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Thermodynamic properties of isomerization reaction between *n*-heptane and isoheptane

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Table S1 Data used for the *n*-heptane partition function using the MS-LH and MS-T methods[a]

Torsion	$\overline{\omega}$	I	W	M
		Structure 1		
C(1)–C(2)	233	3.0	1056	3.00
C(2)–C(3)	96	17.8	1033	3.08
C(3)–C(4)	87	21.2	996	3.08
C(4)–C(5)	87	21.2	996	3.08
C(5)–C(6)	96	17.8	1033	3.08
C(6)–C(7)	233	3.0	1056	3.00
		Structures 2 and 3		
C(1)–C(2)	227	3.0	1019	3.00
C(2)–C(3)	91	20.7	964	3.25
C(3)–C(4)	96	17.4	903	3.25
C(4)–C(5)	75	29.9	950	3.25
C(5)–C(6)	105	16.4	1012	3.25
C(6)–C(7)	231	3.1	1084	3.00
		Structures 4 and 5		
C(1)–C(2)	225	3.1	1021	3.00
C(2)–C(3)	105	15.4	1028	3.13
C(3)–C(4)	88	22.6	1051	3.13
C(4)–C(5)	96	18.8	1048	3.13
C(5)–C(6)	93	21.2	1113	3.13
C(6)–C(7)	229	3.0	1035	3.00
		Structures 6 and 7		
C(1)–C(2)	224	3.1	1015	3.00
C(2)–C(3)	95	18.9	1007	3.18
C(3)–C(4)	89	23.0	1066	3.18
C(4)–C(5)	95	34.3	1824	3.18
C(5)–C(6)	108	27.1	1861	3.18
C(6)–C(7)	243	3.1	1206	3.00
		Structures 8 and 9		
C(1)–C(2)	226	3.1	1030	3.00
C(2)–C(3)	92	22.5	892	3.56
C(3)–C(4)	104	29.2	1480	3.56
C(4)–C(5)	104	29.2	1480	3.56
C(5)–C(6)	92	22.5	892	3.56
C(6)–C(7)	226	3.1	1030	3.00

Structures 10 and 11

C(1)–C(2)	228	3.0	1029	3.00
C(2)–C(3)	95	20.8	1193	3.05
C(3)–C(4)	107	16.8	1226	3.05
C(4)–C(5)	65	46.2	1230	3.05
C(5)–C(6)	110	16.5	1273	3.05
C(6)–C(7)	233	3.1	1106	3.00
		Structures 12 and 13		
C(1)–C(2)	231	3.1	1087	3.00
C(2)–C(3)	94	20.9	1384	2.82
C(3)–C(4)	81	26.2	1295	2.82
C(4)–C(5)	81	26.2	1295	2.82
C(5)–C(6)	94	20.9	1384	2.82
C(6)–C(7)	231	3.1	1087	3.00
		Structures 14 and 15		
C(1)–C(2)	230	3.1	1078	3.00
C(2)–C(3)	96	18.9	1213	2.93
C(3)–C(4)	78	26.8	1123	2.93
C(4)–C(5)	78	26.8	1123	2.93
C(5)–C(6)	96	18.9	1213	2.93
C(6)–C(7)	230	3.1	1078	3.00
		Structures 16 and 17		
C(1)–C(2)	230	3.0	1043	3.00
C(2)–C(3)	89	21.1	1034	3.09
C(3)–C(4)	90	20.2	1006	3.09
C(4)–C(5)	59	43.8	962	3.09
C(5)–C(6)	95	19.1	1069	3.09
C(6)–C(7)	223	3.1	1006	3.00
		Structures 18 and 19		
C(1)–C(2)	224	3.1	1010	3.00
C(2)–C(3)	92	21.3	1020	3.25
C(3)–C(4)	113	27.3	1951	3.25
C(4)–C(5)	90	59.3	2703	3.25
C(5)–C(6)	115	25.7	1908	3.25
C(6)–C(7)	235	3.1	1124	3.00
		Structures 20 and 21		
C(1)–C(2)	231	3.1	1086	3.00
C(2)–C(3)	103	18.2	805	3.76
C(3)–C(4)	62	47.4	770	3.76
C(4)–C(5)	109	28.9	1433	3.76
C(5)–C(6)	114	25.3	1391	3.76
C(6)–C(7)	243	3.1	1211	3.00

		Structures 22 and 23		
C(1)–C(2)	221	3.1	985	3.00
C(2)–C(3)	91	21.0	1083	3.09
C(3)–C(4)	63	42.3	1041	3.09
C(4)–C(5)	95	33.4	1877	3.09
C(5)–C(6)	114	24.1	1952	3.09
C(6)–C(7)	246	3.1	1236	3.00
		Structures 24 and 25		
C(1)–C(2)	239	3.1	1154	3.00
C(2)–C(3)	112	24.1	1677	3.27
C(3)–C(4)	97	53.1	2766	3.27
C(4)–C(5)	97	53.1	2766	3.27
C(5)–C(6)	112	24.1	1677	3.27
C(6)–C(7)	239	3.1	1154	3.00
		Structures 26 and 27		
C(1)–C(2)	224	3.1	1013	3.00
C(2)–C(3)	92	19.9	757	3.65
C(3)–C(4)	79	23.7	652	3.65
C(4)–C(5)	109	34.1	1819	3.65
C(5)–C(6)	136	17.9	1468	3.65
C(6)–C(7)	288	3.1	1693	3.00
		Structures 28 and 29		
C(1)–C(2)	225	3.1	1032	3.00
C(2)–C(3)	100	16.8	889	3.34
C(3)–C(4)	118	19.4	1448	3.34
C(4)–C(5)	118	22.5	1670	3.34
C(5)–C(6)	127	25.9	2227	3.34
C(6)–C(7)	217	3.1	965	3.00
		Structures 30 and 31		
C(1)–C(2)	223	3.1	1007	3.00
C(2)–C(3)	124	18.5	1407	3.46
C(3)–C(4)	128	20.1	1628	3.46
C(4)–C(5)	123	28.3	2135	3.46
C(5)–C(6)	82	23.4	780	3.46
C(6)–C(7)	227	3.1	1041	3.00
		Structures 32 and 33		
C(1)–C(2)	228	3.1	1051	3.00
C(2)–C(3)	90	23.2	1080	3.20
C(3)–C(4)	147	30.5	3848	3.20
C(4)–C(5)	121	47.8	4059	3.20
C(5)–C(6)	143	23.5	2801	3.20

C(6)–C(7)	239	3.1	1160	3.00
		Structures 34 and 35		
C(1)–C(2)	226	3.1	1029	3.00
C(2)–C(3)	95	20.1	901	3.45
C(3)–C(4)	133	24.3	2132	3.45
C(4)–C(5)	115	48.8	3200	3.45
C(5)–C(6)	148	28.0	3052	3.45
C(6)–C(7)	224	3.1	1021	3.00
		Structures 36 and 37		
C(1)–C(2)	217	3.1	965	3.00
C(2)–C(3)	99	18.5	1300	2.88
C(3)–C(4)	55	49.3	1051	2.88
C(4)–C(5)	120	29.8	3068	2.88
C(5)–C(6)	125	22.1	2464	2.88
C(6)–C(7)	291	3.1	1729	3.00
		Structures 38 and 39		
C(1)–C(2)	232	3.1	1098	3.00
C(2)–C(3)	100	19.4	1108	3.21
C(3)–C(4)	83	41.9	1670	3.21
C(4)–C(5)	113	25.2	1864	3.21
C(5)–C(6)	126	25.8	2370	3.21
C(6)–C(7)	218	3.1	974	3.00
		Structures 40 and 41		
C(1)–C(2)	234	3.1	1109	3.00
C(2)–C(3)	97	21.5	1102	3.29
C(3)–C(4)	63	42.8	917	3.29
C(4)–C(5)	121	31.2	2518	3.29
C(5)–C(6)	132	19.9	1896	3.29
C(6)–C(7)	293	3.1	1756	3.00
		Structures 42 and 43		
C(1)–C(2)	225	3.1	1022	3.00
C(2)–C(3)	88	20.7	901	3.25
C(3)–C(4)	104	25.4	1540	3.25
C(4)–C(5)	79	56.9	1999	3.25
C(5)–C(6)	142	17.1	1929	3.25
C(6)–C(7)	285	3.1	1663	3.00
		Structures 44 and 45		
C(1)–C(2)	225	3.0	1015	3.00
C(2)–C(3)	121	18.7	1470	3.32
C(3)–C(4)	139	17.4	1814	3.32
C(4)–C(5)	82	55.9	2015	3.32

C(5)–C(6)	109	23.7	1524	3.32
C(6)–C(7)	219	3.1	967	3.00
		Structures 46 and 47		
C(1)–C(2)	240	3.1	1164	3.00
C(2)–C(3)	108	23.7	1344	3.48
C(3)–C(4)	114	59.6	3770	3.48
C(4)–C(5)	116	51.7	3430	3.48
C(5)–C(6)	139	20.5	1949	3.48
C(6)–C(7)	243	3.1	1198	3.00
		Structures 48 and 49		
C(1)–C(2)	232	3.1	1100	3.00
C(2)–C(3)	156	27.9	3861	3.24
C(3)–C(4)	135	40.0	4127	3.24
C(4)–C(5)	101	54.3	3131	3.24
C(5)–C(6)	116	25.2	1914	3.24
C(6)–C(7)	215	3.1	938	3.00
		Structures 50 and 51		
C(1)–C(2)	229	3.1	1061	3.00
C(2)–C(3)	102	23.4	1643	2.95
C(3)–C(4)	169	30.2	5867	2.95
C(4)–C(5)	165	31.3	5769	2.95
C(5)–C(6)	173	28.0	5689	2.95
C(6)–C(7)	228	3.1	1059	3.00
		Structures 52 and 53		
C(1)–C(2)	286	3.1	1675	3.00
C(2)–C(3)	134	19.1	1725	3.44
C(3)–C(4)	93	50.8	2180	3.44
C(4)–C(5)	93	50.8	2180	3.44
C(5)–C(6)	134	19.1	1725	3.44
C(6)–C(7)	286	3.1	1675	3.00
		Structures 54 and 55		
C(1)–C(2)	220	3.1	983	3.00
C(2)–C(3)	112	21.9	1854	2.96
C(3)–C(4)	116	57.2	5230	2.96
C(4)–C(5)	157	30.9	5185	2.96
C(5)–C(6)	166	27.4	5132	2.96
C(6)–C(7)	229	3.1	1068	3.00
		Structures 56 and 57		
C(1)–C(2)	237	3.1	1145	3.00
C(2)–C(3)	104	22.3	1192	3.48
C(3)–C(4)	95	46.1	2045	3.48

C(4)–C(5)	99	63.0	3033	3.48
C(5)–C(6)	114	20.6	1305	3.48
C(6)–C(7)	291	3.1	1726	3.00
		Structures 58 and 59		
C(1)–C(2)	265	3.1	1428	3.00
C(2)–C(3)	123	21.8	1379	3.75
C(3)–C(4)	134	56.7	4268	3.75
C(4)–C(5)	134	56.7	4268	3.75
C(5)–C(6)	123	21.8	1379	3.75
C(6)–C(7)	265	3.1	1428	3.00

[a]The units are cm^{-1} for torsional barrier heights W and frequencies $\overline{\omega}$. The unit is amu $Å^2$ for internal moments of inertia I, and the local periodicity M is unitless.

Table S2. Data used for the isoheptane partition function using the MS-LH and MS-T methods[a]

Torsion	$\bar{\omega}$	I	W	M
		Structures 1 and 2		
C(1)–C(2)	241	3.1	1167	3.00
C(2)–C(3)	88	26.5	1361	3.00
C(3)–C(4)	94	19.2	962	3.23
C(4)–C(5)	95	19.0	978	3.23
C(5)–C(6)	227	3.0	891	3.23
C(6)–C(7)	247	3.1	1253	3.00
		Structures 3 and 4		
C(1)–C(2)	243	3.1	1190	3.00
C(2)–C(3)	90	43.2	2311	3.00
C(3)–C(4)	119	22.6	1773	3.28
C(4)–C(5)	98	21.0	1101	3.28
C(5)–C(6)	228	3.0	873	3.28
C(6)–C(7)	255	3.1	1335	3.00
		Structures 5 and 6		
C(1)–C(2)	243	3.1	1197	3.00
C(2)–C(3)	93	42.3	2408	3.00
C(3)–C(4)	108	42.2	3335	2.97
C(4)–C(5)	121	24.9	2445	2.97
C(5)–C(6)	238	3.1	1183	2.97
C(6)–C(7)	250	3.1	1279	3.00
		Structures 7 and 8		
C(1)–C(2)	249	3.1	1015	3.00
C(2)–C(3)	96	25.1	1007	3.00
C(3)–C(4)	75	34.0	1066	3.71
C(4)–C(5)	102	19.5	1824	3.71
C(5)–C(6)	236	3.1	1861	3.71
C(6)–C(7)	238	3.1	1206	3.00
		Structures 9 and 10		
C(1)–C(2)	239	3.1	1163	3.00
C(2)–C(3)	83	28.0	1278	3.00
C(3)–C(4)	68	32.8	870	3.20
C(4)–C(5)	94	19.6	1001	3.20
C(5)–C(6)	218	3.1	850	3.20
C(6)–C(7)	241	3.1	1186	3.00
		Structures 11 and 12		

C(1)–C(2)	263	3.1	1412	3.00
C(2)–C(3)	89	24.9	1294	3.00
C(3)–C(4)	63	33.3	536	3.81
C(4)–C(5)	101	19.5	806	3.81
C(5)–C(6)	263	3.1	876	3.81
C(6)–C(7)	279	3.1	1600	3.00
		Structure 13		
C(1)–C(2)	243	3.1	1215	3.00
C(2)–C(3)	82	26.4	1161	3.00
C(3)–C(4)	84	21.6	784	3.39
C(4)–C(5)	95	18.3	862	3.39
C(5)–C(6)	221	3.1	777	3.39
C(6)–C(7)	243	3.1	1215	3.00
		Structures 14 and 15		
C(1)–C(2)	232	3.1	1097	3.00
C(2)–C(3)	90	27.3	1441	3.00
C(3)–C(4)	64	40.9	1115	3.00
C(4)–C(5)	101	19.6	1309	3.00
C(5)–C(6)	234	3.1	1113	3.00
C(6)–C(7)	254	3.1	1326	3.00
		Structures 16 and 17		
C(1)–C(2)	243	3.0	1186	3.00
C(2)–C(3)	100	38.0	2515	3.00
C(3)–C(4)	133	23.4	1852	3.65
C(4)–C(5)	87	21.6	725	3.65
C(5)–C(6)	226	3.0	691	3.65
C(6)–C(7)	298	3.1	1821	3.00
		Structures 18 and 19		
C(1)–C(2)	241	3.1	1173	3.00
C(2)–C(3)	123	43.6	4343	3.00
C(3)–C(4)	132	37.5	4394	2.96
C(4)–C(5)	136	24.1	3012	2.96
C(5)–C(6)	238	3.1	1189	2.96
C(6)–C(7)	236	3.1	1144	3.00
		Structures 20 and 21		
C(1)–C(2)	265	3.1	1415	3.00
C(2)–C(3)	105	42.8	3105	3.00
C(3)–C(4)	121	21.5	1393	3.67
C(4)–C(5)	123	19.7	1317	3.67
C(5)–C(6)	225	3.0	679	3.67

C(6)–C(7)	236	3.1	1138	3.00
		Structures 22 and 23		
C(1)–C(2)	293	3.1	1762	3.00
C(2)–C(3)	111	32.3	2630	3.00
C(3)–C(4)	95	40.8	1264	4.15
C(4)–C(5)	112	23.1	995	4.15
C(5)–C(6)	219	3.1	508	4.15
C(6)–C(7)	244	3.1	1204	3.00
		Structures 24 and 25		
C(1)–C(2)	263	3.1	1393	3.00
C(2)–C(3)	107	41.9	3145	3.00
C(3)–C(4)	122	44.4	3174	3.51
C(4)–C(5)	159	25.7	3129	3.51
C(5)–C(6)	223	3.1	743	3.51
C(6)–C(7)	250	3.1	1278	3.00
		Structures 26 and 27		
C(1)–C(2)	305	3.1	1903	3.00
C(2)–C(3)	111	39.0	3168	3.00
C(3)–C(4)	116	25.3	1747	3.41
C(4)–C(5)	89	20.5	821	3.41
C(5)–C(6)	227	3.1	804	3.41
C(6)–C(7)	226	3.1	1044	3.00
		Structures 28 and 29		
C(1)–C(2)	215	3.1	946	3.00
C(2)–C(3)	121	42.5	4082	3.00
C(3)–C(4)	127	24.0	2180	3.25
C(4)–C(5)	115	19.6	1449	3.25
C(5)–C(6)	227	3.1	884	3.25
C(6)–C(7)	272	3.1	1521	3.00
		Structures 30 and 31		
C(1)–C(2)	254	3.1	1312	3.00
C(2)–C(3)	123	44.8	4433	3.00
C(3)–C(4)	119	51.1	5304	2.85
C(4)–C(5)	154	25.4	4425	2.85
C(5)–C(6)	232	3.1	1216	2.85
C(6)–C(7)	278	3.1	1580	3.00
		Structures 32 and 33		
C(1)–C(2)	248	3.1	1258	3.00
C(2)–C(3)	139	44.0	5633	3.00
C(3)–C(4)	150	36.0	5414	2.97

C(4)–C(5)	181	24.9	5472	2.97
C(5)–C(6)	228	3.1	1078	2.97
C(6)–C(7)	261	3.1	1376	3.00
		Structures 34 and 35		
C(1)–C(2)	294	3.1	1777	3.00
C(2)–C(3)	120	34.7	3310	3.00
C(3)–C(4)	80	46.6	1297	3.70
C(4)–C(5)	115	22.0	1257	3.70
C(5)–C(6)	218	3.1	631	3.70
C(6)–C(7)	227	3.1	1042	3.00
		Structures 36 and 37		
C(1)–C(2)	249	3.1	1262	3.00
C(2)–C(3)	88	40.9	2096	3.00
C(3)–C(4)	97	41.4	1328	4.15
C(4)–C(5)	133	20.4	1233	4.15
C(5)–C(6)	284	3.1	864	4.15
C(6)–C(7)	237	3.1	1145	3.00

[a]The units are cm^{-1} for torsional barrier heights W and frequencies $\overline{\omega}$. The unit is amu $Å^2$ for internal moments of inertia I, and the local periodicity M is unitless.

Table S3. Cartesian coordinates (in Å) of *n*-heptane optimized by M06-2X/6-311+G(2df,2p)[a]

1. apapapap				**2. ap⁻ap⁻g⁻ap⁻**			
C	0.00000	3.80972	−0.35645	C	3.70482	0.03318	0.14493
C	0.00000	2.54654	0.49636	C	2.32533	0.55779	−0.23554
C	0.00000	1.27284	−0.34125	C	1.20585	−0.40400	0.14597
C	0.00000	0.00000	0.49682	C	−0.18077	0.10325	−0.23282
C	0.00000	−1.27284	−0.34125	C	−1.29459	−0.85800	0.17079
C	0.00000	−2.54654	0.49636	C	−2.68343	−0.43892	−0.30847
C	0.00000	−3.80972	−0.35645	C	−3.14650	0.89843	0.26186
H	−0.87456	2.54409	1.15221	H	2.28559	0.74488	−1.31187
H	0.87456	2.54409	1.15221	H	2.15058	1.52175	0.24941
H	0.00000	4.71016	0.25684	H	4.49278	0.73206	−0.13361
H	−0.88024	3.84275	−1.00003	H	3.90870	−0.91667	−0.35137
H	0.88024	3.84275	−1.00003	H	3.77188	−0.13594	1.22058
H	0.87514	1.27381	−0.99892	H	1.24127	−0.58897	1.22448
H	−0.87514	1.27381	−0.99892	H	1.38217	−1.37157	−0.33462
H	0.87524	0.00000	1.15418	H	−0.34091	1.07795	0.23545
H	−0.87524	0.00000	1.15418	H	−0.22264	0.27094	−1.31442
H	0.87514	−1.27381	−0.99892	H	−1.30413	−0.95702	1.26106
H	−0.87514	−1.27381	−0.99892	H	−1.06358	−1.85056	−0.22537
H	0.87456	−2.54409	1.15221	H	−2.68525	−0.39001	−1.40077
H	−0.87456	−2.54409	1.15221	H	−3.40166	−1.21424	−0.03453
H	0.00000	−4.71016	0.25684	H	−4.17474	1.11516	−0.02565
H	0.88024	−3.84275	−1.00003	H	−2.52595	1.72139	−0.09153
H	−0.88024	−3.84275	−1.00003	H	−3.09836	0.89047	1.35245
4. ap⁻ap⁻sc⁻sc⁻				**6. ap⁻ap⁻ap⁻g⁻**			
C	3.44615	−0.80054	0.10562	C	−3.24981	0.64121	0.31338
C	2.45561	0.31905	−0.19118	C	−2.19293	−0.14873	−0.44933
C	1.02048	−0.05752	0.16027	C	−0.84246	−0.15965	0.25833
C	0.02200	1.05246	−0.15370	C	0.22439	−0.93257	−0.50987
C	−1.40196	0.76290	0.31636	C	1.54826	−1.07531	0.24202
C	−2.03599	−0.46513	−0.33082	C	2.18552	0.24908	0.66647
C	−3.49707	−0.63804	0.06802	C	2.42590	1.20314	−0.49917
H	2.50622	0.58548	−1.25031	H	−2.06821	0.27251	−1.45055
H	2.73683	1.21762	0.36411	H	−2.53199	−1.17821	−0.59078
H	4.46627	−0.51377	−0.14746	H	−4.20839	0.63620	−0.20432
H	3.19939	−1.69770	−0.46383	H	−2.94217	1.68034	0.43851
H	3.42544	−1.06563	1.16367	H	−3.40429	0.22112	1.30829
H	0.96222	−0.30666	1.22544	H	−0.95930	−0.59523	1.25666

H	0.75138	−0.96758	−0.38247	H	−0.51634	0.87321	0.41334
H	0.36998	1.97942	0.31021	H	−0.15797	−1.93054	−0.74003
H	0.01621	1.23382	−1.23324	H	0.39435	−0.44649	−1.47464
H	−2.03158	1.63261	0.10893	H	2.25588	−1.62086	−0.38828
H	−1.40550	0.63530	1.40373	H	1.38612	−1.69158	1.13041
H	−1.95666	−0.37768	−1.41836	H	1.55810	0.73769	1.41523
H	−1.47692	−1.36042	−0.05208	H	3.13492	0.03553	1.16122
H	−3.93787	−1.52312	−0.38941	H	2.97117	2.08997	−0.17832
H	−4.08779	0.22697	−0.23663	H	1.48709	1.53621	−0.94305
H	−3.59289	−0.73778	1.15027	H	3.00780	0.71707	−1.28459
8. $ap^+sc^+sc^+ap^+$				**10. $ap^+sc^+sc^+sc^+$**			
C	−1.19864	2.74158	−1.01068	C	3.49387	−0.37437	0.05005
C	−1.16169	1.39248	−0.30213	C	1.98201	−0.53655	−0.05714
C	0.00000	1.28731	0.68094	C	1.26416	0.80415	−0.18394
C	0.00000	0.00000	1.50649	C	−0.24044	0.68329	−0.41712
C	0.00000	−1.28731	0.68094	C	−0.98162	−0.02168	0.71762
C	1.16169	−1.39248	−0.30213	C	−2.50204	0.09012	0.61650
C	1.19864	−2.74158	−1.01068	C	−3.07085	−0.53768	−0.65256
H	−1.08940	0.59516	−1.04574	H	1.61212	−1.07166	0.81973
H	−2.10150	1.22787	0.23297	H	1.73622	−1.15732	−0.92373
H	−2.02474	2.80332	−1.71825	H	3.99647	−1.33574	0.15056
H	−0.27260	2.91389	−1.56139	H	3.75676	0.23293	0.91750
H	−1.31046	3.55464	−0.29209	H	3.89474	0.12325	−0.83408
H	−0.03550	2.14191	1.36202	H	1.71216	1.36562	−1.00849
H	0.94194	1.37980	0.13279	H	1.44463	1.39246	0.72159
H	0.87540	−0.00037	2.16145	H	−0.66546	1.68314	−0.54752
H	−0.87540	0.00037	2.16145	H	−0.41138	0.15119	−1.35684
H	−0.94194	−1.37980	0.13279	H	−0.65188	0.40206	1.67104
H	0.03550	−2.14191	1.36202	H	−0.70562	−1.07955	0.73792
H	1.08940	−0.59516	−1.04574	H	−2.95289	−0.38816	1.48828
H	2.10150	−1.22787	0.23297	H	−2.78728	1.14472	0.66092
H	2.02474	−2.80332	−1.71825	H	−4.16013	−0.52074	−0.64790
H	0.27260	−2.91389	−1.56139	H	−2.75217	−1.57774	−0.74500
H	1.31046	−3.55464	−0.29209	H	−2.73678	−0.00817	−1.54449
12. $sc^+sc^+sc^+sc^+$				**14. $g^+ap^+sc^+sc^+$**			
C	0.00000	2.95767	−0.90229	C	−0.87188	0.76995	2.78083
C	0.99386	2.36114	0.08996	C	0.41363	−0.02185	2.55978
C	0.42359	1.19538	0.89587	C	0.41363	−0.83930	1.26897
C	0.00000	0.00000	0.04714	C	0.30252	0.00067	0.00000
C	−0.42359	−1.19538	0.89587	C	0.41363	−0.83930	−1.26897

C	−0.99386	−2.36114	0.08996	C	0.41363	−0.02185	−2.55978
C	0.00000	−2.95767	−0.90229	C	−0.87188	0.76995	−2.78083
H	1.32540	3.14026	0.77923	H	0.56990	−0.69520	3.40490
H	1.88572	2.02391	−0.44516	H	1.26655	0.66224	2.55001
H	0.40983	3.84257	−1.38796	H	−0.87125	1.25919	3.75425
H	−0.92221	3.25002	−0.39649	H	−1.74244	0.11275	2.73701
H	−0.26213	2.24512	−1.68389	H	−1.00197	1.54353	2.02460
H	−0.43609	1.54451	1.47683	H	−0.41350	−1.55620	1.29649
H	1.17008	0.86309	1.62261	H	1.33135	−1.43157	1.22064
H	−0.82995	0.28078	−0.60782	H	−0.64747	0.53835	0.00000
H	0.82995	−0.28078	−0.60782	H	1.09046	0.76251	0.00000
H	−1.17008	−0.86309	1.62261	H	−0.41350	−1.55620	−1.29649
H	0.43609	−1.54451	1.47683	H	1.33135	−1.43157	−1.22064
H	−1.32540	−3.14026	0.77923	H	1.26655	0.66224	−2.55001
H	−1.88572	−2.02391	−0.44516	H	0.56990	−0.69520	−3.40490
H	−0.40983	−3.84257	−1.38796	H	−0.87125	1.25919	−3.75425
H	0.92221	−3.25002	−0.39649	H	−1.00197	1.54353	−2.02460
H	0.26213	−2.24512	−1.68389	H	−1.74244	0.11275	−2.73701

16. $ap^+g^+ap^+g^+$

C	3.57375	−0.13169	0.16477
C	2.12404	−0.41480	−0.21241
C	1.20604	0.76293	0.10304
C	−0.23389	0.58891	−0.37798
C	−0.97137	−0.57171	0.28494
C	−2.41851	−0.73057	−0.18149
C	−3.31366	0.45300	0.17413
H	1.78188	−1.30603	0.31669
H	2.05732	−0.64440	−1.27984
H	4.22045	−0.98070	−0.05404
H	3.65982	0.08876	1.22985
H	3.95599	0.73132	−0.38212
H	1.62706	1.66378	−0.35201
H	1.20760	0.93809	1.18383
H	−0.77719	1.51751	−0.19257
H	−0.23716	0.44044	−1.46318
H	−0.95579	−0.43107	1.37127
H	−0.43675	−1.50256	0.08628
H	−2.43012	−0.88573	−1.26384
H	−2.83385	−1.63750	0.26233
H	−4.35211	0.25312	−0.08792

18. $g^+ap^+ap^+g^+$

C	−3.02366	−0.75231	0.04347
C	−1.81938	0.10809	0.40796
C	−0.85190	0.27349	−0.76015
C	0.31191	1.22185	−0.47204
C	1.16849	0.82509	0.73369
C	1.71336	−0.60259	0.67803
C	2.55708	−0.87718	−0.56301
H	−1.29916	−0.33878	1.25832
H	−2.15473	1.09550	0.73827
H	−3.70433	−0.87121	0.88577
H	−2.70595	−1.74698	−0.27309
H	−3.58347	−0.30767	−0.78048
H	−1.40528	0.64628	−1.62632
H	−0.47008	−0.71077	−1.04888
H	0.94372	1.29123	−1.36034
H	−0.08383	2.22676	−0.30291
H	0.58846	0.95091	1.65061
H	2.00868	1.52079	0.80787
H	2.31473	−0.78212	1.57126
H	0.88645	−1.31615	0.72197
H	1.96012	−0.81816	−1.47352

H	−3.01260	1.35931	−0.35002	H	3.00419	−1.86989	−0.52579
H	−3.27290	0.65921	1.24531	H	3.36508	−0.14839	−0.65039
20. $g^+ap^+ap^+g^-$				**22. $g^+ap^+sc^-sc^-$**			
C	−2.65874	0.95617	0.33184	C	3.15566	0.24731	−0.21581
C	−2.31691	−0.33525	−0.40576	C	2.11791	−0.81958	0.12082
C	−0.81675	−0.52771	−0.62197	C	0.77808	−0.25075	0.58756
C	−0.01877	−0.62678	0.67572	C	0.05003	0.56425	−0.47744
C	1.44248	−1.02390	0.46232	C	−1.27390	1.16138	0.00356
C	2.22124	−0.09114	−0.46745	C	−2.28483	0.14253	0.53327
C	2.20113	1.36545	−0.01460	C	−2.60901	−0.96130	−0.46828
H	−2.81920	−0.33947	−1.37511	H	2.51605	−1.47034	0.90184
H	−2.71242	−1.18935	0.15055	H	1.95067	−1.45571	−0.75285
H	−3.73604	1.11097	0.37975	H	4.12056	−0.20214	−0.44806
H	−2.21899	1.81760	−0.17503	H	3.29741	0.92665	0.62679
H	−2.28202	0.94516	1.35421	H	2.85674	0.84410	−1.07677
H	−0.43863	0.30342	−1.22515	H	0.93871	0.37540	1.47209
H	−0.64894	−1.43488	−1.21020	H	0.14062	−1.07781	0.90903
H	−0.06246	0.32396	1.21144	H	0.68991	1.38164	−0.81501
H	−0.49469	−1.36412	1.32884	H	−0.12229	−0.06729	−1.35422
H	1.47978	−2.03940	0.05898	H	−1.73115	1.71215	−0.82302
H	1.94646	−1.05623	1.43213	H	−1.06679	1.89569	0.78670
H	3.25456	−0.43866	−0.52387	H	−1.91401	−0.30162	1.45949
H	1.82225	−0.16374	−1.48165	H	−3.20234	0.67083	0.79945
H	2.84567	1.98253	−0.63948	H	−3.40598	−1.60689	−0.10117
H	2.54707	1.45595	1.01686	H	−1.73981	−1.58993	−0.66507
H	1.19549	1.78518	−0.06276	H	−2.93195	−0.53778	−1.42124
24. $ap^+g^+ap^+g^-$				**26. $ap^+sc^+ac^+ap^+$**			
C	0.00000	2.83546	−0.08718	C	−3.27322	0.59917	0.22374
C	0.71313	1.65122	−0.73253	C	−2.16061	−0.17571	−0.47251
C	1.14454	0.58397	0.27467	C	−0.87003	−0.20580	0.33764
C	0.00000	0.00000	1.10607	C	0.23808	−1.01497	−0.33311
C	−1.14454	−0.58397	0.27467	C	1.57827	−0.98686	0.41715
C	−0.71313	−1.65122	−0.73253	C	2.57221	0.04717	−0.11437
C	0.00000	−2.83546	−0.08718	C	2.06212	1.48405	−0.07843
H	1.59773	2.00773	−1.26370	H	−1.95846	0.26827	−1.45102
H	0.06453	1.20493	−1.49041	H	−2.48826	−1.20108	−0.66410
H	−0.20513	3.61840	−0.81634	H	−4.18676	0.61374	−0.36968
H	0.61017	3.26865	0.70761	H	−2.97276	1.63271	0.40164
H	−0.95197	2.53753	0.35307	H	−3.50917	0.15338	1.19104
H	1.88324	1.01834	0.95369	H	−1.07294	−0.63509	1.32399

H	1.65743	−0.22150	−0.25731	H	−0.53339	0.81823	0.51841
H	0.40308	−0.77178	1.76538	H	−0.10993	−2.04572	−0.43195
H	−0.40308	0.77178	1.76538	H	0.38629	−0.64992	−1.35511
H	−1.65743	0.22150	−0.25731	H	2.05043	−1.96919	0.36426
H	−1.88324	−1.01834	0.95369	H	1.39138	−0.79545	1.47853
H	−1.59773	−2.00773	−1.26370	H	3.49633	−0.02144	0.46340
H	−0.06453	−1.20493	−1.49041	H	2.83342	−0.21484	−1.14326
H	0.95197	−2.53753	0.35307	H	2.83080	2.18065	−0.41171
H	0.20513	−3.61840	−0.81634	H	1.76622	1.76860	0.93291
H	−0.61017	−3.26865	0.70761	H	1.19589	1.61485	−0.72795

28. $ap^+g^+sc^+ac^-$

C	3.15493	0.84178	−0.00027
C	2.24557	−0.37463	0.12706
C	0.77953	−0.04168	−0.12822
C	−0.13400	−1.25371	0.02022
C	−1.60145	−1.00715	−0.33227
C	−2.28137	0.09076	0.50024
C	−2.26849	1.46550	−0.16520
H	2.34515	−0.80728	1.12617
H	2.56457	−1.14935	−0.57502
H	4.19819	0.58593	0.18165
H	2.87028	1.61524	0.71446
H	3.08552	1.27442	−0.99935
H	0.67309	0.37701	−1.13474
H	0.47003	0.74415	0.56694
H	0.25002	−2.06236	−0.60810
H	−0.07399	−1.61447	1.05205
H	−2.14022	−1.94764	−0.20459
H	−1.68078	−0.75277	−1.39385
H	−3.31910	−0.18766	0.69037
H	−1.80049	0.14823	1.48105
H	−2.73753	2.21787	0.46881
H	−2.81741	1.43498	−1.10746
H	−1.25566	1.79846	−0.38774

30. $ap^+ap^+ac^-sc^+$

C	−2.98321	−1.04395	−0.11766
C	−1.57626	−0.55757	0.21099
C	−1.37695	0.91008	−0.15395
C	−0.01518	1.49168	0.22739
C	1.18150	0.76796	−0.40733
C	1.82390	−0.28602	0.49293
C	2.95247	−1.03516	−0.20505
H	−0.84735	−1.17157	−0.32333
H	−1.37565	−0.69610	1.27725
H	−3.11595	−2.09520	0.13558
H	−3.19388	−0.92649	−1.18172
H	−3.73041	−0.46932	0.43140
H	−2.16351	1.50053	0.32458
H	−1.52243	1.02596	−1.23292
H	−0.00379	2.54366	−0.06225
H	0.09256	1.47535	1.31652
H	1.95264	1.49294	−0.67853
H	0.86756	0.29983	−1.34656
H	2.20770	0.20790	1.38939
H	1.06807	−0.99418	0.83736
H	3.42160	−1.76400	0.45497
H	3.72530	−0.34367	−0.54436
H	2.57984	−1.56778	−1.08136

32. $ap^+ap^+g^-g^-$

C	2.78195	0.76714	−0.01318
C	1.61469	−0.06383	0.50665
C	0.83060	−0.72604	−0.62183
C	−0.36105	−1.55691	−0.14920
C	−1.46548	−0.78366	0.57770

34. $ap^-ap^-sc^-ac^+$

C	2.92584	−0.67796	0.28071
C	1.55291	−0.41819	−0.32838
C	1.00720	0.95857	0.04806
C	−0.36042	1.30264	−0.55911
C	−1.55702	0.97641	0.33877

C	−2.10311	0.34826	−0.24146	C	−1.71918	−0.49478	0.71982
C	−1.45345	1.71769	−0.04733	C	−1.96620	−1.40595	−0.47831
H	0.95361	0.57244	1.09861	H	0.86129	−1.20083	−0.01332
H	1.98177	−0.83831	1.18582	H	1.61458	−0.48565	−1.41806
H	3.34793	1.22155	0.79922	H	3.31485	−1.65484	−0.00437
H	2.42507	1.56928	−0.66175	H	2.87929	−0.64103	1.37014
H	3.46763	0.15227	−0.59799	H	3.64341	0.07704	−0.04396
H	1.50982	−1.37335	−1.18357	H	1.74232	1.70261	−0.26908
H	0.49385	0.03559	−1.33126	H	0.95156	1.03901	1.13913
H	−0.80675	−2.05492	−1.01452	H	−0.39734	2.37146	−0.77653
H	0.00275	−2.35175	0.50821	H	−0.46558	0.79941	−1.52429
H	−1.08604	−0.37854	1.51975	H	−2.47185	1.30988	−0.15965
H	−2.23836	−1.50326	0.85380	H	−1.47058	1.57044	1.25263
H	−2.08695	0.07820	−1.30147	H	−0.83928	−0.83206	1.27304
H	−3.15646	0.43410	0.03072	H	−2.55877	−0.58215	1.41253
H	−0.41204	1.73098	−0.36589	H	−2.13076	−2.43655	−0.16513
H	−1.47866	2.00489	1.00522	H	−1.12377	−1.40152	−1.17001
H	−1.98212	2.48490	−0.61300	H	−2.84814	−1.07957	−1.03236
36. $sc^+sc^+g^+ac^-$				**38. $g^+g^+ac^-g^-$**			
C	2.51765	0.97559	−0.52730	C	2.91834	−0.05700	0.76881
C	2.33206	−0.28180	0.31782	C	2.23955	−0.48333	−0.52963
C	0.87865	−0.53849	0.71212	C	0.71350	−0.43218	−0.46360
C	−0.02576	−0.90590	−0.46455	C	0.16310	0.96737	−0.20073
C	−1.50135	−1.08748	−0.07646	C	−1.35538	1.09267	−0.33267
C	−2.36997	0.14471	−0.33576	C	−2.15438	0.19957	0.62907
C	−1.90476	1.40326	0.38958	C	−2.56515	−1.14451	0.03100
H	2.93534	−0.19336	1.22346	H	2.54982	−1.49959	−0.78048
H	2.71704	−1.14975	−0.22473	H	2.58374	0.15505	−1.34785
H	3.57164	1.16487	−0.72808	H	3.99699	−0.20011	0.71541
H	2.11435	1.84857	−0.01054	H	2.54402	−0.64290	1.61054
H	2.01060	0.89531	−1.48835	H	2.73644	0.99437	0.98966
H	0.48546	0.34313	1.22523	H	0.37079	−1.11490	0.31970
H	0.83969	−1.35478	1.43823	H	0.30037	−0.80630	−1.40482
H	0.04370	−0.14436	−1.24631	H	0.44992	1.28866	0.80416
H	0.35929	−1.82765	−0.90747	H	0.63935	1.66731	−0.89444
H	−1.56447	−1.35755	0.98239	H	−1.65045	0.86599	−1.36204
H	−1.92762	−1.92581	−0.62981	H	−1.62210	2.13727	−0.16278
H	−2.39018	0.33843	−1.41168	H	−1.56883	0.03765	1.53877
H	−3.39850	−0.07958	−0.04532	H	−3.05836	0.72397	0.94289
H	−1.85030	1.23611	1.46681	H	−3.11745	−1.74645	0.75260

H	−2.58933	2.23231	0.21285	H	−1.70333	−1.72321	−0.29780
H	−0.91585	1.71474	0.05063	H	−3.20834	−0.99226	−0.83691
40. $g^+ap^-ac^+sc^-$				**42. $g^+ap^+ac^-sc^+$**			
C	−3.11027	−0.26406	−0.32251	C	−3.12313	0.69430	−0.28917
C	−2.08408	0.81634	0.00647	C	−2.00658	−0.34318	−0.28586
C	−0.81502	0.27284	0.65975	C	−0.88610	0.00945	0.68867
C	−0.06058	−0.73864	−0.20435	C	0.26844	−0.99589	0.66821
C	1.32964	−1.09907	0.34128	C	1.18062	−0.88620	−0.56520
C	2.47350	−0.30639	−0.29382	C	2.46019	−0.08600	−0.31614
C	2.35736	1.20577	−0.13196	C	2.21766	1.35584	0.11827
H	−2.53806	1.55411	0.67102	H	−1.60130	−0.44670	−1.29521
H	−1.81267	1.35152	−0.90802	H	−2.41260	−1.32231	−0.01809
H	−4.03572	0.17151	−0.69755	H	−3.92373	0.42274	−0.97638
H	−3.35194	−0.85026	0.56621	H	−2.74264	1.67215	−0.58772
H	−2.73844	−0.95137	−1.08198	H	−3.55726	0.79981	0.70617
H	−1.07303	−0.20453	1.61060	H	−1.30724	0.06383	1.69634
H	−0.15518	1.10599	0.90842	H	−0.51282	1.01062	0.45663
H	−0.66396	−1.64321	−0.29202	H	0.87753	−0.87583	1.56836
H	0.03912	−0.34334	−1.22184	H	−0.15781	−2.00024	0.72656
H	1.52494	−2.16090	0.18323	H	0.62911	−0.42663	−1.39077
H	1.34064	−0.94510	1.42500	H	1.46198	−1.88297	−0.90835
H	3.41898	−0.64280	0.13681	H	3.05142	−0.59762	0.44823
H	2.51752	−0.54996	−1.35884	H	3.06416	−0.09098	−1.22596
H	3.22085	1.71219	−0.56223	H	3.15796	1.89390	0.23437
H	2.29645	1.48298	0.92193	H	1.69181	1.40145	1.07246
H	1.46726	1.59243	−0.62989	H	1.61474	1.88889	−0.61925
44. $ap^+sc^+ac^-g^-$				**46. $ap^-g^+ac^+sc^-$**			
C	3.13817	−0.73293	0.00983	C	−2.56760	0.26033	−0.72254
C	1.63033	−0.53716	−0.10030	C	−1.50723	0.86882	0.19048
C	1.24518	0.93792	−0.15519	C	−0.82203	−0.16186	1.08913
C	−0.24874	1.20480	−0.34313	C	−0.15411	−1.31545	0.33877
C	−1.13052	0.62636	0.77589	C	0.91277	−0.91838	−0.68456
C	−1.76305	−0.72863	0.44411	C	2.14723	−0.21766	−0.09848
C	−2.90233	−0.61419	−0.56450	C	2.05134	1.30502	−0.01999
H	1.13991	−1.01468	0.75114	H	−1.96756	1.63087	0.82261
H	1.25569	−1.04170	−0.99567	H	−0.76342	1.38830	−0.41735
H	3.40552	−1.78802	0.05662	H	−3.11238	1.03306	−1.26365
H	3.52600	−0.24903	0.90749	H	−3.29100	−0.31942	−0.14603
H	3.65010	−0.29456	−0.84794	H	−2.12289	−0.40726	−1.46102
H	1.79862	1.41463	−0.96930	H	−1.56915	−0.58202	1.76843

H	1.58004	1.42359	0.76722	H	−0.08654	0.33727	1.72405
H	−0.39621	2.28383	−0.40930	H	0.30394	−1.98689	1.07001
H	−0.56444	0.79815	−1.30830	H	−0.92277	−1.90416	−0.16751
H	−1.93728	1.32497	1.01070	H	0.47250	−0.28734	−1.46292
H	−0.53202	0.54005	1.68700	H	1.23465	−1.83171	−1.18846
H	−1.00047	−1.40778	0.05773	H	2.35175	−0.62613	0.89554
H	−2.14514	−1.18189	1.36114	H	3.01573	−0.46755	−0.71052
H	−3.32596	−1.59025	−0.79885	H	1.26269	1.63698	0.65277
H	−2.56572	−0.16736	−1.50042	H	1.84356	1.72580	−1.00536
H	−3.70292	0.01302	−0.16945	H	2.98868	1.73538	0.33256
48. $sc^+ap^+g^+g^-$				**50. $ap^-ac^+g^-g^+$**			
C	−1.64366	1.53791	−0.25808	C	2.74336	0.71459	−0.06770
C	−1.82307	0.28268	0.58986	C	1.56806	−0.03612	0.54612
C	−1.50991	−1.00861	−0.16571	C	0.83996	−0.90809	−0.47606
C	−0.08342	−1.13579	−0.70773	C	−0.43630	−1.57174	0.05726
C	1.01480	−1.11671	0.36588	C	−1.74115	−0.79918	−0.15899
C	1.59667	0.25841	0.71096	C	−1.84236	0.58205	0.50206
C	2.35927	0.89865	−0.44518	C	−1.29832	1.73090	−0.34564
H	−2.85573	0.23460	0.94164	H	0.87614	0.67412	1.00167
H	−1.20435	0.34546	1.48785	H	1.92062	−0.67621	1.35897
H	−1.93975	2.43200	0.28981	H	3.28328	1.29894	0.67651
H	−2.25352	1.48141	−1.16163	H	2.40083	1.39832	−0.84660
H	−0.60715	1.67053	−0.56985	H	3.44916	0.02092	−0.52741
H	−2.20925	−1.09938	−1.00196	H	1.53918	−1.67885	−0.81005
H	−1.70571	−1.85940	0.49264	H	0.60266	−0.31783	−1.36653
H	−0.02571	−2.07993	−1.25228	H	−0.55557	−2.54836	−0.41588
H	0.10284	−0.35825	−1.45176	H	−0.31257	−1.76890	1.12707
H	1.84474	−1.74779	0.03725	H	−2.55417	−1.42537	0.21436
H	0.62374	−1.58206	1.27552	H	−1.91450	−0.68890	−1.23438
H	0.81055	0.93536	1.04739	H	−2.89292	0.79153	0.71243
H	2.27670	0.13968	1.55729	H	−1.34274	0.55803	1.47416
H	2.81187	1.84255	−0.14291	H	−0.24241	1.61050	−0.58273
H	1.70938	1.10558	−1.29582	H	−1.41569	2.68608	0.16638
H	3.15714	0.24036	−0.79314	H	−1.84085	1.79158	−1.29030
52. $sc^+ac^-ac^-sc^+$				**54. $g^+ac^+g^-ac^+$**			
C	0.00000	2.51958	−0.72127	C	2.72130	−0.38712	−0.60078
C	−1.22449	1.98887	0.01762	C	1.48406	−0.76363	0.20941
C	−1.20574	0.47739	0.25097	C	0.86007	0.44160	0.92148
C	0.00000	0.00000	1.07814	C	0.07650	1.38680	−0.00154
C	1.20574	−0.47739	0.25097	C	−1.42787	1.12015	−0.11154

C	1.22449	−1.98887	0.01762	C	−1.84605	−0.23396	−0.70070
C	0.00000	−2.51958	−0.72127	C	−1.95575	−1.36535	0.32012
H	−2.12469	2.25138	−0.54213	H	1.75942	−1.51895	0.94874
H	−1.30618	2.49154	0.98525	H	0.74966	−1.23093	−0.44911
H	−0.07773	3.59358	−0.88733	H	3.13608	−1.25136	−1.11855
H	0.10826	2.03705	−1.69434	H	3.49737	0.01934	0.04934
H	0.91577	2.33720	−0.15757	H	2.49193	0.36904	−1.35223
H	−1.21466	−0.03320	−0.71534	H	1.66922	0.99485	1.40514
H	−2.13297	0.19654	0.75438	H	0.20339	0.10710	1.72790
H	0.30525	0.81555	1.73875	H	0.20025	2.41321	0.34894
H	−0.30525	−0.81555	1.73875	H	0.51213	1.36049	−1.00485
H	2.13297	−0.19654	0.75438	H	−1.85315	1.91415	−0.72903
H	1.21466	0.03320	−0.71534	H	−1.88279	1.23062	0.87818
H	2.12469	−2.25138	−0.54213	H	−2.82156	−0.11913	−1.17719
H	1.30618	−2.49154	0.98525	H	−1.15455	−0.51168	−1.50090
H	0.07773	−3.59358	−0.88733	H	−2.28935	−2.28876	−0.15350
H	−0.10826	−2.03705	−1.69434	H	−2.68231	−1.10700	1.09205
H	−0.91577	−2.33720	−0.15757	H	−1.00932	−1.57203	0.81636
56. $ac^+g^-ac^-sc^+$				**58. $ac^+g^-g^-ac^+$**			
C	2.10036	1.27170	−0.40816	C	0.36660	1.71858	−1.41730
C	2.08065	−0.22288	−0.09656	C	0.00000	2.08048	0.01988
C	0.96273	−0.63380	0.88116	C	−0.82199	1.02772	0.77841
C	−0.18834	−1.40080	0.21958	C	0.00000	0.00000	1.56220
C	−0.94921	−0.64975	−0.88249	C	0.82199	−1.02772	0.77841
C	−2.16644	0.14033	−0.39797	C	0.00000	−2.08048	0.01988
C	−1.86664	1.20131	0.65660	C	−0.36660	−1.71858	−1.41730
H	3.05101	−0.50231	0.31603	H	−0.56513	3.01411	−0.00417
H	1.97683	−0.78865	−1.02619	H	0.90955	2.29520	0.58815
H	2.89864	1.52500	−1.10574	H	0.91328	2.53267	−1.89340
H	2.25650	1.84986	0.50377	H	−0.53172	1.53252	−2.00820
H	1.15710	1.60140	−0.84447	H	0.98526	0.82542	−1.47432
H	0.58652	0.25772	1.38541	H	−1.51207	0.52841	0.09374
H	1.37716	−1.27007	1.66500	H	−1.45202	1.54564	1.50455
H	0.23386	−2.31594	−0.20265	H	0.67565	0.55307	2.22114
H	−0.89940	−1.72333	0.98643	H	−0.67565	−0.55307	2.22114
H	−1.29661	−1.36916	−1.62649	H	1.45202	−1.54564	1.50455
H	−0.26670	0.01922	−1.41325	H	1.51207	−0.52841	0.09374
H	−2.63821	0.61549	−1.26076	H	0.56513	−3.01411	−0.00417
H	−2.90186	−0.56239	0.00327	H	−0.90955	−2.29520	0.58815
H	−2.75322	1.79760	0.87081	H	−0.91328	−2.53267	−1.89340

H	−1.07891	1.87895	0.32222	H	0.53172	−1.53252	−2.00820
H	−1.54132	0.74998	1.59366	H	−0.98526	−0.82542	−1.47432

[a] The coordinates for mirror image structures are given for only one of the two structures in each case.

Table S4. Cartesian coordinates (in Å) of isoheptane optimized by M06-2X/6-311+G(2df,2p)[a]

1. sc$^-$ap$^-$ap$^-$				**3. g$^+$sc$^-$ap$^-$**			
C	−2.81769	−0.87469	−0.01818	C	−2.75296	−0.50140	−0.45501
C	−1.63376	0.02785	−0.35477	C	−1.34568	0.07297	−0.31537
C	−0.33366	−0.58799	0.16621	C	−0.46497	−0.89187	0.48460
C	0.92967	0.19524	−0.17389	C	0.96654	−0.42056	0.73717
C	2.20603	−0.54053	0.22024	C	1.74478	−0.08941	−0.53268
C	3.46528	0.25636	−0.09912	C	3.20470	0.24157	−0.24545
C	−1.86383	1.43199	0.19948	C	−1.39631	1.45850	0.32326
H	−3.74818	−0.47572	−0.42311	H	−3.38423	0.14074	−1.06994
H	−2.67689	−1.87987	−0.41711	H	−2.73277	−1.49284	−0.90915
H	−2.93407	−0.95804	1.06494	H	−3.22455	−0.59283	0.52621
H	−1.55571	0.09900	−1.44498	H	−0.92310	0.17310	−1.31956
H	−0.40846	−0.69901	1.25422	H	−0.95314	−1.08400	1.44580
H	−0.24030	−1.60094	−0.23776	H	−0.43495	−1.85098	−0.04166
H	0.91468	1.16682	0.32673	H	1.50118	−1.20232	1.28361
H	0.95036	0.40337	−1.24913	H	0.96287	0.45396	1.39381
H	2.17306	−0.76601	1.28951	H	1.68449	−0.93656	−1.22216
H	2.23847	−1.50409	−0.29475	H	1.27606	0.75483	−1.04374
H	3.46611	1.20955	0.43142	H	3.70816	−0.60216	0.22844
H	4.36733	−0.28491	0.18419	H	3.74915	0.48864	−1.15617
H	3.52613	0.47317	−1.16660	H	3.28143	1.09352	0.43193
H	−1.87016	1.41037	1.29236	H	−1.74635	1.38718	1.35630
H	−1.08991	2.12939	−0.11849	H	−0.41830	1.93986	0.33448
H	−2.82468	1.82754	−0.13132	H	−2.08263	2.11103	−0.21729
5. g$^+$sc$^-$sc$^-$				**7. sc$^-$ap$^+$g$^+$**			
C	−2.30612	−1.10547	−0.01181	C	1.91683	1.23423	0.54373
C	−1.12618	−0.16814	−0.25458	C	1.56677	0.02645	−0.32259
C	−0.20036	−0.16500	0.96495	C	0.11212	−0.40818	−0.13178
C	1.02592	0.74322	0.85193	C	−0.91704	0.66862	−0.46795
C	1.88977	0.48933	−0.38443	C	−2.34741	0.13810	−0.55479
C	2.39347	−0.94741	−0.48236	C	−2.84545	−0.47052	0.75272
C	−1.62144	1.23546	−0.59445	C	2.51085	−1.13409	−0.02136
H	−2.95484	−1.16164	−0.88648	H	2.97112	1.49348	0.44186
H	−1.96774	−2.11490	0.22533	H	1.33027	2.11240	0.27638
H	−2.90737	−0.74885	0.82774	H	1.72803	1.01074	1.59698
H	−0.56509	−0.55008	−1.11355	H	1.69517	0.31014	−1.37273
H	−0.78507	0.13968	1.83904	H	−0.07737	−1.28674	−0.75786
H	0.12222	−1.19108	1.16145	H	−0.01611	−0.73668	0.90481

H	1.64151	0.60649	1.74515	H	−0.64662	1.13149	−1.42174
H	0.70943	1.78847	0.85952	H	−0.88024	1.46259	0.28275
H	1.32740	0.74077	−1.28720	H	−3.01196	0.95271	−0.84937
H	2.74256	1.17046	−0.36029	H	−2.40444	−0.60990	−1.35019
H	1.57182	−1.65053	−0.62243	H	−2.74704	0.24333	1.57280
H	3.07869	−1.07005	−1.32032	H	−3.89441	−0.75589	0.68160
H	2.92216	−1.23504	0.42835	H	−2.27842	−1.36208	1.01954
H	−2.13448	1.67388	0.26538	H	2.42051	−1.43386	1.02534
H	−0.80471	1.90181	−0.87169	H	2.28126	−2.00336	−0.63865
H	−2.32685	1.20867	−1.42556	H	3.55014	−0.85617	−0.19931
9. $sc^+ap^-g^+$				**11. $g^+ap^-sc^-$**			
C	2.41597	1.25852	0.10863	C	−2.48236	−1.13274	−0.03916
C	1.51528	0.11253	−0.34496	C	−1.55057	0.02706	−0.32693
C	0.10904	0.28633	0.23479	C	−0.10538	−0.39871	−0.13401
C	−0.90568	−0.75366	−0.23044	C	0.90659	0.69134	−0.42761
C	−2.31523	−0.52688	0.31718	C	2.32762	0.17175	−0.54271
C	−2.96613	0.76449	−0.16993	C	2.80945	−0.51034	0.72165
C	2.13665	−1.22878	0.03842	C	−1.90075	1.21465	0.54810
H	3.41137	1.17796	−0.32915	H	−3.52432	−0.86090	−0.21775
H	1.99896	2.22646	−0.17152	H	−2.24392	−1.99876	−0.65977
H	2.52769	1.24440	1.19539	H	−2.39165	−1.43614	1.00775
H	1.43320	0.15255	−1.43648	H	−1.67526	0.32264	−1.37605
H	0.17416	0.26133	1.32933	H	0.01346	−0.75266	0.89707
H	−0.24612	1.28562	−0.02879	H	0.10057	−1.26131	−0.77964
H	−0.57146	−1.74809	0.07080	H	0.86941	1.45129	0.35971
H	−0.94121	−0.75624	−1.32531	H	0.62531	1.19614	−1.35849
H	−2.94383	−1.37219	0.03034	H	2.38536	−0.52922	−1.38173
H	−2.27874	−0.52885	1.41003	H	2.99603	1.00126	−0.78769
H	−2.96504	0.80918	−1.26060	H	2.23675	−1.41579	0.92785
H	−4.00032	0.83396	0.16570	H	3.85971	−0.79423	0.64717
H	−2.44274	1.64575	0.19901	H	2.70110	0.15313	1.58331
H	2.16124	−1.33654	1.12590	H	−1.70594	0.97638	1.59837
H	1.58144	−2.07161	−0.37066	H	−1.31663	2.09870	0.28958
H	3.16200	−1.29898	−0.32609	H	−2.95757	1.47140	0.45441
13. apapap				**14. $ap^+ap^+g^+$**			
C	−2.08637	1.25564	−0.43482	C	2.26378	−1.14172	0.02605
C	−1.77667	0.00000	0.37818	C	1.59186	0.14706	0.49645
C	−0.34110	−0.00001	0.91912	C	0.07474	−0.01294	0.66515
C	0.76332	0.00000	−0.13423	C	−0.70440	−0.24348	−0.62884
C	2.15734	−0.00001	0.48553	C	−2.17158	−0.60340	−0.39303

C	3.26503	0.00001	−0.56121	C	−2.95705	0.48452	0.33342
C	−2.08638	−1.25563	−0.43484	C	1.94388	1.30689	−0.43308
H	−3.14375	1.29513	−0.69844	H	3.34876	−1.03164	0.02177
H	−1.84311	2.16063	0.12397	H	2.01219	−1.98023	0.67691
H	−1.51697	1.27125	−1.36540	H	1.95941	−1.40002	−0.98921
H	−2.43710	−0.00001	1.25030	H	1.99201	0.38191	1.48710
H	−0.21002	0.87557	1.56263	H	−0.11640	−0.84948	1.34589
H	−0.21002	−0.87562	1.56260	H	−0.31061	0.88174	1.16069
H	0.66541	0.87597	−0.78146	H	−0.23549	−1.04489	−1.20406
H	0.66540	−0.87594	−0.78150	H	−0.65739	0.65466	−1.25106
H	2.26161	0.87448	1.13317	H	−2.64518	−0.80589	−1.35569
H	2.26160	−0.87453	1.13313	H	−2.22417	−1.53422	0.17818
H	3.19333	0.88029	−1.20159	H	−2.86616	1.43956	−0.18771
H	4.25310	0.00000	−0.10219	H	−4.01587	0.23455	0.39082
H	3.19333	−0.88025	−1.20163	H	−2.59707	0.62695	1.35193
H	−1.51697	−1.27123	−1.36542	H	1.64671	1.08776	−1.46000
H	−1.84313	−2.16063	0.12393	H	1.44322	2.22711	−0.12761
H	−3.14376	−1.29511	−0.69847	H	3.01870	1.49052	−0.43468
16. $g^+ac^+ap^-$				**18. $sc^+g^-ac^+$**			
C	−2.90316	−0.30243	0.21630	C	−2.51846	−0.19582	−0.72295
C	−1.53490	0.03305	−0.37023	C	−1.11219	0.15765	−0.24402
C	−0.48500	−0.96442	0.12945	C	−0.40047	−1.10339	0.25173
C	0.93167	−0.73978	−0.41810	C	1.05334	−0.94303	0.70173
C	1.85480	0.02319	0.53034	C	2.01626	−0.44430	−0.38594
C	3.22086	0.29878	−0.08588	C	2.19413	1.07235	−0.43372
C	−1.16505	1.48081	−0.05855	C	−1.17989	1.23433	0.83608
H	−3.67467	0.36370	−0.17113	H	−3.03759	0.68163	−1.10978
H	−3.19325	−1.32828	−0.01362	H	−2.49121	−0.94927	−1.51090
H	−2.88563	−0.19556	1.30341	H	−3.11054	−0.59694	0.10300
H	−1.59374	−0.07265	−1.45891	H	−0.55869	0.55258	−1.10117
H	−0.46102	−0.92840	1.22472	H	−0.98410	−1.51641	1.08167
H	−0.82836	−1.96774	−0.13176	H	−0.43131	−1.85304	−0.54520
H	0.87328	−0.20725	−1.37338	H	1.39158	−1.91958	1.05311
H	1.39994	−1.70099	−0.64233	H	1.11011	−0.27951	1.56898
H	1.38764	0.96340	0.82931	H	2.99767	−0.89310	−0.22314
H	1.97384	−0.56100	1.44652	H	1.67677	−0.80764	−1.36035
H	3.12470	0.91528	−0.98099	H	2.54500	1.44505	0.53015
H	3.87947	0.81853	0.60908	H	2.92995	1.35582	−1.18624
H	3.70933	−0.63199	−0.37846	H	1.26565	1.59046	−0.66779
H	−1.05124	1.62201	1.01923	H	−1.71387	0.85409	1.71062

H	−0.23111	1.77479	−0.53773	H	−0.19126	1.55468	1.16293
H	−1.94445	2.16094	−0.40400	H	−1.71448	2.11440	0.47664
20. $sp^+sc^+ap^+$				**22. $g^-ac^-g^-$**			
C	−2.77115	−0.51657	−0.38539	C	−1.35605	1.42838	−0.22809
C	−1.36135	0.06440	−0.29332	C	−1.52346	0.00846	0.30680
C	−0.45743	−0.83202	0.57181	C	−0.22730	−0.80424	0.22480
C	0.99728	−0.92479	0.11033	C	0.95747	−0.19208	0.98957
C	1.75803	0.39656	0.06044	C	1.94661	0.57659	0.10864
C	3.22703	0.19564	−0.29464	C	2.80935	−0.34571	−0.74768
C	−1.43481	1.49465	0.24267	C	−2.64574	−0.70873	−0.43795
H	−3.42787	0.12513	−0.97412	H	−2.29786	1.97549	−0.17320
H	−2.76327	−1.50696	−0.84125	H	−0.61082	1.99115	0.33394
H	−3.20470	−0.61144	0.61308	H	−1.04301	1.40593	−1.27510
H	−0.94052	0.09429	−1.30439	H	−1.80202	0.07593	1.36405
H	−0.49200	−0.47824	1.60771	H	−0.43609	−1.80779	0.60135
H	−0.86775	−1.84460	0.58450	H	0.03530	−0.92849	−0.83150
H	1.02382	−1.38137	−0.88454	H	1.50998	−0.97891	1.50859
H	1.53326	−1.61065	0.77272	H	0.57044	0.46765	1.77084
H	1.29692	1.05998	−0.67445	H	1.40361	1.27099	−0.53578
H	1.67630	0.89976	1.02814	H	2.59628	1.18494	0.74126
H	3.32641	−0.29628	−1.26345	H	2.19994	−0.97526	−1.39675
H	3.76309	1.14278	−0.34390	H	3.48991	0.22116	−1.38215
H	3.72285	−0.43292	0.44634	H	3.40848	−1.00495	−0.11774
H	−1.92245	1.49770	1.22034	H	−2.40526	−0.78707	−1.50080
H	−0.45042	1.94308	0.36346	H	−2.79544	−1.71851	−0.05421
H	−2.01934	2.13252	−0.42160	H	−3.58872	−0.16832	−0.34935
24. $sp^+g^+g^+$				**26. $ap^-ac^+ap^-$**			
C	−2.71872	−0.30246	0.09659	C	1.27612	1.52416	−0.04970
C	−1.27588	0.01588	−0.29313	C	1.66867	0.07973	−0.35075
C	−0.29701	−0.82909	0.54079	C	0.49343	−0.75834	−0.87727
C	0.98872	−1.24657	−0.17826	C	−0.75316	−0.79079	0.02103
C	1.90673	−0.11419	−0.63783	C	−1.83792	0.20454	−0.38763
C	2.44104	0.73481	0.51122	C	−3.03239	0.18087	0.55826
C	−1.03460	1.51869	−0.14331	C	2.31773	−0.56380	0.87343
H	−3.42675	0.30223	−0.47129	H	2.14871	2.10583	0.24941
H	−2.95329	−1.35337	−0.07420	H	0.82920	2.00690	−0.91984
H	−2.87654	−0.09299	1.15739	H	0.55504	1.57000	0.76934
H	−1.14117	−0.25205	−1.34691	H	2.41922	0.09855	−1.14642
H	−0.06074	−0.29510	1.46642	H	0.20443	−0.38043	−1.86256
H	−0.80440	−1.74613	0.84991	H	0.85880	−1.77502	−1.03767

H	0.71270	−1.85156	−1.04629	H	−0.47437	−0.60644	1.06264
H	1.55808	−1.90445	0.48481	H	−1.19119	−1.79149	0.00739
H	2.74905	−0.55260	−1.17708	H	−1.42101	1.21244	−0.42967
H	1.38561	0.51602	−1.36191	H	−2.16624	−0.03198	−1.40311
H	2.97080	0.11111	1.23351	H	−2.73005	0.45167	1.57106
H	3.13527	1.49452	0.15323	H	−3.80956	0.87673	0.24407
H	1.63887	1.24489	1.04449	H	−3.47283	−0.81645	0.60195
H	−1.18147	1.81663	0.89782	H	1.62629	−0.59743	1.71706
H	−0.02854	1.81398	−0.43398	H	2.63595	−1.58502	0.66045
H	−1.73924	2.08648	−0.75235	H	3.19272	0.00399	1.19170

28. $ap^+g^+ap^+$

C	1.66740	1.42144	−0.22790
C	1.66013	−0.10773	−0.20221
C	0.51919	−0.73386	−1.02440
C	−0.85947	−0.83737	−0.36765
C	−1.52992	0.48006	0.01516
C	−2.99458	0.28241	0.39065
C	1.69118	−0.63097	1.23185
H	2.56957	1.80497	0.25107
H	1.64729	1.79587	−1.25219
H	0.81276	1.84347	0.29851
H	2.58760	−0.42822	−0.68596
H	0.42393	−0.18301	−1.96512
H	0.82345	−1.74812	−1.29648
H	−0.80051	−1.47612	0.51836
H	−1.51720	−1.36271	−1.06640
H	−1.00514	0.93569	0.85622
H	−1.45060	1.18526	−0.81706
H	−3.08865	−0.41994	1.22049
H	−3.46434	1.21863	0.69017
H	−3.55905	−0.12354	−0.44985
H	0.82397	−0.28231	1.79595
H	1.68954	−1.72192	1.25769
H	2.58385	−0.28183	1.75155

30. $ap^+g^+sc^+$

C	−1.10286	1.60217	−0.02534
C	−1.43412	0.17019	0.39741
C	−0.26333	−0.56615	1.07504
C	0.78029	−1.22880	0.16894
C	1.59991	−0.30945	−0.73823
C	2.35853	0.77475	0.02000
C	−2.01562	−0.62196	−0.77149
H	−1.99968	2.10718	−0.38743
H	−0.71209	2.17848	0.81447
H	−0.36460	1.63346	−0.82598
H	−2.21694	0.24898	1.15764
H	0.23103	0.11993	1.76825
H	−0.68820	−1.36001	1.69506
H	0.29013	−1.98782	−0.44500
H	1.47588	−1.77173	0.81551
H	2.31478	−0.92611	−1.28753
H	0.95785	0.14549	−1.49459
H	2.98754	0.33297	0.79519
H	3.00266	1.34652	−0.64733
H	1.68022	1.47594	0.50525
H	−1.31119	−0.66918	−1.60403
H	−2.25523	−1.64553	−0.47865
H	−2.92890	−0.15310	−1.13878

32. $sc^-g^-ac^+$

C	1.02748	1.37014	0.65147
C	1.14920	0.13971	−0.24870
C	0.42377	−1.08365	0.33609
C	−1.05069	−1.26707	−0.03622
C	−2.02266	−0.16350	0.40322

34. $ap^-ac^+g^+$

C	−1.35134	1.50704	−0.03512
C	−1.52128	0.09473	0.51995
C	−0.17942	−0.62795	0.71715
C	0.70060	−0.72987	−0.54077
C	1.80965	0.32425	−0.61469

C	−2.19943	0.95625	−0.62075	C	2.94534	0.05688	0.36854
C	2.62841	−0.17623	−0.46736	C	−2.47974	−0.71330	−0.35304
H	1.48419	2.24372	0.18413	H	−2.31451	2.01440	−0.09928
H	−0.00512	1.61722	0.88969	H	−0.69409	2.10732	0.59565
H	1.54887	1.18727	1.59401	H	−0.92462	1.48410	−1.04006
H	0.70665	0.36738	−1.22355	H	−1.97666	0.18059	1.51095
H	0.94998	−1.98510	0.01136	H	0.37808	−0.11380	1.50479
H	0.51999	−1.05729	1.42720	H	−0.39356	−1.62675	1.10333
H	−1.37507	−2.21403	0.40009	H	0.07490	−0.65906	−1.43283
H	−1.12874	−1.39388	−1.12090	H	1.16844	−1.71617	−0.58495
H	−3.00233	−0.60982	0.58358	H	2.21639	0.34745	−1.62785
H	−1.70091	0.24544	1.36437	H	1.38870	1.31445	−0.42859
H	−2.61122	0.55521	−1.54801	H	3.41726	−0.90379	0.15676
H	−2.88539	1.72096	−0.25603	H	3.71310	0.82764	0.30891
H	−1.25764	1.44410	−0.86686	H	2.58705	0.02742	1.39791
H	3.09243	−0.47574	0.47551	H	−2.09970	−0.81668	−1.37072
H	2.75886	−0.99270	−1.17796	H	−2.63195	−1.71492	0.05093
H	3.16899	0.69336	−0.84316	H	−3.45168	−0.22288	−0.41708

36. $sc^+ac^+g^+$

C	−2.09211	1.21618	−0.42618
C	−1.15639	0.18139	0.19123
C	−0.17135	−0.34886	−0.85858
C	1.05323	−1.07645	−0.28246
C	2.30211	−0.19694	−0.19788
C	2.12729	1.04656	0.66797
C	−1.96339	−0.95828	0.80966
H	−2.81965	1.57917	0.30060
H	−1.53668	2.07338	−0.80903
H	−2.64454	0.77655	−1.26021
H	−0.58488	0.66546	0.98822
H	−0.72701	−1.01375	−1.52620
H	0.17307	0.48196	−1.48256
H	1.28899	−1.95003	−0.89201
H	0.81893	−1.45790	0.71571
H	3.13120	−0.79248	0.18992
H	2.58725	0.10600	−1.20901
H	1.83374	0.77632	1.68397
H	3.05376	1.61686	0.72729
H	1.35858	1.70757	0.26510
H	−2.59114	−1.42805	0.04870

H	−1.32139	−1.73006	1.23443
H	−2.61656	−0.59263	1.60252

[a] The coordinates for mirror image structures are given for only one of the two structures in each case.

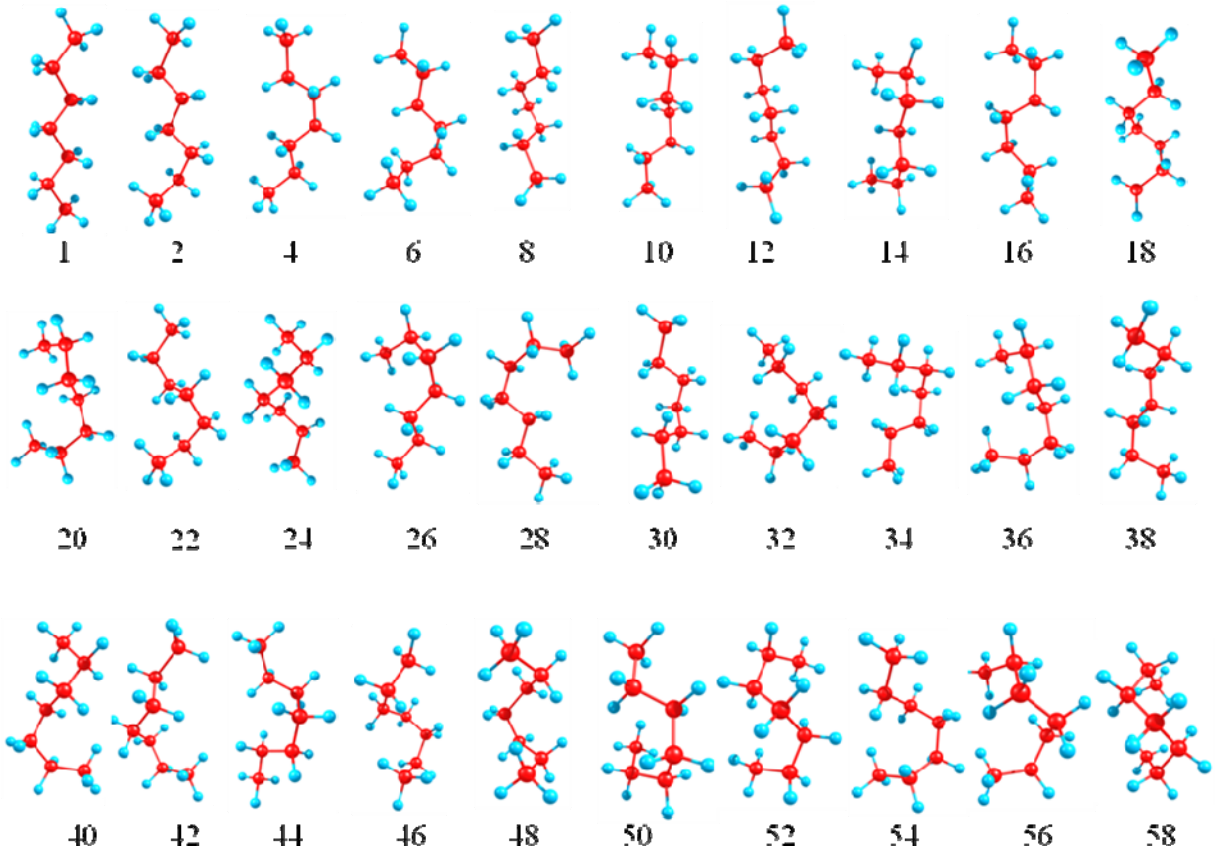

Figure S1. Structures of *n*-heptane. Note that all structures shown except structure 1 also have distinguishable mirror images.

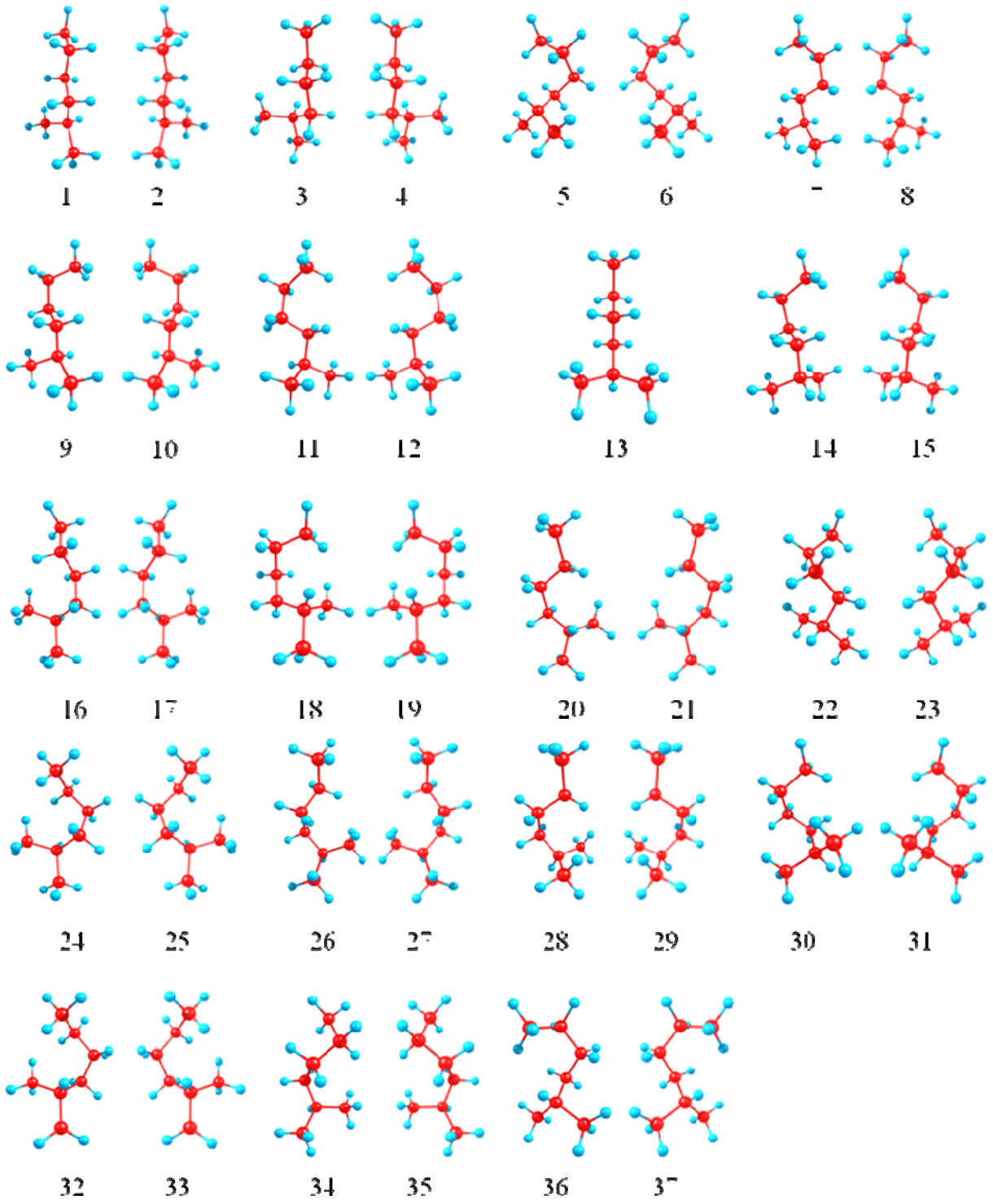

Figure S2. Structures of isoheptane. All structures occur in optically active pairs except structure 13.