Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information: A new method for screening potential sII and sH hydrogen clathrate hydrate promoters with model potentials

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The following tables list some parameters for each of the considered potential promoters. For each atom is listed the Cartesian coordinates (Å) of the optimised geometry, the CHELPG partial charge from MP2/cc-pVTZ calculations and the atom type [as listed in Cornell et al., *J. Am. Chem. Soc.* **117** (1995) 5179] assigned to the atom for the Lennard-Jones interactions. [Types not listed for hydrogen, as the parameters for the hydrogen–water interaction were taken from Hixson et al., *J. Chem. Phys.* **97** (1992) 753.] The oxygen atom of the water molecules was type OW.

1,1-dimethylcyclohexane

Atom	x	y	z	Charge	Type
C	-1.252827	-0.736704	2.093262	0.047225	CT
C	0.000000	-1.443369	2.600226	-0.044935	CT
C	1.252827	-0.736704	2.093262	0.047225	CT
C	1.246667	-0.654860	0.569785	-0.089299	CT
C	0.000000	0.044701	0.011253	0.683125	CT
C	-1.246667	-0.654860	0.569785	-0.089299	CT
C	0.000000	-0.092078	-1.509158	-0.449687	CT
H	0.000000	-1.141979	-1.806236	0.063905	HC
H	-0.882913	0.383625	-1.939690	0.081879	HC
H	0.882913	0.383625	-1.939690	0.081879	HC
H	1.283858	-1.671651	0.164124	-0.009742	HC
H	-1.283858	-1.671651	0.164124	-0.009742	HC
H	2.139580	-0.137109	0.208621	-0.025926	HC
H	-2.139580	-0.137109	0.208621	-0.025926	HC
H	1.293568	0.268918	2.520164	-0.019650	HC
H	-1.293568	0.268918	2.520164	-0.019650	HC
H	2.149443	-1.257051	2.433623	-0.011102	HC
H	-2.149443	-1.257051	2.433623	-0.011102	HC
H	0.000000	-2.476414	2.239345	0.004482	HC
H	0.000000	-1.486475	3.690361	-0.002543	HC
C	0.000000	1.542989	0.388187	-0.418391	CT
H	0.000000	2.166505	-0.505582	0.063031	HC
H	-0.876811	1.818761	0.973465	0.077123	HC
H	0.876811	1.818761	0.973465	0.077123	HC

2-methoxy-2-methyl-propane

Atom	x	y	z	Charge	Type
O	-0.791781	-0.810450	0.000000	-0.529403	OS
C	-0.009355	0.392630	0.000000	0.805981	CT
C	-1.056181	1.493528	0.000000	-0.409873	CT
C	-0.063642	-2.020492	0.000000	0.096163	CT
H	-0.800681	-2.818524	0.000000	0.057197	HC
H	-0.583395	2.474418	0.000000	0.083097	HC
C	0.851165	0.489161	1.254670	-0.354689	CT
C	0.851165	0.489161	-1.254670	-0.354689	CT
H	0.562287	-2.130048	0.887886	0.010230	HC
H	0.562287	-2.130048	-0.887886	0.010230	HC
H	0.234922	0.346558	-2.141413	0.082400	HC
H	0.234922	0.346558	2.141413	0.082400	HC
H	1.315705	1.472963	1.309208	0.054714	HC
H	1.315705	1.472963	-1.309208	0.054714	HC
H	1.648779	-0.251869	1.259364	0.071723	HC
H	1.648779	-0.251869	-1.259364	0.071723	HC
H	-1.686390	1.404731	-0.883042	0.084042	HC
H	-1.686390	1.404731	0.883042	0.084042	HC

2,2-dimethylbutane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.000000	0.706152	CT
C	-1.247400	0.695105	-0.541675	-0.339976	CT
C	1.247400	0.695105	-0.541675	-0.339976	CT
C	0.000000	0.000000	1.535430	0.043150	CT
C	0.000000	-1.452790	-0.471703	-0.473430	CT
C	0.000000	1.371170	2.201400	-0.199455	CT
H	-1.281300	0.619400	-1.629480	0.047814	HC
H	1.281300	0.619400	-1.629480	0.047814	HC
H	-2.152960	0.233600	-0.143900	0.052576	HC
H	2.152960	0.233600	-0.143900	0.052576	HC
H	-1.263200	1.753500	-0.283550	0.054575	HC
H	1.263200	1.753500	-0.283550	0.054575	HC
H	0.000000	-1.507940	-1.561250	0.097523	HC
H	0.882930	-1.979400	-0.106170	0.074955	HC
H	-0.882930	-1.979400	-0.106170	0.074955	HC
H	0.000000	1.267130	3.285530	0.050454	HC
H	0.880800	1.950200	1.929200	0.032013	HC
H	-0.880800	1.950200	1.929200	0.032013	HC
H	-0.875300	-0.562350	1.873040	-0.034154	HC
H	0.875300	-0.562350	1.873040	-0.034154	HC

2,2-dimethylpentane (*gauche*)

Atom	x	y	z	Charge	Type
C	0.321216	-0.051645	-1.516489	-0.354585	CT
C	-0.158816	0.116911	-0.076053	0.768550	CT
C	0.694974	1.181843	0.608160	-0.370677	CT
C	-1.615980	0.576276	-0.097964	-0.438840	CT
C	-0.042779	-1.245902	0.626113	-0.251939	CT
C	-0.331800	-1.271086	2.133467	0.216610	CT
C	0.923068	-1.175020	2.996233	-0.157438	CT
H	0.219781	0.882222	-2.071507	0.061918	HC
H	-0.261239	-0.816616	-2.032397	0.052623	HC
H	1.370335	-0.349750	-1.543282	0.044515	HC
H	-1.706952	1.527521	-0.624448	0.075112	HC
H	0.634592	2.121447	0.056527	0.044558	HC
H	0.356586	1.373673	1.626424	0.078358	HC
H	-2.011836	0.716308	0.907730	0.080349	HC
H	1.743020	0.881007	0.646072	0.062164	HC
H	-2.243492	-0.154727	-0.610342	0.070058	HC
H	0.964979	-1.638768	0.456413	0.021952	HC
H	-0.724229	-1.927434	0.109810	0.016904	HC
H	0.676853	-1.197875	4.057281	0.023859	HC
H	1.477476	-0.259575	2.801473	0.019384	HC
H	1.588652	-2.013482	2.790824	0.033196	HC
H	-1.021980	-0.467526	2.396032	-0.060870	HC
H	-0.848903	-2.198688	2.382383	-0.035761	HC

2,2-dimethylpentane

Atom	x	y	z	Charge	Type
C	0.000000	-0.009903	0.000344	0.666463	CT
C	0.000000	-0.000638	-1.527327	-0.400443	CT
C	-1.247642	0.717569	0.497660	-0.330026	CT
H	0.000000	1.021177	-1.909748	0.077665	HC
H	-0.882957	-0.508570	-1.918387	0.063825	HC
H	0.882957	-0.508570	-1.918387	0.063825	HC
H	-1.283259	1.729738	0.091869	0.052385	HC
H	1.283259	1.729738	0.091869	0.052385	HC
H	1.261976	0.796100	1.584251	0.048079	HC
H	-1.261976	0.796100	1.584251	0.048079	HC
H	2.153011	0.196357	0.181517	0.055746	HC
H	-2.153011	0.196357	0.181517	0.055746	HC
C	0.000000	-1.472832	0.465145	-0.216039	CT
H	0.875973	-1.968361	0.032599	0.021231	HC
H	-0.875973	-1.968361	0.032599	0.021231	HC
C	0.000000	-1.713195	1.970285	0.212009	CT
C	0.000000	-3.202065	2.297053	-0.228042	CT
H	0.000000	-3.377868	3.371715	0.042645	HC
H	0.879746	-3.690112	1.877618	0.048460	HC
H	-0.879746	-3.690112	1.877618	0.048460	HC
C	1.247642	0.717569	0.497660	-0.330026	CT
H	-0.875389	-1.244823	2.422450	-0.036829	HC
H	0.875389	-1.244823	2.422450	-0.036829	HC

2,3-dimethylbutane

Atom	x	y	z	Charge	Type
C	-0.009076	0.143436	0.073435	-0.328096	CT
C	0.868360	-0.760773	-0.788737	0.381404	CT
C	0.526900	-0.634503	-2.280843	0.381404	CT
C	1.404336	-1.538711	-3.143016	-0.328096	CT
C	-0.940609	-0.952474	-2.556778	-0.328096	CT
H	2.456956	-1.270299	-3.090422	0.057751	HC
H	1.100622	-1.482977	-4.188155	0.066883	HC
H	1.303469	-2.578152	-2.823400	0.055070	HC
H	-1.144124	-0.921790	-3.626967	0.066883	HC
H	-1.616644	-0.251898	-2.072020	0.057751	HC
H	-1.182079	-1.956765	-2.202011	0.055070	HC
H	0.715051	0.406363	-2.569105	-0.084620	HC
H	0.091790	1.182877	-0.246181	0.055070	HC
H	-1.061697	-0.124976	0.020842	0.057751	HC
H	0.294637	0.087702	1.118575	0.066883	HC
C	2.335868	-0.442801	-0.512802	-0.328096	CT
H	3.011903	-1.143377	-0.997560	0.057751	HC
H	2.577339	0.561489	-0.867570	0.055070	HC
H	2.539384	-0.473485	0.557387	0.066883	HC
H	0.680209	-1.801638	-0.500475	-0.084620	HC

2,3-dimethylbutene

Atom	x	y	z	Charge	Type
C	0.000000	0.000891	1.334989	-0.584041	CM
C	0.000000	0.012853	-0.003352	0.125896	CM
C	0.000000	-1.265084	-0.792430	-0.097197	CT
C	0.000000	1.315316	-0.764826	0.297394	CT
C	-1.254652	1.464967	-1.625941	-0.222122	CT
C	1.254652	1.464967	-1.625941	-0.222122	CT
H	2.158215	1.351582	-1.028042	0.029218	HC
H	1.276460	2.447444	-2.097542	0.047241	HC
H	1.275101	0.718956	-2.420395	0.052569	HC
H	-1.275101	0.718956	-2.420395	0.052569	HC
H	-1.276460	2.447444	-2.097542	0.047241	HC
H	-2.158215	1.351582	-1.028042	0.029218	HC
H	0.000000	2.117838	-0.023308	-0.027738	HC
H	0.000000	0.922705	1.900988	0.175823	HC
H	-0.877034	-1.333051	-1.436797	0.032843	HC
H	0.877034	-1.333051	-1.436797	0.032843	HC
H	0.000000	-2.127373	-0.128982	0.032534	HC
H	0.000000	-0.928027	1.889000	0.197832	HC

2,3-dimethylbut-2-ene

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.673746	0.015033	CT
C	0.000000	0.000000	-0.673746	0.015033	CT
C	-0.023000	1.247148	1.514214	-0.188930	CT
C	0.023000	-1.247148	1.514214	-0.188930	CT
C	-0.023000	-1.247148	-1.514214	-0.188930	CT
C	0.023000	1.247148	-1.514214	-0.188930	CT
H	-0.217486	2.153443	0.950878	0.061462	HC
H	0.217486	-2.153443	0.950878	0.061462	HC
H	-0.217486	-2.153443	-0.950878	0.061462	HC
H	0.217486	2.153443	-0.950878	0.061462	HC
H	-0.797273	1.159759	2.279131	0.060233	HC
H	0.924322	1.370283	2.044319	0.059718	HC
H	0.797273	-1.159759	2.279131	0.060233	HC
H	-0.924322	-1.370283	2.044319	0.059718	HC
H	-0.797273	-1.159759	-2.279131	0.060233	HC
H	0.924322	-1.370283	-2.044319	0.059718	HC
H	0.797273	1.159759	-2.279131	0.060233	HC
H	-0.924322	1.370283	-2.044319	0.059718	HC

2,3-dimethylpentane

Atom	x	y	z	Charge	Type
H	0.050537	-0.077600	-0.081020	0.084410	HC
C	0.007743	-0.089873	-1.170219	-0.374012	CT
C	-2.020811	1.372469	-1.138710	-0.221629	CT
H	-3.048058	1.520012	-1.469189	0.084410	HC
H	-2.018739	1.384293	-0.048828	0.041445	HC
H	-1.430602	2.224579	-1.476331	0.024949	HC
H	0.636496	0.725043	-1.529196	0.078136	HC
H	0.443047	-1.028325	-1.514347	0.056275	HC
C	-1.430767	0.062893	-1.655418	0.330486	CT
C	-1.540143	-0.090108	-3.183730	0.233919	CT
C	-0.930640	1.087015	-3.948463	0.146890	CT
C	-0.717343	0.797263	-5.430506	-0.255299	CT
H	-1.657636	0.602282	-5.942891	0.055432	HC
H	-0.078081	-0.075925	-5.563230	0.048672	HC
H	-0.240036	1.638795	-5.930588	0.050726	HC
H	-1.579062	1.959428	-3.838326	-0.028581	HC
H	0.029142	1.355665	-3.503861	-0.037291	HC
H	-0.963571	-0.984815	-3.446645	-0.054429	HC
H	-2.010515	-0.758620	-1.222533	-0.061302	HC
C	-2.986851	-0.330152	-3.608275	-0.373370	CT
H	-3.599125	0.553589	-3.425380	0.078934	HC
H	-3.061109	-0.567401	-4.668132	0.084434	HC
H	-3.421912	-1.161168	-3.052629	0.061718	HC

2,4-dimethylpentane (*gauche*)

Atom	x	y	z	Charge	Type
C	-0.165894	-0.009122	2.650803	-0.341925	CT
C	0.012566	-0.806311	1.362061	0.575883	CT
C	-0.881857	-2.045409	1.377422	-0.341642	CT
C	-0.100550	0.024350	0.071706	-0.276347	CT
C	-1.298172	0.954138	-0.190931	0.575919	CT
C	-2.664624	0.298119	-0.015816	-0.341948	CT
C	-1.238630	2.269491	0.584865	-0.341627	CT
H	-1.209204	1.221004	-1.248675	-0.106971	HC
H	1.042961	-1.175393	1.359145	-0.106965	HC
H	-0.774487	-2.620829	0.457660	0.059197	HC
H	-2.880570	0.109205	1.035110	0.064740	HC
H	-0.609905	-2.694043	2.210801	0.052149	HC
H	-3.447329	0.955520	-0.395615	0.053688	HC
H	-1.932347	-1.788708	1.492500	0.061855	HC
H	-2.730667	-0.648593	-0.551285	0.055920	HC
H	-0.042542	-0.682871	-0.761478	0.005280	HC
H	0.798459	0.644087	-0.002023	0.005278	HC
H	0.110183	-0.620215	3.510685	0.053682	HC
H	-1.991571	2.962097	0.207264	0.052141	HC
H	-1.203237	0.294234	2.787390	0.064732	HC
H	-0.263758	2.745987	0.479145	0.059187	HC
H	-1.429329	2.126218	1.645889	0.061852	HC
H	0.453915	0.887025	2.661518	0.055922	HC

2,4-dimethylpentane

Atom	x	y	z	Charge	Type
C	0.000000	0.021370	0.000000	-0.286760	CT
C	0.032957	-0.783832	1.298637	0.508450	CT
C	-0.032957	-0.783832	-1.298637	0.508450	CT
C	0.052043	0.165138	2.492271	-0.345171	CT
C	-0.052043	0.165138	-2.492271	-0.345171	CT
C	-1.150949	-1.738559	1.403450	-0.306214	CT
C	1.150949	-1.738559	-1.403450	-0.306214	CT
H	-0.954686	-1.370921	-1.321091	-0.093346	HC
H	0.954686	-1.370921	1.321091	-0.093346	HC
H	-1.140115	-2.494376	0.619419	0.052184	HC
H	1.140115	-2.494376	-0.619419	0.052184	HC
H	-1.148970	-2.254661	2.363594	0.050639	HC
H	1.148970	-2.254661	-2.363594	0.050639	HC
H	-2.089414	-1.185734	1.323735	0.054767	HC
H	2.089414	-1.185734	-1.323735	0.054767	HC
H	-0.876329	0.678741	0.028522	0.031365	HC
H	0.876329	0.678741	-0.028522	0.031365	HC
H	0.123776	-0.381893	3.432275	0.065767	HC
H	-0.123776	-0.381893	-3.432275	0.065767	HC
H	-0.864433	0.757454	2.519138	0.067711	HC
H	0.864433	0.757454	-2.519138	0.067711	HC
H	-0.894174	0.854931	-2.435884	0.057227	HC
H	0.894174	0.854931	2.435884	0.057227	HC

3,3-dimethylbutene

Atom	x	y	z	Charge	Type
C	-0.059936	0.070470	0.070470	-0.292147	CT
C	0.863851	0.918947	0.918947	0.784504	CT
C	0.618024	0.637971	2.403603	-0.309086	CT
C	2.312214	0.576305	0.576305	-0.364239	CT
C	0.618024	2.403603	0.637971	-0.309086	CT
H	3.001123	1.174011	1.174011	0.062512	HC
H	2.518333	-0.476629	0.772530	0.057706	HC
H	2.518333	0.772530	-0.476629	0.057706	HC
H	1.293137	3.019130	1.235006	0.042903	HC
H	0.784523	2.630982	-0.414991	0.038894	HC
H	-0.406105	2.682087	0.884658	0.050274	HC
H	0.784523	-0.414991	2.630982	0.038894	HC
H	1.293137	1.235006	3.019130	0.042903	HC
H	-0.406105	0.884658	2.682087	0.050274	HC
C	-1.394511	0.111334	0.111334	-0.370404	CT
H	0.411515	-0.621153	-0.621153	0.115490	HC
H	-1.990996	-0.525470	-0.525470	0.149395	HC
H	-1.924715	0.778522	0.778522	0.153504	HC

3,3-dimethylbutyne

Atom	x	y	z	Charge	Type
C	-0.001733	-1.446578	0.482940	-0.297186	CT
C	0.000000	0.000000	-0.021203	0.761844	CT
C	0.000000	0.000000	-1.485898	-0.225900	CT
C	0.000000	0.000000	-2.702514	-0.373286	CT
H	0.000000	0.000000	-3.763620	0.270384	HC
H	0.880673	-1.978527	0.130350	0.052023	HC
H	-0.001745	-1.457100	1.573616	0.048794	HC
H	-0.885410	-1.976412	0.130350	0.052023	HC
C	-1.251908	0.724790	0.482940	-0.297186	CT
H	-2.153791	0.226578	0.130350	0.052023	HC
H	-1.261013	0.730061	1.573616	0.048794	HC
H	-1.268918	1.754993	0.130350	0.052023	HC
C	1.253640	0.721789	0.482940	-0.297186	CT
H	1.273118	1.751949	0.130350	0.052023	HC
H	1.262758	0.727039	1.573616	0.048794	HC
H	2.154327	0.221419	0.130350	0.052023	HC

3,3-dimethylpentane

Atom	x	y	z	Charge	Type
C	2.309381	-1.144135	0.642703	-0.241655	CT
C	0.912203	-1.291323	0.048567	0.090784	CT
C	0.134280	0.017757	-0.151703	0.608191	CT
C	0.930165	0.979666	-1.033333	-0.395423	CT
C	-1.188600	-0.279012	-0.877484	-0.016418	CT
C	-2.151735	-1.223634	-0.166594	-0.165516	CT
C	-0.144129	0.692333	1.191411	-0.368244	CT
H	2.765095	-2.122938	0.786073	0.052454	HC
H	2.282080	-0.651946	1.613751	0.040982	HC
H	2.966845	-0.569916	-0.007259	0.045208	HC
H	-1.724695	-2.216161	-0.036112	0.016738	HC
H	-2.433214	-0.845981	0.815122	0.025881	HC
H	-3.066377	-1.336742	-0.747128	0.045814	HC
H	0.327659	-1.949227	0.694615	-0.030858	HC
H	0.986653	-1.794471	-0.920493	-0.041503	HC
H	-1.693433	0.674932	-1.054967	-0.009496	HC
H	-0.948521	-0.687313	-1.863621	-0.029119	HC
H	-0.788708	1.562301	1.053183	0.059837	HC
H	-0.635593	0.014080	1.888956	0.062256	HC
H	0.778525	1.037685	1.656914	0.058767	HC
H	1.188835	0.511106	-1.984823	0.056845	HC
H	0.339307	1.871602	-1.247629	0.053496	HC
H	1.851900	1.302048	-0.550515	0.080979	HC

Acetic acid

Atom	x	y	z	Charge	Type
C	-0.233267	-0.104144	0.000000	-0.287210	CT
C	1.263632	-0.039671	0.000000	0.821737	C
O	1.935434	0.964575	0.000000	-0.616183	O
O	1.806528	-1.282256	0.000000	-0.635892	OH
H	2.764998	-1.142811	0.000000	0.425354	HO
H	-0.638115	0.900424	0.000000	0.082080	HC
H	-0.574605	-0.648059	0.877491	0.105057	HC
H	-0.574605	-0.648059	-0.877491	0.105057	HC

Acetylene

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.605696	-0.263874	CM
C	0.000000	0.000000	-0.605696	-0.263874	CM
H	0.000000	0.000000	1.667240	0.263874	HC
H	0.000000	0.000000	-1.667240	0.263874	HC

Adamantane

Atom	x	y	z	Charge	Type
C	0.885068	0.885068	0.885068	0.545919	CT
C	-0.885068	-0.885068	0.885068	0.545919	CT
C	-0.885068	0.885068	-0.885068	0.545919	CT
C	0.885068	-0.885068	-0.885068	0.545919	CT
C	0.000000	0.000000	1.765717	-0.388904	CT
C	0.000000	0.000000	-1.765717	-0.388904	CT
C	0.000000	1.765717	0.000000	-0.388904	CT
C	0.000000	-1.765717	0.000000	-0.388904	CT
C	1.765717	0.000000	0.000000	-0.388904	CT
C	-1.765717	0.000000	0.000000	-0.388904	CT
H	1.515877	1.515877	1.515877	-0.097658	HC
H	-1.515877	-1.515877	1.515877	-0.097658	HC
H	-1.515877	1.515877	-1.515877	-0.097658	HC
H	1.515877	-1.515877	-1.515877	-0.097658	HC
H	2.414186	-0.622752	0.622752	0.045032	HC
H	2.414186	0.622752	-0.622752	0.045032	HC
H	-2.414186	-0.622752	-0.622752	0.045032	HC
H	-2.414186	0.622752	0.622752	0.045032	HC
H	-0.622752	2.414186	0.622752	0.045032	HC
H	0.622752	2.414186	-0.622752	0.045032	HC
H	0.622752	-2.414186	0.622752	0.045032	HC
H	-0.622752	-2.414186	-0.622752	0.045032	HC
H	-0.622752	0.622752	2.414186	0.045032	HC
H	0.622752	-0.622752	2.414186	0.045032	HC
H	0.622752	0.622752	-2.414186	0.045032	HC
H	-0.622752	-0.622752	-2.414186	0.045032	HC

Butane (*gauche*)

Atom	x	y	z	Charge	Type
C	0.177079	-0.349408	0.048344	-0.129208	CT
C	-2.070278	1.530985	-0.989599	-0.129208	CT
C	0.096135	0.238052	-1.355742	0.129835	CT
C	-1.334406	0.490067	-1.825115	0.129835	CT
H	-1.517180	2.470642	-0.971841	0.025866	HC
H	-0.399995	-1.272461	0.112709	0.025866	HC
H	-3.059884	1.734383	-1.395560	0.022021	HC
H	1.205834	-0.579864	0.320465	0.022021	HC
H	-2.199400	1.201911	0.039829	0.022908	HC
H	-0.213321	0.339320	0.795286	0.022908	HC
H	-1.314905	0.815744	-2.866453	-0.041891	HC
H	0.586005	-0.440309	-2.056229	-0.041891	HC
H	-1.887034	-0.452422	-1.806141	-0.029591	HC
H	0.654084	1.176857	-1.392895	-0.029591	HC

Butane

Atom	x	y	z	Charge	Type
C	0.046121	-0.027040	0.109972	-0.260501	CT
C	-1.228112	0.721237	-3.491809	-0.260501	CT
C	0.021546	-0.009460	-1.412346	0.180759	CT
C	-1.203537	0.703657	-1.969491	0.180759	CT
H	-2.109026	1.233976	-3.875013	0.059266	HC
H	0.927035	-0.539779	0.493176	0.059266	HC
H	-0.348116	1.228077	-3.887663	0.048737	HC
H	-1.232022	-0.292985	-3.890959	0.048737	HC
H	0.050031	0.987181	0.509122	0.048737	HC
H	-0.833875	-0.533880	0.505826	0.048737	HC
H	-2.104156	0.214764	-1.591115	-0.038499	HC
H	-1.225398	1.726966	-1.587838	-0.038499	HC
H	0.043407	-1.032769	-1.793999	-0.038499	HC
H	0.922165	0.479433	-1.790722	-0.038499	HC

cis-1,2-dimethylcyclohexane

Atom	x	y	z	Charge	Type
C	0.002720	-0.015045	0.022722	-0.188331	CT
C	0.020195	0.023907	1.548778	0.143805	CT
C	1.454725	0.038827	2.067586	-0.065477	CT
C	2.242775	-1.149777	1.525217	0.043119	CT
C	2.214684	-1.197422	-0.002252	0.245540	CT
C	0.773388	-1.214665	-0.537689	0.364375	CT
C	3.051742	-2.355067	-0.531049	-0.356509	CT
H	2.716255	-3.304401	-0.113555	0.061877	HC
H	2.991209	-2.424962	-1.618046	0.070721	HC
H	4.099736	-2.228806	-0.258886	0.073836	HC
H	1.827966	-2.079053	1.926507	-0.025146	HC
C	0.040181	-2.526647	-0.263183	-0.332358	CT
H	3.280260	-1.103976	1.864387	-0.025426	HC
H	0.830719	-1.096983	-1.624635	-0.092574	HC
H	1.940111	0.964654	1.744369	0.005779	HC
H	0.460289	0.905002	-0.353422	0.006346	HC
H	1.467611	0.038555	3.158643	-0.005328	HC
H	-1.025017	-0.031866	-0.346961	0.025688	HC
H	-0.503123	-0.846824	1.950899	-0.042081	HC
H	-0.520296	0.902714	1.903825	-0.029766	HC
H	2.664792	-0.263900	-0.360579	-0.072655	HC
H	0.009606	-2.768000	0.798311	0.078718	HC
H	-0.990045	-2.459714	-0.614275	0.057185	HC
H	0.510079	-3.362237	-0.779150	0.058663	HC

cis-1,2-dimethylcyclopentane

Atom	x	y	z	Charge	Type
C	-0.114948	-0.057768	0.048547	0.223148	CT
C	0.812390	0.882007	0.852517	0.252700	CT
C	0.799137	-1.244745	-0.358260	-0.058629	CT
C	1.801028	-0.079905	1.508095	-0.026907	CT
C	2.144509	-1.029643	0.363258	0.000683	CT
C	0.120483	1.835762	1.811861	-0.324639	CT
C	-1.317032	-0.547301	0.849688	-0.243430	CT
H	2.670344	0.425855	1.928328	-0.013649	HC
H	1.305610	-0.619819	2.319771	-0.003870	HC
H	0.928415	-1.310231	-1.437561	-0.009186	HC
H	0.343099	-2.182377	-0.037759	0.010945	HC
H	2.597228	-1.963627	0.691978	-0.008430	HC
H	2.855080	-0.539064	-0.303605	-0.003466	HC
H	-0.486100	0.463034	-0.835750	-0.063306	HC
H	1.379346	1.473500	0.125908	-0.060486	HC
H	-1.882544	-1.274693	0.267260	0.036991	HC
H	-1.000450	-1.040438	1.770175	0.054067	HC
H	-1.991836	0.265231	1.115779	0.047747	HC
H	-0.397153	1.293112	2.602086	0.059276	HC
H	0.846612	2.496501	2.285224	0.066366	HC
H	-0.611342	2.459796	1.297628	0.064074	HC

Cyclobutane

Atom	x	y	z	Charge	Type
C	0.000000	1.071224	0.152799	-0.011954	CT
C	0.000000	-1.071224	0.152799	-0.011954	CT
C	-1.071224	0.000000	-0.152799	-0.011954	CT
C	1.071224	0.000000	-0.152799	-0.011954	CT
H	0.000000	1.321930	1.212682	0.024978	HC
H	0.000000	1.988010	-0.432048	-0.013024	HC
H	0.000000	-1.321930	1.212682	0.024978	HC
H	0.000000	-1.988010	-0.432048	-0.013024	HC
H	-1.321930	0.000000	-1.212682	0.024978	HC
H	-1.988010	0.000000	0.432048	-0.013024	HC
H	1.321930	0.000000	-1.212682	0.024978	HC
H	1.988010	0.000000	0.432048	-0.013024	HC

Cycloheptane

Atom	x	y	z	Charge	Type
C	1.240265	-0.640890	-1.415973	0.049329	CT
C	1.240265	0.640890	1.415973	0.049329	CT
C	0.006721	-0.016659	-0.762653	0.068566	CT
C	0.006721	0.016659	0.762653	0.068566	CT
C	2.492533	0.228419	-1.274719	0.032811	CT
C	2.492533	-0.228419	1.274719	0.032811	CT
C	3.308902	0.000000	0.000000	0.072765	CT
H	3.151253	0.069273	-2.129973	-0.025455	HC
H	3.151253	-0.069273	2.129973	-0.025455	HC
H	2.182567	1.274825	-1.328714	-0.014755	HC
H	2.182567	-1.274825	1.328714	-0.014755	HC
H	1.024634	0.776587	2.477163	-0.027910	HC
H	1.024634	-0.776587	-2.477163	-0.027910	HC
H	1.421255	-1.640466	-1.010357	-0.021148	HC
H	1.421255	1.640466	1.010357	-0.021148	HC
H	-0.091153	1.004854	-1.142004	-0.028032	HC
H	-0.091153	-1.004854	1.142004	-0.028032	HC
H	-0.886271	-0.552151	-1.092349	-0.037261	HC
H	-0.886271	0.552151	1.092349	-0.037261	HC
H	3.965449	0.860577	0.144868	-0.032528	HC
H	3.965449	-0.860577	-0.144868	-0.032528	HC

Cyclohexane

Atom	x	y	z	Charge	Type
C	0.000000	-1.452263	0.234711	0.039807	CT
C	-1.257697	0.726131	0.234711	0.039807	CT
C	1.257697	0.726131	0.234711	0.039807	CT
C	0.000000	1.452263	-0.234711	0.039807	CT
C	-1.257697	-0.726131	-0.234711	0.039807	CT
C	1.257697	-0.726131	-0.234711	0.039807	CT
H	0.000000	-1.496322	1.327845	-0.013290	HC
H	-1.295853	0.748161	1.327845	-0.013290	HC
H	1.295853	0.748161	1.327845	-0.013290	HC
H	0.000000	1.496322	-1.327845	-0.013290	HC
H	-1.295853	-0.748161	-1.327845	-0.013290	HC
H	1.295853	-0.748161	-1.327845	-0.013290	HC
H	0.000000	-2.482802	-0.123426	-0.025851	HC
H	-2.150169	1.241401	-0.123426	-0.025851	HC
H	2.150169	1.241401	-0.123426	-0.025851	HC
H	0.000000	2.482802	0.123426	-0.025851	HC
H	-2.150169	-1.241401	0.123426	-0.025851	HC
H	2.150169	-1.241401	0.123426	-0.025851	HC

Cyclohexane (*boat*)

Atom	x	y	z	Charge	Type
C	1.236128	-0.782326	-0.451272	-0.002814	CT
C	-1.357210	0.704722	0.022235	-0.002814	CT
C	0.066469	-1.329127	0.383592	0.03330	CT
C	-1.256911	-0.817023	-0.173522	0.03330	CT
C	0.023487	1.377101	-0.051962	0.03330	CT
C	0.924708	0.613549	-1.015702	0.03330	CT
H	1.849707	1.157443	-1.206482	-0.022023	HC
H	0.092793	-2.418564	0.400227	-0.022023	HC
H	-0.081165	2.419911	-0.351048	-0.022023	HC
H	-2.103457	-1.314140	0.299863	-0.022023	HC
H	0.160966	-1.000450	1.421044	-0.002927	HC
H	0.490884	1.382750	0.935355	-0.002927	HC
H	-1.308051	-1.062025	-1.236833	-0.002927	HC
H	0.413684	0.523434	-1.976957	-0.002927	HC
H	-2.013097	1.128564	-0.739633	-0.006932	HC
H	1.453590	-1.467977	-1.271550	-0.006932	HC
H	-1.817535	0.921091	0.987398	-0.006932	HC
H	2.134975	-0.736569	0.165365	-0.006932	HC

Cyclooctane

Atom	x	y	z	Charge	Type
C	1.297652	0.486282	-0.162086	0.080302	CT
C	1.584175	1.244697	1.138657	-0.007852	CT
C	1.315590	0.444448	2.422821	0.104319	CT
C	-0.000006	0.769187	3.134517	0.019965	CT
C	-1.315597	0.444448	2.422812	0.104319	CT
C	-1.584175	1.244696	1.138647	-0.007852	CT
C	-1.297643	0.486282	-0.162095	0.080302	CT
C	0.000005	-0.313173	-0.214885	0.077182	CT
H	1.019598	2.176272	1.170806	-0.009082	HC
H	-1.019598	2.176272	1.170799	-0.009082	HC
H	-2.634211	1.540692	1.114735	-0.017103	HC
H	2.634211	1.540692	1.114752	-0.017103	HC
H	-0.000009	0.248593	4.095227	-0.026691	HC
H	-0.000007	1.838143	3.369803	-0.023421	HC
H	1.323539	1.187841	-1.000245	-0.034348	HC
H	2.120322	-0.214372	-0.326944	-0.034892	HC
H	-1.323525	1.187841	-1.000253	-0.034348	HC
H	-2.120312	-0.214373	-0.326958	-0.034892	HC
H	2.116059	0.648202	3.136148	-0.034169	HC
H	1.372573	-0.627022	2.213937	-0.039431	HC
H	-2.116071	0.648201	3.136134	-0.034169	HC
H	-1.372579	-0.627022	2.213928	-0.039431	HC
H	0.000008	-0.887899	-1.143774	-0.047076	HC
H	0.000002	-1.055499	0.585382	-0.015447	HC

Cyclopentane

Atom	x	y	z	Charge	Type
C	-0.519813	-1.160433	0.000000	0.009209	CT
C	0.129536	-0.453835	1.188372	0.034253	CT
C	0.129536	-0.453835	-1.188372	0.034253	CT
C	0.129536	1.027953	0.775509	0.037428	CT
C	0.129536	1.027953	-0.775509	0.037428	CT
H	-0.767593	1.518675	1.150903	-0.014542	HC
H	0.981902	1.564404	1.187714	-0.014542	HC
H	-0.767593	1.518675	-1.150903	-0.024117	HC
H	0.981902	1.564404	-1.187714	-0.024117	HC
H	1.154784	-0.812392	1.297341	-0.002957	HC
H	1.154784	-0.812392	-1.297341	-0.002957	HC
H	-0.382981	-0.628492	-2.132863	-0.027397	HC
H	-0.382981	-0.628492	2.132863	-0.027397	HC
H	-0.365990	-2.238502	0.000000	-0.021834	HC
H	-1.596212	-0.972697	0.000000	0.007291	HC

Dimethylpropane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.000000	0.794756	CT
C	0.880947	0.880947	0.880947	-0.365015	CT
C	-0.880947	-0.880947	0.880947	-0.365015	CT
C	-0.880947	0.880947	-0.880947	-0.365015	CT
C	0.880947	-0.880947	-0.880947	-0.365015	CT
H	1.521361	0.272912	1.521361	0.055442	HC
H	1.521361	1.521361	0.272912	0.055442	HC
H	0.272912	1.521361	1.521361	0.055442	HC
H	-1.521361	-1.521361	0.272912	0.055442	HC
H	-0.272912	-1.521361	1.521361	0.055442	HC
H	-1.521361	-0.272912	1.521361	0.055442	HC
H	-1.521361	0.272912	-1.521361	0.055442	HC
H	-1.521361	1.521361	-0.272912	0.055442	HC
H	-0.272912	1.521361	-1.521361	0.055442	HC
H	1.521361	-1.521361	-0.272912	0.055442	HC
H	0.272912	-1.521361	-1.521361	0.055442	HC
H	1.521361	-0.272912	-1.521361	0.055442	HC

Ethane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.761599	0.013142	CT
C	0.000000	0.000000	-0.761599	0.013142	CT
H	0.000000	1.014465	1.155591	-0.004381	HC
H	-0.878553	-0.507234	1.155593	-0.004381	HC
H	0.878553	-0.507234	1.155593	-0.004381	HC
H	0.000000	-1.014465	-1.155591	-0.004381	HC
H	-0.878553	0.507234	-1.155593	-0.004381	HC
H	0.878553	0.507234	-1.155593	-0.004381	HC

Ethene

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.665903	-0.289676	CM
C	0.000000	0.000000	-0.665903	-0.289676	CM
H	0.000000	0.922479	1.228298	0.144838	HC
H	0.000000	-0.922479	1.228298	0.144838	HC
H	0.000000	-0.922479	-1.228298	0.144838	HC
H	0.000000	0.922479	-1.228298	0.144838	HC

Fluoromethane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	-0.634658	0.192739	CT
F	0.000000	0.000000	0.745806	-0.283249	F
H	0.000000	1.026664	-0.991216	0.030170	H1
H	0.889117	-0.513332	-0.991216	0.030170	H1
H	-0.889117	-0.513332	-0.991216	0.030170	H1

Formaldehyde

Atom	x	y	z	Charge	Type
O	0.000000	0.000000	0.672817	-0.471837	O
C	0.000000	0.000000	-0.537846	0.445072	CT
H	0.000000	0.934306	-1.119086	0.013382	HC
H	0.000000	-0.934306	-1.119086	0.013382	HC

Glyoxyl

Atom	x	y	z	Charge	Type
C	0.000000	-0.013037	0.756780	0.437137	C
C	0.000000	0.013037	-0.756780	0.437137	C
H	0.000000	1.019483	-1.204512	0.030685	HC
H	0.000000	-1.019483	1.204512	0.030685	HC
O	0.000000	1.010289	1.408093	-0.467822	O
O	0.000000	-1.010289	-1.408093	-0.467822	O

Hydrogen

Atom	x	y	z	Charge
H	-0.371500	0.000000	0.000000	0.420000
X	0.000000	0.000000	0.000000	-0.840000
H	0.371500	0.000000	0.000000	0.420000

Methane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.000000	-0.349881	CT
H	0.626577	0.626577	0.626577	0.087470	HC
H	-0.626577	-0.626577	0.626577	0.087470	HC
H	-0.626577	0.626577	-0.626577	0.087470	HC
H	0.626577	-0.626577	-0.626577	0.087470	HC

Methanol

Atom	x	y	z	Charge	Type
C	-0.229157	0.150094	0.150094	0.255445	CT
H	0.366449	0.791828	0.791828	0.035466	HC
H	-0.864396	-0.471064	0.783653	-0.024492	HC
H	-0.864396	0.783653	-0.471064	-0.024492	HC
O	0.681763	-0.619253	-0.619253	-0.635494	OH
H	0.163806	-1.190415	-1.190415	-0.635494	HO

Methylbutane

Atom	x	y	z	Charge	Type
C	0.159740	-0.045809	-0.071711	-0.383317	CT
C	0.277597	-0.306353	-1.568892	0.437169	CT
C	1.408423	-1.291837	-1.842288	-0.272206	CT
C	-1.056739	-0.802731	-2.123701	0.077251	CT
C	-1.076276	-0.981393	-3.636778	-0.198324	CT
H	-0.074809	-0.972841	0.454734	0.067493	HC
H	1.091630	0.343204	0.338131	0.085623	HC
H	-0.632025	0.671142	0.144993	0.064217	HC
H	1.577327	-1.439021	-2.907397	0.044120	HC
H	1.175325	-2.262736	-1.400066	0.052634	HC
H	2.342488	-0.941878	-1.403138	0.043802	HC
H	0.515754	0.639281	-2.066559	-0.083900	HC
H	-0.393551	-1.765472	-3.958601	0.040942	HC
H	-0.784066	-0.057986	-4.137845	0.032740	HC
H	-2.071829	-1.249140	-3.987399	0.046267	HC
H	-1.304632	-1.750025	-1.635415	-0.027304	HC
H	-1.837065	-0.094571	-1.835455	-0.027207	HC

Methylcyclohexane

Atom	x	y	z	Charge	Type
C	-0.008974	0.000000	-0.003123	0.384483	CT
C	-0.000611	0.000000	1.516430	-0.410826	CT
C	1.358816	0.000000	-2.623129	0.021574	CT
C	0.666870	-1.248616	-0.558870	-0.082573	CT
C	0.666870	1.248616	-0.558870	-0.082573	CT
C	0.684026	-1.254093	-2.082284	0.014212	CT
C	0.684026	1.254093	-2.082284	0.014212	CT
H	-1.048740	0.000000	-0.348408	-0.065674	HC
H	1.024587	0.000000	1.887566	0.074786	HC
H	-0.500052	0.881908	1.915044	0.083701	HC
H	-0.500052	-0.881908	1.915044	0.083701	HC
H	1.695615	-1.280550	-0.185783	0.012436	HC
H	1.695615	1.280550	-0.185783	0.012436	HC
H	0.166131	-2.140848	-0.178694	-0.004010	HC
H	0.166131	2.140848	-0.178694	-0.004010	HC
H	-0.343861	-1.294805	-2.451662	-0.007780	HC
H	-0.343861	1.294805	-2.451662	-0.007780	HC
H	1.188083	-2.147172	-2.452139	-0.007030	HC
H	1.188083	2.147172	-2.452139	-0.007030	HC
H	2.408904	0.000000	-2.319513	-0.007010	HC
H	1.344001	0.000000	-3.713130	-0.015247	HC

Methylcyclopentane

Atom	x	y	z	Charge	Type
C	-0.779677	-0.910793	-2.118116	0.003357	CT
C	-1.189250	-0.729419	-0.640371	-0.023951	CT
C	0.000000	0.007007	-0.004948	0.334599	CT
C	1.189250	-0.729419	-0.640371	-0.023951	CT
C	0.779677	-0.910793	-2.118116	0.003357	CT
C	0.000000	0.017761	1.520947	-0.389917	CT
H	1.160972	-0.069950	-2.722376	-0.007930	HC
H	-1.160972	-0.069950	-2.722376	-0.007930	HC
H	1.199706	-1.832489	-2.553209	-0.006949	HC
H	-1.199706	-1.832489	-2.553209	-0.006949	HC
H	-2.147957	-0.196869	-0.518915	-0.021284	HC
H	2.147957	-0.196869	-0.518915	-0.021284	HC
H	1.291963	-1.714909	-0.146331	-0.003203	HC
H	-1.291963	-1.714909	-0.146331	-0.003203	HC
H	0.000000	1.051894	-0.378466	-0.059963	HC
H	0.000000	-1.015633	1.911722	0.075545	HC
H	-0.891943	0.530859	1.919509	0.079828	HC
H	0.891943	0.530859	1.919509	0.079828	HC

Methylpropane

Atom	x	y	z	Charge	Type
C	0.000000	0.000018	0.384134	0.562835	CT
H	0.000000	0.000018	1.477238	-0.109575	HC
C	0.000000	1.446675	-0.094632	-0.311953	CT
C	1.252842	-0.723311	-0.094632	-0.311953	CT
C	-1.252842	-0.723311	-0.094632	-0.311953	CT
H	0.000000	1.481857	-1.185527	0.055682	HC
H	1.283311	-0.740902	-1.185527	0.055682	HC
H	-1.283311	-0.740902	-1.185527	0.055682	HC
H	0.882320	1.981159	0.256668	0.052592	HC
H	-0.882320	1.981159	0.256668	0.052592	HC
H	1.274558	-1.754664	0.256668	0.052592	HC
H	2.156878	-0.226441	0.256668	0.052592	HC
H	-2.156878	-0.226441	0.256668	0.052592	HC
H	-1.274558	-1.754664	0.256668	0.052592	HC

Methylpropene

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.120317	0.316559	CT
C	0.000000	0.000000	1.456701	-0.641536	CT
H	0.000000	0.924762	2.016730	0.200880	HC
H	0.000000	-0.924762	2.016730	0.200880	HC
C	0.000000	1.270608	-0.675799	-0.231644	CT
C	0.000000	-1.270608	-0.675799	-0.231644	CT
H	0.000000	2.146982	-0.031615	0.063420	HC
H	0.876212	1.317574	-1.324637	0.064917	HC
H	-0.876212	1.317574	-1.324637	0.064917	HC
H	0.000000	-2.146982	-0.031615	0.063420	HC
H	-0.876212	-1.317574	-1.324637	0.064917	HC
H	0.876212	-1.317574	-1.324637	0.064917	HC

Nitrogen

Atom	x	y	z	Charge	Type
N	0.565350	0.000000	0.000000	0.000000	N
N	-0.565350	0.000000	0.000000	0.000000	N

Oxetane

Atom	x	y	z	Charge	Type
O	-0.009454	0.000000	0.000000	-0.580131	O
C	1.002562	-1.033034	0.000000	0.520816	CT
C	1.002562	1.033034	0.000000	0.520816	CT
C	2.138670	0.000000	0.000000	-0.376991	CT
H	0.934925	1.659427	0.889132	-0.059820	HC
H	0.934925	1.659427	-0.889132	-0.059820	HC
H	0.934925	-1.659427	0.889132	-0.059820	HC
H	0.934925	-1.659427	-0.889132	-0.059820	HC
H	2.762979	0.000000	0.887341	0.077384	HC
H	2.762979	0.000000	-0.887341	0.077384	HC

Propane

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	0.592517	0.324164	CT
C	0.000000	1.262458	-0.259240	-0.197189	CT
C	0.000000	-1.262458	-0.259240	-0.197189	CT
H	0.873520	0.000000	1.245962	-0.066705	HC
H	-0.873520	0.000000	1.245962	-0.066705	HC
H	0.000000	2.162702	0.353058	0.028922	HC
H	0.000000	-2.162702	0.353058	0.028922	HC
H	0.879491	1.294409	-0.902194	0.036445	HC
H	-0.879491	1.294409	-0.902194	0.036445	HC
H	-0.879491	-1.294409	-0.902194	0.036445	HC
H	0.879491	-1.294409	-0.902194	0.036445	HC

Pyridine

Atom	x	y	z	Charge	Type
C	0.000000	0.000000	2.802669	0.249562	CA
C	1.193985	0.000000	2.089257	-0.457479	CA
C	1.141136	0.000000	0.697788	0.469781	CA
N	0.000000	0.000000	-0.004678	-0.663730	NC
C	-1.141136	0.000000	0.697788	0.469781	CA
C	-1.193985	0.000000	2.089257	-0.457479	CA
H	0.000000	0.000000	3.883865	0.061025	HA
H	2.148613	0.000000	2.595560	0.152003	HA
H	-2.148613	0.000000	2.595560	0.152003	HA
H	2.054614	0.000000	0.116239	0.012266	HA
H	-2.054614	0.000000	0.116239	0.012266	HA

Pyrrole

Atom	x	y	z	Charge	Type
H	0.000000	0.000000	0.001946	0.286700	HA
N	0.000000	0.000000	1.005902	-0.146060	NA
C	1.122127	0.000000	1.788750	-0.207229	CW
C	-1.122127	0.000000	1.788750	-0.207229	CW
C	0.708001	0.000000	3.107458	-0.132305	C$*$
C	-0.708001	0.000000	3.107458	-0.132305	C$*$
H	-2.105430	0.000000	1.353810	0.158444	HA
H	2.105430	0.000000	1.353810	0.158444	HA
H	1.356438	0.000000	3.966079	0.110769	HA
H	-1.356438	0.000000	3.966079	0.110769	HA

Sulfur hexafluoride

Atom	x	y	z	Charge	Type
S	0.000000	0.000000	0.000000	0.928914	S
F	0.000000	0.000000	1.571975	-0.154819	F
F	0.000000	1.571975	0.000000	-0.154819	F
F	1.571975	0.000000	0.000000	-0.154819	F
F	0.000000	-1.571975	0.000000	-0.154819	F
F	-1.571975	0.000000	0.000000	-0.154819	F
F	0.000000	0.000000	-1.571975	-0.154819	F

trans-1,2-dimethylcyclohexane

Atom	x	y	z	Charge	Type
C	2.204742	-1.237487	0.009852	0.336491	CT
C	0.769710	-1.237389	-0.530446	0.336491	CT
C	-0.002938	-0.033908	0.009438	-0.075338	CT
C	-0.001827	0.019253	1.532288	0.004880	CT
C	1.425660	0.025237	2.066025	0.004880	CT
C	2.199118	-1.176472	1.537290	-0.075338	CT
C	0.720615	-1.249426	-2.053874	-0.399189	CT
C	3.005004	-2.445908	-0.462047	-0.399189	CT
H	3.991294	-2.457744	0.002445	0.079256	HC
H	2.494323	-3.369423	-0.181445	0.065239	HC
H	3.146606	-2.453640	-1.540933	0.083441	HC
H	1.744269	-2.097070	1.919583	-0.001040	HC
H	3.227900	-1.159366	1.904160	-0.001163	HC
H	0.281859	-2.146820	-0.156039	-0.077889	HC
H	1.925264	0.943776	1.744438	-0.013564	HC
H	0.456662	0.878971	-0.385476	-0.001040	HC
H	1.427553	0.028394	3.157143	-0.001123	HC
H	-1.026770	-0.059057	-0.370582	-0.001163	HC
H	-0.527341	-0.857190	1.922698	-0.013564	HC
H	-0.546287	0.897630	1.882389	-0.001123	HC
H	2.691697	-0.326600	-0.362176	-0.077889	HC
H	-0.308366	-1.168228	-2.404964	0.079256	HC
H	1.277003	-0.400175	-2.455888	0.065239	HC
H	1.143725	-2.159212	-2.475035	0.083441	HC

trans-1,2-dimethylcyclopentane

Atom	x	y	z	Charge	Type
C	0.936795	0.000000	0.000000	0.032833	CT
C	0.000000	0.000000	-1.228390	-0.098868	CT
C	-1.385700	0.349000	-0.680800	0.318530	CT
C	-1.385700	-0.349000	0.680800	0.318530	CT
C	0.000000	0.000000	1.228390	-0.098868	CT
C	-2.526130	-0.047500	-1.600900	-0.382418	CT
C	-2.526130	0.047500	1.600900	-0.382418	CT
H	-0.045550	0.998900	1.668500	0.003443	HC
H	0.326400	-0.682300	2.012500	0.002803	HC
H	0.326400	0.682300	-2.012500	0.002803	HC
H	-0.045550	-0.998900	-1.668500	0.003443	HC
H	1.585300	-0.874300	-0.004945	-0.010199	HC
H	1.585300	0.874300	0.004945	-0.010199	HC
H	-1.428500	1.428700	-0.491600	-0.070581	HC
H	-1.428500	-1.428700	0.491600	-0.070581	HC
H	-2.438100	0.439000	-2.572210	0.075727	HC
H	-2.516500	-1.126300	-1.766190	0.069770	HC
H	-2.516500	1.126300	1.766190	0.069770	HC
H	-2.438100	-0.439000	2.572210	0.075727	HC
H	-3.495600	0.220500	-1.182280	0.075376	HC
H	-3.495600	-0.220500	1.182280	0.075376	HC

Tetrahydrofuran

Atom	x	y	z	Charge	Type
O	0.011551	0.000000	-0.037731	-0.481481	OS
C	0.600697	1.119263	0.608587	0.250261	CT
C	0.600697	-1.119263	0.608587	0.250261	CT
C	2.087263	0.772643	0.751370	-0.022186	CT
C	2.087263	-0.772643	0.751370	-0.022186	CT
H	0.407355	1.998513	0.000585	-0.000288	HC
H	0.144100	1.261659	1.595041	-0.009630	HC
H	0.407355	-1.998513	0.000585	-0.000288	HC
H	0.144100	-1.261659	1.595041	-0.009630	HC
H	2.650040	1.156376	-0.095615	-0.009206	HC
H	2.514770	1.192472	1.658898	0.031789	HC
H	2.650040	-1.156376	-0.095615	-0.009206	HC
H	2.514770	-1.192472	1.658898	0.031789	HC

Tetramethylbutane

Atom	x	y	z	Charge	Type
C	-1.237931	-1.330052	0.716987	-0.337006	CT
C	1.237931	-1.330052	0.716987	-0.337006	CT
C	0.000000	-0.783004	-0.003479	0.579255	CT
C	0.000000	0.783004	0.003479	0.579255	CT
C	-1.237931	1.330052	-0.716987	-0.337006	CT
C	1.237931	1.330052	-0.716987	-0.337006	CT
H	-1.188340	-2.419592	0.741862	0.060792	HC
H	1.188340	-2.419592	0.741862	0.060792	HC
H	-1.188340	2.419592	-0.741862	0.060792	HC
H	1.188340	2.419592	-0.741862	0.060792	HC
H	-1.308330	-0.979754	1.746259	0.039627	HC
H	1.308330	0.979754	-1.746259	0.039627	HC
H	1.308330	-0.979754	1.746259	0.039627	HC
H	-1.308330	0.979754	-1.746259	0.039627	HC
H	-2.156594	-1.057776	0.199458	0.048223	HC
H	2.156594	-1.057776	0.199458	0.048223	HC
H	-2.156594	1.057776	-0.199458	0.048223	HC
H	2.156594	1.057776	-0.199458	0.048223	HC
C	0.000000	-1.343426	-1.448200	-0.429157	CT
H	-0.877221	-1.963947	-1.629332	0.071411	HC
H	0.877221	-1.963947	-1.629332	0.071411	HC
H	0.000000	-0.565270	-2.207024	0.083808	HC
C	0.000000	1.343426	1.448200	-0.429157	CT
H	-0.877221	1.963947	1.629332	0.071411	HC
H	0.877221	1.963947	1.629332	0.071411	HC
H	0.000000	0.565270	2.207024	0.083808	HC

Trimethylbutane

Atom	x	y	z	Charge	Type
C	-0.036994	0.011114	0.125091	-0.365783	CT
C	0.794262	-0.849762	-0.829635	0.628921	CT
C	0.327862	-0.603268	-2.282011	-0.394423	CT
C	2.296160	-0.521537	-0.640640	0.363383	CT
C	0.544060	-2.313102	-0.455963	-0.365783	CT
H	-1.085302	-0.287199	0.078946	0.064785	HC
H	0.303166	-0.109418	1.155619	0.046311	HC
H	0.014935	1.067801	-0.131685	0.064820	HC
H	-0.469310	0.138438	-2.322256	0.061791	HC
H	1.131412	-0.242460	-2.921695	0.072708	HC
H	-0.055561	-1.516563	-2.736006	0.061791	HC
H	-0.525481	-2.526486	-0.480876	0.064785	HC
H	1.031326	-2.997768	-1.148077	0.064820	HC
H	0.907357	-2.526186	0.551427	0.046311	HC
C	2.627375	0.946868	-0.900156	-0.336455	CT
C	3.214362	-1.401083	-1.487143	-0.336455	CT
H	2.387262	1.230131	-1.925727	0.055613	HC
H	2.092954	1.617582	-0.231095	0.049725	HC
H	3.693905	1.119736	-0.756629	0.070015	HC
H	2.517502	-0.729482	0.412483	-0.092231	HC
H	3.012871	-1.272306	-2.551336	0.055613	HC
H	4.255167	-1.125313	-1.317891	0.070015	HC
H	3.111756	-2.457630	-1.249898	0.049725	HC