Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Effect of hindered internal rotation treatments on predicting thermodynamic properties of alkanes.

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Content

1. The Cartetian coordinates, and symmetry numbers for all the molecules we studied at the B3LYP/6-31G (d) level.

Table S1 The Cartetian coordinates (coordinate units: Angstrom), and symmetry numbers (σ) for all the molecules we studied at the B3LYP/6-31G (d) level.(Mirror image=0 means that this structure has no mirror image structure, and Mirror image=1 means this structure has a mirror image structure but only one structure is presented here.)

butane

Structure 1			σ=2	Mirror image=0	Structure 2			σ=2	Mirror image=1
C	-0.70484	1.83073		0.00000	C	0.58807	1.46363		-0.55952
H	-1.72385	2.23366		0.00000	H	1.41260	2.18133		-0.48364
H	-0.18962	2.22489		0.88453	H	0.69655	0.93799		-1.51450
H	-0.18962	2.22489		-0.88453	H	-0.34844	2.03403		-0.59956
C	-0.70484	0.30026		0.00000	C	0.58807	0.49382		0.62622
H	-1.25361	-0.06854		-0.87815	H	0.56623	1.07034		1.56061
H	-1.25361	-0.06854		0.87815	H	1.53144	-0.07067		0.63690
C	0.70484	-0.30026		0.00000	C	-0.58807	-0.49382		0.62622
C	0.70484	-1.83073		0.00000	C	-0.58807	-1.46363		-0.55952
H	1.25361	0.06854		0.87815	H	-1.53144	0.07067		0.63690
H	1.25361	0.06854		-0.87815	H	-0.56623	-1.07034		1.56061
H	1.72385	-2.23366		0.00000	H	-1.41260	-2.18133		-0.48364
H	0.18962	-2.22489		0.88453	H	-0.69655	-0.93799		-1.51450
H	0.18962	-2.22489		-0.88453	H	0.34844	-2.03403		-0.59956

pentane

Structure 1			σ=2	Mirror image=0	Structure 2			σ=1	Mirror image=1
C	0.00000	2.55438		0.32470	C	2.43994	-0.17503		0.12501
H	0.00000	3.45480		-0.29983	H	3.09676	-0.94186		-0.30085
H	-0.88449	2.59650		0.97203	H	2.83017	0.80491		-0.17598
H	0.88449	2.59650		0.97203	H	2.51664	-0.23873		1.21740
C	0.00000	1.28092		-0.52437	C	0.99129	-0.35603		-0.33535
H	0.87812	1.27933		-1.18540	H	0.64478	-1.35821		-0.05253
H	-0.87812	1.27933		-1.18540	H	0.94542	-0.31491		-1.43311
C	0.00000	0.00000		0.31555	C	0.04895	0.70445		0.24559

H	-0.87845	0.00000	0.97793	H	0.44339	1.69994	-0.00293
H	0.87845	0.00000	0.97793	H	0.06302	0.63685	1.34375
C	0.00000	-1.28092	-0.52437	C	1.40130	0.60562	-0.24854
C	0.00000	-2.55438	0.32470	C	2.11907	-0.68038	0.17359
H	0.87812	-1.27933	-1.18540	H	1.41492	0.68927	-1.34457
H	-0.87812	-1.27933	-1.18540	H	1.96340	1.46957	0.13009
H	0.00000	-3.45480	-0.29983	H	3.16591	-0.67347	-0.15014
H	0.88449	-2.59650	0.97203	H	1.64712	-1.56986	-0.25765
H	-0.88449	-2.59650	0.97203	H	2.10767	-0.79531	1.26474
Structure 3		σ=2	Mirror image=1	Structure 4		σ=1	Mirror image=1
C	0.00000	1.88251	-0.69044	C	1.80845	0.79861	0.15046
H	0.62762	2.62510	-1.19569	H	2.67773	1.11066	-0.44004
H	-0.50407	1.29537	-1.46617	H	1.09606	1.62881	0.15820
H	-0.77341	2.42343	-0.13088	H	2.14567	0.64612	1.18304
C	0.83279	0.99573	0.24004	C	1.19276	-0.48841	-0.41136
H	1.39711	1.63207	0.93440	H	1.97154	-1.26186	-0.42098
H	1.58449	0.45381	-0.34853	H	0.90915	-0.33701	-1.46268
C	0.00000	0.00000	1.06237	C	-0.02613	-1.01545	0.37413
H	-0.67461	0.56387	1.72217	H	0.09781	-0.77272	1.43978
H	0.67461	-0.56387	1.72217	H	-0.04056	-2.11160	0.31523
C	-0.83279	-0.99573	0.24004	C	-1.39481	-0.50911	-0.10814
C	0.00000	-1.88251	-0.69044	C	-1.60502	1.00554	-0.02264
H	-1.58449	-0.45381	-0.34853	H	-2.17469	-1.01016	0.48117
H	-1.39711	-1.63207	0.93440	H	-1.54489	-0.83426	-1.14752
H	-0.62762	-2.62510	-1.19569	H	-2.63408	1.27293	-0.28885
H	0.50407	-1.29537	-1.46617	H	-1.41523	1.37602	0.99223
H	0.77341	-2.42343	-0.13088	H	-0.94001	1.54600	-0.70434

2-methylbutane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=0
C	2.09213	-0.03638	-0.10839	C	-0.35380	-1.83869	0.00000
H	2.20770	-0.00068	-1.19887	H	-0.98877	-1.71825	0.88456
H	2.93523	-0.60703	0.29676	H	0.01665	-2.86983	0.00000
H	2.17847	0.98852	0.26794	H	-0.98877	-1.71825	-0.88456
C	0.75699	-0.67697	0.28110	C	0.81424	-0.84623	0.00000
H	0.65347	-0.67613	1.37634	H	1.44567	-1.03884	-0.87837
H	0.76556	-1.73287	-0.02249	H	1.44567	-1.03884	0.87837
C	-0.48248	-0.00295	-0.33373	C	-0.42011	0.64551	0.00000

H	0.35302	-0.00409	-1.42729	H	1.36214	1.21364	0.00000
C	-1.74732	-0.80637	-0.00656	C	0.35380	1.04304	-1.26406
H	-1.91986	-0.83478	1.07725	H	1.33525	0.55607	-1.30293
H	-2.63436	-0.36136	-0.47223	H	0.52455	2.12544	-1.29396
H	-1.66484	-1.84173	-0.35769	H	-0.19461	0.76369	-2.17172
C	-0.63849	1.45355	0.12227	C	0.35380	1.04304	1.26406
H	-0.73343	1.50839	1.21484	H	1.33525	0.55607	1.30293
H	-0.21740	2.07030	-0.17048	H	-0.19461	0.76369	2.17172
H	-1.53732	1.90621	-0.31227	H	0.52455	2.12544	1.29396

hexane

Structure 1		σ=2	Mirror image=0	Structure 2		σ=1	Mirror image=1
C	-1.41527	2.89580	0.00000	C	-2.97340	0.53760	0.11282
H	-2.43440	3.29848	0.00000	H	-3.94101	0.16137	-0.23785
H	-0.90004	3.28995	0.88449	H	-3.03729	0.66159	1.20080
H	-0.90004	3.28995	-0.88449	H	-2.82335	1.53250	-0.32403
C	-1.41527	1.36524	0.00000	C	-1.83116	-0.40776	-0.26677
H	-1.96431	0.99712	-0.87808	H	-1.80892	-0.53843	-1.35788
H	-1.96431	0.99712	0.87808	H	-2.02242	-1.40463	0.15476
C-	-0.00567	0.76560	0.00000	C	-0.46106	0.08626	0.20849
H	0.54480	1.13371	0.87843	H	-0.47903	0.21020	1.30177
H-	0.54480	1.13371	-0.87843	H	-0.27945	1.08627	-0.20807
C-	0.00567	-0.76560	0.00000	C	0.68488	-0.85671	-0.17373
H-	-0.54480	-1.13371	-0.87843	H	0.72971	-0.94547	-1.26943
H-	-0.54480	-1.13371	0.87843	H	0.45514	-1.86297	0.20407
C-	1.41527	-1.36524	0.00000	C	2.06172	-0.42933	0.35462
C-	1.41527	-2.89580	0.00000	C	2.56790	0.89667	-0.22199
H-	1.96431	-0.99712	0.87808	H	2.78889	-1.21968	0.12589
H-	1.96431	-0.99712	-0.87808	H	2.02118	-0.35966	1.45093
H	2.43440	-3.29848	0.00000	H	3.57770	1.12437	0.13741
H	0.90004	-3.28995	0.88449	H	2.60404	0.85897	-1.31801
H	0.90004	-3.28995	-0.88449	H	1.92151	1.73516	0.05903

Structure 3		σ=2	Mirror image=1	Structure 4		σ=1	Mirror image=1
C	-0.70339	2.95414	-0.32351	C	2.76374	-0.47521	0.11872
H	-1.22710	3.40558	-1.17364	H	3.18008	-1.47978	-0.01646
H	-1.19634	3.29755	0.59424	H	3.29706	0.20266	-0.55890
H	0.32040	3.34789	-0.31461	H	2.98560	-0.15699	1.14482
C	-0.70339	1.42586	-0.40964	C	1.25680	-0.44950	-0.15066

H	-0.23889	1.11696	-1.35471	H	0.76085	-1.16742	0.51419
H	-1.73907	1.05836	-0.44347	H	1.05912	-0.79179	-1.17623
C	0.02376	0.76702	0.76846	C	0.65065	0.94444	0.04645
H	-0.41720	1.13700	1.70487	H	1.23525	1.66589	-0.54254
H	1.07301	1.09792	0.77544	H	0.77862	1.24062	1.09831
C	-0.02376	-0.76702	0.76846	C	0.83009	1.09439	-0.33541
H	-1.07301	-1.09792	0.77544	H	0.95380	0.88514	-1.40809
H	0.41720	-1.13700	1.70487	H	1.09893	2.15044	-0.20294
C	0.70339	-1.42586	-0.40964	C	1.81768	0.22337	0.46841
C	0.70339	-2.95414	-0.32351	C	2.10336	-1.15256	-0.14486
H	1.73907	-1.05836	-0.44347	H	2.77123	0.75927	0.55998
H	0.23889	-1.11696	-1.35471	H	1.44261	0.10280	1.49473
H	1.22710	-3.40558	-1.17364	H	2.82323	-1.71346	0.46251
H	1.19634	-3.29755	0.59424	H	2.52860	-1.04607	-1.15035
H	-0.32040	-3.34789	-0.31461	H	1.19859	-1.76096	-0.23494
Structure 5		σ=1	Mirror image=1	Structure 6		σ=1	Mirror image=0
C	-2.75059	-0.51583	-0.03413	C	2.74035	-0.49260	-0.08704
H	-3.36107	-0.96078	0.75968	H	3.76464	-0.30314	0.25311
H	-3.31413	0.32357	-0.45949	H	2.38604	-1.39444	0.42375
H	-2.63175	-1.26693	-0.82475	H	2.78073	-0.71417	-1.16092
C	-1.38979	-0.05439	0.49341	C	1.83534	0.71237	0.18895
H	-0.86983	-0.90810	0.94718	H	2.28382	1.60614	-0.26470
H	-1.53531	0.67777	1.30057	H	1.80112	0.90428	1.27084
C	-0.51232	0.56722	-0.59859	C	0.40154	0.55778	-0.33984
H	-1.07323	1.37744	-1.08530	H	0.43387	0.36861	-1.42354
H	-0.32894	-0.18106	-1.38194	H	0.12188	1.51372	-0.21201
C	0.82320	1.13320	-0.09304	C	0.40154	-0.55778	0.33984
H	0.61733	1.95081	0.61214	H	0.43387	-0.36861	1.42354
H	1.35701	1.58645	-0.94029	H	0.12188	-1.51372	0.21201
C	1.75241	0.11613	0.58815	C	1.83534	-0.71237	-0.18895
C	2.14996	-1.05980	-0.30886	C	2.74035	0.49260	0.08704
H	1.27877	-0.26592	1.50177	H	2.28382	-1.60614	0.26470
H	2.65896	0.64113	0.91692	H	1.80112	-0.90428	-1.27084
H	2.87158	-1.71400	0.19301	H	3.76464	0.30314	-0.25311
H	1.28350	-1.67295	-0.58082	H	2.78073	0.71417	1.16092
H	2.60990	-0.70669	-1.24032	H	2.38604	1.39444	-0.42375
Structure 7		σ=2	Mirror image=1	Structure 8		σ=1	Mirror image=1

C	0.06460	2.53356	0.75142	C	1.90882	0.96805	0.45962
H	0.14541	3.62373	0.67594	H	2.49571	1.80663	0.06828
H	-0.99857	2.28761	0.84657	H	1.06126	1.38749	1.01177
H	0.56030	2.22532	1.68056	H	2.53680	0.42759	1.17888
C	0.70012	1.84637	-0.46145	C	1.44905	0.04035	-0.66844
H	1.73582	2.19520	-0.56843	H	2.32708	-0.28688	-1.24136
H	0.17585	2.15968	-1.37548	H	0.82357	0.59826	-1.37652
C	0.70012	0.31303	-0.38097	C	0.70169	-1.21075	-0.18319
H	1.24658	0.00496	0.52089	H	1.38721	-1.80141	0.44162
H	1.26534	-0.08919	-1.23404	H	0.46749	-1.83924	-1.05415
C	-0.70012	-0.31303	-0.38097	C	0.59625	-0.98479	0.61110
H	-1.26534	0.08919	-1.23404	H	0.38455	-0.41909	1.52884
H	-1.24658	-0.00496	0.52089	H	0.94248	-1.97140	0.94579
C	-0.70012	-1.84637	-0.46145	C	1.74334	-0.29900	-0.15782
C	-0.06460	-2.53356	0.75142	C	1.73860	1.23364	-0.10848
H	-0.17585	-2.15968	-1.37548	H	2.69890	-0.64673	0.25599
H	-1.73582	-2.19520	-0.56843	H	1.73002	-0.63605	-1.20417
H	-0.14541	-3.62373	0.67594	H	2.61291	1.64484	-0.62631
H	0.99857	-2.28761	0.84657	H	1.77133	1.58801	0.92917
H	-0.56030	-2.22532	1.68056	H	0.84715	1.66304	-0.57457

Structure 9		σ=2	Mirror image=1	Structure 10		σ=1	Mirror image=1
C	0.76265	2.24667	-0.51408	C	-1.85133	1.28616	0.00908
H	1.24687	2.75732	-1.35396	H	-2.74249	1.83307	-0.31954
H	-0.31417	2.22958	-0.71551	H	-1.69732	1.50598	1.07265
H	0.92095	2.85641	0.38425	H	-0.99614	1.69213	-0.54173
C	1.32597	0.83503	-0.32549	C	-2.01426	-0.21795	-0.22797
H	2.41771	0.89324	-0.22420	H	-2.12956	-0.40087	-1.30580
H	1.13981	0.24449	-1.23237	H	-2.95056	-0.55323	0.23824
C	0.76265	0.09752	0.89881	C	-0.86780	-1.09448	0.30076
H	1.04123	0.65238	1.80574	H	-1.13770	-2.14195	0.11458
H	1.25545	-0.87993	0.98062	H	-0.80372	-0.99024	1.39379
C	-0.76265	-0.09752	0.89881	C	0.51624	-0.81125	-0.31866
H	-1.25545	0.87993	0.98062	H	0.38878	-0.45157	-1.35066
H	-1.04123	-0.65238	1.80574	H	1.07779	-1.75195	-0.39973
C	-1.32597	-0.83503	-0.32549	C	1.38012	0.18518	0.46619
C	-0.76265	-2.24667	-0.51408	C	2.73102	0.45004	-0.20237
H	-1.13981	-0.24449	-1.23237	H	1.54179	-0.20990	1.47896
H	-2.41771	-0.89324	-0.22420	H	0.84350	1.13246	0.59413

H	-1.24687	-2.75732	-1.35396	H	3.34104	1.14648	0.38388
H	0.31417	-2.22958	-0.71551	H	3.30277	-0.47891	-0.31920
H	-0.92095	-2.85641	0.38425	H	2.59786	0.88239	-1.20174

Structure 11		σ=2	Mirror image=1
C	0.06383	1.78905	-1.14535
H	-0.52661	2.24794	-1.94693
H	0.82972	2.51259	-0.84059
H	0.58245	0.92406	-1.56898
C	-0.82134	1.41136	0.04817
H	-1.63093	0.74438	-0.27747
H	-1.31431	2.32541	0.40399
C	-0.06383	0.76677	1.22718
H	-0.56814	1.04535	2.16194
H	0.94128	1.20951	1.28806
C	0.06383	-0.76677	1.22718
H	-0.94128	-1.20951	1.28806
H	0.56814	-1.04535	2.16194
C	0.82134	-1.41136	0.04817
C	-0.06383	-1.78905	-1.14535
H	1.31431	-2.32541	0.40399
H	1.63093	-0.74438	-0.27747
H	0.52661	-2.24794	-1.94693
H	-0.82972	-2.51259	-0.84059
H	-0.58245	-0.92406	-1.56898

2-methylpentane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=0
C	-1.49043	0.36711	-0.28978	C	-1.32192	0.25496	0.00000
C	-2.83672	-0.21838	0.14439	C	-2.38532	1.35669	0.00000
H	-1.46907	0.46795	-1.38432	H	-1.46724	-0.38729	0.87800
H	-1.39254	1.38299	0.11301	H	-1.46724	-0.38729	-0.87800
H	-2.89358	-0.30729	1.23621	H	-2.28826	1.99829	-0.88440
H	-3.67298	0.40934	-0.18336	H	-3.39817	0.93840	0.00000
H	-2.98532	-1.22058	-0.27586	H	-2.28826	1.99829	0.88440
C	-0.30275	-0.49079	0.15951	C	0.10240	0.82387	0.00000
C	1.07279	-0.01453	-0.33817	C	1.24601	-0.21114	0.00000
H	-0.46352	-1.52167	-0.18836	H	0.21986	1.47505	0.87853
H	-0.28647	-0.54149	1.25921	H	0.21986	1.47505	-0.87853

H	1.02790	0.04269	-1.43683	H	2.18291	0.36535	0.00000
C	2.15942	-1.02995	0.03726	C	1.24601	-1.08113	-1.26432
H	3.14004	-0.72456	-0.34603	H	2.13261	-1.72505	-1.29570
H	2.24324	-1.12375	1.12782	H	0.36608	-1.73385	-1.30211
H	1.93349	-2.02412	-0.36592	H	1.24500	-0.46538	-2.17175
C	1.43441	1.37868	0.19336	C	1.24601	-1.08113	1.26432
H	0.71972	2.14156	-0.13186	H	1.24500	-0.46538	2.17175
H	1.45089	1.38104	1.29128	H	0.36608	-1.73385	1.30211
H	2.42786	1.68499	-0.15437	H	2.13261	-1.72505	1.29570
Structure 3		σ=1	Mirror image=1	Structure 4		σ=1	Mirror image=1
C	-1.59658	-0.09119	0.63663	C	1.48945	-0.62924	0.11307
C	-2.28203	0.04002	-0.72678	C	1.96306	0.65605	-0.57376
H	-1.53669	0.89609	1.11238	H	1.30429	-1.39951	-0.64677
H	-2.22462	-0.70389	1.29674	H	2.31077	-1.01600	0.73130
H	-2.33605	-0.93090	-1.23495	H	2.06214	1.47760	0.14608
H	-3.30468	0.41884	-0.62048	H	2.94083	0.50618	-1.04604
H	-1.74289	0.72818	-1.38725	H	1.27058	0.98271	-1.35542
C	-0.19972	-0.72679	0.57474	C	0.25787	-0.49871	1.02560
C	0.83891	0.00788	-0.29245	C	-1.09708	-0.11397	0.38547
H	-0.29799	-1.75645	0.20090	H	0.48306	0.22121	1.82576
H	0.19863	-0.81003	1.59685	H	0.12286	-1.46927	1.52319
H	0.46725	0.03247	-1.32684	H	-1.85938	-0.36926	1.13661
C	2.16457	-0.76374	-0.29510	C	-1.40616	-0.93952	-0.86991
H	2.90468	-0.28255	-0.94511	H	-2.42692	-0.74870	-1.22086
H	2.58962	-0.81056	0.71600	H	-0.72448	-0.68896	-1.69130
H	2.02599	-1.79335	-0.64560	H	-1.31309	-2.01482	-0.67564
C	1.05767	1.45512	0.16584	C	-1.25236	1.38945	0.11085
H	0.14390	2.05356	0.08714	H	-1.02180	1.98048	1.00504
H	1.38746	1.48504	1.21270	H	-0.59514	1.73316	-0.69337
H	1.82851	1.94570	-0.43978	H	-2.28232	1.62081	-0.18649
Structure 5		σ=1	Mirror image=1				
C	1.54026	-0.58809	-0.45855				
C	2.40213	0.36478	0.37805				
H	1.41101	-0.18056	-1.47113				
H	2.09457	-1.52671	-0.58504				
H	2.59564	-0.06106	1.37014				
H	3.37141	0.54572	-0.10095				

H	1.91792	1.33469	0.52730
C	0.15579	-0.89871	0.14849
C	-1.00763	-0.02303	-0.35345
H	0.21286	-0.82336	1.24502
H	-0.10458	-1.94368	-0.06583
H	-1.08013	-0.17145	-1.44211
C	-0.79286	1.47460	-0.10263
H	-1.66072	2.05338	-0.44031
H	-0.65411	1.67618	0.96743
H	0.08491	1.85616	-0.63357
C	-2.32859	-0.48695	0.27333
H	-2.51455	-1.54904	0.07462
H	-2.31089	-0.34996	1.36238
H	-3.17801	0.08403	-0.11939

3-methylpentane

Structure 1		σ=1	Mirror image=0	Structure 2		σ=1	Mirror image=1
C	0.30957	-0.67946	1.26127	C	0.80130	-0.75992	0.37549
C	0.30957	0.10145	2.57857	C	2.23567	-0.90193	-0.14326
H	-0.47087	-1.45406	1.29306	H	0.81679	-0.61009	1.46543
H	1.26449	-1.21443	1.16636	H	0.27585	-1.70724	0.20536
H	1.06081	0.90089	2.56140	H	2.24902	-1.01230	-1.23484
H	-0.66213	0.56373	2.78185	H	2.85213	-0.03309	0.10973
H	0.54278	-0.55577	3.42377	H	2.72169	-1.78537	0.28569
C	0.10615	0.18012	0.00000	C	-0.00173	0.38511	-0.26818
C	0.30957	-0.67946	-1.26127	C	-1.46442	0.40195	0.21505
H	0.88510	0.95993	0.00000	H	-0.01348	0.21318	-1.35682
H	1.26449	-1.21443	-1.16636	H	-1.47636	0.53416	1.30707
H	-0.47087	-1.45406	-1.29306	H	-1.95526	1.29171	-0.20221
C	0.30957	0.10145	-2.57857	C	-2.28575	-0.83472	-0.16179
H	1.06081	0.90089	-2.56140	H	-1.91407	-1.74158	0.32647
H	0.54278	-0.55577	-3.42377	H	-3.33428	-0.71186	0.13175
H	-0.66213	0.56373	-2.78185	H	-2.26148	-1.00693	-1.24508
C	-1.26129	0.87610	0.00000	C	0.64892	1.75118	-0.01200
H	-2.07080	0.13395	0.00000	H	0.71795	1.95161	1.06539
H	-1.39170	1.51211	0.88117	H	1.65970	1.81069	-0.42752
H	-1.39170	1.51211	-0.88117	H	0.05785	2.55705	-0.46236

Structure 3	σ=1	Mirror image=1	Structure 4	σ=1	Mirror image=1

C	-0.95361	-0.76529	-0.12248	C	-0.98766	0.98012	0.13937
C	-2.44427	-0.41439	-0.09943	C	-0.00584	2.14213	-0.03115
H	-0.64070	-0.94241	-1.16032	H	-1.89583	1.19488	-0.44045
H	-0.80207	-1.71525	0.40905	H	-1.30594	0.92839	1.19121
H	-2.78593	-0.21611	0.92413	H	0.86152	2.04167	0.62957
H	-2.66234	0.47542	-0.69980	H	0.36413	2.20309	-1.06184
H	-3.04888	-1.23623	-0.49907	H	-0.48908	3.09679	0.20594
C	-0.04437	0.30263	0.51306	C	-0.46689	-0.40823	-0.27837
C	1.39537	-0.21540	0.71295	C	0.80645	-0.83973	0.48926
H	-0.44204	0.50704	1.51938	H	-0.21673	-0.36423	-1.34996
H	1.96492	0.54507	1.26474	H	0.79018	-0.39748	1.49567
H	1.35957	-1.10126	1.36205	H	0.77882	-1.92660	0.64251
C	2.15447	-0.56997	-0.57077	C	2.12483	-0.49402	-0.21209
H	2.25275	0.29508	-1.23572	H	2.23454	0.58137	-0.37976
H	3.16578	-0.92044	-0.33634	H	2.98573	-0.82953	0.37777
H	1.65285	-1.36584	-1.13197	H	2.18094	-0.98586	-1.19089
C	-0.07152	1.62435	-0.26790	C	-1.58358	-1.44680	-0.10154
H	0.22104	1.47659	-1.31430	H	-1.84553	-1.55855	0.95871
H	-1.07020	2.07275	-0.26619	H	-2.49320	-1.15416	-0.63918
H	0.61885	2.35398	0.17180	H	-1.27335	-2.43054	-0.47217
Structure 5		σ=1	Mirror image=1	Structure 6		σ=1	Mirror image=1
C	-1.12941	0.48649	-0.45851	C	-1.39733	0.03588	0.57848
C	-2.19656	-0.47044	0.07940	C	-1.67937	-1.03657	-0.47976
H	-1.57230	1.48372	-0.58529	H	-1.52324	-0.41175	1.57403
H	-0.82226	0.16690	-1.46372	H	-2.16642	0.81717	0.49969
H	-1.83712	-1.50481	0.11090	H	-1.50695	-0.66526	-1.49600
H	-2.49723	-0.19362	1.09757	H	-1.05359	-1.92293	-0.33644
H	-3.09394	-0.45308	-0.54907	H	-2.72407	-1.36305	-0.42262
C	0.11516	0.62583	0.43734	C	-0.01897	0.73123	0.53185
C	0.82045	-0.71714	0.72297	C	1.18055	-0.21648	0.77771
H	-0.22877	1.00916	1.41059	H	-0.02620	1.42713	1.38378
H	1.68005	-0.51915	1.37766	H	2.00189	0.38054	1.19722
H	0.14623	-1.36146	1.30103	H	0.90302	-0.93534	1.56117
C	1.30021	-1.48281	-0.51490	C	1.73207	-0.97538	-0.43661
H	1.99902	-0.88977	-1.11499	H	2.11694	-0.28712	-1.19671
H	1.81721	-2.40366	-0.22301	H	2.56235	-1.62290	-0.13220
H	0.46478	-1.76739	-1.16431	H	0.97938	-1.60706	-0.91601
C	1.08230	1.66350	-0.14857	C	0.15569	1.58671	-0.73021

H	1.43270	1.36845	-1.14466	H	0.13044	0.98375	-1.64392
H	0.59495	2.64024	-0.24982	H	-0.64286	2.33406	-0.80510
H	1.96379	1.79189	0.49071	H	1.11356	2.12042	-0.71565

2,3-dimethylbutane

Structure 1		σ=2	Mirror image=0	Structure 2		σ=2	Mirror image=1
C	-0.23336	0.73851	0.00000	C	0.71897	-0.29062	-0.38237
C	0.23336	1.49404	1.25342	C	1.55148	0.12314	0.83940
H	-1.33519	0.73099	0.00000	H	1.21423	0.12476	-1.27319
H	1.32748	1.46260	1.34100	H	1.14072	-0.29905	1.76392
H	-0.06352	2.54781	1.20257	H	2.58034	-0.24218	0.74273
H	-0.18851	1.07779	2.17273	H	1.59711	1.21075	0.95804
C	0.23336	-0.73851	0.00000	C	-0.71897	0.29062	-0.38237
C	-0.23336	-1.49404	-1.25342	C	-0.71897	1.81775	-0.53529
H	1.33519	-0.73099	0.00000	H	-1.21423	-0.12476	-1.27319
H	0.06352	-2.54781	-1.20257	H	-1.73955	2.19704	-0.66239
H	-1.32748	-1.46260	-1.34100	H	-0.29576	2.31076	0.34774
H	0.18851	-1.07779	-2.17273	H	-0.13257	2.13143	-1.40722
C	0.23336	1.49404	-1.25342	C	0.71897	-1.81775	-0.53529
H	1.32748	1.46260	-1.34100	H	0.29576	-2.31076	0.34774
H	-0.18851	1.07779	-2.17273	H	0.13257	-2.13143	-1.40722
H	-0.06352	2.54781	-1.20257	H	1.73955	-2.19704	-0.66239
C	-0.23336	-1.49404	1.25342	C	-1.55148	-0.12314	0.83940
H	0.18851	-1.07779	2.17273	H	-1.59711	-1.21075	0.95804
H	-1.32748	-1.46260	1.34100	H	-1.14072	0.29905	1.76392
H	0.06352	-2.54781	1.20257	H	-2.58034	0.24218	0.74273

heptane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	-3.52280	-0.64662	0.07704	C	-3.50751	-0.38632	0.16655
H	-3.97689	-1.51026	-0.42169	H	-3.99317	-1.32197	0.46575
H	-4.13166	0.23475	-0.15891	H	-3.94437	-0.07303	-0.78959
H	-3.58938	-0.81283	1.15926	H	-3.76448	0.37649	0.91177
C	-2.06953	-0.44475	-0.35921	C	-1.99023	-0.55177	0.05075
H	-1.49752	-1.35638	-0.14462	H	-1.58998	-0.90204	1.01066
H	-2.02734	-0.30673	-1.44918	H	-1.75967	-1.33850	-0.68191
C	-1.40841	0.75805	0.32401	C	-1.28384	0.74352	-0.36627
H	-1.40844	0.59942	1.41270	H	-1.47412	1.51813	0.39152
H	-2.02889	1.64789	0.14689	H	-1.74071	1.10949	-1.29663

C	0.02356	1.04881	-0.14566	C	0.22982	0.60094	-0.57719
H	0.36381	1.98849	0.31168	H	0.62437	1.54549	-0.97840
H	0.02043	1.22318	-1.23183	H	0.41139	-0.15850	-1.34981
C	1.03607	-0.05338	0.18465	C	1.00868	0.24584	0.69585
H	0.75072	-0.98824	-0.31637	H	0.70641	-0.74800	1.05321
H	1.00297	-0.26400	1.26423	H	0.72881	0.95448	1.48860
C	2.46997	0.30729	-0.21635	C	2.53408	0.26843	0.52270
H	2.76418	1.23689	0.29092	H	3.00399	0.11352	1.50301
H	2.49923	0.52637	-1.29305	H	2.84440	1.26896	0.18933
C	3.47877	-0.79661	0.10947	C	3.06512	-0.78264	-0.45729
H	3.22635	-1.72783	-0.41234	H	2.69562	-0.61279	-1.47436
H	4.49527	-0.51327	-0.18591	H	4.16005	-0.76864	-0.49766
H	3.49137	-1.01419	1.18449	H	2.75474	-1.79112	-0.15618
Structure 3		σ=1	Mirror image=1	Structure 4		σ=2	Mirror image=1
C	-3.59892	-0.14265	0.18400	C	1.21148	2.79671	-1.00575
H	-4.25061	-0.98594	-0.07091	H	2.07173	2.88352	-1.67897
H	-4.00078	0.75175	-0.30770	H	1.25928	3.62829	-0.29213
H	-3.66830	0.01760	1.26694	H	0.30294	2.92967	-1.60594
C	-2.15139	-0.40146	-0.24128	C	1.19748	1.44881	-0.28054
H	-1.79375	-1.32202	0.23705	H	1.18963	0.63954	-1.02224
H	-2.11242	-0.58460	-1.32467	H	2.12775	1.32769	0.29272
C	-1.21699	0.76424	0.10341	C	0.00000	1.29818	0.66385
H	-1.21984	0.91931	1.19265	H	-0.92854	1.37211	0.08127
H	-1.62887	1.68441	-0.33460	H	-0.01390	2.15055	1.35754
C	0.23008	0.58967	-0.37940	C	0.00000	0.00000	1.48552
H	0.77060	1.52847	-0.20490	H	-0.87861	0.00104	2.14582
H	0.23278	0.43341	-1.46867	H	0.87861	-0.00104	2.14582
C	0.98335	-0.56392	0.29433	C	0.00000	-1.29818	0.66385
H	0.44742	-1.50422	0.11376	H	0.01390	-2.15055	1.35754
H	0.97490	-0.41094	1.38415	H	0.92854	-1.37211	0.08127
C	2.43432	-0.73030	-0.18131	C	-1.19748	-1.44881	-0.28054
H	2.44089	-0.88367	-1.26985	H	-1.18963	-0.63954	-1.02224
H	2.84588	-1.64870	0.25792	H	-2.12775	-1.32769	0.29272
C	3.35112	0.44462	0.17395	C	-1.21148	-2.79671	-1.00575
H	3.35163	0.62769	1.25581	H	-1.25928	-3.62829	-0.29213
H	4.38454	0.24509	-0.13099	H	-2.07173	-2.88352	-1.67897
H	3.03649	1.37116	-0.31825	H	-0.30294	-2.92967	-1.60594
Structure 5		σ=1	Mirror	Structure 6		σ=1	Mirror

			image=1				image=1
C	3.07919	-0.76288	0.03938	C	-2.85467	0.76730	0.00551
H	3.77827	-0.85608	0.87806	H	-3.40860	1.22037	0.83535
H	3.63108	-0.34624	-0.81206	H	-3.55010	0.12849	-0.55258
H	2.75630	-1.77332	-0.24012	H	-2.53950	1.57569	-0.66592
C	1.87930	0.11592	0.40106	C	-1.64864	-0.03275	0.50348
H	1.37296	-0.30680	1.27842	H	-0.98973	0.62849	1.07951
H	2.22927	1.11364	0.70231	H	-1.98397	-0.81248	1.20209
C	0.88260	0.25980	-0.75423	C	-0.86289	-0.68773	-0.63718
H	0.50220	-0.73486	-1.02578	H	-0.52775	0.08478	-1.34202
H	1.41856	0.62669	-1.64086	H	-1.54599	-1.33240	-1.20841
C	-0.29128	1.20669	-0.46517	C	0.33333	-1.53507	-0.18098
H	-0.91565	1.27978	-1.36498	H	0.78104	-2.01186	-1.06438
H	0.10236	2.21756	-0.28935	H	-0.04077	-2.35506	0.44876
C	-1.16942	0.81209	0.73428	C	1.44844	-0.80678	0.58934
H	-1.98776	1.54083	0.81932	H	2.18169	-1.56762	0.88717
H	-0.58641	0.90434	1.65972	H	1.05317	-0.39396	1.52748
C	-1.76902	-0.60059	0.66605	C	2.18251	0.30495	-0.18724
H	-2.35374	-0.77464	1.57892	H	2.26572	0.01428	-1.24422
H	-0.96302	-1.34631	0.67915	H	3.21268	0.37159	0.18619
C	-2.66128	-0.83861	-0.55574	C	1.55293	1.69945	-0.08257
H	-2.09444	-0.76979	-1.49082	H	1.47990	2.01373	0.96585
H	-3.12200	-1.83222	-0.52211	H	2.16063	2.44400	-0.60984
H	-3.46859	-0.09712	-0.60357	H	0.54555	1.73568	-0.50726
	Structure 7	σ=1	Mirror image=1		Structure 8	σ=1	Mirror image=1
C	3.03824	-1.02348	-0.12611	C	-3.13642	-0.75539	0.03744
H	3.19314	-2.07484	0.14109	H	-3.39287	-1.81777	0.11706
H	3.78524	-0.42731	0.41210	H	-3.65278	-0.35087	-0.84168
H	3.24288	-0.91768	-1.19861	H	-3.54197	-0.24672	0.92068
C	1.61819	-0.56063	0.21026	C	-1.62333	-0.54796	-0.06912
H	0.89745	-1.20232	-0.31195	H	-1.13571	-0.99851	0.80428
H	1.42993	-0.69741	1.28446	H	-1.23812	-1.08500	-0.94751
C	1.37467	0.90492	-0.16601	C	-1.23998	0.93253	-0.17095
H	1.49429	1.01546	-1.25410	H	-1.56449	1.44669	0.74607
H	2.16538	1.51930	0.28817	H	-1.81439	1.38696	-0.99107
C	0.01159	1.48283	0.24500	C	0.25148	1.22025	-0.40237
H	0.00361	2.54405	-0.03479	H	0.36577	2.30462	-0.52666
H	-0.07871	1.46084	1.34087	H	0.56006	0.77847	-1.35968

C	-1.21520	0.78725	-0.37978	C	1.19228	0.74236	0.72421
H	-0.94735	0.39518	-1.37228	H	0.65186	0.78781	1.68017
H	-2.00344	1.53156	-0.55739	H	2.02889	1.44805	0.82021
C	-1.81725	-0.34030	0.46940	C	1.78639	-0.66534	0.54161
H	-2.12634	0.07504	1.43887	H	0.98557	-1.39327	0.36696
H	-1.05350	-1.09394	0.69378	H	2.27214	-0.96501	1.47991
C	-3.01483	-1.01269	-0.20570	C	2.80994	-0.75409	-0.59467
H	-2.72353	-1.47047	-1.15910	H	3.64506	-0.06327	-0.42463
H	-3.44349	-1.79959	0.42507	H	3.22356	-1.76549	-0.67727
H	-3.80795	-0.28529	-0.41858	H	2.36527	-0.50088	-1.56374
Structure 9		σ=2	Mirror image=0	Structure 10		σ=1	Mirror image=1
C	0.00000	3.83452	-0.35349	C	3.73017	0.04527	0.16769
H	0.00000	4.73497	0.27099	H	4.52137	0.73533	-0.14637
H	-0.88449	3.87658	-1.00083	H	3.94929	-0.93620	-0.27029
H	0.88449	3.87658	-1.00083	H	3.79106	-0.05932	1.25788
C	0.00000	2.56111	0.49564	C	2.34747	0.54245	-0.26071
H	0.87809	2.55942	1.15667	H	2.16674	1.53957	0.16487
H	-0.87809	2.55942	1.15667	H	2.32365	0.66898	-1.35224
C	0.00000	1.28023	-0.34451	C	1.21458	-0.39798	0.16180
H	0.87840	1.28102	-1.00671	H	1.23703	-0.52432	1.25439
H	-0.87840	1.28102	-1.00671	H	1.39497	-1.39691	-0.26213
C	0.00000	0.00000	0.49573	C	-0.17340	0.09057	-0.26286
H	-0.87842	0.00000	1.15776	H	-0.19871	0.20868	-1.35653
H	0.87842	0.00000	1.15776	H	-0.34223	1.09195	0.15544
C	0.00000	-1.28023	-0.34451	C	-1.30134	-0.85331	0.16803
H	0.87840	-1.28102	-1.00671	H	-1.30402	-0.93616	1.26507
H	-0.87840	-1.28102	-1.00671	H	-1.08344	-1.86101	-0.21282
C	0.00000	-2.56111	0.49564	C	-2.69839	-0.43215	-0.30971
H	-0.87809	-2.55942	1.15667	H	-3.41423	-1.22302	-0.04924
H	0.87809	-2.55942	1.15667	H	-2.69983	-0.36829	-1.40713
C	0.00000	-3.83452	-0.35349	C	-3.18573	0.89573	0.27873
H	0.88449	-3.87658	-1.00083	H	-2.55260	1.73424	-0.03099
H	0.00000	-4.73497	0.27099	H	-4.20902	1.11916	-0.04326
H	-0.88449	-3.87658	-1.00083	H	-3.18017	0.86380	1.37552
Structure 11		σ=1	Mirror image=1	Structure 12		σ=1	Mirror image=1
C	-3.30329	0.63727	0.31610	C	3.19784	0.83004	-0.01196
H	-4.25130	0.66657	-0.23273	H	4.24167	0.55986	0.18346

H	-3.00126	1.67244	0.51715	H	2.92373	1.63107	0.68545
H	-3.49161	0.15520	1.28321	H	3.14379	1.24359	-1.02646
C	-2.22159	-0.10863	-0.46869	C	2.26659	-0.37484	0.14084
H	-2.56236	-1.13067	-0.68601	H	2.58299	-1.17473	-0.54327
H	-2.07425	0.37627	-1.44408	H	2.36159	-0.78732	1.15526
C	-0.88051	-0.17070	0.26919	C	0.79718	-0.03388	-0.12820
H	-1.02297	-0.66485	1.24200	H	0.69768	0.36503	-1.14853
H	-0.55105	0.85292	0.49466	H	0.49268	0.77546	0.54832
C	0.20679	-0.90717	-0.51979	C	-0.13575	-1.23687	0.04501
H	0.38263	-0.38129	-1.46816	H	-0.09651	-1.56842	1.09321
H	-0.16693	-1.90322	-0.79530	H	0.25720	-2.07352	-0.55043
C	1.53304	-1.07597	0.23672	C	-1.60356	-1.01029	-0.34899
H	2.23075	-1.64096	-0.39749	H	-2.12762	-1.96773	-0.23169
H	1.35711	-1.69607	1.12699	H	-1.66080	-0.76538	-1.41969
C	2.21136	0.23229	0.67280	C	-2.35157	0.07029	0.45897
H	3.13538	-0.01885	1.21007	H	-1.97019	0.08111	1.48999
H	1.57527	0.75634	1.39789	H	-3.40970	-0.21158	0.53491
C	2.54449	1.17556	-0.48680	C	-2.27764	1.48123	-0.13666
H	1.63962	1.53344	-0.99061	H	-2.70330	1.49605	-1.14750
H	3.09529	2.05525	-0.13554	H	-2.84287	2.19645	0.47219
H	3.16386	0.67150	-1.23922	H	-1.24884	1.84600	-0.20930
Structure 13		σ=1	Mirror image=1	Structure 14		σ=1	Mirror image=1
C	3.29074	0.63959	0.19791	C	2.96105	-0.70134	0.27009
H	4.22913	0.58088	-0.36492	H	3.31616	-1.70930	0.02776
H	3.49713	0.31929	1.22646	H	2.97286	-0.59656	1.36195
H	2.98872	1.69343	0.23533	H	3.68437	0.01564	-0.13746
C	2.19804	-0.22318	-0.43794	C	1.55942	-0.44884	-0.29066
H	2.03433	0.09722	-1.47661	H	1.56819	-0.59295	-1.38031
H	2.53760	-1.26724	-0.49228	H	0.86903	-1.20010	0.10895
C	0.86949	-0.16318	0.32172	C	1.04831	0.96514	0.01722
H	0.53075	0.87903	0.37232	H	1.78339	1.67813	-0.38124
H	1.03267	-0.47762	1.36314	H	1.04176	1.12195	1.10624
C	-0.21949	-1.04809	-0.29827	C	-0.34106	1.30607	-0.55735
H	0.14771	-2.08333	-0.29974	H	-0.46656	0.80659	-1.52773
H	-0.35290	-0.77853	-1.35655	H	-0.37761	2.38175	-0.77273
C	-1.58353	-0.99229	0.42000	C	-1.53518	0.98928	0.35929
H	-1.42188	-0.79755	1.49030	H	-2.44784	1.37328	-0.11889
H	-2.06027	-1.97932	0.36311	H	-1.41600	1.56179	1.29006

C	-2.57794	0.03682	-0.14070	C	-1.76167	-0.48689	0.71748
H	-3.52449	-0.06145	0.40776	H	-2.61252	-0.54486	1.40950
H	-2.80373	-0.22387	-1.18451	H	-0.89838	-0.87222	1.27477
C	-2.11658	1.49576	-0.07868	C	-2.04151	-1.38506	-0.49070
H	-1.24316	1.67136	-0.71569	H	-1.18689	-1.42546	-1.17428
H	-2.91026	2.17180	-0.41683	H	-2.26292	-2.41174	-0.17809
H	-1.84573	1.78337	0.94461	H	-2.90325	-1.01609	-1.06079
Structure 15		σ=1	Mirror image=1	Structure 16		σ=1	Mirror image=1
C	2.79848	0.73208	-0.06268	C	-3.11623	0.72382	-0.23845
H	3.31763	1.33977	0.68694	H	-3.87787	0.56630	-1.01040
H	2.49168	1.39836	-0.87856	H	-2.74621	1.75157	-0.33874
H	3.52237	0.01870	-0.47560	H	-3.60881	0.64516	0.73850
C	1.59147	0.00756	0.53683	C	-1.97255	-0.28595	-0.36144
H	1.91604	-0.61427	1.38274	H	-2.37241	-1.30761	-0.29323
H	0.89572	0.74358	0.95561	H	-1.52158	-0.20256	-1.35908
C	0.87159	-0.88778	-0.48045	C	-0.89702	-0.09731	0.71460
H	1.58440	-1.65548	-0.81157	H	-1.36987	-0.19992	1.70161
H	0.62459	-0.30641	-1.37984	H	-0.51729	0.93089	0.66534
C	-0.39917	-1.57514	0.05793	C	0.26613	-1.09882	0.61293
H	-0.26758	-1.77744	1.13108	H	-0.16340	-2.10858	0.56055
H	-0.49856	-2.55890	-0.41913	H	0.85169	-1.07244	1.54252
C	-1.73296	-0.83668	-0.15237	C	1.22045	-0.88777	-0.58228
H	-2.52628	-1.49301	0.22930	H	0.67100	-0.44658	-1.42521
H	-1.92106	-0.73814	-1.23168	H	1.57340	-1.86470	-0.93654
C	-1.88479	0.54885	0.50745	C	2.45622	-0.02562	-0.27964
H	-1.36696	0.55310	1.47624	H	3.09549	-0.00920	-1.17269
H	-2.94593	0.71215	0.73685	H	3.04611	-0.51713	0.50716
C	-1.40486	1.72481	-0.35160	C	2.15806	1.41548	0.14443
H	-1.95868	1.76000	-1.29767	H	1.62374	1.45430	1.09956
H	-1.56455	2.67968	0.16258	H	3.08468	1.98867	0.26304
H	-0.34143	1.65610	-0.59799	H	1.54093	1.92895	-0.60327
Structure 17		σ=1	Mirror image=1	Structure 18		σ=1	Mirror image=1
C	2.54759	-1.18841	0.01373	C	2.65669	-1.07803	-0.32922
H	3.16955	-1.77590	0.69912	H	3.43751	-1.64732	0.18846
H	3.10138	-1.07959	-0.92684	H	3.00710	-0.88619	-1.35076
H	1.64768	-1.77175	-0.20150	H	1.77124	-1.71668	-0.40170
C	2.21958	0.18598	0.60899	C	2.36111	0.24030	0.39577

H	1.70455	0.06086	1.57218	H	2.06758	0.03563	1.43520
H	3.16668	0.69063	0.83992	H	3.29612	0.81189	0.45693
C	1.37726	1.10227	-0.30222	C	1.28157	1.11486	-0.27603
H	1.65478	0.92329	-1.35142	H	1.31603	0.95947	-1.36426
H	1.64342	2.14697	-0.09484	H	1.52925	2.17229	-0.11642
C	-0.14646	0.97586	-0.14733	C	-0.15542	0.89723	0.22408
H	-0.62315	1.73963	-0.77927	H	-0.80448	1.62347	-0.28203
H	-0.41349	1.22980	0.88750	H	-0.20060	1.14481	1.29529
C	-0.73894	-0.39176	-0.50883	C	-0.71832	-0.51443	0.02334
H	-0.39946	-1.14659	0.21289	H	-0.11204	-1.22929	0.59300
H	-0.34820	-0.70300	-1.48777	H	-0.62026	-0.80056	-1.03453
C	-2.27385	-0.40912	-0.55570	C	-2.18491	-0.66867	0.45494
H	-2.60586	-1.39077	-0.91886	H	-2.28501	-0.36324	1.50626
H	-2.61984	0.32485	-1.29737	H	-2.45178	-1.73322	0.42067
C	-2.94102	-0.12342	0.79353	C	-3.17953	0.11960	-0.40325
H	-2.71345	0.88591	1.15306	H	-3.09421	-0.16296	-1.45999
H	-4.03100	-0.21035	0.72244	H	-4.21136	-0.07315	-0.08873
H	-2.59848	-0.83244	1.55778	H	-3.01216	1.19990	-0.33511

Structure 19		σ=1	Mirror image=1	Structure 20		σ=1	Mirror image=1
C	-2.09173	1.30809	-0.01571	C	1.88112	1.34807	-0.47095
H	-3.04638	1.74164	0.30429	H	2.72911	1.73040	-1.05107
H	-1.83505	1.75220	-0.98538	H	1.75650	1.99728	0.40424
H	-1.32965	1.62312	0.70263	H	0.98386	1.45584	-1.08730
C	-2.19555	-0.21754	-0.12830	C	2.12165	-0.10336	-0.03910
H	-2.46066	-0.64373	0.84982	H	2.25935	-0.73642	-0.92709
H	-3.03769	-0.44940	-0.79351	H	3.07592	-0.13840	0.50230
C	-0.93920	-0.93028	-0.66661	C	1.02359	-0.71349	0.85808
H	-0.49396	-0.32538	-1.46886	H	0.60232	0.07115	1.49691
H	-1.25320	-1.86812	-1.14341	H	1.49532	-1.43049	1.54306
C	0.12987	-1.29468	0.37758	C	-0.08967	-1.48109	0.12050
H	0.88456	-1.92462	-0.11158	H	-0.72783	-1.97567	0.86744
H	-0.33706	-1.93057	1.14289	H	0.39791	-2.29349	-0.43687
C	0.83993	-0.12953	1.08529	C	-0.99828	-0.71446	-0.85904
H	1.57945	-0.55309	1.77992	H	-1.43895	-1.45256	-1.54282
H	0.12165	0.41477	1.71084	H	-0.39840	-0.05051	-1.49349
C	1.55411	0.86402	0.15680	C	-2.16348	0.07361	-0.23766
H	2.00571	1.65246	0.77343	H	-2.77011	-0.61549	0.36739
H	0.82045	1.36743	-0.48503	H	-2.81627	0.40980	-1.05478

C	2.63857	0.22645	-0.71696	C	-1.78636	1.29068	0.61344
H	2.21628	-0.49618	-1.42400	H	-1.13027	1.97443	0.06267
H	3.17215	0.98477	-1.30079	H	-2.68232	1.85097	0.90492
H	3.37746	-0.30448	-0.10372	H	-1.26760	1.00344	1.53282
Structure 21		σ=1	Mirror image=1	Structure 22		σ=1	Mirror image=1
C	2.03055	1.39036	0.37608	C	-2.01286	-1.35453	0.33114
H	2.76305	2.18008	0.17343	H	-2.33667	-2.28959	-0.14061
H	2.01070	1.22271	1.45992	H	-2.77336	-1.07436	1.07018
H	1.04721	1.77134	0.08048	H	-1.08765	-1.56214	0.87603
C	2.38878	0.10594	-0.37701	C	-1.84129	-0.24198	-0.70979
H	2.36433	0.30563	-1.45777	H	-1.12167	-0.55328	-1.47939
H	3.42633	-0.16800	-0.14274	H	-2.79947	-0.11931	-1.23141
C	1.48763	-1.10303	-0.07914	C	-1.41774	1.12355	-0.13081
H	1.58099	-1.37475	0.98247	H	-1.88772	1.25311	0.85529
H	1.88124	-1.95798	-0.64378	H	-1.83543	1.91578	-0.76617
C	-0.00309	-0.90990	-0.42701	C	0.09182	1.39598	-0.00782
H	-0.42149	-1.86222	-0.78082	H	0.20492	2.43220	0.33649
H	-0.08554	-0.21478	-1.27350	H	0.53858	1.37025	-1.01127
C	-0.86950	-0.42465	0.74395	C	0.88923	0.47194	0.93623
H	-0.47413	0.51808	1.14270	H	0.23997	0.15851	1.76420
H	-0.78612	-1.15654	1.55954	H	1.70285	1.04804	1.39832
C	-2.35154	-0.23636	0.39056	C	1.51710	-0.76538	0.27030
H	-2.91363	-0.04306	1.31383	H	0.75914	-1.31485	-0.29979
H	-2.74907	-1.17644	-0.01799	H	1.86530	-1.45099	1.05443
C	-2.61487	0.90299	-0.59961	C	2.69458	-0.42821	-0.64998
H	-2.14389	0.71580	-1.57067	H	3.49203	0.08132	-0.09518
H	-3.68840	1.03560	-0.77483	H	3.12185	-1.33384	-1.09502
H	-2.21937	1.85246	-0.21725	H	2.39233	0.23083	-1.47180
Structure 23		σ=1	Mirror image=0	Structure 24		σ=2	Mirror image=1
C	-0.88145	0.76493	2.82216	C	0.00000	3.03731	-0.85151
H	-0.85559	1.27657	3.79081	H	0.43132	3.90769	-1.35857
H	-1.75267	0.09787	2.81991	H	-0.86959	3.38186	-0.27785
H	-1.04597	1.52639	2.05210	H	-0.36427	2.35250	-1.62496
C	0.41039	-0.02150	2.57752	C	1.02793	2.36492	0.06404
H	1.26400	0.67109	2.56858	H	1.87967	2.01586	-0.53692
H	0.57942	-0.70299	3.42177	H	1.43142	3.11288	0.75939
C	0.41039	-0.83708	1.27671	C	0.46807	1.18751	0.87474

H	-0.43314	-1.54328	1.29287	H	-0.36873	1.54063	1.49561
H	1.32098	-1.45157	1.24121	H	1.24014	0.83834	1.57484
C	0.33484	0.00756	0.00000	C	0.00000	0.00000	0.02613
H	1.15796	0.73829	0.00000	H	0.82173	-0.31080	-0.63358
H	-0.59297	0.59207	0.00000	H	-0.82173	0.31080	-0.63358
C	0.41039	-0.83708	-1.27671	C	-0.46807	-1.18751	0.87474
H	-0.43314	-1.54328	-1.29287	H	-1.24014	-0.83834	1.57484
H	1.32098	-1.45157	-1.24121	H	0.36873	-1.54063	1.49561
C	0.41039	-0.02150	-2.57752	C	-1.02793	-2.36492	0.06404
H	0.57942	-0.70299	-3.42177	H	-1.87967	-2.01586	-0.53692
H	1.26400	0.67109	-2.56858	H	-1.43142	-3.11288	0.75939
C	-0.88145	0.76493	-2.82216	C	0.00000	-3.03731	-0.85151
H	-1.04597	1.52639	-2.05210	H	0.86959	-3.38186	-0.27785
H	-0.85559	1.27657	-3.79081	H	-0.43132	-3.90769	-1.35857
H	-1.75267	0.09787	-2.81991	H	0.36427	-2.35250	-1.62496
Structure 25		σ=1	Mirror image=1	Structure 26		σ=1	Mirror image=1
C	3.20421	0.23678	-0.24849	C	-2.66871	1.02670	0.27733
H	4.15704	-0.23266	-0.51774	H	-3.74875	1.18177	0.37795
H	3.39392	0.92200	0.58721	H	-2.27132	1.83857	-0.34490
H	2.88160	0.83976	-1.10409	H	-2.22699	1.12770	1.27456
C	2.15896	-0.81582	0.13415	C	-2.36070	-0.33921	-0.34459
H	1.97795	-1.48034	-0.72275	H	-2.75299	-1.13410	0.30552
H	2.56809	-1.45113	0.93086	H	-2.90028	-0.42872	-1.29674
C	0.81998	-0.23115	0.60787	C	-0.86627	-0.58481	-0.59680
H	0.99782	0.43411	1.46631	H	-0.48587	0.20224	-1.26270
H	0.19511	-1.05182	0.98306	H	-0.74518	-1.53129	-1.14295
C	0.05312	0.53686	-0.47476	C	-0.01835	-0.63967	0.67947
H	-0.13031	-0.13233	-1.32692	H	-0.46599	-1.36783	1.37078
H	0.67986	1.35006	-0.86167	H	-0.05889	0.32767	1.19502
C	-1.27350	1.14470	0.00707	C	1.44782	-1.02957	0.43839
H	-1.72451	1.70528	-0.82395	H	1.48200	-2.04516	0.01941
H	-1.06018	1.88223	0.79364	H	1.96319	-1.07967	1.40798
C	-2.30669	0.13935	0.53982	C	2.23091	-0.08616	-0.48845
H	-3.19912	0.69554	0.85571	H	1.80025	-0.11578	-1.49771
H	-1.92088	-0.34727	1.44492	H	3.25528	-0.46876	-0.58742
C	-2.71449	-0.92969	-0.47808	C	2.28040	1.36437	0.00057
H	-1.87144	-1.57638	-0.74580	H	2.68642	1.42363	1.01818
H	-3.50870	-1.57172	-0.08103	H	2.91421	1.97911	-0.64825

H	-3.08583	-0.47143	-1.40326	H	1.28430	1.82071	0.01577
Structure 27		σ=1	Mirror image=1	Structure 28		σ=2	Mirror image=1
C	-2.34626	0.97810	-0.42827	C	0.00000	2.90962	-0.07493
H	-2.76278	1.93323	-0.08925	H	-0.22812	3.68671	-0.81300
H	-3.17242	0.37280	-0.82163	H	0.63552	3.35903	0.69835
H	-1.67010	1.19329	-1.26333	H	-0.94356	2.62008	0.40078
C	-1.63012	0.25118	0.71407	C	0.69517	1.71200	-0.72926
H	-0.82848	0.88807	1.10429	H	0.03075	1.27429	-1.48581
H	-2.33737	0.11365	1.54295	H	1.58110	2.06339	-1.27443
C	-1.07659	-1.12936	0.31905	C	1.13463	0.62696	0.26570
H	-1.91569	-1.72070	-0.07338	H	1.87105	1.05863	0.95805
H	-0.73764	-1.65429	1.22342	H	1.66449	-0.16227	-0.28387
C	0.06544	-1.14075	-0.71746	C	0.00000	0.00000	1.09186
H	-0.09440	-0.35250	-1.46360	H	-0.43220	0.76004	1.75531
H	0.01574	-2.08403	-1.27652	H	0.43220	-0.76004	1.75531
C	1.48655	-1.03501	-0.13768	C	-1.13463	-0.62696	0.26570
H	2.20353	-1.16997	-0.96040	H	-1.66449	0.16227	-0.28387
H	1.64511	-1.88159	0.54541	H	-1.87105	-1.05863	0.95805
C	1.84046	0.26388	0.60190	C	-0.69517	-1.71200	-0.72926
H	2.86890	0.17435	0.97676	H	-0.03075	-1.27429	-1.48581
H	1.20787	0.37154	1.49189	H	-1.58110	-2.06339	-1.27443
C	1.73483	1.52293	-0.26317	C	0.00000	-2.90962	-0.07493
H	0.70652	1.70617	-0.59240	H	-0.63552	-3.35903	0.69835
H	2.06747	2.41028	0.28701	H	0.22812	-3.68671	-0.81300
H	2.35787	1.43393	-1.16188	H	0.94356	-2.62008	0.40078
Structure 29		σ=1	Mirror image=1	Structure 30		σ=2	Mirror image=1
C	3.18775	-0.28102	-0.20519	C	0.00000	2.50973	-0.80061
H	4.12480	0.12147	-0.60604	H	0.08508	3.58242	-1.00865
H	2.86193	-1.08463	-0.87440	H	-0.94851	2.35002	-0.27658
H	3.40824	-0.73146	0.77080	H	-0.06051	1.98699	-1.76319
C	2.12622	0.81592	-0.07413	C	1.19266	2.01544	0.02328
H	2.53652	1.64123	0.52285	H	2.12191	2.28169	-0.49833
H	1.91046	1.23574	-1.06711	H	1.21601	2.55475	0.98104
C	0.81315	0.34723	0.56853	C	1.20562	0.50514	0.30719
H	0.16131	1.21638	0.71412	H	2.13397	0.27211	0.84492
H	1.02231	-0.04596	1.57452	H	1.26237	-0.03862	-0.64406
C	0.06828	-0.72828	-0.23508	C	0.00000	0.00000	1.13001

H	0.69340	-1.62810	-0.27938	H	-0.32547	0.81088	1.79568
H	-0.04616	-0.39205	-1.27673	H	0.32547	-0.81088	1.79568
C	-1.31490	-1.10269	0.33802	C	-1.20562	-0.50514	0.30719
H	-1.30741	-0.95600	1.42798	H	-1.26237	0.03862	-0.64406
H	-1.49395	-2.17405	0.18075	H	-2.13397	-0.27211	0.84492
C	-2.50137	-0.33838	-0.27071	C	-1.19266	-2.01544	0.02328
H	-3.42896	-0.72879	0.16927	H	-2.12191	-2.28169	-0.49833
H	-2.55445	-0.56836	-1.34438	H	-1.21601	-2.55475	0.98104
C	-2.46468	1.18149	-0.08699	C	0.00000	-2.50973	-0.80061
H	-1.61441	1.63196	-0.61031	H	0.94851	-2.35002	-0.27658
H	-3.37585	1.64541	-0.48174	H	-0.08508	-3.58242	-1.00865
H	-2.38451	1.45153	0.97314	H	0.06051	-1.98699	-1.76319

2-methylhexane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	-2.30911	-1.11228	-0.01615	C	1.77362	-0.68024	1.19063
H	-2.09000	-1.96797	0.63374	H	1.80001	-1.77624	1.16363
H	-1.99243	-1.37425	-1.03237	H	0.91981	-0.38254	1.81071
H	-3.39665	-0.97624	-0.03790	H	2.68273	-0.33463	1.69618
C	-1.60951	0.15956	0.48210	C	1.67433	-0.08660	-0.22028
H	-2.02523	0.39259	1.47358	H	2.59250	-0.36991	-0.75609
C	-0.09355	-0.04154	0.68736	C	0.51301	-0.70003	-1.03829
H	0.05624	-0.85450	1.41325	H	0.81980	-1.71195	-1.33738
H	0.31043	0.86505	1.15673	H	0.40471	-0.13034	-1.97250
C	0.71420	-0.36048	-0.57741	C	-0.86627	-0.82855	-0.37036
H	0.63438	0.47150	-1.29037	H	-0.78707	-1.45868	0.52598
H	0.28116	-1.23630	-1.07706	H	-1.51384	-1.38434	-1.06381
C	2.20041	-0.63927	-0.30580	C	-1.57671	0.47906	-0.00045
H	2.67290	-0.97122	-1.23979	H	-1.54510	1.16732	-0.85655
H	2.28703	-1.48078	0.39623	H	-1.04137	0.98003	0.81444
C	2.97390	0.56401	0.24275	C	-3.03001	0.25097	0.42425
H	2.60174	0.87425	1.22506	H	-3.08627	-0.42125	1.28938
H	4.03919	0.33200	0.35267	H	-3.52162	1.19078	0.69968
H	2.88753	1.42538	-0.43151	H	-3.61052	-0.20635	-0.38630
C	-1.91959	1.35107	-0.43418	C	1.66079	1.44871	-0.17493
H	-1.42111	2.26308	-0.08427	H	1.58444	1.87308	-1.18295
H	-1.58837	1.16261	-1.46204	H	0.82448	1.83748	0.41369
H	-2.99735	1.54840	-0.46807	H	2.58472	1.82764	0.27842
Structure 3		σ=1	Mirror	Structure 4		σ=1	Mirror

			image=1				image=1
C	-2.09862	-0.61523	-0.73439	C	-1.89979	1.43681	0.20966
H	-2.35503	-1.63312	-0.41693	H	-1.11051	2.14147	-0.07137
H	-1.42819	-0.69442	-1.59816	H	-1.95399	1.41394	1.30614
H	-3.01913	-0.12837	-1.07667	H	-2.85020	1.83754	-0.16161
C	-1.45203	0.18171	0.40589	C	-1.64238	0.03066	-0.34754
H	-2.20776	0.28129	1.19926	H	-1.55316	0.11056	-1.44205
C	-0.26693	-0.57154	1.05630	C	-0.33230	-0.57692	0.18309
H	-0.68976	-1.37908	1.66993	H	-0.24883	-1.60814	-0.18962
H	0.23381	0.10446	1.76226	H	-0.39464	-0.65511	1.27941
C	0.77906	-1.22441	0.13408	C	0.93965	0.18659	-0.19896
H	0.27961	-1.95735	-0.51238	H	0.91768	1.19615	0.23255
H	1.45719	-1.80732	0.77392	H	0.96891	0.32169	-1.29057
C	1.63590	-0.29750	-0.74211	C	2.22153	-0.51849	0.25644
H	1.00759	0.20750	-1.48553	H	2.25588	-1.52561	-0.18224
H	2.33127	-0.92386	-1.31724	H	2.18665	-0.66252	1.34553
C	2.43891	0.74150	0.04502	C	3.49190	0.24823	-0.11867
H	3.07066	0.25764	0.80045	H	3.49828	1.24675	0.33529
H	3.09365	1.31945	-0.61684	H	4.39313	-0.27701	0.21704
H	1.78635	1.45050	0.56462	H	3.56661	0.37959	-1.20510
C	-1.11321	1.61093	-0.04353	C	-2.82598	-0.89416	-0.03685
H	-0.66529	2.18721	0.77445	H	-2.67263	-1.89445	-0.45865
H	-0.41325	1.62495	-0.88453	H	-2.95717	-1.00617	1.04730
H	-2.02009	2.13772	-0.36418	H	-3.76181	-0.49495	-0.44507
	Structure 5	σ=1	Mirror image=1		Structure 6	σ=1	Mirror image=1
C	-1.90858	1.28496	0.49554	C	2.16789	-1.23088	0.06119
H	-1.28787	2.13523	0.19513	H	1.59528	-2.08787	-0.30758
H	-1.74444	1.11235	1.56747	H	2.23405	-1.31691	1.15385
H	-2.95720	1.57543	0.36250	H	3.18440	-1.31410	-0.34066
C	-1.58278	0.02086	-0.31070	C	1.52923	0.10614	-0.33701
H	-1.71884	0.25485	-1.37798	H	1.44628	0.12936	-1.43469
C	-0.12620	-0.43456	-0.11548	C	0.11260	0.27602	0.24045
H	0.02169	-1.37932	-0.65935	H	-0.23554	1.28899	-0.00025
H	0.02726	-0.66814	0.94766	H	0.16733	0.22564	1.33913
C	0.92928	0.57228	-0.58804	C	-0.91472	-0.74533	-0.26052
H	0.88790	1.47734	0.03281	H	-0.58263	-1.75775	0.00070
H	0.68199	0.89014	-1.61105	H	-0.95363	-0.70896	-1.35968
C	2.36383	0.02491	-0.57030	C	-2.32966	-0.53771	0.30075

H	3.03290	0.77130	-1.01865	H	-2.29018	-0.57287	1.39876
H	2.41924	-0.86300	-1.21602	H	-2.95809	-1.38338	-0.00849
C	2.87683	-0.33002	0.82893	C	-2.99833	0.76681	-0.14439
H	2.29425	-1.13995	1.28112	H	-3.03742	0.83316	-1.23892
H	3.92299	-0.65437	0.79647	H	-4.02597	0.83129	0.23049
H	2.81618	0.53615	1.49983	H	-2.45944	1.64738	0.22148
C	-2.55166	-1.11147	0.05184	C	2.42467	1.27507	0.09297
H	-2.35254	-2.01232	-0.54050	H	2.00134	2.23759	-0.21747
H	-2.45482	-1.38125	1.11156	H	2.53687	1.29700	1.18481
H	-3.59304	-0.81612	-0.12173	H	3.42733	1.19071	-0.34216
Structure 7		σ=1	Mirror image=1	Structure 8		σ=1	Mirror image=1
C	-1.44116	1.50884	0.21892	C	-1.05784	1.52352	-0.17397
H	-0.44959	1.96642	0.27252	H	-0.05750	1.81000	-0.50842
H	-1.87420	1.53807	1.22724	H	-1.16478	1.84642	0.86983
H	-2.06647	2.13512	-0.42850	H	-1.78358	2.08891	-0.77058
C	-1.39015	0.06271	-0.29595	C	-1.30925	0.01301	-0.29382
H	-0.99925	0.07811	-1.32493	H	-1.20948	-0.26779	-1.35359
C	-0.45860	-0.83442	0.55319	C	-0.30095	-0.83267	0.51796
H	-0.86079	-1.85628	0.55945	H	-0.79515	-1.76580	0.81991
H	-0.48678	-0.49531	1.59923	H	-0.06207	-0.31002	1.45470
C	1.00012	-0.92023	0.07858	C	0.99080	-1.23219	-0.21573
H	1.01834	-1.34322	-0.93694	H	0.71348	-1.80272	-1.11346
H	1.52861	-1.64448	0.71510	H	1.54586	-1.93058	0.42708
C	1.78956	0.39339	0.07904	C	1.94357	-0.10057	-0.62858
H	1.71221	0.86567	1.06850	H	1.44716	0.56500	-1.34582
H	1.34163	1.09671	-0.63381	H	2.78704	-0.54653	-1.17251
C	3.26406	0.18829	-0.27859	C	2.48720	0.71509	0.54778
H	3.36868	-0.26324	-1.27282	H	2.99296	0.06528	1.27281
H	3.81297	1.13666	-0.28333	H	3.21141	1.46454	0.20921
H	3.75487	-0.47959	0.43983	H	1.68929	1.24370	1.07991
C	-2.80949	-0.51970	-0.34561	C	-2.74758	-0.30417	0.13986
H	-2.81329	-1.52409	-0.78475	H	-2.98535	-1.36355	-0.01093
H	-3.23207	-0.59606	0.66478	H	-2.88915	-0.07931	1.20513
H	-3.48085	0.11221	-0.93910	H	-3.47591	0.29037	-0.42423
Structure 9		σ=1	Mirror image=1	Structure 10		σ=1	Mirror image=1
C	-1.48008	1.48100	0.25880	C	-1.70789	1.23340	-0.57045
H	-0.51290	1.99396	0.28618	H	-0.91209	1.93794	-0.83391

H	-1.87469	1.45715	1.28313	H	-2.24377	1.64329	0.29579
H	-2.16163	2.09026	-0.34609	H	-2.41141	1.19794	-1.41037
C	-1.36233	0.06157	-0.31002	C	-1.15829	-0.16339	-0.25550
H	-0.92014	0.13449	-1.31387	H	-0.59724	-0.51210	-1.13467
C	-0.45599	-0.83755	0.55103	C	-0.20349	-0.15454	0.95168
H	-0.41961	-1.83577	0.09108	H	0.12797	-1.18439	1.14070
H	-0.93400	-0.97204	1.53266	H	-0.77325	0.14498	1.84358
C	0.98092	-0.34031	0.76380	C	1.02569	0.75991	0.82710
H	1.50680	-1.06247	1.40406	H	1.63207	0.64747	1.73685
H	0.97287	0.60411	1.32474	H	0.70274	1.80868	0.80907
C	1.78413	-0.15120	-0.52783	C	1.91663	0.49374	-0.39592
H	1.31044	0.61833	-1.15104	H	2.74811	1.21067	-0.38253
H	1.75029	-1.08092	-1.11365	H	1.35535	0.70189	-1.31637
C	3.24069	0.23907	-0.26520	C	2.48036	-0.92900	-0.45601
H	3.75540	-0.53048	0.32296	H	1.68582	-1.67490	-0.56922
H	3.79680	0.37394	-1.19973	H	3.16649	-1.04751	-1.30203
H	3.30067	1.17871	0.29767	H	3.03348	-1.17203	0.45985
C	-2.74889	-0.57684	-0.45983	C	-2.30466	-1.15368	-0.01538
H	-2.68008	-1.58388	-0.88799	H	-1.92455	-2.16273	0.18355
H	-3.24491	-0.66294	0.51573	H	-2.90756	-0.84849	0.84975
H	-3.39598	0.02312	-1.11032	H	-2.97225	-1.20939	-0.88317
Structure 11		σ=1	Mirror image=1	Structure 12		σ=1	Mirror image=1
C	-1.23537	1.22173	0.86413	C	2.92323	-0.32705	0.20053
H	-0.25083	1.56854	1.19282	H	3.19691	-1.36118	-0.03975
H	-1.75638	0.81558	1.74110	H	2.93412	-0.22495	1.29350
H	-1.79840	2.09675	0.51897	H	3.70216	0.33089	-0.20218
C	-1.13544	0.16268	-0.24026	C	1.54318	0.03222	-0.36416
H	-0.58799	0.59781	-1.08762	H	1.58716	-0.07711	-1.45893
C	-0.38492	-1.09725	0.22680	C	0.48179	-0.95862	0.14961
H	-0.38594	-1.82551	-0.59735	H	0.45867	-0.91858	1.24920
H	-0.97012	-1.55835	1.03681	H	0.82468	-1.97007	-0.10470
C	1.06349	-0.92740	0.71439	C	-0.94431	-0.75043	-0.40074
H	1.39198	-1.90829	1.08214	H	-1.41567	-1.72743	-0.57267
H	1.09567	-0.25997	1.58621	H	-0.89026	-0.27030	-1.38899
C	2.07616	-0.43933	-0.34095	C	-1.86939	0.06463	0.51271
H	1.81893	-0.87446	-1.31719	H	-1.41440	1.03608	0.73966
H	3.06609	-0.83999	-0.08653	H	-1.96310	-0.45733	1.47530
C	2.20398	1.08313	-0.47124	C	-3.25859	0.27952	-0.09194

H	2.47866	1.53286	0.49088	H	-3.74855	-0.67833	-0.30622
H	2.98238	1.34984	-1.19553	H	-3.90977	0.84397	0.58494
H	1.27263	1.55316	-0.79996	H	-3.19563	0.83527	-1.03566
C	-2.53336	-0.21891	-0.74487	C	1.20277	1.49562	-0.05718
H	-2.47774	-0.95461	-1.55590	H	0.26863	1.80711	-0.53545
H	-3.13195	-0.65877	0.06347	H	1.09702	1.65395	1.02388
H	-3.07428	0.65755	-1.12032	H	1.99597	2.16268	-0.41498

Structure 13		σ=1	Mirror image=0
C	0.21508	-2.13918	1.26425
H	-0.33068	-1.85407	2.17171
H	1.20004	-1.65941	1.30178
H	0.37738	-3.22285	1.29575
C	-0.55691	-1.73791	0.00000
H	-1.50067	-2.30309	0.00000
C	-0.94744	-0.24574	0.00000
H	-1.57934	-0.05013	0.87852
H	-1.57934	-0.05013	-0.87852
C	0.21508	0.75386	0.00000
H	0.85353	0.58791	-0.87827
H	0.85353	0.58791	0.87827
C	-0.25921	2.21110	0.00000
H	-0.89748	2.38350	0.87803
H	-0.89748	2.38350	-0.87803
C	0.89530	3.21580	0.00000
H	1.53087	3.08584	-0.88451
H	0.53017	4.24900	0.00000
H	1.53087	3.08584	0.88451
C	0.21508	-2.13918	-1.26425
H	-0.33068	-1.85407	-2.17171
H	1.20004	-1.65941	-1.30178
H	0.37738	-3.22285	-1.29575

3-methylhexane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	2.31501	-1.49572	-0.16031	C	2.74604	-0.89130	0.00753
H	2.29386	-1.59328	-1.25294	H	2.83300	-1.05572	-1.07382
H	1.59831	-2.21432	0.25064	H	2.29856	-1.78984	0.44480
H	3.31184	-1.79657	0.18099	H	3.76026	-0.80082	0.41233

C	2.00163	-0.05893	0.26776	C	1.92461	0.36637	0.30680
H	1.99423	0.00560	1.36585	H	1.81316	0.48329	1.39492
H	2.81792	0.59511	-0.06787	H	2.48755	1.24551	-0.03533
C	0.67505	0.50779	-0.27313	C	0.52812	0.40577	-0.34259
H	0.69163	0.40054	-1.36984	H	0.66449	0.27251	-1.42813
C	-0.53945	-0.27656	0.25413	C	-0.36159	-0.75131	0.15081
H	-0.56897	-0.19056	1.35153	H	-0.44030	-0.69754	1.24749
H	-0.40240	-1.34375	0.03689	H	0.15485	-1.69291	-0.06698
C	-1.89201	0.15601	-0.32378	C	-1.77774	-0.81212	-0.46203
H	-1.83531	0.14409	-1.42167	H	-2.05984	-1.86255	-0.60787
H	-2.10924	1.19299	-0.03978	H	-1.76005	-0.36747	-1.46692
C	-3.04166	-0.74274	0.13919	C	-2.86614	-0.14077	0.38356
H	-3.13381	-0.73217	1.23219	H	-2.66010	0.92049	0.55274
H	-4.00057	-0.41735	-0.27965	H	-3.84707	-0.21793	-0.09970
H	-2.87789	-1.78307	-0.16747	H	-2.94103	-0.62096	1.36684
C	0.57454	2.00386	0.05443	C	-0.10952	1.78322	-0.12045
H	-0.30636	2.46709	-0.40078	H	-1.05217	1.89078	-0.66572
H	0.51088	2.15955	1.13950	H	-0.31549	1.95313	0.94419
H	1.45724	2.54391	-0.30730	H	0.56149	2.58087	-0.46060
Structure 3		σ=1	Mirror image=1	Structure 4		σ=1	Mirror image=1
C	2.43088	-1.20465	-0.19708	C	-1.70593	-1.80593	0.07632
H	2.15969	-1.56563	-1.19711	H	-2.12049	-1.82111	1.09199
H	2.00991	-1.90358	0.53307	H	-0.71744	-2.27655	0.11606
H	3.52185	-1.25704	-0.10936	H	-2.34475	-2.43496	-0.55358
C	1.93298	0.22707	0.02244	C	-1.63344	-0.37664	-0.46730
H	2.18089	0.55094	1.04408	H	-1.18322	-0.38707	-1.46927
H	2.48286	0.89944	-0.65017	H	-2.65328	0.00847	-0.60271
C	0.42489	0.43426	-0.21398	C	-0.86440	0.61081	0.42998
H	0.20561	0.08675	-1.23481	H	-1.39178	0.64589	1.39590
C	-0.42026	-0.39618	0.77010	C	0.57987	0.16474	0.73973
H	-0.13713	-0.11161	1.79465	H	0.55389	-0.76064	1.33062
H	-0.15642	-1.45626	0.66268	H	1.04148	0.92085	1.39107
C	-1.94397	-0.26625	0.62098	C	1.48715	-0.05739	-0.47647
H	-2.25732	0.76165	0.84294	H	1.52681	0.85429	-1.08621
H	-2.41837	-0.89559	1.38549	H	1.06137	-0.83762	-1.12061
C	-2.46914	-0.67389	-0.75888	C	2.90870	-0.45818	-0.07306
H	-2.15221	-1.69264	-1.01492	H	2.90507	-1.38532	0.51327
H	-3.56410	-0.64685	-0.78936	H	3.54586	-0.61980	-0.94984

H	-2.10074	-0.00681	-1.54612	H	3.37755	0.31888	0.54295
C	0.08245	1.92788	-0.13874	C	-0.90999	2.02384	-0.16759
H	-0.95934	2.12557	-0.41105	H	-0.38605	2.74363	0.47237
H	0.23979	2.31260	0.87747	H	-0.44205	2.05634	-1.15852
H	0.71795	2.50960	-0.81649	H	-1.94469	2.36718	-0.28313
Structure 5		σ=1	Mirror image=1	Structure 6		σ=1	Mirror image=1
C	1.10086	2.03067	0.23776	C	-2.26054	-1.10227	-0.16703
H	1.73966	2.03794	1.12967	H	-2.91219	-0.80504	0.66398
H	0.07408	2.22166	0.56504	H	-1.63487	-1.92970	0.18460
H	1.40643	2.87016	-0.39682	H	-2.89915	-1.48924	-0.96895
C	1.22517	0.70146	-0.51099	C	-1.42032	0.08208	-0.65308
H	0.57559	0.70692	-1.39610	H	-0.77305	-0.23824	-1.48109
H	2.24956	0.60778	-0.89738	H	-2.08895	0.84492	-1.07464
C	0.92609	-0.54507	0.34105	C	-0.56368	0.74248	0.44137
H	1.62808	-0.52191	1.18947	H	-1.25338	1.04485	1.24502
C	-0.48539	-0.58990	0.97074	C	0.44241	-0.22971	1.10380
H	-0.61084	0.26516	1.64837	H	-0.12152	-0.90013	1.76541
H	-0.51135	-1.48071	1.61281	H	1.09968	0.35369	1.76439
C	-1.69540	-0.64952	0.01605	C	1.31426	-1.11525	0.19644
H	-2.51976	-1.14582	0.54453	H	0.67358	-1.74851	-0.43063
H	-1.46673	-1.29450	-0.84183	H	1.86216	-1.80682	0.85061
C	-2.20730	0.70686	-0.48366	C	2.32669	-0.38615	-0.69319
H	-1.47287	1.22800	-1.10420	H	2.91976	0.33173	-0.11375
H	-3.11658	0.58283	-1.08329	H	3.02125	-1.09813	-1.15387
H	-2.45398	1.36443	0.35901	H	1.83963	0.16433	-1.50355
C	1.22799	-1.82030	-0.45879	C	0.08326	2.03484	-0.07984
H	1.03793	-2.72019	0.13806	H	0.71395	2.49945	0.68708
H	0.61195	-1.88465	-1.36342	H	0.70774	1.85923	-0.96072
H	2.27674	-1.84231	-0.77687	H	-0.68710	2.76146	-0.36471
Structure 7		σ=1	Mirror image=1	Structure 8		σ=1	Mirror image=1
C	-1.43435	1.98456	-0.18880	C	-0.52606	2.18145	-0.10267
H	-1.96613	1.94349	-1.14723	H	-0.65366	2.29362	-1.18638
H	-0.40985	2.30678	-0.39664	H	0.54813	2.16514	0.10137
H	-1.91072	2.76009	0.42217	H	-0.93959	3.07795	0.37363
C	-1.48279	0.62244	0.51244	C	-1.23718	0.91884	0.39750
H	-1.00536	0.69195	1.50030	H	-1.12679	0.83545	1.48822
H	-2.53557	0.37949	0.70793	H	-2.31274	1.04678	0.21704

C	-0.83960	-0.53885	-0.28391	C	-0.77900	-0.40437	-0.26168
H	-0.89870	-0.28773	-1.35445	H	-0.43586	-0.17590	-1.28131
C	0.64283	-0.76922	0.06391	C	0.36803	-1.10126	0.49744
H	1.00871	-1.61926	-0.53038	H	0.58179	-2.05611	-0.00479
H	0.70941	-1.08734	1.11588	H	-0.00170	-1.36303	1.49990
C	1.58676	0.41746	-0.15462	C	1.68759	-0.33087	0.64471
H	1.30509	1.24494	0.50808	H	2.36641	-0.93359	1.26278
H	1.47296	0.79175	-1.18158	H	1.52026	0.59656	1.20642
C	3.05172	0.05025	0.09757	C	2.37791	-0.01753	-0.68598
H	3.38013	-0.74892	-0.57807	H	1.77215	0.64420	-1.31382
H	3.71382	0.91013	-0.05397	H	3.34456	0.47293	-0.52497
H	3.19678	-0.30640	1.12472	H	2.56058	-0.93682	-1.25622
C	-1.62258	-1.84157	-0.06660	C	-1.96161	-1.37718	-0.38213
H	-1.17889	-2.67466	-0.62439	H	-1.65820	-2.32161	-0.84889
H	-1.62848	-2.11848	0.99568	H	-2.37327	-1.61321	0.60791
H	-2.66517	-1.73630	-0.38804	H	-2.77018	-0.94679	-0.98406
Structure 9		σ=1	Mirror image=1	Structure 10		σ=1	Mirror image=1
C	-0.22041	2.17248	-0.35565	C	-2.40567	-1.05161	-0.57628
H	-0.79934	2.36447	-1.26717	H	-1.67212	-1.75234	-0.98966
H	0.80050	1.92918	-0.66278	H	-2.65135	-0.32622	-1.35963
H	-0.18139	3.10729	0.21555	H	-3.31653	-1.62006	-0.35782
C	-0.86980	1.05207	0.46431	C	-1.88218	-0.36400	0.68975
H	-0.33195	0.91086	1.41146	H	-2.67131	0.28398	1.09546
H	-1.87776	1.38598	0.74447	H	-1.68912	-1.12742	1.45604
C	-0.98599	-0.30553	-0.26853	C	-0.60320	0.48008	0.50754
H	-1.07681	-0.09549	-1.34583	H	-0.36350	0.89519	1.49877
C	0.21836	-1.25182	-0.08251	C	0.59533	-0.38487	0.07762
H	-0.01721	-2.17489	-0.62876	H	0.43806	-0.75032	-0.94711
H	0.27665	-1.54187	0.97778	H	0.63261	-1.27909	0.71737
C	1.60385	-0.75493	-0.54295	C	1.95284	0.32341	0.14845
H	1.49103	-0.11271	-1.42644	H	2.09635	0.72831	1.16036
H	2.18906	-1.62027	-0.88010	H	1.96023	1.18590	-0.52993
C	2.41835	-0.03208	0.53620	C	3.11959	-0.60308	-0.20332
H	2.59047	-0.69385	1.39374	H	3.01408	-1.00027	-1.22035
H	3.39792	0.27505	0.15170	H	4.08045	-0.07918	-0.14768
H	1.91417	0.86334	0.91064	H	3.16449	-1.45876	0.48146
C	-2.26414	-1.03528	0.17163	C	-0.83310	1.66434	-0.44250
H	-2.37435	-1.99879	-0.33967	H	0.01684	2.35422	-0.43939

H	-2.24600	-1.23246	1.25147	H	-0.97798	1.32579	-1.47530
H	-3.15637	-0.43530	-0.04112	H	-1.72283	2.23467	-0.15014
Structure 11		σ=1	Mirror image=1	Structure 12		σ=1	Mirror image=1
C	3.09882	-0.42211	-0.25470	C	2.45648	-0.40569	0.92732
H	3.43396	0.56129	0.09145	H	1.87223	-1.15298	1.47512
H	3.10412	-0.40783	-1.35175	H	2.39008	0.53833	1.47924
H	3.84443	-1.15569	0.07183	H	3.50388	-0.72663	0.95025
C	1.70944	-0.77750	0.28233	C	1.97137	-0.25155	-0.51862
H	1.47573	-1.81379	0.00223	H	2.61997	0.46938	-1.03512
H	1.72349	-0.75583	1.38204	H	2.09999	-1.20865	-1.04279
C	0.57067	0.13018	-0.21868	C	0.50689	0.20691	-0.68505
H	0.59042	0.10938	-1.32039	H	0.33276	0.29259	-1.76889
C	-0.78837	-0.43366	0.23338	C	-0.48097	-0.85434	-0.16348
H	-0.84188	-0.40145	1.33252	H	-0.34065	-0.99294	0.91742
H	-0.83359	-1.49791	-0.04015	H	-0.20810	-1.81175	-0.62747
C	-2.01720	0.27023	-0.35265	C	-1.97167	-0.56605	-0.44177
H	-1.93164	0.29258	-1.44844	H	-2.48739	-1.51412	-0.64069
H	-2.04306	1.31727	-0.02631	H	-2.06341	0.02232	-1.36564
C	-3.32922	-0.41140	0.04491	C	-2.70669	0.14426	0.70098
H	-3.45071	-0.42576	1.13498	H	-2.25831	1.11328	0.94009
H	-4.19636	0.10596	-0.38078	H	-3.75913	0.31692	0.44757
H	-3.35536	-1.45124	-0.30314	H	-2.67978	-0.46365	1.61357
C	0.76297	1.58453	0.23164	C	0.27738	1.59885	-0.08004
H	-0.02619	2.23621	-0.15619	H	-0.69391	2.00799	-0.37486
H	0.74524	1.65339	1.32754	H	0.30738	1.57358	1.01539
H	1.71870	1.99182	-0.11291	H	1.04769	2.30206	-0.41927
Structure 13		σ=1	Mirror image=1	Structure 14		σ=1	Mirror image=1
C	-2.67802	-0.56116	-0.35254	C	-1.79514	-1.44510	-0.45404
H	-2.26820	-1.33177	-1.01435	H	-0.84676	-1.80701	-0.86045
H	-2.88073	0.32693	-0.96119	H	-2.33477	-0.94954	-1.26816
H	-3.63975	-0.92861	0.02249	H	-2.38394	-2.32061	-0.15725
C	-1.73143	-0.24611	0.81125	C	-1.60346	-0.50532	0.74365
H	-2.21355	0.48890	1.47049	H	-2.60045	-0.19719	1.08720
H	-1.59328	-1.15357	1.41528	H	-1.15891	-1.06480	1.57843
C	-0.34061	0.29505	0.41669	C	-0.76468	0.77457	0.50677
H	0.18392	0.49357	1.36208	H	-1.04253	1.46507	1.31667
C	0.47654	-0.75495	-0.35856	C	0.75799	0.57347	0.66456

H	-0.03500	-0.98339	-1.30313	H	0.95939	0.24205	1.69361
H	0.48186	-1.68960	0.22165	H	1.23748	1.55913	0.56793
C	1.92864	-0.36552	-0.67653	C	1.45417	-0.39677	-0.29830
H	1.94257	0.50392	-1.34639	H	1.18811	-0.15728	-1.33584
H	2.38805	-1.18655	-1.24262	H	1.10010	-1.41838	-0.11612
C	2.78417	-0.07099	0.55922	C	2.97768	-0.36220	-0.14584
H	2.76738	-0.91533	1.25971	H	3.27703	-0.61647	0.87844
H	3.82829	0.11213	0.28180	H	3.46620	-1.07227	-0.82258
H	2.42777	0.81290	1.09964	H	3.37291	0.63704	-0.36584
C	-0.43844	1.62599	-0.34175	C	-1.12349	1.47861	-0.80901
H	0.54318	2.09835	-0.45287	H	-0.60802	2.44315	-0.88485
H	-0.85036	1.48511	-1.34814	H	-0.84276	0.88450	-1.68488
H	-1.08718	2.33315	0.18878	H	-2.20156	1.66901	-0.87306
Structure 15		σ=1	Mirror image=1	Structure 16		σ=1	Mirror image=1
C	-1.47929	1.52660	0.30352	C	1.57482	1.60411	-0.57984
H	-0.46975	1.94537	0.33058	H	0.63049	1.81589	-1.09367
H	-1.75370	1.25834	1.32935	H	2.23363	1.09707	-1.29329
H	-2.15849	2.32457	-0.01772	H	2.03670	2.56634	-0.33241
C	-1.59370	0.32249	-0.64014	C	1.35559	0.76868	0.68606
H	-2.63936	-0.01413	-0.62454	H	2.31541	0.64701	1.20635
H	-1.39998	0.64919	-1.67133	H	0.71053	1.32850	1.37474
C	-0.69624	-0.90056	-0.33432	C	0.75322	-0.63398	0.45581
H	-1.15751	-1.74109	-0.87422	H	0.58491	-1.06764	1.45367
C	0.72667	-0.80819	-0.93634	C	-0.60806	-0.60697	-0.26205
H	0.61420	-0.86041	-2.02844	H	-0.96605	-1.64206	-0.35974
H	1.27460	-1.71792	-0.64903	H	-0.47490	-0.24121	-1.29031
C	1.61910	0.40883	-0.63813	C	-1.69099	0.22440	0.43310
H	1.11925	1.32700	-0.97120	H	-1.38893	1.27902	0.46510
H	2.50934	0.31404	-1.27488	H	-1.78026	-0.09939	1.47986
C	2.08493	0.56947	0.81269	C	-3.05279	0.11196	-0.25703
H	2.51113	-0.36614	1.19474	H	-3.40470	-0.92680	-0.26913
H	2.85754	1.34332	0.88896	H	-3.81264	0.71700	0.25029
H	1.26780	0.85707	1.48026	H	-2.99526	0.45231	-1.29826
C	-0.72319	-1.29921	1.14858	C	1.72982	-1.55710	-0.28573
H	-0.15889	-2.22528	1.30861	H	1.33114	-2.57600	-0.35370
H	-0.29247	-0.53599	1.80104	H	1.91288	-1.20900	-1.30912
H	-1.75338	-1.47450	1.48263	H	2.69731	-1.60765	0.22774
Structure 17		σ=1	Mirror	Structure 18		σ=1	Mirror

			image=1				image=1
C	1.76042	-1.52038	0.32888	C	0.98116	1.83260	-0.44399
H	1.09606	-1.75721	1.16725	H	0.14136	1.72370	-1.13823
H	2.60839	-0.95319	0.72805	H	1.90235	1.64497	-1.00605
H	2.15171	-2.46785	-0.05796	H	1.00379	2.87799	-0.11632
C	1.02814	-0.74777	-0.77364	C	0.85231	0.89217	0.75903
H	1.71297	-0.59375	-1.61868	H	1.70793	1.05576	1.42872
H	0.21068	-1.36964	-1.16053	H	-0.03630	1.16510	1.34113
C	0.46406	0.62647	-0.35580	C	0.79258	-0.61193	0.42246
H	-0.07218	1.02178	-1.23032	H	0.71030	-1.13932	1.38546
C	-0.53827	0.54662	0.81149	C	-0.42942	-1.03626	-0.41661
H	-0.92522	1.55862	0.99949	H	-0.32787	-2.11352	-0.60363
H	-0.00153	0.25757	1.72544	H	-0.38449	-0.56133	-1.40700
C	-1.72644	-0.40496	0.60942	C	-1.81095	-0.77553	0.21848
H	-2.34496	-0.38260	1.51635	H	-1.73142	-0.86839	1.31089
H	-1.36579	-1.43779	0.51796	H	-2.49819	-1.57068	-0.09794
C	-2.60048	-0.06204	-0.60075	C	-2.45233	0.57019	-0.14016
H	-2.04981	-0.16769	-1.54200	H	-2.56291	0.66904	-1.22702
H	-3.47568	-0.71905	-0.65546	H	-3.45067	0.65884	0.30379
H	-2.96173	0.97239	-0.54397	H	-1.85964	1.42083	0.20846
C	1.58127	1.62551	-0.02487	C	2.08715	-1.09037	-0.25033
H	1.16919	2.62212	0.17205	H	2.09434	-2.18135	-0.35618
H	2.14151	1.32172	0.86724	H	2.19936	-0.66385	-1.25399
H	2.29419	1.71391	-0.85328	H	2.96907	-0.80296	0.33458
Structure 19		σ=1	Mirror image=1	Structure 20		σ=1	Mirror image=1
C	-3.09029	0.03622	0.12121	C	-2.90842	-0.21805	0.57305
H	-3.15146	1.10949	-0.08763	H	-3.16743	0.83211	0.40148
H	-3.18153	-0.09685	1.20641	H	-2.68950	-0.33588	1.64165
H	-3.96051	-0.43804	-0.34619	H	-3.79888	-0.81576	0.34823
C	-1.78721	-0.57748	-0.39888	C	-1.71902	-0.66318	-0.28256
H	-1.83124	-1.66707	-0.26486	H	-1.57344	-1.74435	-0.15188
H	-1.70738	-0.40796	-1.48278	H	-1.95474	-0.51502	-1.34674
C	-0.50859	-0.05417	0.28166	C	-0.39142	0.04860	0.03748
H	-0.63005	-0.19563	1.36790	H	-0.20525	-0.07895	1.11448
C	0.69950	-0.90463	-0.15623	C	0.75771	-0.62873	-0.73298
H	0.80324	-0.84248	-1.25006	H	0.54109	-0.56317	-1.80953
H	0.45802	-1.95336	0.06131	H	0.75470	-1.70047	-0.48631
C	2.04798	-0.54888	0.50573	C	2.16632	-0.07264	-0.47641

H	2.60982	-1.47269	0.69297	H	2.23004	0.96477	-0.82859
H	1.86367	-0.10781	1.49537	H	2.87670	-0.64089	-1.09127
C	2.93466	0.38804	-0.32286	C	2.60515	-0.14206	0.98935
H	2.44172	1.34240	-0.53248	H	2.53192	-1.16710	1.37379
H	3.87586	0.60478	0.19565	H	3.64410	0.18555	1.10718
H	3.18408	-0.07055	-1.28749	H	1.98412	0.49483	1.62901
C	-0.30119	1.44406	0.02786	C	-0.46424	1.55237	-0.25645
H	0.56672	1.82757	0.57289	H	0.46124	2.06490	0.02538
H	-0.14135	1.63954	-1.04057	H	-0.63027	1.72902	-1.32748
H	-1.16880	2.02960	0.34862	H	-1.28084	2.03263	0.29180
Structure 21		σ=1	Mirror image=1	Structure 22		σ=1	Mirror image=1
C	-2.88246	-0.73459	-0.13057	C	-2.69295	-0.71221	-0.03610
H	-3.22473	0.09220	-0.76228	H	-2.93820	-0.18578	-0.96498
H	-3.27822	-0.56691	0.87888	H	-3.19831	-0.18880	0.78518
H	-3.33650	-1.65350	-0.51804	H	-3.12352	-1.71747	-0.10562
C	-1.35474	-0.84076	-0.11060	C	-1.18065	-0.77607	0.20092
H	-1.06624	-1.73913	0.45291	H	-0.98566	-1.39014	1.09062
H	-0.99007	-0.99273	-1.13541	H	-0.70837	-1.29850	-0.63899
C	-0.64654	0.37695	0.51177	C	-0.52577	0.60469	0.40450
H	-1.10169	0.54249	1.50069	H	-1.13475	1.11864	1.16482
C	0.85034	0.10377	0.76499	C	0.90073	0.53316	0.99975
H	0.93972	-0.75777	1.44278	H	0.89750	-0.18778	1.83013
H	1.27602	0.96140	1.30610	H	1.11641	1.51156	1.45137
C	1.70672	-0.16229	-0.47949	C	2.07380	0.20340	0.06061
H	1.63911	0.68987	-1.16777	H	2.99756	0.32610	0.64194
H	1.31288	-1.02950	-1.02465	H	2.12735	0.95276	-0.73962
C	3.17604	-0.41185	-0.12855	C	2.07298	-1.19879	-0.55703
H	3.28117	-1.27945	0.53439	H	1.28151	-1.31847	-1.30291
H	3.77743	-0.60121	-1.02483	H	3.02677	-1.40329	-1.05707
H	3.60988	0.45245	0.38917	H	1.92539	-1.96975	0.20899
C	-0.86347	1.65523	-0.31112	C	-0.57135	1.46181	-0.86782
H	-0.30857	2.49740	0.11915	H	-0.08107	2.42973	-0.70937
H	-0.52519	1.52692	-1.34619	H	-0.06252	0.96382	-1.70188
H	-1.92038	1.93872	-0.34336	H	-1.60092	1.66145	-1.18152
Structure 23		σ=1	Mirror image=1	Structure 24		σ=1	Mirror image=1
C	-2.72086	-0.45937	-0.46920	C	2.69181	-1.08851	-0.10423
H	-2.85249	0.46129	-1.04773	H	3.38306	-0.29083	0.18690

H	-3.26934	-0.34031	0.47352	H	2.73423	-1.18278	-1.19658
H	-3.19605	-1.27140	-1.03089	H	3.07003	-2.02331	0.32448
C	-1.24200	-0.76103	-0.20953	C	1.26092	-0.81001	0.36651
H	-1.15811	-1.74068	0.28159	H	0.64958	-1.69674	0.16079
H	-0.71840	-0.85629	-1.17059	H	1.25121	-0.67869	1.45889
C	-0.52741	0.28861	0.65990	C	0.60060	0.41983	-0.28353
H	-1.12794	0.40597	1.57562	H	0.60837	0.26470	-1.37460
C	0.85795	-0.20739	1.13843	C	-0.86720	0.58129	0.15336
H	0.68405	-0.98099	1.89951	H	-1.25081	1.52510	-0.26045
H	1.36406	0.61869	1.65855	H	-0.90487	0.69534	1.24770
C	1.82419	-0.80574	0.10127	C	-1.81031	-0.55015	-0.27103
H	1.35789	-1.67591	-0.37826	H	-1.50650	-1.49324	0.19962
H	2.68731	-1.20067	0.65395	H	-1.72092	-0.70608	-1.35558
C	2.33742	0.15324	-0.97803	C	-3.27067	-0.26046	0.08623
H	2.72248	1.07992	-0.53539	H	-3.62268	0.65582	-0.40325
H	3.15121	-0.30660	-1.55057	H	-3.93024	-1.07940	-0.22215
H	1.55292	0.42778	-1.68947	H	-3.39150	-0.12340	1.16781
C	-0.48858	1.67161	-0.01007	C	1.37913	1.70831	0.01540
H	0.10187	2.37729	0.58564	H	0.88853	2.57650	-0.43965
H	-0.04799	1.63255	-1.01110	H	1.43326	1.88631	1.09754
H	-1.49569	2.08983	-0.11099	H	2.40361	1.66887	-0.36773
Structure 25		σ=1	Mirror image=1	Structure 26		σ=1	Mirror image=1
C	2.31950	-1.31202	-0.11312	C	-2.25110	-1.42501	0.16701
H	3.14551	-0.59333	-0.11521	H	-3.04404	-0.88593	-0.36152
H	2.12847	-1.60149	-1.15417	H	-2.44858	-1.33587	1.24271
H	2.66194	-2.20474	0.42210	H	-2.33933	-2.48404	-0.10002
C	1.05729	-0.73492	0.53508	C	-0.85937	-0.88744	-0.18145
H	0.31593	-1.53818	0.62563	H	-0.11067	-1.55045	0.26761
H	1.28417	-0.41239	1.56225	H	-0.70532	-0.94110	-1.26936
C	0.42982	0.44509	-0.22792	C	-0.59502	0.55326	0.28990
H	0.18892	0.09428	-1.24271	H	-0.70532	0.56377	1.38647
C	-0.87387	0.92979	0.43568	C	0.83599	1.02973	-0.02933
H	-1.26293	1.77500	-0.15039	H	0.92693	2.05955	0.33984
H	-0.62928	1.33604	1.42830	H	0.95543	1.09354	-1.12145
C	-1.99249	-0.11232	0.58747	C	1.97980	0.17735	0.56198
H	-2.85292	0.37697	1.06266	H	1.62371	-0.33536	1.46651
H	-1.67961	-0.90330	1.28071	H	2.78640	0.84181	0.89649
C	-2.44095	-0.74118	-0.73509	C	2.57748	-0.84461	-0.41215

H	-1.64081	-1.33194	-1.19469	H	3.00155	-0.33946	-1.28847
H	-3.29817	-1.40713	-0.58579	H	3.38084	-1.42142	0.06070
H	-2.73789	0.03000	-1.45683	H	1.82654	-1.55334	-0.77530
C	1.40420	1.62304	-0.36449	C	-1.61129	1.54344	-0.29493
H	0.92953	2.46448	-0.88255	H	-1.38922	2.56777	0.02618
H	1.72409	1.97922	0.62369	H	-1.58253	1.52579	-1.39243
H	2.30199	1.35165	-0.92865	H	-2.63536	1.31438	0.01580

2,2-dimethylpentane

Structure 1		σ=1	Mirror image=0	Structure 2		σ=1	Mirror image=1
C	2.16135	-0.69045	0.00000	C	-2.15964	-0.48581	-0.57135
H	2.55157	-0.17535	0.88623	H	-2.32430	-1.53758	-0.30823
H	2.55157	-0.17535	-0.88623	H	-2.17312	-0.40786	-1.66550
H	2.56380	-1.71060	0.00000	H	-3.00522	0.09504	-0.18378
C	0.62251	-0.70356	0.00000	C	-0.82568	0.02930	0.00290
C	0.13203	0.76429	0.00000	C	0.31277	-0.80155	-0.64873
H	0.56068	1.27005	-0.87805	H	0.40051	-0.49613	-1.70181
H	0.56068	1.27005	0.87805	H	-0.01920	-1.84919	-0.66864
C	-1.38403	0.99092	0.00000	C	1.71281	-0.79568	-0.01060
H	-1.83485	0.51171	0.87807	H	2.31240	-1.53689	-0.55603
H	-1.83485	0.51171	-0.87807	H	1.64957	-1.16974	1.01920
C	-1.74316	2.47968	0.00000	C	2.47108	0.53582	-0.02077
H	-1.33484	2.98394	-0.88440	H	2.04651	1.25838	0.68262
H	-2.82844	2.63111	0.00000	H	3.51925	0.38492	0.26217
H	-1.33484	2.98394	0.88440	H	2.45683	0.99409	-1.01706
C	0.13203	-1.44363	1.25655	C	-0.83835	-0.15434	1.52916
H	0.44521	-0.92104	2.16882	H	-0.89523	-1.21582	1.80016
H	-0.95944	-1.53184	1.27687	H	0.06024	0.26373	1.99579
H	0.54567	-2.45854	1.29363	H	-1.70588	0.35005	1.97125
C	0.13203	-1.44363	-1.25655	C	-0.71302	1.52704	-0.33817
H	0.44521	-0.92104	-2.16882	H	-0.68826	1.67956	-1.42398
H	0.54567	-2.45854	-1.29363	H	-1.57867	2.07409	0.05509
H	-0.95944	-1.53184	-1.27687	H	0.18472	1.98465	0.08404

3,3-dimethylpentane

Structure 1		σ=2	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	1.13755	1.41292	-1.34212	C	1.28248	1.81562	-0.02401
H	1.11044	0.61036	-2.08725	H	2.00857	1.29324	-0.65447
H	2.12117	1.38623	-0.86114	H	1.54714	1.62632	1.02208

H	1.06227	2.36367	-1.88159	H	1.40900	2.88929	-0.20438
C	0.00000	1.28324	-0.32464	C	-0.15554	1.39409	-0.34125
H	0.02712	2.14734	0.35377	H	-0.84301	2.07283	0.18311
H	-0.95916	1.35174	-0.85418	H	-0.33575	1.55435	-1.41369
C	0.00000	0.00000	0.54226	C	-0.58206	-0.05617	0.00323
C	0.00000	-1.28324	-0.32464	C	0.30202	-1.11667	-0.71204
H	-0.02712	-2.14734	0.35377	H	0.51069	-0.75856	-1.73009
H	0.95916	-1.35174	-0.85418	H	-0.29964	-2.02747	-0.83683
C	-1.13755	-1.41292	-1.34212	C	1.61614	-1.52682	-0.03492
H	-1.11044	-0.61036	-2.08725	H	1.43325	-2.00755	0.93181
H	-1.06227	-2.36367	-1.88159	H	2.15092	-2.24935	-0.66217
H	-2.12117	-1.38623	-0.86114	H	2.28667	-0.68179	0.13936
C	1.24705	-0.03166	1.44407	C	-0.58880	-0.26760	1.52639
H	1.22149	-0.90266	2.10995	H	-0.90009	-1.28846	1.77922
H	2.17122	-0.09246	0.85915	H	0.39579	-0.10218	1.97419
H	1.30272	0.86684	2.07067	H	-1.29305	0.42329	2.00531
C	-1.24705	0.03166	1.44407	C	-2.02341	-0.22939	-0.51523
H	-1.22149	0.90266	2.10995	H	-2.68779	0.54029	-0.10427
H	-2.17122	0.09246	0.85915	H	-2.05973	-0.15395	-1.60909
H	-1.30272	-0.86684	2.07067	H	-2.42798	-1.20864	-0.23311
Structure 3		σ=1	Mirror image=1	Structure 4		σ=2	Mirror image=0
C	2.30659	-0.88517	-0.02318	C	0.00000	2.61510	-0.18565
H	1.88708	-1.86055	-0.29077	H	0.88470	2.76129	0.44304
H	2.41587	-0.85602	1.06630	H	-0.88470	2.76129	0.44304
H	3.31260	-0.83342	-0.45444	H	0.00000	3.41107	-0.93876
C	1.44731	0.27299	-0.54079	C	0.00000	1.24258	-0.86599
H	1.95557	1.21905	-0.30723	H	-0.87761	1.17565	-1.52449
H	1.40004	0.21773	-1.63767	H	0.87761	1.17565	-1.52449
C	-0.00266	0.36490	0.00076	C	0.00000	0.00000	0.06137
C	-0.78319	-0.91167	-0.39778	C	0.00000	-1.24258	-0.86599
H	-0.29502	-1.78000	0.06185	H	0.87761	-1.17565	-1.52449
H	-0.68684	-1.04741	-1.48465	H	-0.87761	-1.17565	-1.52449
C	-2.26931	-0.94188	-0.02494	C	0.00000	-2.61510	-0.18565
H	-2.83287	-0.14415	-0.51985	H	-0.88470	-2.76129	0.44304
H	-2.71804	-1.89504	-0.32634	H	0.00000	-3.41107	-0.93876
H	-2.42010	-0.83683	1.05500	H	0.88470	-2.76129	0.44304
C	0.01383	0.53698	1.53025	C	1.25677	0.00000	0.94859
H	-0.98984	0.73715	1.91989	H	1.28712	-0.88069	1.59847

H	0.39246	-0.35814	2.03582	H	2.16906	0.00000	0.33895
H	0.65227	1.38111	1.81825	H	1.28712	0.88069	1.59847
C	-0.65156	1.60797	-0.63456	C	-1.25677	0.00000	0.94859
H	-0.06072	2.50586	-0.41714	H	-1.28712	0.88069	1.59847
H	-0.71548	1.50602	-1.72508	H	-2.16906	0.00000	0.33895
H	-1.66308	1.77995	-0.25243	H	-1.28712	-0.88069	1.59847

2,3-dimethylpentane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	1.54190	-1.20316	0.78056	C	0.94541	-1.07266	1.23139
H	0.79625	-1.96449	1.03222	H	0.00065	-1.33618	1.71858
H	1.70991	-0.58920	1.67304	H	1.43475	-0.30543	1.84263
H	2.48214	-1.72102	0.55868	H	1.58581	-1.96205	1.24938
C	1.10789	-0.34362	-0.41545	C	0.73562	-0.59242	-0.21132
H	0.99802	-1.01588	-1.27986	H	0.25358	-1.41163	-0.76183
C	-0.27371	0.33636	-0.22499	C	-0.20953	0.63206	-0.32713
H	-0.43302	0.95667	-1.12138	H	-0.30886	0.83692	-1.40510
C	-1.41229	-0.70116	-0.19242	C	-1.62917	0.35949	0.20792
H	-1.35250	-1.28414	0.73655	H	-2.23196	1.26094	0.03327
H	-1.25798	-1.41594	-1.01268	H	-1.59270	0.23452	1.29872
C	-2.81559	-0.09996	-0.31776	C	-2.34064	-0.84157	-0.42122
H	-2.90470	0.50390	-1.22941	H	-1.86049	-1.78919	-0.15471
H	-3.57716	-0.88650	-0.36354	H	-3.38275	-0.89721	-0.08730
H	-3.06164	0.54495	0.53255	H	-2.34505	-0.76877	-1.51597
C	2.20498	0.66930	-0.77038	C	2.08701	-0.33949	-0.89452
H	1.91163	1.29230	-1.62378	H	1.95326	0.03524	-1.91658
H	2.42720	1.33641	0.07059	H	2.68812	0.39395	-0.34504
H	3.13728	0.15613	-1.03334	H	2.67225	-1.26468	-0.95009
C	-0.32677	1.26813	0.99463	C	0.35433	1.90035	0.32993
H	-1.26172	1.83673	1.01620	H	-0.32558	2.74581	0.17388
H	-0.26525	0.70118	1.93106	H	0.47221	1.77257	1.41237
H	0.49304	1.99362	0.98793	H	1.32854	2.18059	-0.08250

Structure 3		σ=1	Mirror image=1	Structure 4		σ=1	Mirror image=1
C	0.99875	-1.30610	0.84647	C	-2.27358	0.77290	0.18530
H	0.03376	-1.73869	1.12253	H	-2.16262	1.79437	-0.18883
H	1.38010	-0.76203	1.71821	H	-2.28527	0.81550	1.28250
H	1.69161	-2.13251	0.64951	H	-3.25427	0.40869	-0.14122
C	0.90817	-0.38736	-0.38250	C	-1.15854	-0.16095	-0.31152

H	0.63338	-1.01202	-1.24569	H	-1.13050	-0.09592	-1.41095
C	-0.16519	0.73489	-0.27644	C	0.23993	0.26427	0.21020
H	0.15791	1.52693	-0.96816	H	0.21695	0.17302	1.30907
C	-1.55878	0.30807	-0.78759	C	1.35185	-0.67055	-0.30870
H	-1.46731	0.03962	-1.84918	H	1.36641	-0.62869	-1.40808
H	-2.21292	1.19061	-0.75442	H	1.10512	-1.70449	-0.04615
C	-2.25056	-0.84399	-0.05092	C	2.75318	-0.36841	0.23324
H	-2.33163	-0.65304	1.02494	H	2.75189	-0.33799	1.33012
H	-3.26656	-0.98729	-0.43602	H	3.46310	-1.14380	-0.07584
H	-1.71540	-1.78965	-0.18428	H	3.14112	0.59033	-0.12508
C	2.29203	0.21162	-0.67520	C	-1.51278	-1.60795	0.06717
H	2.28885	0.78680	-1.60827	H	-0.84611	-2.34091	-0.39539
H	2.60751	0.88562	0.13130	H	-1.46342	-1.74772	1.15516
H	3.05316	-0.57247	-0.76437	H	-2.53359	-1.84898	-0.25041
C	-0.23749	1.37735	1.11604	C	0.55318	1.72823	-0.13447
H	-0.90621	2.24580	1.10219	H	1.54135	2.02248	0.23053
H	-0.61502	0.68174	1.87251	H	0.54057	1.88145	-1.22194
H	0.74713	1.72368	1.45005	H	-0.17016	2.41749	0.30909
Structure 5		σ=1	Mirror image=1	Structure 6		σ=1	Mirror image=1
C	-2.23882	-0.04722	-0.41314	C	-2.24042	0.52275	-0.28109
H	-2.36412	0.85349	-1.02118	H	-2.15102	1.50847	-0.74691
H	-2.67485	0.14914	0.57443	H	-2.59975	0.66775	0.74634
H	-2.82858	-0.84608	-0.87769	H	-3.01329	-0.03070	-0.82670
C	-0.76853	-0.47855	-0.29721	C	-0.91250	-0.24973	-0.28875
H	-0.40134	-0.64584	-1.32158	H	-0.56876	-0.30662	-1.33229
C	0.16635	0.58329	0.36353	C	0.18142	0.48010	0.53077
H	0.24574	0.33046	1.43257	H	-0.20559	0.57745	1.55779
C	1.59052	0.56764	-0.23355	C	1.50271	-0.31373	0.63734
H	2.17836	1.34190	0.27797	H	1.32698	-1.24517	1.18813
H	1.52235	0.88831	-1.28377	H	2.19757	0.27097	1.25514
C	2.36528	-0.75092	-0.16656	C	2.18044	-0.64055	-0.69791
H	1.90185	-1.53230	-0.77728	H	2.40357	0.26559	-1.27168
H	3.38763	-0.61162	-0.53638	H	3.12714	-1.16675	-0.53243
H	2.43317	-1.12391	0.86245	H	1.55262	-1.28307	-1.32520
C	-0.71468	-1.81766	0.45686	C	-1.15110	-1.68269	0.20899
H	0.30415	-2.19057	0.58284	H	-0.26775	-2.31740	0.09062
H	-1.15008	-1.70320	1.45807	H	-1.42511	-1.68505	1.27219
H	-1.29247	-2.58737	-0.06850	H	-1.97175	-2.15283	-0.34481

C	-0.36462	2.02324	0.27847	C	0.44566	1.89955	0.00223
H	0.33565	2.71388	0.76226	H	1.28770	2.35990	0.53219
H	-0.47549	2.34632	-0.76432	H	0.69146	1.89009	-1.06652
H	-1.33496	2.13852	0.76964	H	-0.42134	2.55307	0.13463
Structure 7		σ=1	Mirror image=1	Structure 8		σ=1	Mirror image=1
C	1.78756	-1.26658	-0.63073	C	1.59672	-0.99270	-0.91682
H	1.47020	-1.58460	-1.63098	H	1.42735	-0.88444	-1.99465
H	1.43775	-2.01861	0.08604	H	1.11273	-1.91948	-0.59612
H	2.88342	-1.27942	-0.60578	H	2.67520	-1.11411	-0.75895
C	1.25236	0.13227	-0.29467	C	1.07679	0.23352	-0.15126
H	1.69598	0.82849	-1.02227	H	1.67511	1.08647	-0.50453
C	-0.28449	0.23343	-0.48818	C	-0.40065	0.59343	-0.48362
H	-0.49597	-0.19676	-1.48000	H	-0.54873	0.37413	-1.55231
C	-1.08279	-0.58771	0.54247	C	-1.48044	-0.18499	0.29539
H	-0.99778	-0.11348	1.52940	H	-2.45399	0.22457	-0.00633
H	-0.63365	-1.58350	0.64212	H	-1.38679	0.03931	1.36649
C	-2.56420	-0.75660	0.18966	C	-1.51637	-1.70313	0.09461
H	-2.68195	-1.21960	-0.79794	H	-0.65942	-2.20214	0.55657
H	-3.07166	-1.39676	0.92004	H	-2.42145	-2.12899	0.54287
H	-3.09276	0.20242	0.17108	H	-1.51823	-1.96359	-0.97063
C	1.72533	0.56564	1.10037	C	1.34540	0.09481	1.35364
H	1.37731	1.57143	1.35843	H	0.99075	0.96726	1.91369
H	1.36681	-0.12271	1.87442	H	0.85425	-0.79178	1.77049
H	2.82029	0.57154	1.14934	H	2.42006	-0.00621	1.54390
C	-0.74721	1.69747	-0.51998	C	-0.63464	2.10066	-0.29092
H	-1.79887	1.78165	-0.81170	H	-1.65742	2.38199	-0.56696
H	-0.64037	2.17265	0.46251	H	-0.48465	2.39562	0.75515
H	-0.15820	2.27970	-1.23835	H	0.05441	2.69177	-0.90479
Structure 9		σ=1	Mirror image=1				
C	1.77799	-0.97916	-0.69851				
H	1.66949	-1.08491	-1.78474				
H	1.32887	-1.86302	-0.23050				
H	2.84891	-0.99357	-0.46530				
C	1.12776	0.31526	-0.19340				
H	1.68941	1.15209	-0.63672				
C	-0.32316	0.48223	-0.72619				
H	-0.20603	0.61473	-1.81299				

C	-1.25852	-0.73990	-0.58060
H	-0.83201	-1.58541	-1.13413
H	-2.19310	-0.48815	-1.10095
C	-1.60523	-1.20469	0.83881
H	-1.95261	-0.37879	1.46897
H	-2.40520	-1.95333	0.80850
H	-0.74808	-1.66573	1.33845
C	1.29948	0.44656	1.32827
H	0.89037	1.38867	1.70627
H	0.81634	-0.36981	1.87264
H	2.36524	0.42500	1.58537
C	-0.98479	1.76412	-0.20196
H	-1.92500	1.95847	-0.73107
H	-1.21599	1.70442	0.86657
H	-0.33171	2.63280	-0.34888

2,4-dimethylpentane

Structure 1		σ=2	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	0.00000	1.85233	-1.06343	C	1.15289	1.33285	0.66921
H	0.51041	1.24496	-1.81826	H	0.25340	1.58876	1.23571
H	0.76695	2.40517	-0.50513	H	1.19031	1.98372	-0.21359
H	-0.62030	2.58580	-1.59156	H	2.01748	1.57584	1.29846
C	-0.84990	0.99771	-0.11476	C	1.18042	-0.14627	0.26199
H	-1.56778	0.42825	-0.72170	H	1.01847	-0.74799	1.16749
C	0.00000	0.00000	0.69179	C	0.10390	-0.53755	-0.76999
H	-0.66742	-0.57179	1.35439	H	0.27423	-1.59452	-1.01922
H	0.66742	0.57179	1.35439	H	0.29068	0.02235	-1.69872
C	0.84990	-0.99771	-0.11476	C	-1.39051	-0.38897	-0.39595
H	1.56778	-0.42825	-0.72170	H	-1.93311	-1.01611	-1.11882
C	1.65626	-1.89046	0.83728	C	-1.70557	-0.94097	1.00040
H	0.98788	-2.49611	1.46302	H	-1.25073	-0.32748	1.78683
H	2.30677	-2.57746	0.28348	H	-2.78703	-0.95456	1.17880
H	2.28710	-1.29288	1.50588	H	-1.33260	-1.96531	1.11940
C	-1.65626	1.89046	0.83728	C	2.56613	-0.51138	-0.29068
H	-2.28710	1.29288	1.50588	H	2.62472	-1.57331	-0.55664
H	-0.98788	2.49611	1.46302	H	2.79063	0.07081	-1.19392
H	-2.30677	2.57746	0.28348	H	3.35324	-0.30280	0.44323
C	0.00000	-1.85233	-1.06343	C	-1.94457	1.03327	-0.57035
H	0.62030	-2.58580	-1.59156	H	-3.03497	1.03562	-0.45332

H	-0.76695	-2.40517	-0.50513	H	-1.53617	1.73313	0.16430
H	-0.51041	-1.24496	-1.81826	H	-1.71469	1.42597	-1.56782
Structure 3		σ=1	Mirror image=1	Structure 4		σ=2	Mirror image=1
C	-1.56345	1.35028	-0.33499	C	0.00000	2.21200	-0.19244
H	-0.78350	1.88579	-0.88530	H	-0.69905	2.61833	0.54804
H	-1.57964	1.73866	0.69159	H	-0.58268	1.89219	-1.06094
H	-2.52520	1.59854	-0.79924	H	0.65265	3.03034	-0.51966
C	-1.33325	-0.16588	-0.34252	C	0.83639	1.06701	0.40064
H	-1.27217	-0.48816	-1.39369	H	1.45790	1.52288	1.18637
C	-0.01952	-0.59103	0.33939	C	0.00000	0.00000	1.14970
H	0.02970	-1.68757	0.29597	H	-0.68384	0.54669	1.81473
H	-0.06999	-0.33686	1.40907	H	0.68384	-0.54669	1.81473
C	1.27819	-0.00477	-0.26680	C	-0.83639	-1.06701	0.40064
H	1.07325	0.26184	-1.31476	H	-1.45790	-1.52288	1.18637
C	1.74499	1.26138	0.46632	C	-1.80296	-0.50357	-0.64939
H	2.01549	1.02202	1.50291	H	-1.26835	-0.13428	-1.53126
H	2.62987	1.69331	-0.01615	H	-2.49327	-1.28410	-0.99105
H	0.96929	2.03176	0.49761	H	-2.40114	0.32209	-0.24824
C	-2.52212	-0.88984	0.30236	C	1.80296	0.50357	-0.64939
H	-2.39157	-1.97800	0.27314	H	2.40114	-0.32209	-0.24824
H	-2.63182	-0.59562	1.35424	H	1.26835	0.13428	-1.53126
H	-3.46079	-0.64809	-0.20974	H	2.49327	1.28410	-0.99105
C	2.40233	-1.04997	-0.26704	C	0.00000	-2.21200	-0.19244
H	3.32726	-0.64269	-0.69238	H	-0.65265	-3.03034	-0.51966
H	2.62414	-1.38054	0.75603	H	0.58268	-1.89219	-1.06094
H	2.12266	-1.93546	-0.84964	H	0.69905	-2.61833	0.54804

3-ethylpentane

Structure 1		σ=1	Mirror image=1	Structure 2		σ=1	Mirror image=1
C	-0.75574	2.16169	-0.21526	C	-1.75908	-1.73200	0.04314
H	-1.71902	1.85012	-0.63171	H	-2.54616	-0.97236	0.06945
H	-0.10393	2.42402	-1.05740	H	-1.67564	-2.15249	1.05276
H	-0.92367	3.07160	0.37263	H	-2.09161	-2.53502	-0.62494
C	-0.11851	1.05820	0.63542	C	-0.41489	-1.15301	-0.41264
H	0.83075	1.43790	1.03248	H	0.31650	-1.97176	-0.43398
H	-0.74608	0.85839	1.51512	H	-0.49608	-0.80054	-1.45003
C	0.12803	-0.26983	-0.12447	C	0.12452	-0.01213	0.48665
H	0.13278	-0.04923	-1.20425	H	-0.34613	-0.12143	1.47626

C	1.50070	-0.87717	0.22344	C	1.64588	-0.14012	0.71603
H	1.54813	-1.90190	-0.16939	H	1.84143	-1.10946	1.19473
H	1.58459	-0.96619	1.31644	H	1.96212	0.62667	1.43668
C	2.69024	-0.08465	-0.32529	C	2.50842	-0.02651	-0.54612
H	2.70718	0.94370	0.05326	H	2.42020	0.96110	-1.01117
H	3.64101	-0.55291	-0.04700	H	3.56625	-0.18414	-0.30814
H	2.65123	-0.03183	-1.42020	H	2.22404	-0.77341	-1.29614
C	-0.98227	-1.30590	0.13207	C	-0.23857	1.39135	-0.03431
H	-0.74021	-2.22044	-0.42635	H	0.22906	2.13594	0.62515
H	-0.96079	-1.58508	1.19597	H	0.21212	1.53669	-1.02509
C	-2.39679	-0.85676	-0.24324	C	-1.73856	1.68394	-0.12765
H	-2.45100	-0.55853	-1.29738	H	-2.23750	1.51675	0.83472
H	-3.11740	-1.66789	-0.08913	H	-1.91530	2.72569	-0.41857
H	-2.72752	-0.00525	0.36089	H	-2.22969	1.04874	-0.87236
Structure 3		σ=1	Mirror image=1	Structure 4		σ=1	Mirror image=0
C	2.16296	-1.28837	-0.41417	C	-2.08334	0.28926	0.00000
H	2.63753	-0.35094	-0.71933	H	-2.19394	-0.34892	0.88381
H	1.85001	-1.80982	-1.32699	H	-2.19394	-0.34892	-0.88381
H	2.92536	-1.90503	0.07599	H	-2.91856	0.99836	0.00000
C	0.96300	-1.05297	0.50981	C	-0.74297	1.03165	0.00000
H	0.55259	-2.03196	0.79028	H	-0.70038	1.69457	-0.87270
H	1.30032	-0.59335	1.44944	H	-0.70038	1.69457	0.87270
C	-0.16516	-0.19010	-0.10905	C	0.50807	0.12804	0.00000
H	-0.08343	-0.26068	-1.20604	H	1.37933	0.80301	0.00000
C	-1.54389	-0.75854	0.28290	C	0.61750	-0.75227	1.25982
H	-1.64399	-0.72519	1.37799	H	1.54476	-1.33662	1.18626
H	-1.56312	-1.82238	0.01038	H	-0.19805	-1.48830	1.26443
C	-2.74578	-0.06394	-0.36366	C	0.61750	0.01665	2.58378
H	-2.64155	-0.03465	-1.45566	H	-0.34238	0.51040	2.76977
H	-3.67476	-0.59729	-0.13278	H	0.80930	-0.65562	3.42752
H	-2.86511	0.96663	-0.01399	H	1.39506	0.79066	2.59086
C	-0.04824	1.29760	0.27365	C	0.61750	-0.75227	-1.25982
H	-0.85901	1.85527	-0.21000	H	1.54476	-1.33662	-1.18626
H	-0.21793	1.39093	1.35692	H	-0.19805	-1.48830	-1.26443
C	1.27983	1.96876	-0.08770	C	0.61750	0.01665	-2.58378
H	1.49326	1.87486	-1.15942	H	1.39506	0.79066	-2.59086
H	1.25212	3.03757	0.15306	H	0.80930	-0.65562	-3.42752
H	2.12140	1.53140	0.45942	H	-0.34238	0.51040	-2.76977

Structure 5		σ=1	Mirror image=1	Structure 6		σ=1	Mirror image=1
C	-0.32801	2.54897	0.33552	C	1.50894	-1.69771	-0.54805
H	-0.12055	2.51110	1.41194	H	1.97399	-0.96852	-1.22089
H	-1.41471	2.49819	0.20705	H	0.73084	-2.22119	-1.11423
H	0.00000	3.52753	-0.03277	H	2.27511	-2.43460	-0.28258
C	0.39359	1.41436	-0.39782	C	0.94377	-1.02842	0.70968
H	0.20393	1.48989	-1.47863	H	0.54604	-1.80305	1.37933
H	1.47397	1.55385	-0.27071	H	1.76479	-0.55148	1.25901
C	0.00000	0.00000	0.07260	C	-0.17156	0.00986	0.46138
H	0.00000	0.00000	1.17528	H	-0.42360	0.43656	1.44585
C	-1.42166	-0.36632	-0.39782	C	0.28127	1.17727	-0.43611
H	-1.39225	-0.56834	-1.47863	H	-0.54284	1.89537	-0.52242
H	-2.08266	0.49957	-0.27071	H	0.46207	0.80487	-1.45390
C	-2.04347	-1.55856	0.33552	C	1.52342	1.91913	0.06620
H	-2.11441	-1.35995	1.41194	H	2.41550	1.28397	0.04709
H	-3.05493	-1.76376	-0.03277	H	1.73239	2.79841	-0.55336
H	-1.45614	-2.47428	0.20705	H	1.38520	2.26442	1.09840
C	1.02808	-1.04804	-0.39782	C	-1.44868	-0.66208	-0.08019
H	0.60869	-2.05342	-0.27071	H	-1.27209	-1.01450	-1.10547
H	1.18832	-0.92155	-1.47863	H	-1.64943	-1.56043	0.51982
C	2.37148	-0.99042	0.33552	C	-2.69362	0.23051	-0.06178
H	2.23496	-1.15115	1.41194	H	-2.59274	1.09049	-0.73220
H	3.05493	-1.76376	-0.03277	H	-3.58140	-0.32842	-0.37835
H	2.87086	-0.02392	0.20705	H	-2.88507	0.61672	0.94713
Structure 7		σ=1	Mirror image=1	Structure 8		σ=1	Mirror image=1
C	2.24253	-0.42536	-0.67338	C	-0.45175	1.88546	-0.81096
H	2.43815	0.65095	-0.69845	H	-1.49718	1.60910	-0.98354
H	1.71946	-0.69265	-1.59813	H	0.15095	1.41214	-1.59045
H	3.21412	-0.93247	-0.68697	H	-0.37624	2.97073	-0.94670
C	1.44686	-0.83271	0.57223	C	0.00000	1.50036	0.60361
H	1.43836	-1.92990	0.63627	H	1.00693	1.90251	0.78385
H	1.98545	-0.48329	1.46391	H	-0.65780	2.02333	1.31122
C	-0.01748	-0.35081	0.67033	C	0.00000	0.00000	0.98706
H	-0.38551	-0.76414	1.62250	H	0.00000	0.00000	2.08678
C	-0.16818	1.18571	0.79831	C	-1.29935	-0.75018	0.60361
H	0.62655	1.55455	1.46118	H	-2.15109	-0.07923	0.78385
H	-1.10956	1.39761	1.32158	H	-1.42336	-1.58133	1.31122

C	-0.16086	2.00242	-0.50083	C	-1.40698	-1.33396	-0.81096
H	-1.00060	1.73435	-1.15090	H	-0.64493	-2.10115	-0.98354
H	-0.25268	3.07095	-0.27470	H	-2.38461	-1.81120	-0.94670
H	0.75666	1.86525	-1.07880	H	-1.29842	-0.57534	-1.59045
C	-0.90001	-0.96163	-0.43272	C	1.29935	-0.75018	0.60361
H	-0.61497	-0.55820	-1.41222	H	2.08116	-0.44200	1.31122
H	-0.69627	-2.04022	-0.48048	H	1.14416	-1.82328	0.78385
C	-2.40057	-0.74847	-0.21183	C	1.85873	-0.55150	-0.81096
H	-2.66795	0.31379	-0.22768	H	2.14211	0.49205	-0.98354
H	-2.99018	-1.24878	-0.98821	H	2.76085	-1.15953	-0.94670
H	-2.71478	-1.15256	0.75847	H	1.14747	-0.83680	-1.59045

octane

C	0.16366	4.49221	0.00000	C	3.11844	-0.62778	-0.30055
H	-0.47252	4.61913	0.88449	H	3.47469	-0.20983	0.64701
H	-0.47252	4.61913	-0.88449	H	3.40858	0.06579	-1.09958
H	0.90126	5.30260	0.00000	H	3.65455	-1.56910	-0.46562
C	0.83773	3.11807	0.00000	C	1.60327	-0.85320	-0.29243
H	1.49281	3.02941	-0.87808	H	1.31595	-1.36670	-1.22046
H	1.49281	3.02941	0.87808	H	1.34748	-1.53756	0.52745
C	-0.16366	1.95890	0.00000	C	0.77380	0.43971	-0.17057
H	-0.82003	2.04679	-0.87839	H	1.14156	1.12471	-0.95083
H	-0.82003	2.04679	0.87839	C	-0.72556	0.19431	-0.49102
C	0.50080	0.57924	0.00000	H	-0.74589	-0.37091	-1.43629
H	1.15707	0.49206	0.87837	C	-1.44059	-0.66764	0.56730
H	1.15707	0.49206	-0.87837	H	-1.52647	-0.09836	1.50256
C	-0.50080	-0.57924	0.00000	H	-0.82352	-1.54449	0.79839
H	-1.15707	-0.49206	-0.87837	C	-2.83106	-1.15023	0.14150
H	-1.15707	-0.49206	0.87837	H	-2.78149	-1.70612	-0.80309
C	0.16366	-1.95890	0.00000	H	-3.26407	-1.81559	0.89686
H	0.82003	-2.04679	0.87839	H	-3.52809	-0.31754	-0.00022
H	0.82003	-2.04679	-0.87839	C	0.99584	1.12671	1.18530
C	-0.83773	-3.11807	0.00000	H	0.38792	2.03172	1.28580
H	-1.49281	-3.02941	-0.87808	H	0.74065	0.45794	2.01574
H	-1.49281	-3.02941	0.87808	H	2.04178	1.42344	1.31167
C	-0.16366	-4.49221	0.00000	C	-1.47017	1.51463	-0.73876
H	0.47252	-4.61913	0.88449	H	-1.58245	2.09348	0.18571
H	-0.90126	-5.30260	0.00000	H	-0.93102	2.13935	-1.46059
H	0.47252	-4.61913	-0.88449	H	-2.47392	1.34072	-1.13915

3-ethyl-2-methylpentane

2,2,3,3-tetramethylbutane

C	1.86597	-1.13921	-1.04186	C	0.84534	1.16303	1.35092
H	1.50794	-1.07124	-2.07605	H	0.53814	2.13137	0.94188
H	1.60757	-2.13500	-0.66364	H	1.91140	1.03072	1.14205
H	2.96008	-1.07313	-1.05995	H	0.72932	1.21644	2.43969
C	1.27008	-0.02208	-0.17320	C	0.00000	0.00000	0.79177
H	1.63778	0.92399	-0.59169	C	0.00000	0.00000	-0.79177
C	-0.27901	0.02065	-0.26223	C	-0.84534	1.16303	-1.35092
H	-0.52466	-0.00628	-1.33656	H	-0.53814	2.13137	-0.94188
C	-0.95041	-1.20542	0.39184	H	-0.72932	1.21644	-2.43969
H	-0.93951	-1.08547	1.48358	H	-1.91140	1.03072	-1.14205
H	-0.36091	-2.10537	0.18061	C	-1.42988	0.15057	1.35092
C	-2.38765	-1.45294	-0.07813	H	-1.84832	1.13996	1.14205
H	-2.42241	-1.60615	-1.16372	H	-2.11489	-0.59964	0.94188
H	-2.80892	-2.34547	0.39813	H	-1.41813	0.02339	2.43969
H	-3.04958	-0.61286	0.15828	C	0.58454	-1.31360	1.35092
C	-0.87332	1.32776	0.30087	H	1.57675	-1.53173	0.94188
H	-1.96654	1.26728	0.23871	H	0.68881	-1.23983	2.43969
H	-0.64088	1.40254	1.37191	H	-0.06307	-2.17067	1.14205
C	-0.42078	2.60548	-0.41244	C	1.42988	0.15057	-1.35092
H	-0.96940	3.47665	-0.03716	H	2.11489	-0.59964	-0.94188
H	0.64610	2.80504	-0.26742	H	1.41813	0.02339	-2.43969
H	-0.60166	2.53810	-1.49249	H	1.84832	1.13996	-1.14205
C	1.79429	-0.12133	1.26628	C	-0.58454	-1.31360	-1.35092
H	1.41867	0.69134	1.89734	H	-1.57675	-1.53173	-0.94188
H	1.50214	-1.06937	1.73257	H	-0.68881	-1.23983	-2.43969
H	2.88917	-0.07207	1.28077	H	0.06307	-2.17067	-1.14205
		nonane				2,2,3,3-tetramethylpentane	
C	-5.11469	0.36985	-0.00012	C	-1.42458	-0.95541	1.30778
H	-5.15672	1.01723	-0.88458	H	-1.42415	-0.29300	2.17882
H	-5.15676	1.01717	0.88440	H	-0.71326	-1.76542	1.50018
H	-6.01517	-0.25461	-0.00016	H	-2.42157	-1.40600	1.23944
C	-3.84128	-0.47929	-0.00011	C	-1.10668	-0.19255	0.00460
H	-3.83963	-1.14036	0.87795	C	0.39323	0.32962	-0.00784
H	-3.83959	-1.14030	-0.87822	C	1.36875	-0.85954	-0.23716
C	-2.56037	0.36082	-0.00005	H	1.24781	-1.21691	-1.26640
H	-2.56116	1.02300	0.87837	H	1.07964	-1.69606	0.41070
H	-2.56111	1.02306	-0.87843	C	2.85654	-0.57341	0.00041
C	-1.28018	-0.47945	-0.00005	H	3.06704	-0.34045	1.04899
H	-1.28006	-1.14145	-0.87845	H	3.45414	-1.45243	-0.26611

H	-1.28011	-1.14151	0.87831	H	3.22074	0.26292	-0.60624
C	0.00000	0.36103	0.00001	C	-2.10877	0.97628	-0.10274
H	-0.00002	1.02302	0.87838	H	-1.93379	1.74495	0.65732
H	0.00002	1.02308	-0.87831	H	-2.07255	1.45768	-1.08468
C	1.28018	-0.47945	0.00002	H	-3.12922	0.60232	0.04048
H	1.28011	-1.14145	-0.87839	C	-1.38492	-1.14587	-1.17674
H	1.28006	-1.14151	0.87838	H	-1.11486	-0.69961	-2.13979
C	2.56037	0.36082	0.00008	H	-0.84417	-2.09188	-1.07913
H	2.56111	1.02300	0.87849	H	-2.45441	-1.38348	-1.21521
H	2.56116	1.02306	-0.87830	C	0.59958	1.35869	-1.13867
C	3.84128	-0.47929	0.00008	H	1.65763	1.62544	-1.22650
H	3.83963	-1.14030	-0.87802	H	0.27800	0.97098	-2.11122
H	3.83959	-1.14035	0.87814	H	0.05067	2.28547	-0.94677
C	5.11469	0.36985	0.00014	C	0.73454	1.02365	1.32713
H	5.15672	1.01717	0.88465	H	0.81621	0.30900	2.15245
H	6.01517	-0.25461	0.00014	H	1.69095	1.55070	1.25271
H	5.15676	1.01723	-0.88433	H	-0.02108	1.76705	1.60027
	2,4-dimethyl-3-ethylpentane				5-methylnonane		
C	2.55544	0.30805	0.04007	C	-0.40766	-0.00352	-5.11473
H	2.47539	1.24456	0.60022	H	0.35476	0.76094	-5.30830
H	2.69106	0.56282	-1.01909	H	-1.38244	0.49926	-5.10077
H	3.46472	-0.20258	0.37746	H	-0.40356	-0.70082	-5.96004
C	1.32425	-0.59255	0.22495	C	-0.14124	-0.72333	-3.79061
H	1.23936	-0.82384	1.29717	H	-0.89805	-1.50548	-3.63763
C	0.02786	0.14300	-0.20585	C	-0.14124	0.22160	-2.58434
H	0.19371	0.46513	-1.24674	H	-1.11348	0.73341	-2.52523
C	-1.22189	-0.77558	-0.25025	C	0.13290	-0.49918	-1.26050
H	-0.98076	-1.61294	-0.91681	H	-0.57529	-1.33494	-1.16503
C	-1.58957	-1.36803	1.11687	C	0.02505	0.37810	0.00000
H	-1.83902	-0.58368	1.84117	H	-0.97596	0.83871	0.00000
H	-2.46351	-2.02404	1.03071	C	0.13290	-0.49918	1.26050
H	-0.77009	-1.96013	1.53810	H	1.13473	-0.95397	1.29489
C	1.54909	-1.91221	-0.52681	H	-0.57529	-1.33494	1.16503
H	0.78822	-2.66300	-0.29408	C	-0.14124	0.22160	2.58434
H	1.53984	-1.74979	-1.61266	H	-1.11348	0.73341	2.52523
H	2.52375	-2.34055	-0.26601	H	0.60729	1.00743	2.75081
C	-2.42583	-0.05989	-0.87962	C	-0.14124	-0.72333	3.79061
H	-2.77828	0.77433	-0.26210	H	0.82613	-1.24258	3.84213
H	-2.17391	0.34105	-1.86870	H	-0.89805	-1.50548	3.63763

H	-3.26683	-0.75240	-1.00175	C	-0.40766	-0.00352	5.11473
C	-0.20724	1.41998	0.64892	H	-1.38244	0.49926	5.10077
H	-1.22084	1.41584	1.06418	H	-0.40356	-0.70082	5.96004
H	0.45946	1.41234	1.52019	H	0.35476	0.76094	5.30830
C	-0.01123	2.72376	-0.13038	H	0.82613	-1.24258	-3.84213
H	-0.71366	2.78331	-0.97031	H	0.60729	1.00743	-2.75081
H	-0.17499	3.60141	0.50590	H	1.13473	-0.95397	-1.29489
H	1.00108	2.79307	-0.54437	C	1.06586	1.50579	0.00000
				H	2.08256	1.09061	0.00000
				H	0.96735	2.14704	-0.88145
				H	0.96735	2.14704	0.88145

3,4,5-trimethylheptane

C	3.38093	-0.97517	-0.32657
H	3.28269	-1.73766	0.45647
H	4.05408	-0.19816	0.05053
H	3.86990	-1.44420	-1.18777
C	2.01141	-0.40789	-0.71410
C	1.21174	0.16204	0.47196
C	-0.24702	0.55217	0.09955
C	-1.11051	-0.65363	-0.35867
C	-2.57936	-0.26652	-0.65068
C	-3.34855	0.34200	0.52677
H	-2.91911	1.29923	0.84236
H	1.42938	-1.20347	-1.19506
H	-3.34993	-0.32342	1.39721
H	-3.10186	-1.17274	-0.98543
H	-0.70184	-1.01030	-1.31518
H	-4.39295	0.52612	0.25133
H	-2.61535	0.42640	-1.49920
H	-0.69285	0.92763	1.03269
H	1.14324	-0.63159	1.22760
C	-0.29987	1.69467	-0.92807
H	-0.00236	1.34842	-1.92504
H	-1.30812	2.11034	-1.01259
H	0.36426	2.51823	-0.64988
C	-1.05362	-1.82848	0.63137
H	-0.06754	-2.30198	0.65037
H	-1.28359	-1.50609	1.65401
H	-1.78134	-2.60039	0.35512

2,4-dimethyl-3-ethylhexane

C	-1.96807	-0.92704	1.27885
H	-2.82611	-0.32317	0.96317
H	-1.52191	-0.43979	2.14960
H	-2.35668	-1.89951	1.60316
C	-0.96469	-1.11818	0.12940
H	-0.20399	-1.82780	0.47903
C	-0.22716	0.17886	-0.31994
H	0.07808	0.00493	-1.36124
C	1.09402	0.47006	0.44438
H	1.52136	1.36631	-0.02726
C	2.15686	-0.63663	0.28260
H	1.84611	-1.53674	0.82991
H	3.07136	-0.29064	0.78330
C	2.49538	-1.01137	-1.16282
H	2.74594	-0.12177	-1.75415
H	3.35637	-1.68814	-1.19843
H	1.66162	-1.51630	-1.66198
C	-1.67123	-1.77795	-1.06500
H	-2.42675	-1.11034	-1.49789
H	-0.95874	-2.03260	-1.85828
H	-2.18234	-2.69962	-0.76273
C	0.91460	0.78754	1.93564
H	0.17159	1.57309	2.10727
H	0.60301	-0.09912	2.49878
H	1.86238	1.12946	2.36784
C	-1.17078	1.39782	-0.37149
H	-1.48341	1.68390	0.63972

H	2.14506	0.37413	-1.47370	H	-2.08938	1.10009	-0.89360
C	1.95134	1.33099	1.14258	C	-0.58527	2.62135	-1.08354
H	2.23020	2.10741	0.42083	H	0.25436	3.05668	-0.53156
H	1.32703	1.79923	1.91289	H	-0.22266	2.35876	-2.08526
H	2.87207	0.99180	1.62759	H	-1.34219	3.40543	-1.19785

2,2,3,3,4-pentamethylpentane

C	-2.39586	-0.28063	0.74249
H	-2.31504	0.16690	1.73783
H	-2.43502	-1.36764	0.86245
H	-3.35745	0.03401	0.32055
C	-1.25030	0.17525	-0.18828
C	0.15322	-0.40495	0.29487
C	1.35760	0.28419	-0.46321
H	1.00309	0.53433	-1.47114
C	2.58443	-0.62849	-0.64864
H	2.37415	-1.50711	-1.26326
H	3.38880	-0.06859	-1.13935
H	2.97475	-0.97622	0.31594
C	-1.29471	1.71643	-0.21042
H	-1.05359	2.15113	0.76487
H	-0.61595	2.14104	-0.95537
H	-2.30781	2.04575	-0.46979
C	0.32896	-0.22424	1.81703
H	0.16484	0.80689	2.14350
H	-0.36163	-0.86512	2.37292
H	1.34359	-0.50774	2.11871
C	1.87070	1.58828	0.18103
H	2.57535	2.07944	-0.50011
H	1.08429	2.30597	0.41336
H	2.41359	1.37896	1.10943
C	0.17650	-1.92902	0.03220
H	-0.71523	-2.41292	0.44095
H	0.22683	-2.17203	-1.03264
H	1.04072	-2.39152	0.51745
C	-1.59041	-0.31158	-1.61383
H	-1.79032	-1.38656	-1.64368
H	-2.49129	0.19828	-1.97422
H	-0.78747	-0.09866	-2.32782

2. Standard enthalpy of formation for the 15 C4-C7 compounds using different methods

Table S2 Standard enthalpy of formation for the 15 C4-C7 compounds

	$H_{f,298K}$/kcal·mol^{-1}						
Molecule	Exp.[a]	GA[b]	SS-HO	MS-T	PO-N	PI-N	PI-A
butane	-30.02±0.16	-30.26	-30.58	-30.20	-30.06	-30.21	-30.40
pentane	-35.09±0.14	-35.19	-35.74	-35.13	-34.87	-35.10	-35.50
2-methylbutane	-36.74±0.14	-36.63	-36.79	-36.52	-36.24	-36.49	-36.56
hexane	-39.94	-40.12	-40.83	-40.03	-39.60	-39.92	-40.53
2-methylpentane	-41.66±0.24	-41.56	-41.87	-41.48	-41.03	-41.37	-41.58
3-methylpentane	-41.01±0.23	-40.76	-41.18	-40.79	-40.33	-40.67	-40.93
2,3-dimethylbutane	-42.50±0.24	-43.00	-42.16	-41.93	-41.51	-41.83	-41.92
heptane	-44.89±0.19	-45.05	-46.01	-44.94	-44.47	-44.84	-45.66
2-methylhexane	-46.61±0.31	-46.49	-47.01	-46.39	-45.82	-46.26	-46.67
3-methylhexane	-45.96±0.31	-45.69	-46.15	-45.57	-44.97	-45.41	-45.79
2,2-dimethylpentane	-49.28±0.31	-48.56	-48.77	-48.50	-47.89	-48.33	-48.57
3,3-dimethylpentane	-48.16±0.22	-46.96	-48.16	-47.49	-46.94	-47.40	-47.77
2,3-dimethylpentane	-47.61±0.31	-47.13	-46.77	-46.27	-45.66	-46.13	-46.42
2,4-dimethylpentane	-48.30±0.23	-47.93	-48.46	-48.12	-47.28	-47.75	-48.06
3-ethylpentane	-45.34±0.29	-44.89	-45.70	-45.01	-44.32	-44.75	-45.34

[a] Experimental data from NIST Chemistry WebBook.[1]

[b] Group additivity data from THERM.[2]

3. The heat capacity and entropy for the 15 compounds using different methods

Table S3 Heat capacity for the 15 C4-C7 molecules

	Cp/cal·mol^{-1}·K^{-1}								
T (K)	Exp.[a]	Exp.[b]	Exp.[c]	GA[d]	SS-HO	MS-T	PO-N	PI-N	PI-A
				butane					
300	23.65	23.65		23.38	21.97	23.33	24.39	23.27	22.80
400	29.82	29.82		29.59	28.30	29.24	30.39	29.23	28.98
500	35.53	35.53		35.30	34.40	34.82	35.94	34.82	34.78
600	40.46	40.46		40.27	39.79	39.71	40.79	39.70	39.87
700	44.70	44.70			44.46	43.94	44.98	43.92	44.27

800	48.37	48.37		48.18	48.51	47.62	48.62	47.59	48.09
900	51.56	51.56			52.03	50.83	51.79	50.80	51.40
1000	54.34	54.34		54.23	55.09	53.64	54.55	53.61	54.28
				pentane					
300	28.83	28.83		28.87	26.91	28.87	30.63	28.86	27.87
400	36.46	36.46		36.52	34.83	36.38	37.97	36.16	35.67
500	43.64	43.64	43.59	43.55	42.41	43.41	44.72	43.01	43.01
600	49.90	49.90	50.01	49.64	49.08	49.50	50.58	48.98	49.42
700	55.30	55.30	55.66		54.84	54.72	55.64	54.13	54.95
800	59.90	59.90		59.25	59.80	59.24	60.02	58.60	59.71
900	63.79	63.80			64.11	63.16	63.83	62.49	63.80
1000	67.30	67.30		66.56	67.84	66.57	67.15	65.89	67.33
				2-methylbutane					
300.00	28.56	28.56		28.61	27.46	28.77	30.85	28.86	28.67
400.00	36.54	36.54		36.47	35.35	36.21	38.54	36.43	36.33
500.00	43.80	43.80		43.62	42.84	43.15	45.37	43.35	43.35
600.00	50.19	50.20		49.76	49.41	49.20	51.21	49.31	49.45
700.00	55.46	55.70			55.09	54.39	56.21	54.43	54.71
800.00	60.50	60.50		59.44	60.00	58.89	60.53	58.86	59.28
900.00	64.70	64.70			64.25	62.79	64.28	62.72	63.27
1000.00	68.40	68.40		66.71	67.95	66.19	67.53	66.08	66.73
				hexane					
300.00	34.24	34.24		34.37	31.87	34.29	36.25	34.31	32.96
400.00	43.39	43.39		43.48	41.37	43.35	44.89	42.99	42.39
500.00	51.93	51.93		51.79	50.43	51.77	52.95	51.14	51.27
600.00	59.30	59.30		58.99	58.38	59.01	59.96	58.23	59.02
700.00	65.50	65.50			65.21	65.19	65.99	64.32	65.67
800.00	70.80	70.80		70.32	71.10	70.50	71.20	69.59	71.37
900.00	75.30	75.30			76.19	75.09	75.72	74.17	76.25
1000.00	79.20	79.20		78.90	80.59	79.08	79.63	78.17	80.42
				2-methylpentane					
300.00	34.18	34.18		34.11	32.42	34.20	37.32	34.75	33.73
400.00	43.86	43.86		43.43	41.89	43.28	46.43	43.78	43.01
500.00	52.54	52.54		51.86	50.85	51.64	54.44	51.93	51.56
600.00	60.00	60.00		59.13	58.71	58.86	61.25	58.92	58.98
700.00	66.30	66.30			65.46	65.05	67.09	64.91	65.36
800.00	71.80	71.80		70.51	71.29	70.37	72.12	70.09	70.86
900.00	76.50	76.50			76.33	74.98	76.50	74.60	75.63
1000.00	80.60	80.60		79.04	80.70	78.99	80.30	78.52	79.74

			3-methylpentane					
300.00	33.67	33.67	34.11	32.43	33.63	36.63	34.00	33.75
400.00	43.30	43.30	43.43	41.90	42.66	45.59	42.85	43.01
500.00	51.98	51.98	51.86	50.86	51.10	53.64	51.07	51.53
600.00	59.50	59.50	59.13	58.70	58.41	60.57	58.19	58.95
700.00	65.90	65.90		65.45	64.67	66.51	64.31	65.34
800.00	71.40	71.40	70.51	71.27	70.05	71.64	69.60	70.88
900.00	76.20	76.20		76.31	74.70	76.09	74.20	75.67
1000.00	80.30	80.30	79.04	80.68	78.72	79.95	78.19	79.83
			2,3-dimethylbutane					
300.00	33.51	33.51	33.84	32.94	33.86	36.95	34.32	34.50
400.00	43.43	43.43	43.36	42.40	42.99	46.30	43.38	43.65
500.00	52.19	52.19	51.94	51.27	51.41	54.40	51.56	51.88
600.00	59.80	59.80	59.25	59.03	58.67	61.25	58.59	58.96
700.00	66.30	66.30		65.70	64.86	67.08	64.61	65.05
800.00	72.10	72.10	70.70	71.46	70.18	72.11	69.82	70.33
900.00	77.10	77.10		76.45	74.76	76.47	74.35	74.95
1000.00	81.40	81.40	79.18	80.78	78.74	80.26	78.30	78.98
			heptane					
300.00	39.67	39.67	39.89	36.81	39.99	42.14	39.78	38.05
400.00	50.35	50.35	50.43	47.90	50.47	52.16	49.83	49.11
500.00	60.25	60.25	60.04	58.44	60.19	61.45	59.26	59.54
600.00	68.70	68.70	68.33	67.67	68.56	69.52	67.45	68.64
700.00	75.80	75.80		75.59	75.68	76.45	74.49	76.42
800.00	81.80	81.80	81.38	82.40	81.80	82.43	80.56	83.06
900.00	86.90	86.90		88.27	87.08	87.61	85.84	88.72
1000.00	91.20	91.20	91.23	93.35	91.66	92.10	90.42	93.54
			2-methylhexane					
300.00	39.52	39.52	39.60	37.37	39.86	43.23	40.30	38.81
400.00	50.66	50.66	50.36	48.42	50.23	53.62	50.64	49.71
500.00	60.66	60.66	60.11	58.87	59.84	62.88	60.06	59.80
600.00	69.20	69.20	68.48	68.00	68.15	70.80	68.15	68.55
700.00	76.40	76.40		75.84	75.27	77.56	75.08	76.06
800.00	82.60	82.60	81.57	82.59	81.41	83.40	81.07	82.51
900.00	87.90	87.90		88.41	86.72	88.45	86.26	88.05
1000.00	92.40	92.40	91.37	93.45	91.33	92.83	90.79	92.82
			3-methylhexane					
300.00	39.31	39.31	39.60	37.26	38.88	43.67	40.61	38.67
400.00	50.60	50.60	50.36	48.36	49.29	54.31	51.17	49.58

500.00	60.65	60.65	60.11	58.82	58.97	63.53	60.58	59.66
600.00	69.20	69.20	68.48	67.95	67.34	71.34	68.61	68.43
700.00	76.40	76.40		75.79	74.52	77.99	75.47	75.96
800.00	82.60	82.60	81.57	82.53	80.70	83.74	81.40	82.46
900.00	87.90	87.90		88.36	86.05	88.72	86.55	88.07
1000.00	92.40	92.40	91.37	93.40	90.69	93.05	91.03	92.90
			2,2-dimethylpentane					
300.00	40.07	40.07	40.13	38.31	39.93	44.47	41.22	39.87
400.00	51.81	51.81	51.39	49.33	50.91	55.22	51.96	50.87
500.00	62.09	62.09	61.45	59.61	60.83	64.36	61.33	60.74
600.00	70.90	70.90	69.98	68.57	69.25	72.06	69.28	69.17
700.00	78.40	78.40		76.27	76.35	78.62	76.05	76.35
800.00	84.90	84.90	82.98	82.90	82.40	84.28	81.88	82.52
900.00	90.60	90.60		88.64	87.61	89.19	86.96	87.84
1000.00	95.60	95.60	92.52	93.62	92.11	93.46	91.38	92.44
			3,3-dimethylpentane					
300.00	39.84	39.84	40.13	38.25	40.03	44.96	41.51	39.95
400.00	51.47	51.47	51.39	49.30	50.42	55.78	52.25	50.83
500.00	61.77	61.77	61.45	59.58	60.17	64.99	61.68	60.62
600.00	70.70	70.70	69.98	68.53	68.64	72.65	69.62	69.03
700.00	78.30	78.30		76.23	75.88	79.12	76.34	76.23
800.00	84.90	84.90	82.98	82.86	82.08	84.68	82.11	82.44
900.00	90.70	90.70		88.59	87.40	89.50	87.13	87.82
1000.00	95.70	95.70	92.52	93.57	92.00	93.69	91.49	92.47
			2,3-dimethylpentane					
300.00	38.68	38.68	39.34	37.87	38.98	44.76	41.35	39.54
400.00	50.44	50.44	50.31	48.90	49.41	55.19	51.70	50.27
500.00	60.64	60.64	60.18	59.24	59.12	64.15	60.90	60.00
600.00	69.30	69.30	68.62	68.27	67.53	71.76	68.78	68.41
700.00	76.80	76.80		76.02	74.71	78.28	75.55	75.64
800.00	83.10	83.10	81.76	82.70	80.87	83.93	81.41	81.90
900.00	88.70	88.70		88.48	86.20	88.85	86.53	87.34
1000.00	93.50	93.50	91.52	93.48	90.81	93.14	90.99	92.08
			2,4-dimethylpentane					
300.00	41.04	41.04	39.34	37.85	40.98	46.34	42.84	39.60
400.00	52.60	52.60	50.31	48.89	52.59	57.20	53.66	50.35
500.00	62.47	62.47	60.18	59.25	62.52	66.01	62.72	60.12
600.00	70.80	70.80	68.62	68.29	70.66	73.34	70.33	68.56
700.00	78.00	78.00		76.06	77.45	79.60	76.84	75.82

800.00	84.20	84.20	81.76	82.75	83.24	85.04	82.49	82.09
900.00	89.50	89.50		88.53	88.25	89.79	87.43	87.53
1000.00	94.20	94.20	91.52	93.54	92.61	93.94	91.75	92.25
			3-ethylpentane					
300.00	39.87	39.87	39.60	37.21	39.73	44.91	41.77	38.68
400.00	50.56	50.56	50.36	48.33	50.41	54.92	51.69	49.58
500.00	60.38	60.38	60.11	58.80	60.36	63.78	60.78	59.65
600.00	68.90	68.90	68.48	67.93	68.96	71.42	68.68	68.42
700.00	76.10	76.10		75.76	76.26	77.99	75.50	75.97
800.00	82.20	82.20	81.57	82.50	82.49	83.68	81.41	82.50
900.00	87.50	87.50		88.32	87.83	88.63	86.55	88.15
1000.00	92.10	92.10	91.37	93.36	92.43	92.94	91.03	93.03

[a] Experimental data from Ref. 3.

[b] Experimental data from NIST Chemistry WebBook.

[c] Experimental data from direct experimental measurement from Ref 4.

[d] Group additivity data from NIST structures and properties.[5]

Table S4 Entropy for the 15 C4-C7 molecules at 1 atm

	S/cal·mol^{-1}·K^{-1}						
T (K)	Exp.[a]	GA[b]	SS-HO	MS-T	PO-N	PI-N	PI-A
			butane				
300.00	74.22	74.08	72.08	74.71	75.46	74.74	73.80
400.00	81.87	81.70	79.26	82.23	83.30	82.25	81.21
500.00	89.15	88.94	86.24	89.37	90.69	89.38	88.31
600.00	96.08	95.83	93.00	96.16	97.68	96.17	95.11
700.00	102.60		99.49	102.61	104.29	102.62	101.60
800.00	108.80	108.55	105.70	108.72	110.54	108.73	107.76
900.00	114.70		111.62	114.52	116.45	114.52	113.62
1000.00	120.30	119.98	117.27	120.02	122.06	120.02	119.19
			pentane				
300.00	83.70	83.54	79.80	84.04	85.63	84.49	82.49
400.00	93.03	92.94	88.62	93.37	95.45	93.79	91.57
500.00	101.95	101.88	97.22	102.26	104.66	102.61	100.34
600.00	110.50	110.37	105.56	110.73	113.35	110.99	108.76
700.00	118.60		113.56	118.76	121.53	118.94	116.80
800.00	126.30	126.03	121.22	126.37	129.26	126.47	124.46
900.00	133.60		128.52	133.58	136.55	133.60	131.74
1000.00	140.50	140.07	135.47	140.41	143.45	140.36	138.65
			2-methylbutane				
300.00	82.30	82.23	80.04	83.01	84.39	83.16	81.94
400.00	91.63	91.59	89.02	92.31	94.33	92.50	91.24
500.00	100.57	100.52	97.72	101.15	103.69	101.39	100.12
600.00	109.10	109.04	106.13	109.56	112.49	109.84	108.58
700.00	117.30		114.18	117.55	120.77	117.83	116.61
800.00	125.00	124.74	121.87	125.11	128.57	125.40	124.22
900.00	132.40		129.19	132.28	135.92	132.56	131.44
1000.00	139.40	138.82	136.15	139.07	142.86	139.34	138.29
			hexane				
300.00	93.12	92.99	87.54	93.39	95.80	94.12	90.91
400.00	104.22	104.19	98.00	104.50	107.41	105.17	101.68
500.00	114.84	114.82	108.22	115.09	118.31	115.66	112.12
600.00	125.00	124.92	118.14	125.19	128.60	125.63	122.17
700.00	134.60		127.66	134.76	138.31	135.07	131.78
800.00	143.70	143.52	136.77	143.82	147.47	144.01	140.93

900.00	152.30		145.44	152.40	156.12	152.48	149.62
1000.00	160.50	160.17	153.70	160.52	164.30	160.51	157.88
			2-methylpentane				
300.00	91.24	91.68	87.78	91.80	94.13	92.39	90.66
400.00	102.42	102.83	98.40	102.88	106.14	103.64	101.64
500.00	113.15	113.47	108.73	113.46	117.38	114.31	112.18
600.00	123.40	123.58	118.71	123.53	127.92	124.41	122.25
700.00	133.10		128.28	133.08	137.82	133.95	131.83
800.00	142.40	142.23	137.41	142.12	147.11	142.97	140.93
900.00	151.10		146.11	150.68	155.86	151.49	149.56
1000.00	159.40	158.92	154.38	158.80	164.12	159.56	157.74
			3-methylpentane				
300.00	91.72	91.68	87.89	92.48	94.98	93.18	90.09
400.00	102.75	102.83	98.51	103.40	106.75	104.17	101.08
500.00	113.36	113.47	108.84	113.84	117.81	114.64	111.61
600.00	123.50	123.58	118.82	123.82	128.22	124.59	121.68
700.00	133.20		128.39	133.31	138.01	134.04	131.26
800.00	142.40	142.23	137.52	142.30	147.24	142.98	140.35
900.00	151.00		146.21	150.83	155.94	151.45	148.98
1000.00	159.30	158.92	154.49	158.91	164.16	159.48	157.18
			2,3-dimethylbutane				
300.00	87.63	87.61	85.36	88.54	90.41	88.81	86.91
400.00	98.66	98.71	96.13	99.54	102.35	99.94	98.10
500.00	109.31	109.35	106.57	110.06	113.58	110.52	108.74
600.00	119.50	119.48	116.62	120.09	124.12	120.56	118.84
700.00	129.20		126.23	129.61	134.01	130.05	128.40
800.00	138.50	138.17	135.39	138.63	143.30	139.03	137.44
900.00	147.30		144.10	147.16	152.05	147.52	146.00
1000.00	155.60	154.90	152.39	155.25	160.31	155.56	154.11
			heptane				
300.00	102.53	102.43	95.25	102.72	105.68	103.72	99.25
400.00	115.41	115.42	107.35	115.66	119.17	116.53	111.71
500.00	127.72	127.74	119.20	127.99	131.83	128.68	123.81
600.00	139.50	139.45	130.69	139.72	143.77	140.23	135.49
700.00	150.60		141.73	150.84	155.02	151.17	146.67
800.00	161.20	160.98	152.28	161.36	165.63	161.52	157.32
900.00	171.10		162.33	171.30	175.64	171.33	167.44
1000.00	180.50	180.24	171.90	180.72	185.11	180.61	177.05
			2-methylhexane				

300.00	100.72	101.12	95.53	101.16	104.23	101.85	98.96
400.00	113.63	114.06	107.79	114.05	118.11	114.87	111.62
500.00	126.03	126.39	119.74	126.32	131.09	127.21	123.82
600.00	137.90	138.11	131.30	137.98	143.27	138.89	135.51
700.00	149.10		142.39	149.04	154.71	149.93	146.66
800.00	159.70	159.69	152.97	159.50	165.46	160.35	157.25
900.00	169.80		163.04	169.40	175.58	170.21	167.29
1000.00	179.30	178.99	172.62	178.78	185.13	179.54	176.82
			3-methylhexane				
300.00	102.04	102.51	95.61	102.67	104.50	102.26	99.72
400.00	114.92	115.45	107.84	115.28	118.55	115.40	112.34
500.00	127.31	127.77	119.78	127.34	131.68	127.86	124.51
600.00	139.20	139.49	131.33	138.85	143.98	139.63	136.18
700.00	150.40		142.41	149.79	155.48	150.74	147.31
800.00	161.00	161.08	152.98	160.15	166.28	161.21	157.89
900.00	171.00		163.05	169.97	176.44	171.10	167.94
1000.00	180.50	180.37	172.62	179.28	186.02	180.46	177.47
			2,2-dimethylpentane				
300.00	94.07	94.73	93.49	95.02	97.81	95.58	94.42
400.00	107.24	107.89	106.03	108.03	112.12	108.93	107.41
500.00	119.92	120.48	118.16	120.48	125.45	121.56	119.85
600.00	132.00	132.46	129.84	132.34	137.88	133.47	131.69
700.00	143.60		141.01	143.56	149.50	144.67	142.90
800.00	154.50	154.46	151.63	154.16	160.38	155.21	153.51
900.00	164.80		161.74	164.17	170.59	165.16	163.55
1000.00	174.60	174.04	171.34	173.64	180.22	174.55	173.04
			3,3-dimethylpentane				
300.00	95.40	95.54	90.46	96.48	97.86	95.52	94.47
400.00	108.48	108.70	102.98	109.42	112.31	108.95	107.47
500.00	121.09	121.29	115.11	121.73	125.78	121.66	119.89
600.00	133.10	133.27	126.78	133.47	138.32	133.62	131.71
700.00	144.60		137.94	144.61	150.02	144.87	142.90
800.00	155.50	155.28	148.56	155.16	160.96	155.45	153.50
900.00	165.90		158.66	165.14	171.22	165.42	163.52
1000.00	175.70	174.86	168.26	174.60	180.87	174.83	173.02
			2,3-dimethylpentane				
300.00	99.31	99.81	94.52	99.77	102.02	99.60	97.84
400.00	112.09	112.71	106.92	112.42	116.36	112.93	110.70
500.00	124.50	125.04	118.97	124.51	129.66	125.48	122.99

600.00	136.30	136.78	130.58	136.05	142.05	137.30	134.69
700.00	147.60		141.71	147.01	153.61	148.42	145.79
800.00	158.30	158.41	152.30	157.40	164.44	158.90	156.31
900.00	168.40		162.39	167.24	174.62	168.79	166.28
1000.00	177.90	177.74	171.97	176.57	184.21	178.15	175.73
			2,4-dimethylpentane				
300.00	95.11	97.06	91.87	94.84	97.48	95.13	95.77
400.00	108.54	109.96	104.27	108.25	112.36	108.98	108.64
500.00	121.36	122.29	116.32	121.08	126.10	121.96	120.95
600.00	133.50	134.03	127.94	133.23	138.80	134.09	132.68
700.00	145.00		139.07	144.64	150.59	145.43	143.81
800.00	155.80	155.66	149.67	155.37	161.58	156.07	154.35
900.00	166.00		159.76	165.47	171.88	166.08	164.34
1000.00	175.70	174.99	169.35	175.00	181.56	175.52	173.81
			3-ethylpentane				
300.00	98.60	98.95	94.00	98.52	102.59	100.28	97.70
400.00	111.54	111.89	106.23	111.07	116.90	113.66	110.33
500.00	123.89	124.22	118.16	123.19	130.13	126.20	122.50
600.00	135.70	135.94	129.70	134.86	142.45	137.99	134.17
700.00	146.80		140.78	146.02	153.97	149.11	145.30
800.00	157.40	157.52	151.35	156.65	164.76	159.58	155.88
900.00	167.40		161.41	166.75	174.91	169.47	165.93
1000.00	176.90	176.82	170.98	176.36	184.48	178.83	175.48

[a] Experimental data from Ref. 3.

[b] Group additivity data from NIST structures and properties.[5]

4. The maximum absolute deviation of different approaches for the 15 C4-C7 molecules

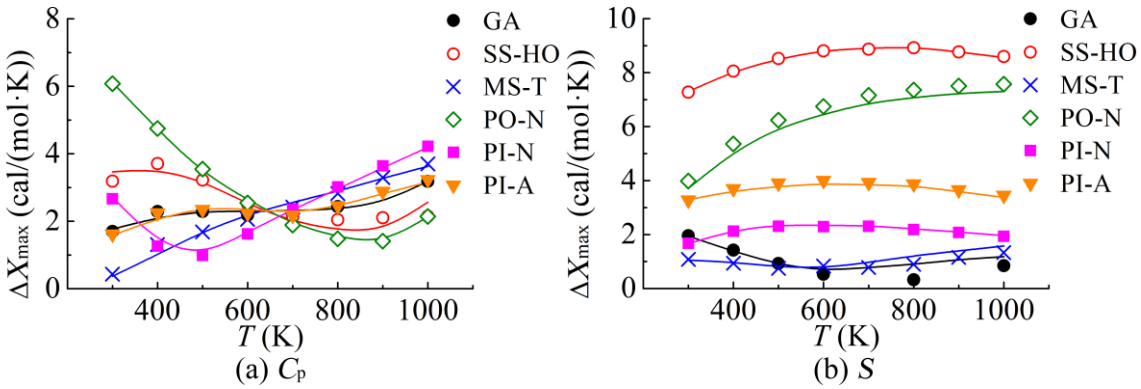
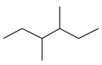
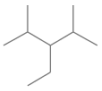
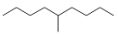
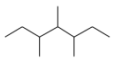
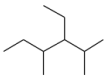


Fig. S1 The maximum absolute deviation(ΔX_{max}, $\Delta X_{max} = \max_i \left|X_i^{calc} - X_i^{exp}\right|_T$, X represents C_p or S) of the predicted values from the experimental data. The lines use the polynomial fitted values.

5. Heat capacity for the 11 representative C8-C10 molecules

Table S5 Heat capacity (units: cal·mol^{-1}·K^{-1}) for the 11 representative C8-C10 molecules

Name	Structure	Temperature/K					
		Method	300	400	500	600	800	1000
octane		Exp.[a]	45.10	57.30	68.55	78.1	92.8	103.1
		GA[b]	45.39	57.39	68.31	77.68	92.47	103.58
		PI-A	43.17	55.88	67.86	78.30	94.80	106.71
		PI-N	45.22	56.66	67.38	76.68	91.53	102.68
3,4-dimethylhexane		Exp.	43.85	57.42	69.02	78.8	94.1	105.4
		GA	44.84	57.27	68.45	77.96	92.83	103.86
		PI-A	44.66	56.96	68.19	77.89	93.42	105.07
		PI-N	46.91	58.38	68.74	77.71	92.16	103.11
3-ethyl-2-methylpentane		Exp.	46.14	58.48	69.39	78.8	93.9	105.2
		GA	44.84	57.27	68.45	77.96	92.83	103.86
		PI-A	44.62	56.93	68.16	77.87	93.43	105.12
		PI-N	48.31	59.35	69.37	78.12	92.35	103.21
2,2,3,3-tetramethylbutane		Exp.	45.00	58.32	70.21	80.6	97.8	111.2
		GA	45.89	59.30	71.13	80.98	95.65	106.14
		PI-A	48.30	60.76	71.30	80.03	93.69	104.02
		PI-N	45.89	58.25	69.20	78.46	93.01	103.86
nonane		Exp.	50.53	64.25	76.85	87.5	103.7	115.1
		GA	50.88	64.34	76.55	87.02	103.53	115.92
		PI-A	48.27	62.62	76.17	87.96	106.54	119.88
		PI-N	50.74	63.54	75.55	85.96	102.54	114.97
2,2,3,3-tetramethylpentane		Exp.	50.99	66.31	79.52	90.9	109.4	123.6
		GA	51.39	66.25	79.37	90.32	106.73	118.48
		PI-A	52.42	66.35	78.43	88.57	104.54	116.53
		PI-N	51.76	65.28	77.24	87.42	103.61	115.80
2,4-dimethyl-3-ethylpentane		Exp.	49.95	64.62	77.41	88.3	105.6	118.4
		GA	50.07	64.15	76.77	87.45	104.10	116.34
		PI-A	50.38	64.14	76.58	87.28	104.39	117.30
		PI-N	53.46	67.28	79.31	89.36	105.08	116.82
5-methylnonane		Exp.	55.61	71.52	85.65	97.5	115.6	128.4
		GA	56.12	71.22	84.87	96.51	114.79	128.40
		PI-A	54.13	69.90	84.60	97.36	117.53	132.19
		PI-N	56.83	71.26	84.47	95.87	114.03	127.62

3,4,5-trimethylheptane		Exp.	56.14	72.67	86.70	98.5	117.1	130.8
		GA	55.57	71.10	85.01	96.80	115.17	128.68
		PI-A	55.41	70.81	84.76	96.78	115.96	130.35
		PI-N	59.22	74.94	88.33	99.38	116.54	129.39
2,4-dimethyl-3-ethylhexane		Exp.	55.26	71.56	85.69	97.7	116.5	130.3
		GA	55.57	71.10	85.01	96.80	115.17	128.68
		PI-A	55.55	70.91	84.86	96.89	116.12	130.55
		PI-N	59.56	75.31	88.58	99.49	116.55	129.40
2,2,3,3,4-pentamethylpentane		Exp.	56.00	73.10	87.86	100.6	121.0	136.9
		GA	56.62	73.14	87.69	99.81	117.99	130.96
		PI-A	58.18	73.64	86.95	98.10	115.64	128.82
		PI-N	58.16	73.13	86.60	98.07	116.07	129.38

[a] Experimental data from Ref. 3.

[b] Group additivity data from NIST structures and properties.[5]

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