Supplementary Information

Table 1: Absolute energies (hartree) from BP86/LANL2DZ calculations.

No.	E_{tot}	E_o	H_{298}	G_{298}	E_{sov}
8a	-607.881301	-607.610489	-607.585842	-607.667950	-607.940782
9a	-243.025510	-242.937435	-242.930485	-242.968672	-243.028047
11a	-850.939210	-850.578854	-850.546031	-850.651409	-850.988715
[11a-12a]$^{\neq}$	-850.919111	-850.558888	-850.527631	-850.627270	-850.974042
12a	-850.921901	-850.561383	-850.528952	-850.634030	-850.975142
[12a-13a]$^{\neq}$	-850.918319	-850.558476	-850.526870	-850.630133	-850.971472
13a	-850.934655	-850.574101	-850.542458	-850.640999	-850.986859
[13a-14a]$^{\neq}$	-850.923911	-850.564064	-850.532836	-850.630018	-850.975809
14a	-850.939706	-850.578700	-850.546997	-850.645792	-850.991435
[14a-15a]$^{\neq}$	-850.926165	-850.565612	-850.534472	-850.629343	-850.980665
15a	-839.454556	-839.090886	-839.061612	-839.15165	-839.464231
16a	-839.472299	-839.108235	-839.078986	-839.169775	-839.477312
Iodide (I^-)	-11.504977	-11.504978	-11.502617	-11.521826	-11.584167

E_{tot} total energy
E_o total energy plus zero-point vibrational energy
H_{298} enthalpy at 298 K
G_{298} Gibbs free enthalpy at 298 K
E_{sov} total energy plus CPCM solvation energy (THF)

Table 2: Relative energies (kcal mol^{-1}) from BP86 calculations.

No.	ΔE_{tot}	ΔG_{298}	ΔE_{sov}	ΔE_{ext}
8a+9a	0.0	0.0	0.0	0.0
11a	-20.3	-9.3	-12.5	-15.2
[11a-12a]$^{\neq}$	-7.7	5.9	-3.3	-5.5
12a	-9.5	1.6	-4.0	-6.1
[12a-13a]$^{\neq}$	-7.2	4.1	-1.7	-4.1
13a	-17.5	-2.7	-11.3	-13.4
[13a-14a]$^{\neq}$	-10.7	4.1	-4.4	-5.7
14a	-20.6	-5.8	-14.2	-15.2
[14a-15a]$^{\neq}$	-12.1	4.6	-7.4	-4.7
15a+I^-	-33.1	-23.1	-49.9	-21.3
16a+I^-	-44.2	-34.4	-58.3	-30.3

ΔE_{tot}, ΔG_{298}, ΔE_{sov}: BP86/LANL2DZ results based on Table 1.
E_{ext}: BP86/EXT single-point results (see text)

Optimized Cartesian coordinates (Å) from BP86/LANL2DZ calculations.

Structure **8a**

Pd	0.166230	-0.040140	0.264797
P	0.295319	0.010795	2.584416
P	-1.663611	-0.020513	-1.270903
C	1.930830	0.112583	3.632431
H	2.469604	1.031607	3.338809
H	1.733860	0.122084	4.724672
H	2.560759	-0.756508	3.369996
C	-0.504195	-1.457495	3.543878
H	-0.458024	-1.308004	4.641667
H	-1.555057	-1.548243	3.217685
H	0.027687	-2.386614	3.271636
C	-0.638134	1.449301	3.464318
H	-1.699000	1.402497	3.161087
H	-0.555386	1.387258	4.568556
H	-0.216830	2.407322	3.111125
C	-3.496156	-0.085522	-0.670034
H	-3.666169	0.753979	0.028287
H	-4.211556	-0.019202	-1.515130
H	-3.655284	-1.033193	-0.123582
C	-1.767024	1.506753	-2.418791
H	-1.831172	2.424589	-1.807384
H	-0.818555	1.495202	-2.985292
H	-2.637760	1.445853	-3.102616
C	-1.738650	-1.385315	-2.613209
H	-0.800395	-1.274691	-3.184852
H	-1.771157	-2.378293	-2.129947
H	-2.618716	-1.258177	-3.275640
O	2.036052	-0.061817	-1.107500
C	2.071073	0.037800	-2.417138
O	1.070722	0.183914	-3.229694
C	3.503179	-0.052113	-3.025274
H	4.172351	0.660503	-2.507222
H	3.906137	-1.069920	-2.856212
H	3.482752	0.161444	-4.108524

Structure **9a**

C	1.224087	-2.687775	0.000000
C	1.232629	-1.270433	0.000000
C	0.000000	-0.576419	0.000000
C	-1.232629	-1.270433	0.000000
C	-1.224087	-2.687775	0.000000
C	0.000000	-3.398458	0.000000
H	2.177796	-3.228186	0.000000
H	2.181519	-0.724696	0.000000
H	-2.181519	-0.724696	0.000000
H	-2.177796	-3.228186	0.000000
H	0.000000	-4.494375	0.000000
I	0.000000	1.580149	0.000000

Structure **11a**

Pd	0.046709	-0.233703	-1.260716
P	2.431556	-0.336616	-1.169203
P	-2.329685	-0.366265	-1.387713
O	0.657049	0.365307	-3.541563
C	-0.124410	0.849438	-4.487547

O	-1.413300	0.954768	-4.455238
C	3.228450	1.335829	-1.603463
H	3.009890	2.060222	-0.800068
H	4.323277	1.246359	-1.742776
H	2.743697	1.670830	-2.535684
C	3.115533	-1.421087	-2.574887
H	2.582877	-1.093003	-3.483705
H	4.210343	-1.302101	-2.689772
H	2.872478	-2.478610	-2.371364
C	3.511906	-0.894606	0.299869
H	4.588403	-0.812758	0.054271
H	3.271303	-0.269727	1.176423
H	3.262872	-1.940484	0.549768
C	-3.196589	1.293113	-1.716050
H	-2.967925	1.993757	-0.894680
H	-2.772110	1.664792	-2.664906
H	-4.292457	1.161499	-1.806083
C	-2.956871	-1.381581	-2.868688
H	-2.557602	-0.872799	-3.763882
H	-2.559401	-2.409494	-2.805693
H	-4.063821	-1.405752	-2.892833
C	-3.397814	-1.084830	0.020451
H	-3.177168	-0.539940	0.953587
H	-4.474537	-1.006607	-0.225610
H	-3.124752	-2.144130	0.170082
C	0.604861	1.373104	-5.757065
H	1.633287	0.976942	-5.817402
H	0.030561	1.094487	-6.659394
H	0.648688	2.479358	-5.714030
I	-0.049868	-0.102767	1.683802
C	-0.073348	0.224279	4.061937
C	-0.041010	-0.885333	4.946689
C	-0.037972	-0.691112	6.354176
C	-0.067254	0.620872	6.892098
C	-0.100152	1.734569	6.014556
C	-0.103002	1.534228	4.608089
H	-0.017448	-1.904857	4.537153
H	-0.012522	-1.559838	7.028123
H	-0.064406	0.773163	7.979795
H	-0.123276	2.755186	6.423411
H	-0.127860	2.401799	3.933891

Structure **[11a-12a]**$^{\neq}$

Pd	0.386113	-0.341969	0.248518
P	2.093759	0.685535	1.538957
P	-1.785966	-1.015584	0.918233
O	-0.157966	-0.700827	4.829598
C	-0.743759	0.424053	5.152908
O	-1.060745	1.401505	4.345483
C	2.574045	-0.386346	3.034053
H	2.988490	-1.349366	2.682163
H	3.321688	0.134508	3.667361
H	1.650919	-0.574664	3.623913
C	1.485648	2.251802	2.427510
H	0.578483	1.983306	3.010593
H	2.264575	2.644678	3.113265
H	1.226077	3.023411	1.678950
C	3.822616	1.265371	0.933580
H	4.405140	1.709025	1.766668
H	4.370630	0.398869	0.518992

H	3.693760	2.016066	0.131660
C	-1.706299	-2.247877	2.363273
H	-1.197513	-3.172233	2.032002
H	-1.119702	-1.775092	3.180299
H	-2.724631	-2.492326	2.729840
C	-2.778539	0.389221	1.726350
H	-2.169041	0.802750	2.558301
H	-2.972359	1.183142	0.981159
H	-3.742518	0.010995	2.125001
C	-3.137733	-1.827046	-0.178721
H	-2.740996	-2.766908	-0.605723
H	-4.049333	-2.044447	0.414327
H	-3.390390	-1.142540	-1.009827
C	-1.110571	0.592234	6.661034
H	-0.217077	0.391215	7.283903
H	-1.497004	1.607704	6.860987
H	-1.879650	-0.158827	6.932495
I	1.040013	-1.015564	-2.944686
C	-0.383615	0.540390	-3.420706
C	-0.881769	1.318259	-2.352529
C	-1.812481	2.347754	-2.641320
C	-2.231617	2.589829	-3.973677
C	-1.716830	1.796554	-5.029943
C	-0.782425	0.763481	-4.759049
H	-0.551550	1.093598	-1.311401
H	-2.205068	2.958035	-1.817623
H	-2.953475	3.389459	-4.187198
H	-2.037714	1.975629	-6.065058
H	-0.380832	0.148704	-5.573565

Structure **12a**

Pd	0.029894	0.369660	-0.757731
P	-2.197501	0.317711	-1.536562
P	2.203781	0.055283	-1.620889
O	-0.162045	-1.635074	-4.648845
C	-0.093786	-0.610399	-5.457043
O	-0.071148	0.654221	-5.121597
C	-2.551483	-1.343030	-2.390628
H	-2.550040	-2.151701	-1.637913
H	-3.529163	-1.316472	-2.911667
H	-1.734314	-1.518222	-3.122005
C	-2.417144	1.517403	-2.994246
H	-1.605052	1.300932	-3.721017
H	-3.405665	1.377336	-3.475078
H	-2.320508	2.557411	-2.633910
C	-3.824793	0.597104	-0.557498
H	-4.705460	0.490971	-1.220687
H	-3.885248	-0.143818	0.259454
H	-3.813540	1.609867	-0.116394
C	2.334793	-1.645824	-2.459714
H	2.261422	-2.439650	-1.695158
H	1.479583	-1.731411	-3.161797
H	3.291348	-1.741631	-3.010900
C	2.488008	1.202039	-3.110896
H	1.612896	1.089839	-3.785101
H	2.549208	2.249439	-2.764381
H	3.419403	0.928353	-3.645130
C	3.897165	0.167956	-0.723736
H	3.919706	-0.570607	0.097318
H	4.729042	-0.033106	-1.426749

H	4.012616	1.178843	-0.293493
C	0.013949	-0.920586	-6.982506
H	-0.353473	-1.939096	-7.200890
H	-0.550877	-0.169529	-7.565054
H	1.078037	-0.854590	-7.287109
I	-0.127552	-1.623998	4.210806
C	0.069861	0.503524	3.806148
C	0.097607	0.959185	2.474259
C	0.223285	2.352415	2.236070
C	0.319180	3.264483	3.312534
C	0.289999	2.783181	4.646050
C	0.164696	1.394877	4.902604
H	0.025952	0.290833	1.589390
H	0.241717	2.680235	1.187468
H	0.415466	4.339621	3.117515
H	0.363818	3.479840	5.490779
H	0.141553	1.021805	5.932363

Structure: **[12a-13a]**$^{\neq}$

Pd	0.573631	0.231126	0.444170
P	2.132260	-0.673441	1.996024
P	-1.680994	0.932904	0.755875
O	-1.300886	-1.271835	4.348816
C	-1.181402	-0.224190	5.121022
O	-0.551954	0.888064	4.841697
C	1.447424	-2.229069	2.848544
H	1.295058	-3.024448	2.097055
H	2.144492	-2.583040	3.634011
H	0.471828	-1.957761	3.305420
C	2.383245	0.465588	3.497252
H	1.381724	0.673732	3.932234
H	3.028676	-0.023345	4.253971
H	2.845363	1.413850	3.167938
C	3.944903	-1.220594	1.651571
H	4.416512	-1.614708	2.573096
H	3.946359	-2.004580	0.872695
H	4.524848	-0.353726	1.285584
C	-2.766670	-0.448511	1.483377
H	-2.843647	-1.274860	0.754593
H	-2.271683	-0.814497	2.406276
H	-3.778272	-0.065696	1.724356
C	-1.827606	2.245964	2.124182
H	-1.337882	1.842427	3.034789
H	-1.305715	3.166239	1.805345
H	-2.891314	2.474041	2.336654
C	-2.854193	1.662191	-0.576917
H	-2.965471	0.931013	-1.396988
H	-3.847095	1.893612	-0.143617
H	-2.403681	2.584467	-0.985241
C	-1.901995	-0.284457	6.503159
H	-2.022751	-1.331907	6.833125
H	-1.340208	0.299358	7.255001
H	-2.909140	0.168183	6.401136
I	-0.966513	-1.298204	-3.798138
C	0.412589	0.310925	-3.339371
C	1.271308	0.189404	-2.221501
C	2.195037	1.243433	-1.964857
C	2.223385	2.394445	-2.785541
C	1.333314	2.503017	-3.884889
C	0.422768	1.454745	-4.171746

H	1.266902	-0.701928	-1.570530
H	2.865441	1.142139	-1.103132
H	2.927666	3.206084	-2.565737
H	1.342824	3.395298	-4.523476
H	-0.261543	1.533961	-5.023378

Structure **13a**

Pd	0.710313	-0.552449	0.041264
P	-1.654641	-0.586787	0.718275
P	1.912977	-0.150404	2.156519
O	-1.273524	1.699879	4.244533
C	-1.451469	0.774877	5.152576
O	-1.172955	-0.496670	5.032149
C	-2.419966	1.062800	1.271436
H	-2.231647	1.830738	0.500604
H	-3.511005	0.946939	1.422620
H	-1.950122	1.362701	2.231631
C	-2.123490	-1.709268	2.180306
H	-1.695644	-1.298257	3.118864
H	-3.225505	-1.760205	2.280962
H	-1.722919	-2.723831	2.002746
C	-2.931050	-1.178250	-0.577747
H	-3.957599	-1.122301	-0.166279
H	-2.852232	-0.550689	-1.481656
H	-2.704489	-2.223315	-0.855913
C	1.649569	1.574738	2.905977
H	1.817253	2.337080	2.124316
H	0.605249	1.644685	3.278852
H	2.349278	1.742270	3.748161
C	1.635969	-1.260819	3.676130
H	0.621697	-1.062372	4.084221
H	1.718969	-2.321023	3.375875
H	2.389388	-1.036747	4.456606
C	3.824147	-0.198411	2.035899
H	4.151210	0.523643	1.267528
H	4.284339	0.060974	3.008796
H	4.146212	-1.211441	1.734418
C	-2.046117	1.252629	6.509674
H	-2.996752	1.789830	6.328292
H	-2.217080	0.398667	7.187814
H	-1.347199	1.970105	6.982440
I	-1.223618	0.287612	-4.140231
C	0.637963	0.293050	-2.995190
C	0.919023	-0.843877	-2.149665
C	2.244637	-0.855134	-1.492825
C	3.150245	0.250837	-1.714011
C	2.785588	1.345939	-2.504008
C	1.506118	1.372714	-3.167166
H	0.390872	-1.786726	-2.334544
H	2.668073	-1.820676	-1.179184
H	4.147175	0.212288	-1.254923
H	3.472604	2.190389	-2.642756
H	1.237008	2.217740	-3.809109

Structure **[13a-14a]**$^{\neq}$

Pd	0.343583	0.516666	0.208636
P	-1.713848	0.942784	-1.072491
P	1.921810	-0.660676	-1.251265

O	-0.771237	-1.481726	-4.401705
C	-0.400091	-0.533187	-5.222925
O	0.139892	0.611788	-4.897655
C	-2.578087	-0.551163	-1.873194
H	-2.740783	-1.329313	-1.106531
H	-3.550186	-0.248118	-2.310003
H	-1.922434	-0.945833	-2.678046
C	-1.544408	2.099391	-2.573842
H	-0.872913	1.617728	-3.316323
H	-2.533188	2.281257	-3.039735
H	-1.106755	3.060255	-2.246728
C	-3.200268	1.756941	-0.169516
H	-4.043361	1.916974	-0.869015
H	-3.527712	1.099007	0.655259
H	-2.888987	2.730384	0.252106
C	1.337938	-2.272550	-2.071857
H	0.940083	-2.952716	-1.297475
H	0.538693	-2.025039	-2.802454
H	2.178576	-2.762331	-2.601541
C	2.557643	0.297444	-2.764893
H	1.702252	0.489275	-3.447085
H	2.991694	1.257675	-2.432424
H	3.326817	-0.293781	-3.299810
C	3.573235	-1.237926	-0.468502
H	3.355641	-1.958806	0.339505
H	4.222703	-1.715378	-1.228174
H	4.089092	-0.365124	-0.031042
C	-0.652737	-0.800408	-6.736545
H	-1.744322	-0.804083	-6.926803
H	-0.175440	-0.023095	-7.358369
H	-0.266015	-1.800693	-7.008868
I	-1.181010	-1.195952	3.343359
C	0.363083	0.241499	2.796567
C	-0.054929	1.451664	2.116372
C	1.019607	2.400556	1.854514
C	2.328501	2.206477	2.360549
C	2.650807	1.056143	3.130445
C	1.667755	0.052681	3.322616
H	-1.100987	1.774487	2.127211
H	0.768229	3.334544	1.337295
H	3.097497	2.962353	2.153775
H	3.662142	0.909779	3.528009
H	1.911418	-0.868081	3.864473

Structure **14a**

Pd	0.518648	0.066560	-0.308090
P	1.920963	-0.615469	1.604444
P	-1.526441	0.870623	0.785275
O	-1.118105	-1.119197	4.463088
C	-0.814093	-0.104120	5.231337
O	-0.168637	0.974207	4.872128
C	1.329573	-2.090660	2.641441
H	1.063941	-2.925080	1.967806
H	2.126549	-2.414066	3.339081
H	0.434242	-1.779950	3.222829
C	2.368241	0.644348	2.953324
H	1.464599	0.844459	3.568742
H	3.166294	0.235528	3.603413
H	2.719109	1.578274	2.479096
C	3.658480	-1.204557	1.065101

H	4.262882	-1.499656	1.944300
H	3.552611	-2.066402	0.382685
H	4.162580	-0.384744	0.524054
C	-2.604528	-0.410128	1.678096
H	-2.794259	-1.259850	0.999263
H	-2.064924	-0.757080	2.584427
H	-3.566874	0.046706	1.980719
C	-1.345098	2.211513	2.117940
H	-0.843580	1.781324	3.009783
H	-0.742171	3.044721	1.714708
H	-2.343780	2.587496	2.414108
C	-2.786834	1.695756	-0.387528
H	-3.026904	0.998181	-1.208356
H	-3.709382	1.968021	0.160098
H	-2.332199	2.606127	-0.817074
C	-1.275123	-0.204190	6.713994
H	-0.846510	-1.116272	7.172369
H	-0.961808	0.686696	7.285207
H	-2.377194	-0.304742	6.750058
I	-1.416522	-0.983662	-3.204410
C	0.337588	0.317232	-2.374260
C	1.621032	-0.382773	-2.212044
C	2.836762	0.315794	-2.558331
C	2.809179	1.642485	-3.008763
C	1.551769	2.320223	-3.163677
C	0.339640	1.670692	-2.887742
H	1.641506	-1.478115	-2.157615
H	3.789431	-0.228610	-2.496198
H	3.742612	2.161697	-3.261318
H	1.534112	3.366438	-3.497778
H	-0.616452	2.184135	-3.039408

Structure **[14a-15a]**$^{\neq}$

Pd	0.471592	-0.300360	-0.627706
P	0.631212	0.049093	-3.079219
P	-1.373442	-1.815008	-0.375273
O	-0.284482	2.201307	-1.039646
C	-1.579676	2.454669	-0.975553
O	-2.495868	1.903130	-1.717346
C	1.663949	1.603519	-3.432367
H	2.695674	1.448237	-3.070737
H	1.671760	1.847503	-4.512095
H	1.188993	2.405367	-2.842494
C	-0.959316	0.415887	-4.049729
H	-1.600700	1.031728	-3.381523
H	-0.730207	0.946158	-4.994066
H	-1.476115	-0.534216	-4.282585
C	1.494435	-1.223746	-4.222406
H	1.570558	-0.843046	-5.259041
H	2.506111	-1.429926	-3.829877
H	0.917596	-2.165807	-4.220810
C	-2.992005	-0.887483	-0.041770
H	-2.910284	-0.441942	0.965622
H	-3.084312	-0.063494	-0.773939
H	-3.858944	-1.574907	-0.090186
C	-1.863354	-2.933618	-1.843967
H	-2.106212	-2.290683	-2.707309
H	-1.015066	-3.589380	-2.107730
H	-2.745529	-3.551885	-1.589737
C	-1.335636	-3.086733	1.038920

H	-1.151921	-2.532709	1.976932
H	-2.300796	-3.623938	1.106794
H	-0.516728	-3.806849	0.865181
C	-2.013487	3.461139	0.113493
H	-1.334349	4.333799	0.124193
H	-3.057216	3.785609	-0.041342
H	-1.924774	2.958216	1.096608
I	-0.702562	0.348934	3.097500
C	1.301169	-0.168290	1.212551
C	1.977136	1.038361	0.809878
C	3.395401	1.118913	0.959372
C	4.123608	0.044651	1.516143
C	3.440650	-1.136907	1.930449
C	2.038697	-1.246538	1.797608
H	1.387536	1.902433	0.468580
H	3.910088	2.043935	0.664073
H	5.211922	0.120610	1.642218
H	4.007293	-1.976598	2.356883
H	1.514976	-2.144917	2.140962

Structure **15a**

Pd	-0.016892	-0.234609	-0.135641
P	-0.013394	-0.227880	-2.630536
P	-2.280899	0.247968	0.337838
O	2.046343	-0.671939	-0.202396
C	2.820020	0.368642	-0.552714
O	2.377824	1.474718	-1.028740
C	1.583851	-0.922422	-3.382140
H	1.799804	-1.907911	-2.939581
H	1.484942	-1.008702	-4.479710
H	2.407498	-0.235020	-3.134387
C	-0.065742	1.515058	-3.377295
H	0.733782	2.088221	-2.879766
H	0.099071	1.488165	-4.469775
H	-1.039643	1.989905	-3.165132
C	-1.310546	-1.167508	-3.666809
H	-1.090631	-1.061279	-4.744809
H	-1.282413	-2.237247	-3.395943
H	-2.320982	-0.774900	-3.466382
C	-2.524746	1.879265	1.268167
H	-1.944770	1.842347	2.203997
H	-2.143779	2.709267	0.649825
H	-3.595113	2.041296	1.489722
C	-3.519353	0.446689	-1.089955
H	-3.148615	1.202984	-1.802133
H	-3.636917	-0.517269	-1.611979
H	-4.500621	0.768033	-0.696287
C	-3.184433	-1.001761	1.438243
H	-2.619969	-1.116443	2.377245
H	-4.210675	-0.654238	1.655215
H	-3.225000	-1.977489	0.925182
C	4.315062	0.134181	-0.315276
H	4.578570	-0.924286	-0.477673
H	4.912743	0.790376	-0.969104
H	4.547802	0.380793	0.737943
C	0.269564	-0.180042	1.883498
C	0.736440	1.016722	2.494042
C	1.061001	1.040800	3.875445
C	0.923498	-0.128274	4.663523
C	0.470200	-1.326083	4.058772

C	0.143685	-1.352188	2.677315
H	0.877498	1.920916	1.888621
H	1.429445	1.970112	4.329553
H	1.177295	-0.108893	5.730512
H	0.378024	-2.242931	4.655846
H	-0.180261	-2.295812	2.219126

Structure **16a**

Pd	0.094650	-0.126714	0.198214
P	2.475777	-0.039055	-0.053240
P	-2.299720	-0.167565	0.458071
C	-3.067652	1.529697	0.777723
H	-2.848784	2.196506	-0.073325
H	-4.162294	1.439277	0.902852
H	-2.598760	1.914982	1.695962
C	-2.972787	-1.238261	1.866816
H	-2.570370	-2.261201	1.777555
H	-2.638675	-0.786989	2.813488
H	-4.077083	-1.268580	1.824625
C	-3.301917	-0.803931	-1.021857
H	-3.063229	-0.204635	-1.914916
H	-3.031890	-1.853487	-1.226792
H	-4.383094	-0.737372	-0.801493
C	3.287721	0.019334	-1.760200
H	2.948751	0.923591	-2.292196
H	4.388686	0.027863	-1.668331
H	2.966830	-0.858223	-2.345074
C	3.301198	-1.509738	0.803189
H	3.102158	-2.429275	0.227241
H	4.392128	-1.358365	0.893832
H	2.837029	-1.599123	1.798844
C	3.219728	1.450977	0.844645
H	4.324091	1.412288	0.830136
H	2.874879	2.380387	0.361644
H	2.853328	1.431321	1.883611
O	0.658589	-0.320546	2.271551
C	-0.002183	0.277654	3.270278
O	-1.081297	0.955505	3.137057
C	0.612880	0.070491	4.663112
H	-0.010999	-0.645712	5.230675
H	1.638437	-0.326364	4.596743
H	0.605503	1.025728	5.216443
C	-0.166029	0.030445	-1.800326
C	-0.145276	-1.117112	-2.646263
C	-0.303665	-0.993068	-4.051039
C	-0.484863	0.281728	-4.642206
C	-0.505172	1.431352	-3.814842
C	-0.346484	1.306953	-2.409690
H	-0.011329	-2.116117	-2.210296
H	-0.287020	-1.892415	-4.680903
H	-0.607912	0.377388	-5.727808
H	-0.644575	2.425614	-4.259572
H	-0.361884	2.212261	-1.788157