0.40964
F	2.76679	-3.48569	0.23731
O	-1.63102	-1.29315	1.62639
F	-3.26820	-3.41464	1.42625
F	-2.73237	-3.55922	-0.67832
C	0.15665	-0.08774	-2.59021
H	-3.94139	3.85604	-0.18877
H	-1.62707	5.10374	-1.06429
H	2.76471	4.50546	0.39811
H	3.71768	2.77480	2.34231
H	-3.85509	0.46632	-0.27334
H	-3.14643	0.65746	1.35078
H	-4.47032	1.73004	0.82894
H	2.58985	0.71949	3.42662
H	1.44955	-0.24948	2.45763
H	3.18719	-0.29702	2.08042
H	0.82161	2.82152	-1.99354

H	0.77155	4.39743	-1.17356
H	-0.06314	-1.14639	-2.56378
H	0.95720	0.25133	-3.23041
H	-0.68790	0.57656	-2.45682

ts13_14

C	1.97245	0.83432	-0.59296
N	1.88908	2.08124	-1.13344
C	3.13466	2.51919	-1.55677
C	4.00380	1.51972	-1.26443
N	3.27767	0.49851	-0.66523
C	0.64014	2.83369	-1.23721
N	-0.01987	2.85825	0.06094
C	-0.52952	3.95038	0.75100
C	-1.11154	3.44598	1.87061
N	-0.94851	2.06512	1.84042
C	-0.28148	1.71375	0.72823
Pd	0.23604	-0.08852	-0.02439
Br	0.79494	-2.39847	-0.87858
C	-1.42164	1.14260	2.88434
C	3.89992	-0.75998	-0.23077
Br	1.03720	-1.90312	1.81152
O	-1.75909	-0.71730	0.26081
C	-2.32016	-0.22333	-0.78470
O	-1.72902	0.45237	-1.64094
C	-3.84093	-0.47313	-0.89106
F	-4.46433	0.32286	0.00393
F	-4.28993	-0.17850	-2.11085
F	-4.13640	-1.74586	-0.60723
H	-1.62432	3.94068	2.68097
H	-0.44629	4.96289	0.38735
H	3.28769	3.48150	-2.02042
H	5.06853	1.44277	-1.42162
H	-1.80088	0.23876	2.40872
H	-0.60257	0.89902	3.56507
H	-2.22484	1.63272	3.43579
H	3.86683	-1.49116	-1.04098
H	4.93614	-0.55139	0.03936
H	3.36990	-1.14646	0.63680
H	-0.02312	2.35700	-1.96373
H	0.86793	3.85325	-1.54657

ts14_16

C	-0.07384	1.83661	-0.01179
N	-0.90996	2.67080	-0.67676
C	-0.62492	3.99717	-0.37852
C	0.41167	3.96606	0.49506
N	0.73265	2.63315	0.71780
C	-1.93013	2.21181	-1.60401
N	-2.74254	1.15691	-1.01238
C	-4.13069	1.14386	-1.01698
C	-4.49674	-0.00487	-0.39959
N	-3.33898	-0.67157	-0.02322
C	-2.25816	0.03716	-0.40865
Pd	-0.25127	-0.24119	-0.16982
Br	-0.36361	-2.73360	-0.42399
C	-3.39835	-1.95886	0.69502
C	1.80561	2.22767	1.64219
O	1.80984	-0.50630	0.27713
C	2.64204	-0.23432	-0.63046
C	4.14069	-0.33713	-0.24541

F	4.56493	0.90966	0.06837
Br	-0.66921	-0.32649	2.30250
C	-0.02752	-0.35949	-2.62811
H	0.13755	0.46571	-3.33336
O	2.37866	0.16916	-1.78936
F	4.31955	-1.12640	0.80975
F	4.85849	-0.78846	-1.27058
H	-5.47394	-0.40954	-0.18705
H	-4.71729	1.93728	-1.45360
H	-1.17082	4.82268	-0.80868
H	0.94543	4.76661	0.98359
H	-3.33814	-2.78042	-0.01871
H	-2.57229	-2.01952	1.39815
H	-4.34726	-1.98673	1.23269
H	2.76374	2.21562	1.11975
H	1.83837	2.95285	2.45663
H	1.58083	1.24177	2.04029
H	-1.46406	1.85074	-2.52236
H	-2.58387	3.04992	-1.84416
H	-1.09557	-0.53278	-2.53482
H	1.05141	-0.01286	-1.95058
H	0.41236	-1.29850	-2.97468

ts18_28

C	-1.57785	-0.15609	-0.02397
N	-2.78995	-0.15368	0.57342
C	-3.42719	1.07379	0.42167
H	-4.40714	1.27127	0.82891
N	-1.45910	1.10176	-0.55188
C	-2.58719	1.86938	-0.28813
H	-2.69893	2.88804	-0.62745
C	1.42529	0.21502	-0.12321
N	0.95356	1.42259	-0.60038
C	1.53507	2.47816	0.10814
H	1.30358	3.51022	-0.10588
N	2.30940	0.54395	0.85961
C	2.38597	1.92891	1.00176
H	3.05112	2.38766	1.71714
C	-0.29361	1.51764	-1.34669
C	-3.36610	-1.29160	1.28892
H	-2.65120	-2.11358	1.25465
H	-3.55975	-1.02002	2.33006
H	-4.30034	-1.59916	0.81167
C	3.06836	-0.39492	1.68488
H	2.64319	-1.39200	1.57578
H	4.12187	-0.40370	1.38872
H	2.98931	-0.09436	2.73227
H	-0.22626	0.88555	-2.23320
H	-0.43637	2.55396	-1.65463
Pd	0.16791	-1.27846	-0.30833
C	2.18683	-1.26625	-1.27387
H	3.14371	-1.36760	-0.76714
H	1.82670	-2.27387	-1.54971
H	2.28175	-0.66972	-2.18016

ts19_20

C	-0.65536	1.62366	0.08594
N	-1.92315	1.95515	-0.29587
C	-2.27958	3.22311	0.14702
C	-1.20333	3.69353	0.82523
N	-0.22979	2.70215	0.78232

C	-2.76223	1.05862	-1.08165
N	-2.86703	-0.24589	-0.44006
C	-4.02300	-0.84340	0.04811
C	-3.62790	-1.99188	0.65251
N	-2.24437	-2.06582	0.53078
C	-1.77234	-0.99673	-0.14578
Pd	0.10114	-0.34784	-0.54165
Br	2.48354	0.39738	-0.99819
C	-1.43490	-3.14757	1.09985
C	1.08956	2.84957	1.40329
Br	2.10216	-0.93857	1.26757
H	-4.19965	-2.75736	1.15417
H	-5.00364	-0.41354	-0.08626
H	-3.24125	3.66888	-0.05625
H	-1.04712	4.63147	1.33576
H	-0.39379	-2.82888	1.13080
H	-1.78174	-3.35335	2.11485
H	-1.52794	-4.05065	0.49106
H	1.76588	3.38630	0.73301
H	0.98061	3.40694	2.33591
H	1.49452	1.86274	1.61903
H	-2.33610	0.93474	-2.07994
H	-3.75987	1.48893	-1.16898
H	1.39549	-2.61058	-1.08688
C	0.50331	-2.16361	-1.52522
H	0.68891	-1.82386	-2.54790
H	-0.34132	-2.85023	-1.49696

ts20_23

C	1.70522	-0.57591	-0.05862
N	2.55608	0.18024	0.68937
C	3.87361	-0.21539	0.49569
C	3.82710	-1.23649	-0.39564
N	2.49435	-1.43607	-0.73433
C	2.10078	1.31234	1.48296
N	1.30897	2.21572	0.65710
C	0.26325	1.77843	-0.09718
N	-0.14373	2.85918	-0.79584
C	0.62943	3.96792	-0.47049
C	1.55158	3.56625	0.43958
Pd	-0.30949	-0.20358	-0.02968
C	-1.38662	-0.19073	2.14373
C	-1.22527	2.90981	-1.78886
C	2.07255	-2.45123	-1.71095
H	4.61740	-1.83441	-0.82268
H	4.70499	0.24964	1.00269
H	2.33645	4.10918	0.94339
H	0.45767	4.93410	-0.91957
H	2.00066	-3.42584	-1.22569
H	1.09664	-2.18486	-2.10877
H	2.81212	-2.47812	-2.51391
H	-0.90220	3.54087	-2.61927
H	-1.42952	1.90397	-2.14835
H	-2.13007	3.32075	-1.33627
H	1.50104	0.95916	2.32497
H	2.96798	1.84959	1.86647
H	-0.38408	-0.52411	2.39334
H	-2.14465	-0.95348	2.26056
H	-1.64919	0.81753	2.43595
Br	-0.78728	-2.64941	0.08782
Br	-2.74409	0.33962	-0.00561

ts21_22

C	-4.40559	1.39978	-0.17962
N	-3.41002	0.47188	-0.45859
C	-2.17816	1.05102	-0.39368
N	-2.40652	2.34128	-0.06476
C	-3.77050	2.57445	0.06076
C	-3.59822	-0.95093	-0.71511
N	-2.82360	-1.73919	0.23573
C	-1.50524	-1.49769	0.45072
N	-1.13118	-2.38084	1.39785
C	-2.20602	-3.17994	1.76899
C	-3.27937	-2.77558	1.04089
Pd	-0.51432	0.00664	-0.64773
O	1.23184	1.09295	1.67195
S	2.30537	1.85127	1.05073
O	2.84995	1.17866	-0.25943
O	3.18839	-0.67506	0.25898
S	2.58346	-1.61519	-0.80541
O	2.78637	-2.97688	-0.32183
C	0.21612	-2.48377	1.97385
C	-1.38341	3.37295	0.14064
C	0.09756	1.32348	-2.20697
O	1.22378	-1.21987	-1.21410
O	3.42148	-1.38033	-2.16077
O	2.07724	3.23736	0.62980
O	3.52510	1.79304	2.10192
H	-2.11512	-3.95064	2.51899
H	-4.29992	-3.12609	1.02588
H	-5.45490	1.14824	-0.18450
H	-4.16175	3.54823	0.31166
H	0.82109	-3.18971	1.40048
H	0.68142	-1.49755	1.96298
H	0.12804	-2.82595	3.00651
H	-1.24040	3.95172	-0.77534
H	-1.71249	4.03465	0.94387
H	-0.44719	2.90174	0.42977
H	-3.27630	-1.18348	-1.73284
H	-4.65524	-1.19294	-0.60434
H	0.39300	0.63954	-3.00260
H	-0.66495	2.03073	-2.52596
H	0.95236	1.78921	-1.70238
H	4.29632	-1.81125	-2.07685
H	4.23659	2.39756	1.80861

ts2_3

C	3.53919	2.89486	0.51787
N	2.99656	1.75604	-0.06321
C	1.70829	1.58460	0.32680
N	1.43938	2.60384	1.16459
C	2.55265	3.42763	1.28443
C	3.65624	0.80143	-0.94686
N	3.44798	-0.54926	-0.43831
C	4.42832	-1.48098	-0.12266
C	3.77824	-2.53854	0.42442
N	2.42268	-2.23203	0.44636
C	2.21655	-1.01592	-0.09781
Pd	0.58707	0.06927	-0.38473
O	-0.99338	1.59763	-0.74981
S	-2.44923	1.81981	-0.83492
O	-2.80698	1.31771	-2.32299

C	1.40323	-3.13093	1.00859
C	0.16682	2.83820	1.86353
Br	-0.68651	-1.86475	-1.44205
O	-3.26577	0.88383	0.12815
O	-2.93872	3.16618	-0.60800
O	-2.45656	-0.71273	-0.11125
S	-2.34118	-1.23694	1.48104
O	-3.83155	-0.97662	2.02500
O	-1.47107	-0.32269	2.19422
O	-2.08494	-2.66418	1.43315
H	2.54446	4.30902	1.90701
H	4.55174	3.22021	0.33543
H	5.47611	-1.31413	-0.31889
H	4.15374	-3.47631	0.80354
H	-0.46168	3.51241	1.27791
H	-0.34464	1.88700	2.00702
H	0.38650	3.28297	2.83567
H	1.02516	-3.80078	0.23497
H	1.86591	-3.70452	1.81348
H	0.57898	-2.54388	1.40714
H	3.24441	0.88492	-1.95546
H	4.72536	1.01174	-0.96997
H	-3.72790	1.57100	-2.53798
H	-4.40051	-1.73082	1.76801

ts25_26_prot

C	3.48042	-1.79044	0.65302
C	3.76643	-0.69315	-0.09114
N	2.54175	-0.15772	-0.47170
C	1.51069	-0.89492	0.02072
N	2.09484	-1.89508	0.71744
Pd	-0.41409	-0.38598	-0.26426
C	2.31773	1.06252	-1.23406
N	1.42695	1.94978	-0.49731
C	0.23051	1.53328	0.00178
N	-0.29393	2.62349	0.60209
C	0.56027	3.71194	0.47558
C	1.64816	3.29182	-0.21753
C	-1.55444	2.66824	1.35138
C	1.39816	-2.93581	1.47903
H	0.31784	4.67935	0.88755
H	2.53152	3.81964	-0.54240
H	4.71031	-0.26122	-0.38615
H	4.13077	-2.49855	1.14310
H	-2.21587	1.90128	0.95496
H	-1.36235	2.50023	2.41477
H	-2.00852	3.65141	1.21340
H	1.74914	-2.92297	2.51370
H	0.32961	-2.73011	1.45546
H	1.59407	-3.91565	1.03631
H	1.87614	0.81651	-2.20281
H	3.27241	1.56544	-1.38873
C	-0.90697	-2.52408	-1.03108
H	0.14821	-2.62332	-1.28988
H	-1.79171	-1.97637	-0.12507
O	-2.41776	0.25621	-0.48743
C	-3.28770	-0.57778	-0.06188
O	-2.98450	-1.74318	0.33808
C	-4.73718	-0.16235	-0.03903
H	-5.31294	-0.84283	-0.67466
H	-4.86113	0.86285	-0.38944

H	-5.12908	-0.26403	0.97811
H	-1.18179	-3.48896	-0.58326
H	-1.47412	-2.40104	-1.95883

ts5_3

Br	-1.74867	-1.67778	0.00703
O	2.30173	-0.04085	1.50964
S	2.45473	-0.15296	0.06316
O	3.78604	-0.05001	-0.53135
O	1.90848	-1.62701	-0.39225
O	1.53178	0.84281	-0.71908
O	-0.21143	0.14081	-0.32211
S	-1.06158	1.53275	0.08431
O	-1.35270	1.50198	1.50820
O	-2.42564	1.28301	-0.76559
O	-0.45734	2.69782	-0.52633
H	0.97136	-1.69653	-0.11092
H	-2.70549	0.35354	-0.58387

ts6_7prot

C	4.09496	-1.75964	0.68024
C	4.37527	-0.65716	-0.05831
N	3.14886	-0.13587	-0.45212
C	2.12290	-0.88874	0.02685
N	2.71036	-1.88290	0.72854
Pd	0.20436	-0.40621	-0.28535
C	2.92263	1.08502	-1.21408
N	2.01272	1.96084	-0.48700
C	0.81756	1.52788	-0.00132
N	0.26837	2.61053	0.59124
C	1.10833	3.71071	0.47179
C	2.21085	3.30637	-0.20796
C	-0.99973	2.64269	1.33274
C	2.02112	-2.93571	1.48082
H	0.84724	4.67516	0.87914
H	3.08977	3.84713	-0.52338
H	5.31690	-0.21235	-0.34116
H	4.74860	-2.46023	1.17673
H	-1.72998	2.01293	0.83036
H	-0.84030	2.29614	2.35746
H	-1.36058	3.67213	1.35133
H	2.36753	-2.92453	2.51694
H	0.95075	-2.74125	1.45364
H	2.23010	-3.91062	1.03333
H	2.49819	0.83774	-2.19016
H	3.87460	1.59739	-1.35322
C	-0.25659	-2.53039	-1.04036
H	0.79692	-2.64385	-1.30100
H	-1.22955	-2.01346	-0.13194
O	-1.82270	0.22003	-0.51924
C	-2.65634	-0.61813	-0.08715
O	-2.39229	-1.79817	0.27925
C	-4.11993	-0.13483	0.00412
F	-4.56640	0.17363	-1.21924
F	-4.15723	0.97545	0.76943
F	-4.91172	-1.05610	0.54421
H	-0.52990	-3.48946	-0.57764
H	-0.82129	-2.42564	-1.97262

ts6_7

C	-4.43508	1.70320	-0.51906
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C	-4.69239	0.39698	-0.26106
N	-3.46137	-0.24487	-0.27012
C	-2.44562	0.63483	-0.52341
N	-3.05882	1.83262	-0.66684
Pd	-0.54565	-0.03758	-0.57184
C	-3.21539	-1.65465	0.01863
N	-2.25614	-1.77876	1.10468
C	-1.05583	-1.15254	1.02548
N	-0.40177	-1.48612	2.15602
C	-1.18059	-2.34070	2.92925
C	-2.35461	-2.52592	2.27197
C	0.95506	-1.04565	2.50652
C	-2.39611	3.11459	-0.93222
H	-0.83404	-2.73112	3.87337
H	-3.22623	-3.10978	2.52362
H	-5.62065	-0.12316	-0.08233
H	-5.09901	2.54927	-0.60474
H	1.13497	-0.06079	2.07747
H	1.02944	-0.99172	3.59483
H	1.69070	-1.74746	2.11052
H	-1.35105	3.05714	-0.62688
H	-2.45823	3.35223	-1.99795
H	-2.90454	3.89168	-0.35626
H	-2.80693	-2.14609	-0.86781
H	-4.15533	-2.12573	0.30867
O	1.32652	-0.97001	-0.61027
C	1.25603	-2.22039	-0.90165
O	0.27149	-2.90385	-1.17257
C	2.63796	-2.91751	-0.79527
F	2.65034	-4.10295	-1.42040
F	3.63825	-2.17360	-1.28845
F	2.91273	-3.15219	0.52119
C	0.01427	0.96763	-2.54116
H	-0.29100	-0.02214	-2.90767
H	-0.62304	1.70976	-3.03213
H	1.05565	1.09184	-2.85950
H	0.32588	1.66024	-1.39122
O	0.66666	2.51940	-0.47689
C	1.94433	2.74669	-0.39275
O	2.80813	2.61035	-1.23896
C	2.33076	3.21838	1.03408
F	1.54064	4.22720	1.46276
F	3.60160	3.63050	1.10907
F	2.18097	2.19522	1.92135

ts6_8

C	-3.86391	-1.31086	-1.57598
C	-3.60995	-2.36401	-0.76124
N	-2.26062	-2.28521	-0.44086
C	-1.69405	-1.19210	-1.01413
N	-2.67496	-0.60711	-1.72867
Pd	0.22829	-0.72920	-0.68660
C	-1.52156	-3.12429	0.49704
N	-1.02505	-2.32123	1.59585
C	-0.25716	-1.21716	1.36604
N	-0.12737	-0.63787	2.57616
C	-0.81332	-1.35758	3.54664
C	-1.39352	-2.41775	2.93334
C	0.47124	0.67451	2.84244
C	-2.58879	0.67016	-2.44020
H	-0.82492	-1.04848	4.58027

H	-1.99472	-3.22618	3.31985
H	-4.24851	-3.15405	-0.39830
H	-4.77620	-0.99247	-2.05560
H	1.01807	0.62482	3.78766
H	1.15656	0.93530	2.03392
H	-0.32998	1.41525	2.90921
H	-2.96655	0.54394	-3.45805
H	-3.17707	1.41819	-1.90339
H	-1.55234	0.99623	-2.45303
H	-0.68278	-3.58694	-0.02781
H	-2.18879	-3.89673	0.88067
O	2.30727	-0.63911	-0.48140
O	-0.28303	1.52612	-0.44223
C	0.74676	-0.58084	-2.78779
H	1.75505	-0.94331	-2.98516
H	0.59154	-1.87914	-1.69369
H	0.01927	-0.96228	-3.50392
H	0.74990	0.51168	-2.75696
C	3.03028	0.27018	0.07229
O	2.73583	1.20002	0.80719
C	4.52580	0.04752	-0.29787
F	4.69616	0.01215	-1.63801
F	5.31100	1.01791	0.18893
F	4.96870	-1.12949	0.19991
C	-1.30785	1.83111	0.23681
C	-1.61073	3.35366	0.31872
O	-2.13125	1.10362	0.81383
F	-1.78698	3.74058	1.60056
F	-2.76881	3.61913	-0.34722
F	-0.65829	4.13159	-0.21583

ts7_27

C	4.45104	-0.30579	0.28534
C	4.10374	0.54794	-0.69824
N	2.76683	0.27203	-1.03317
C	2.26110	-0.74132	-0.20844
N	3.33892	-1.09244	0.58528
Pd	0.36724	-0.74844	0.18530
C	1.85981	1.24182	-1.60705
N	1.07730	1.96656	-0.58413
C	0.29257	1.30111	0.30896
N	-0.42239	2.26606	0.92782
C	-0.09953	3.52345	0.42664
C	0.84372	3.33504	-0.53268
C	-1.43397	1.99546	1.94839
C	3.24021	-1.98157	1.72812
H	-0.56176	4.42768	0.79259
H	1.34874	4.04098	-1.17442
H	4.69082	1.27206	-1.24260
H	5.39985	-0.46159	0.77652
H	-1.68481	0.93537	1.90081
H	-1.05428	2.25310	2.94230
H	-2.33145	2.58071	1.73374
H	2.51341	-2.76780	1.51036
H	4.21590	-2.43728	1.91955
H	2.90831	-1.44504	2.62458
H	1.15357	0.73364	-2.26755
H	2.43557	1.97281	-2.17776
O	-1.76863	-1.12773	0.42970
C	-2.46020	-0.62012	-0.51737
O	-2.09189	-0.11876	-1.58113

C	-3.97536	-0.57611	-0.18131
F	-4.73862	-0.32680	-1.25801
F	-4.42152	-1.71764	0.37916
F	-4.20657	0.42655	0.71512
C	1.49910	-2.38338	-1.05929
H	0.49877	-2.83394	-1.02211
H	1.71423	-2.10677	-2.09128
H	2.22645	-3.10761	-0.69258

ts7_9

C	1.34277	1.63386	-0.40863
N	1.15881	2.77970	0.30684
C	2.36220	3.31028	0.76505
H	2.41577	4.22194	1.34153
N	2.70860	1.47810	-0.39331
C	3.34493	2.48035	0.33349
H	4.41639	2.52837	0.46037
C	1.72016	-1.37247	-0.05369
N	3.01448	-0.91317	-0.17382
C	3.89924	-1.61722	0.63560
H	4.95663	-1.40197	0.67522
N	1.84628	-2.39734	0.84503
C	3.16181	-2.56103	1.27029
H	3.45399	-3.32419	1.97594
C	3.32326	0.28247	-0.94700
C	-0.15355	3.36576	0.55515
H	-0.91013	2.67175	0.18575
H	-0.29626	3.52283	1.62927
H	-0.24818	4.32651	0.03713
C	0.72947	-3.20042	1.32362
H	-0.18414	-2.78537	0.89502
H	0.84900	-4.24690	1.02056
H	0.66745	-3.14832	2.41533
H	2.94349	0.14463	-1.95970
H	4.40707	0.41482	-0.97186
Pd	0.15262	-0.17727	-0.63329
C	-1.50947	-2.05516	-1.80128
H	-0.99321	-1.31778	-2.41179
O	-1.96538	0.65891	-0.69071
C	-2.71111	-0.22300	-0.22738
O	-2.60422	-1.48992	-0.31004
C	-3.99235	0.23554	0.50471
F	-4.16187	-0.42565	1.66651
F	-3.96087	1.54889	0.78604
F	-5.07465	0.00085	-0.26598
H	-2.47013	-2.36292	-2.20050
H	-0.89618	-2.86268	-1.42657

ts9_17

N	2.70853	-0.08815	0.56485
C	1.51408	-0.08582	-0.09722
N	1.40037	-1.38828	-0.52066
C	2.48194	-2.17009	-0.12815
C	3.31087	-1.34283	0.55597
C	0.23985	-1.83270	-1.27635
N	-0.99663	-1.67941	-0.52802
C	-1.79614	-2.70618	-0.03488
C	-2.79502	-2.10189	0.65504
N	-2.56408	-0.73084	0.56877
C	-1.44549	-0.43629	-0.15463
H	4.26292	-1.53499	1.02747

H	2.57340	-3.21706	-0.37658
H	-1.60062	-3.75075	-0.22689
H	-3.63758	-2.52045	1.18497
H	0.16707	-1.23444	-2.18620
H	0.36991	-2.88506	-1.53777
Pd	-0.06946	1.29286	-0.28284
C	-3.40378	0.28452	1.18684
H	-4.43179	0.20917	0.81618
H	-3.40546	0.17164	2.27628
H	-2.98788	1.25754	0.92488
C	3.26994	1.09144	1.20646
H	3.28452	0.96930	2.29497
H	4.29021	1.26684	0.84886
H	2.62866	1.93434	0.94146
C	-1.10547	3.24757	-0.50711
H	-1.76548	2.98048	-1.33938
H	0.38021	2.84118	-0.37717
H	-1.67961	3.31178	0.42409
H	-0.71527	4.24935	-0.71494