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Non-Dynamic Kinetic Resolution of Configurationally Stable Biaryl Lactones by Reduction with Oxazaborolidine-Activated Borane: AM1 Studies and Experimental Verification[†]

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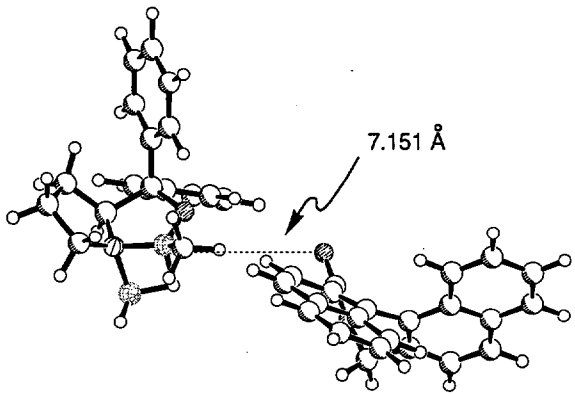
Supporting Information

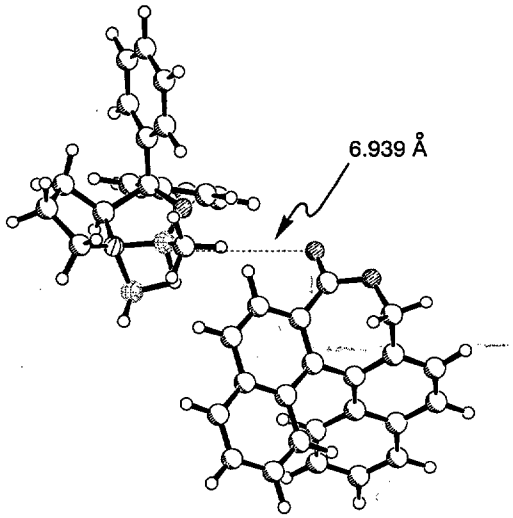
Chromatographic resolution of 6f, 7f and 14. HPLC analyses were carried out with a combination of a Waters HPLC pump 510, a 20 µL injection loop, and a Chiralcel OD-H column (25x0.46 cm) with UV detection at 280 nm. For lactone **6f**, hexane:isopropanol 99:1 (0.5 mL/min) was used as the eluent, the retention times were: (*P*)-**6f** 14 min, (*M*)-**6f** 22 min. The enantiomers of alcohol **7f** were separated using hexane:isopropanol 90:10 (1mL/min), retention times: (*M*)-**7f** 7 min, (*P*)-**7f** 26 min. Hydroxy aldehyde (*M*)-**14** was eluted after 9 min, (*P*)-**14** after 13 min, using hexane:isopropanol 96:4 (1mL/min).

Reduction of an enantiomerically enriched sample of **14** by $LiAlH_4$ and HPLC analysis of the resulting alcohol **7f** was used to assign the configuration of **14**.

Figure 1



(*M*)-**13**



(*P*)-**13**

Figure 1. Minimum structures of weakly bonded Coulomb pairs **13** between (*S*)-**4**·BH_3 and the two atropisomeric forms of lactone **3**.

Table 1. Selected Dihedral Angles (deg) of Minimum Structures 8-13[a]

	∢ O_I-C_J-O_O-B_N	∢ C_J-O_O-B_N-N_M	∢ O_I-B_L-N_M-B_N	∢ B_L-O_I-C_J-O_O	∢ B_L-N_M-B_N-O_O
(*M*)-**13**	142.2	-120.8	-48.4	-110.5	64.8
(*M*)-**13**	153.4	-71.0	-64.2	-120.7	60.4
(*P*)-**13**	-122.9	-122.5	-36.2	118.6	61.2
(*P*)-**13**	-132.4	-108.5	-78.4	121.1	60.3
(*M*)-**8**	-6.8	-85.4	10.3	55.2	37.0
(*M*)-**8**	-168.3	-113.7	-33.7	-52.8	42.7
(*M*)-**8**	33.7	40.3	-55.9	-67.0	24.5
(*P*)-**8**	-16.9	-79.3	13.4	62.4	34.0
(*P*)-**8**	178.1	-52.5	-31.0	-75.9	36.7
(*P*)-**8**	2.3	47.9	-58.7	-48.4	29.1
(*S,M*)-**9**	76.9	113.2	-17.7	-4.1	2.6
(*R,M*)-**9**	-133.9	117.3	-50.5	-32.5	2.8
(*S,P*)-**9**	68.8	-131.1	45.6	17.5	8.7
(*R,P*)-**9**	-77.1	-121.5	6.2	7.1	9.4
(*S,M*)-**10**	82.0	-62.0	49.9	-29.0	-11.0
(*R,M*)-**10**	-78.8	38.0	-29.5	61.9	21.5
(*S,P*)-**10**	55.0	-86.2	31.9	18.2	24.4
(*R,P*)-**10**	67.7	-68.2	37.6	-9.5	2.3
(*M*)-**11**	-74.0	56.2	-57.4	34.4	30.1
(*M*)-**11**	69.3	-85.3	57.4	-3.4	2.7
(*P*)-**11**	39.1	-76.3	66.2	33.0	27.5
(*P*)-**11**	-74.7	61.9	35.4	74.4	-20.7
(*M*)-**12**	-103.3	113.5	-119.9	2.0	7.9
(*M*)-**12**	103.0	-143.0	102.5	12.9	8.1
(*P*)-**12**	92.3	-130.4	99.3	9.2	10.5
(*P*)-**12**	-140.3	123.1	117.6	64.4	-6.7

[a] For the atom denotation, see Scheme 4 in body text.

Z-matrices and total energies of all calculated compounds

(M)-13 HEAT OF FORMATION = -5.357950 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0	
O	1.445265	1	.000000	0	.000000	0	1	0	0	
N	1.566374	1	107.779698	1	.000000	0	1	2	0	
C	1.553620	1	115.773565	1	-141.584633	1	1	2	3	
O	7.151353	1	46.904143	1	114.448310	1	1	2	3	
C	1.446142	1	111.775751	1	4.697807	1	2	1	3	
C	1.492093	1	106.407678	1	.067540	1	3	1	2	
C	1.466167	1	122.768058	1	-127.243199	1	3	1	2	
B	1.554686	1	77.344635	1	114.724635	1	3	1	2	
C	1.232673	1	79.410905	1	152.245311	1	5	1	2	
C	1.512840	1	107.728859	1	-125.924822	1	6	2	1	
C	1.512162	1	107.755758	1	115.073076	1	6	2	1	
C	1.534662	1	107.827379	1	-131.416078	1	7	3	1	
C	1.534584	1	108.589339	1	124.693844	1	8	3	1	
O	1.374693	1	112.273715	1	142.206839	1	10	5	1	
C	1.476415	1	126.598025	1	-32.903538	1	10	5	1	
C	1.400480	1	121.542818	1	155.470094	1	11	6	2	
C	1.400022	1	119.339523	1	-25.226883	1	11	6	2	
C	1.401344	1	120.855919	1	159.058985	1	12	6	2	
C	1.400577	1	120.231708	1	-19.556181	1	12	6	2	
C	1.431435	1	117.613835	1	172.585576	1	15	10	5	
C	1.387051	1	123.777787	1	-134.875909	1	16	10	5	
C	1.420566	1	115.401829	1	44.904841	1	16	10	5	
C	1.393851	1	120.298197	1	-179.820430	1	17	11	6	
C	1.394767	1	120.522220	1	179.339687	1	18	11	6	
C	1.393557	1	120.497446	1	-179.287709	1	19	12	6	
C	1.394219	1	120.501599	1	179.193524	1	20	12	6	
C	1.493534	1	110.391436	1	-64.032227	1	21	15	10	
C	1.468699	1	120.278438	1	4.412807	1	22	16	10	
C	1.433472	1	118.928239	1	-173.592047	1	22	16	10	
C	1.369462	1	120.635083	1	177.387370	1	23	16	10	
C	1.394699	1	120.250028	1	.026584	1	24	17	11	
C	1.394626	1	120.228328	1	.324432	1	26	19	12	
C	1.415691	1	119.336461	1	-107.599494	1	28	21	15	
C	1.430713	1	121.684390	1	127.297089	1	29	22	16	
C	1.419724	1	119.481569	1	-5.746899	1	30	22	16	
C	1.423959	1	92.311058	1	-50.375611	-1	30	29	35	
C	1.371297	1	120.365025	1	174.989687	1	34	28	21	
C	1.419834	1	119.095841	1	175.810751	1	35	29	22	
C	1.423793	1	93.050311	1	-51.166879	1	35	22	30	
C	1.422500	1	119.565603	1	-179.860045	1	36	30	22	
C	1.372927	1	121.015961	1	-179.243112	1	37	30	22	
C	1.422605	1	119.502897	1	-179.811286	1	39	35	29	
C	1.372830	1	120.950385	1	-179.292493	1	40	35	29	
C	1.372267	1	120.658472	1	-1.523969	1	41	36	30	
C	1.372236	1	120.646999	1	-1.507689	1	43	39	35	
H	1.129455	1	107.247941	1	111.137177	1	7	3	1	
H	1.118077	1	111.868393	1	116.940527	1	13	7	3	
H	1.118844	1	109.272531	1	-124.149661	1	13	7	3	
H	1.117768	1	110.144228	1	119.188416	1	14	8	3	
H	1.117690	1	110.239828	1	-121.989138	1	14	8	3	
H	1.124868	1	108.876389	1	-114.506535	1	8	3	1	
H	1.124709	1	109.259873	1	3.568884	1	8	3	1	
H	1.102697	1	119.255142	1	-.401110	1	18	11	6	
H	1.103883	1	119.943812	1	-178.729422	1	25	18	11	
H	1.099900	1	120.177756	1	179.471716	1	32	24	17	
H	1.099739	1	119.736573	1	179.875792	1	24	17	11	
H	1.100861	1	120.394738	1	.413240	1	17	11	6	
H	1.102310	1	119.508687	1	.228394	1	20	12	6	
H	1.099810	1	119.708184	1	-179.696527	1	27	20	12	
H	1.099545	1	120.139796	1	179.707789	1	33	26	19	
H	1.099882	1	119.728056	1	179.830850	1	26	19	12	
H	1.101058	1	119.984945	1	-.050226	1	19	12	6	
H	1.200475	1	111.961327	1	102.916402	1	9	3	1	
H	1.341584	1	95.418490	1	-6.155862	1	9	3	1	
H	1.199336	1	113.952271	1	-114.434667	1	9	3	1	
H	1.108090	1	109.962983	1	-171.356689	1	4	1	2	
H	1.109688	1	107.937983	1	67.531177	1	4	1	2	
H	1.109894	1	106.760723	1	-51.044463	1	4	1	2	
H	1.104646	1	118.296686	1	-3.173040	1	23	16	10	
H	1.104444	1	120.520202	1	178.508290	1	31	23	16	
H	1.101331	1	118.336595	1	178.935610	1	41	36	30	
H	1.100038	1	120.801303	1	-179.697507	1	45	41	36	
H	1.100186	1	120.455410	1	179.685265	1	42	37	30	
H	1.101844	1	118.718467	1	.409958	1	37	30	22	
H	1.101936	1	118.593741	1	.323189	1	40	35	29	
H	1.100262	1	120.470910	1	179.587376	1	44	40	35	
H	1.100031	1	120.779656	1	-179.681929	1	46	43	39	
H	1.100488	1	118.461154	1	179.043191	1	43	39	35	
H	1.100641	1	120.848687	1	179.232248	1	38	34	28	
H	1.100881	1	118.909272	1	-4.537347	1	34	28	21	

(M)-13 Heat of formation = -5.301979 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.440490	1	0.000000	0	0.000000	0	1	0	0
N	1.566648	1	107.868916	1	0.000000	0	1	2	0
C	1.552426	1	116.136606	1	-142.562358	1	1	2	3
O	7.055020	1	50.231182	1	109.255451	1	1	2	3
C	1.445959	1	111.891417	1	4.040412	1	2	1	3
C	1.492122	1	106.407405	1	-0.486198	1	3	1	2
C	1.466184	1	122.659476	1	-127.665625	1	3	1	2
B	1.554498	1	77.435837	1	114.236424	1	3	1	2
C	1.232549	1	92.586586	1	-163.215264	1	5	1	2
C	1.512739	1	107.858153	1	-124.171471	1	6	2	1
C	1.512344	1	107.498322	1	116.529709	1	6	2	1
C	1.534834	1	107.791246	1	-129.868232	1	7	3	1
C	1.524641	1	106.852868	1	-5.495855	1	13	7	3
O	1.375481	1	112.067712	1	153.422995	1	10	5	1
C	1.476243	1	126.830481	1	-21.542439	1	10	5	1
C	1.400880	1	121.250699	1	158.104884	1	11	6	2
C	1.400176	1	119.621035	1	-22.512883	1	11	6	2
C	1.401012	1	121.107004	1	159.486977	1	12	6	2
C	1.401126	1	120.030533	1	-19.264328	1	12	6	2
C	1.431137	1	117.746162	1	171.867580	1	15	10	5
C	1.387286	1	123.544984	1	-135.046478	1	16	10	5
C	1.421052	1	115.625298	1	45.232191	1	16	10	5
C	1.393601	1	120.367515	1	179.420539	1	17	11	6
C	1.394982	1	120.412999	1	-179.698929	1	18	11	6
C	1.393742	1	120.519973	1	-179.367170	1	19	12	6
C	1.394076	1	120.527138	1	179.268542	1	20	12	6
C	1.493413	1	110.364334	1	-63.507299	1	21	15	10
C	1.387682	1	119.722719	1	69.906856	1	28	21	15
C	1.433118	1	119.012319	1	-172.742891	1	22	16	10
C	1.369662	1	120.461816	1	175.900396	1	23	16	10
C	1.394297	1	120.108582	1	0.392456	1	25	18	11
C	1.393929	1	120.234350	1	-0.085428	1	27	20	12
C	1.415594	1	119.451165	1	-107.361745	1	28	21	15
C	1.430485	1	119.452492	1	-171.190951	1	29	28	21
C	1.419492	1	119.423746	1	-5.316674	1	30	22	16
C	1.423901	1	122.236802	1	172.472554	1	30	22	16
C	1.371340	1	120.340573	1	174.870605	1	34	28	21
C	1.419842	1	119.083952	1	-5.396776	1	35	29	28
C	1.423767	1	122.467127	1	172.532349	1	35	29	28
C	1.422630	1	119.588629	1	179.837511	1	36	30	22
C	1.372914	1	120.996290	1	-179.050967	1	37	30	22
C	1.422574	1	119.484911	1	180.025971	1	39	35	29
C	1.372788	1	120.936658	1	-179.184414	1	40	35	29
C	1.372304	1	120.619018	1	-1.328590	1	41	36	30
C	1.372238	1	120.649869	1	-1.386528	1	43	39	35
H	1.129223	1	107.367893	1	112.694947	1	7	3	1
H	1.118215	1	111.823326	1	115.499580	1	13	7	3
H	1.118694	1	109.313440	1	-125.561343	1	13	7	3
H	1.117766	1	110.937448	1	-115.869841	1	14	13	7
H	1.117664	1	110.869372	1	124.398724	1	14	13	7
H	1.124809	1	108.894910	1	-115.497860	1	8	3	1
H	1.124749	1	109.220247	1	2.576429	1	8	3	1
H	1.102352	1	119.541312	1	0.513932	1	18	11	6
H	1.103893	1	119.788317	1	-179.388108	1	25	18	11
H	1.099882	1	120.039427	1	179.815570	1	32	25	18
H	1.099681	1	119.768118	1	-179.887065	1	24	17	11
H	1.100974	1	120.339140	1	-0.366635	1	17	11	6
H	1.102487	1	119.531442	1	0.310184	1	20	12	6
H	1.099845	1	119.699573	1	-179.658429	1	27	20	12
H	1.099535	1	120.225733	1	-179.802168	1	33	27	20
H	1.099874	1	119.707373	1	179.814044	1	26	19	12
H	1.100765	1	120.121746	1	-0.146042	1	19	12	6
H	1.330225	1	95.884009	1	-6.029183	1	9	3	1
H	1.200405	1	113.840170	1	-114.990848	1	9	3	1
H	1.200849	1	111.976774	1	103.879492	1	9	3	1
H	1.107980	1	110.036040	1	-171.651166	1	4	1	2
H	1.109848	1	107.640001	1	67.312202	1	4	1	2
H	1.109354	1	106.825003	1	-51.216651	1	4	1	2
H	1.105597	1	118.450676	1	-4.660453	1	23	16	10
H	1.103589	1	120.733210	1	179.594543	1	31	23	16
H	1.101088	1	118.381114	1	179.066191	1	41	36	30
H	1.100078	1	120.777104	1	-179.795739	1	45	41	36
H	1.100160	1	120.454062	1	179.718275	1	42	37	30
H	1.101810	1	118.722111	1	0.648325	1	37	30	22
H	1.101953	1	118.590083	1	0.435185	1	40	35	29
H	1.100252	1	120.475827	1	179.596085	1	44	40	35
H	1.100008	1	120.778574	1	-179.663431	1	46	43	39
H	1.100487	1	118.463677	1	179.138008	1	43	39	35
H	1.100648	1	120.842571	1	179.343836	1	38	34	28
H	1.100845	1	118.920773	1	-4.608224	1	34	28	21

(P)-13 HEAT OF FORMATION = -5.385052 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.440652	1	.000000	0	.000000	0	1	0	0
N	1.566644	1	107.871862	1	.000000	0	1	2	0
C	1.492150	1	106.420018	1	-.171563	1	3	1	2
C	1.446130	1	111.918933	1	3.258748	1	2	1	3
C	1.466181	1	122.668049	1	-127.362254	1	3	1	2
C	1.534702	1	108.576656	1	124.043720	1	6	3	1
C	1.524639	1	106.856925	1	-2.215673	1	7	6	3
B	1.554484	1	77.416965	1	114.514423	1	3	1	2
C	1.552551	1	116.000922	1	-142.342520	1	1	2	3
C	1.512094	1	107.490597	1	117.388187	1	5	2	1
C	1.401070	1	120.068068	1	-19.418544	1	11	5	2
C	1.401001	1	121.043715	1	159.379366	1	11	5	2
C	1.393736	1	120.504060	1	-179.385175	1	13	11	5
C	1.394083	1	120.512426	1	179.279987	1	12	11	5
C	1.393949	1	120.231201	1	-.067984	1	15	12	11
C	1.512826	1	107.841195	1	-123.311900	1	5	2	1
C	1.400164	1	119.547797	1	-22.807823	1	17	5	2
C	1.400780	1	121.340102	1	157.661324	1	17	5	2
C	1.393641	1	120.354259	1	179.930937	1	19	17	5
C	1.394897	1	120.451112	1	179.715615	1	18	17	5
C	1.394271	1	120.075359	1	.575928	1	21	18	17
O	6.938885	1	49.788819	1	113.298139	1	1	2	3
C	1.232616	1	77.910369	1	148.116150	1	23	1	2
O	1.375124	1	112.102840	1	-122.860213	1	24	23	1
C	1.476390	1	126.797062	1	52.253202	1	24	23	1
C	1.387341	1	123.534671	1	134.808520	1	26	24	23
C	1.431231	1	117.710516	1	-171.906805	1	25	24	23
C	1.493518	1	110.310625	1	63.684123	1	28	25	24
C	1.387744	1	119.735214	1	-69.887593	1	29	28	25
C	1.430517	1	119.445180	1	171.128974	1	30	29	28
C	1.433161	1	119.011340	1	172.917415	1	27	26	24
C	1.420959	1	115.634534	1	-45.434564	1	26	24	23
C	1.369689	1	120.473806	1	-176.085118	1	33	26	24
C	1.420904	1	120.229590	1	1.125908	1	34	33	26
C	1.422621	1	120.708970	1	176.626926	1	35	34	33
C	1.372276	1	120.621019	1	-177.862922	1	36	35	34
C	1.423934	1	122.240173	1	-172.486259	1	32	27	26
C	1.415137	1	120.027734	1	.107707	1	37	36	35
C	1.415590	1	119.436806	1	107.328314	1	29	28	25
C	1.371349	1	120.346035	1	-174.808903	1	40	29	28
C	1.420768	1	120.388029	1	1.972334	1	41	40	29
C	1.423785	1	122.466895	1	-172.545946	1	31	30	29
C	1.422602	1	120.829532	1	176.328429	1	42	41	40
C	1.372217	1	120.650076	1	-177.473167	1	44	42	41
C	1.415444	1	120.048246	1	.062726	1	45	44	42
H	1.129171	1	107.331772	1	112.991431	1	4	3	1
H	1.118286	1	110.439688	1	-116.627338	1	8	7	6
H	1.118599	1	110.930847	1	124.252405	1	8	7	6
H	1.117596	1	110.270821	1	-122.822175	1	7	6	3
H	1.117801	1	110.123806	1	118.345294	1	7	6	3
H	1.124780	1	108.908374	1	-115.143526	1	6	3	1
H	1.124767	1	109.213473	1	2.933246	1	6	3	1
H	1.200793	1	111.970983	1	103.758117	1	9	3	1
H	1.200401	1	113.886853	1	-114.993028	1	9	3	1
H	1.331024	1	95.843597	1	-6.139553	1	9	3	1
H	1.107972	1	110.031578	1	-172.014094	1	10	1	2
H	1.109299	1	106.849597	1	-51.581087	1	10	1	2
H	1.109855	1	107.619579	1	66.939612	1	10	1	2
H	1.102446	1	119.521677	1	.296198	1	12	11	5
H	1.099833	1	119.702913	1	-179.655921	1	15	12	11
H	1.099538	1	120.220192	1	-179.810613	1	16	15	12
H	1.099872	1	119.711453	1	179.815017	1	14	13	11
H	1.100821	1	120.099318	1	-.171087	1	13	11	5
H	1.100909	1	120.370468	1	.090708	1	19	17	5
H	1.099701	1	119.755498	1	179.991600	1	20	19	17
H	1.099846	1	120.016852	1	-179.957763	1	22	21	18
H	1.103807	1	119.891450	1	-178.946316	1	21	18	17
H	1.102228	1	119.435220	1	-.138724	1	18	17	5
H	1.105490	1	118.480036	1	4.451362	1	33	26	24
H	1.103527	1	120.714160	1	-179.757407	1	34	33	26
H	1.101046	1	118.383848	1	1.714413	1	36	35	34
H	1.100084	1	120.777405	1	179.786027	1	37	36	35
H	1.100159	1	119.110655	1	179.016111	1	39	37	36
H	1.101811	1	118.725087	1	-.618827	1	38	32	27
H	1.101939	1	118.589356	1	-.445125	1	43	31	30
H	1.100238	1	119.090524	1	178.955045	1	46	45	44
H	1.100015	1	120.778903	1	179.680174	1	45	44	42
H	1.100489	1	118.462519	1	2.010563	1	44	42	41
H	1.100643	1	120.843868	1	-179.337385	1	41	40	29
H	1.100873	1	118.915779	1	4.675872	1	40	29	28

(P)-13 Heat of formation = -5.211964 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.440991	1	0.000000	0	0.000000	0	1	0	0
N	1.567054	1	107.844363	1	0.000000	0	1	2	0
C	1.491967	1	106.453649	1	-0.044234	1	3	1	2
C	1.445875	1	111.969718	1	1.956661	1	2	1	3
C	1.466144	1	122.640325	1	-127.209015	1	3	1	2
C	1.534806	1	108.560801	1	123.919122	1	6	3	1
C	1.524636	1	106.820013	1	-3.051225	1	7	6	3
B	1.555046	1	77.350274	1	114.652958	1	3	1	2
C	1.552630	1	115.791127	1	-142.019079	1	1	2	3
C	1.511759	1	107.487438	1	119.218093	1	5	2	1
C	1.401122	1	120.055180	1	-19.305395	1	11	5	2
C	1.400884	1	121.029563	1	159.578188	1	11	5	2
C	1.393760	1	120.489036	1	-179.421013	1	13	11	5
C	1.394072	1	120.494062	1	179.308696	1	12	11	5
C	1.393996	1	120.228733	1	-0.041383	1	15	12	11
C	1.512983	1	107.797915	1	-121.457149	1	5	2	1
C	1.400453	1	119.435461	1	-22.728835	1	17	5	2
C	1.400650	1	121.477588	1	157.469949	1	17	5	2
C	1.393818	1	120.408519	1	-178.945780	1	19	17	5
C	1.394154	1	120.324332	1	178.872667	1	18	17	5
C	1.394754	1	120.340377	1	0.288393	1	21	18	17
O	8.347657	1	56.883261	1	75.914176	1	1	2	3
C	1.232560	1	84.263555	1	138.962267	1	23	1	2
O	1.375247	1	112.114516	1	-132.384640	1	24	23	1
C	1.476476	1	126.829548	1	42.681002	1	24	23	1
C	1.387315	1	123.555497	1	134.608085	1	26	24	23
C	1.431205	1	117.690883	1	-171.717183	1	25	24	23
C	1.493491	1	110.366381	1	63.515269	1	28	25	24
C	1.387802	1	119.768072	1	-69.917742	1	29	28	25
C	1.430553	1	119.436186	1	171.294455	1	30	29	28
C	1.433274	1	118.992543	1	173.127397	1	27	26	24
C	1.420955	1	115.606126	1	-45.563511	1	26	24	23
C	1.369585	1	120.500669	1	-176.521839	1	33	26	24
C	1.421029	1	120.201049	1	1.430003	1	34	33	26
C	1.422593	1	120.684393	1	176.545588	1	35	34	33
C	1.372316	1	120.610667	1	-177.717472	1	36	35	34
C	1.423941	1	122.243738	1	-172.371316	1	32	27	26
C	1.415152	1	120.026252	1	0.100611	1	37	36	35
C	1.415643	1	119.405690	1	107.408066	1	29	28	25
C	1.371312	1	120.353281	1	-175.006310	1	40	29	28
C	1.420793	1	120.381523	1	1.995519	1	41	40	29
C	1.423827	1	122.471295	1	-172.561108	1	31	30	29
C	1.422589	1	120.820819	1	176.436951	1	42	41	40
C	1.372248	1	120.645468	1	-177.498617	1	44	42	41
C	1.415396	1	120.048921	1	0.110475	1	45	44	42
H	1.128919	1	107.310103	1	114.141049	1	4	3	1
H	1.118377	1	110.388655	1	-115.075805	1	8	7	6
H	1.118414	1	111.000073	1	125.748279	1	8	7	6
H	1.117516	1	110.295914	1	-123.680520	1	7	6	3
H	1.117836	1	110.115122	1	117.472688	1	7	6	3
H	1.124736	1	108.926057	1	-115.253907	1	6	3	1
H	1.124779	1	109.207864	1	2.833486	1	6	3	1
H	1.330992	1	95.823754	1	-6.031549	1	9	3	1
H	1.200687	1	111.961724	1	103.948775	1	9	3	1
H	1.200801	1	113.821602	1	-114.942884	1	9	3	1
H	1.109282	1	106.859711	1	-52.583566	1	10	1	2
H	1.109834	1	107.582270	1	65.916031	1	10	1	2
H	1.107958	1	110.043841	1	-173.013475	1	10	1	2
H	1.102439	1	119.510801	1	0.269767	1	12	11	5
H	1.099828	1	119.706951	1	-179.667633	1	15	12	11
H	1.099547	1	120.215816	1	-179.832325	1	16	15	12
H	1.099888	1	119.709397	1	179.824129	1	14	13	11
H	1.100823	1	120.096663	1	-0.200628	1	13	11	5
H	1.101018	1	120.385561	1	1.004858	1	19	17	5
H	1.099965	1	119.859415	1	179.496794	1	20	19	17
H	1.103024	1	120.231698	1	-178.234346	1	22	21	18
H	1.100133	1	119.748036	1	-179.696961	1	21	18	17
H	1.101994	1	119.448793	1	-0.519601	1	18	17	5
H	1.105749	1	118.354622	1	3.937361	1	33	26	24
H	1.102740	1	120.824926	1	-179.312422	1	34	33	26
H	1.101084	1	118.386670	1	1.833157	1	36	35	34
H	1.100109	1	120.774793	1	179.759243	1	37	36	35
H	1.100195	1	119.111478	1	178.968214	1	39	37	36
H	1.101840	1	118.727481	1	-0.500445	1	38	32	27
H	1.101874	1	118.596883	1	-0.320306	1	43	31	30
H	1.100266	1	119.093861	1	178.928990	1	46	45	44
H	1.100013	1	120.772503	1	179.735634	1	45	44	42
H	1.100522	1	118.468581	1	2.001170	1	44	42	41
H	1.100679	1	120.849508	1	-179.298167	1	41	40	29
H	1.100861	1	118.908166	1	4.520508	1	40	29	28

TS (M)-[13 -> 8]A Heat of formation = 8.854323 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.381810	1	0.000000	0	0.000000	0	1	0	0
N	1.538124	1	111.033310	1	0.000000	0	1	2	0
C	1.542582	1	121.550930	1	-162.259352	1	1	2	3
O	2.015446	1	84.687613	1	108.747721	1	1	2	3
C	1.460394	1	111.633468	1	-1.110195	1	2	1	3
C	1.506477	1	103.842551	1	9.257032	1	3	1	2
C	1.492160	1	112.519881	1	-105.580843	1	3	1	2
B	1.602531	1	112.407076	1	130.873904	1	3	1	2
C	1.238753	1	152.506993	1	-145.447879	1	5	1	2
C	1.507299	1	108.372695	1	-126.292265	1	6	2	1
C	1.512662	1	107.019935	1	114.560117	1	6	2	1
C	1.531310	1	107.925900	1	-138.286222	1	7	3	1
C	1.533990	1	108.991097	1	127.175353	1	8	3	1
O	1.369983	1	111.970478	1	105.879603	1	10	5	1
C	1.476825	1	127.316301	1	-72.789390	1	10	5	1
C	1.400763	1	120.753669	1	154.865552	1	11	6	2
C	1.399860	1	119.889827	1	-26.447651	1	11	6	2
C	1.401295	1	120.769429	1	155.900098	1	12	6	2
C	1.400907	1	120.419438	1	-22.874023	1	12	6	2
C	1.433921	1	117.441521	1	167.119012	1	15	10	5
C	1.388495	1	122.724627	1	-127.888064	1	16	10	5
C	1.419500	1	116.257309	1	52.907540	1	16	10	5
C	1.393605	1	120.267559	1	178.369813	1	17	11	6
C	1.394542	1	120.191450	1	-178.341588	1	18	11	6
C	1.393664	1	120.531349	1	-179.392929	1	19	12	6
C	1.394032	1	120.586800	1	179.231255	1	20	12	6
C	1.494282	1	109.931617	1	-63.510815	1	21	15	10
C	1.469028	1	120.148315	1	2.865526	1	22	16	10
C	1.432344	1	119.063864	1	-174.372978	1	22	16	10
C	1.370268	1	120.255820	1	177.358360	1	23	16	10
C	1.394744	1	120.168342	1	0.020608	1	24	17	11
C	1.394440	1	120.258844	1	0.359936	1	26	19	12
C	1.415580	1	119.433875	1	-107.506596	1	28	21	15
C	1.430110	1	121.839929	1	127.155570	1	29	22	16
C	1.419751	1	119.372445	1	-4.499347	1	30	22	16
C	1.424330	1	122.322237	1	173.254981	1	30	22	16
C	1.371628	1	120.354364	1	174.320576	1	34	28	21
C	1.419915	1	119.096888	1	175.597620	1	35	29	22
C	1.423842	1	122.425098	1	-6.469314	1	35	29	22
C	1.422939	1	119.556296	1	-179.845260	1	36	30	22
C	1.372622	1	121.035482	1	-179.339110	1	37	30	22
C	1.422704	1	119.457254	1	179.965287	1	39	35	29
C	1.372705	1	120.926779	1	-179.104219	1	40	35	29
C	1.371982	1	120.670054	1	-1.484261	1	41	36	30
C	1.372203	1	120.652692	1	-1.394505	1	43	39	35
H	1.127814	1	107.050212	1	102.624927	1	7	3	1
H	1.116642	1	111.742214	1	139.333475	1	13	7	3
H	1.120105	1	108.939624	1	-101.667013	1	13	7	3
H	1.117530	1	110.268427	1	116.989006	1	14	8	3
H	1.117817	1	110.160607	1	-123.905147	1	14	8	3
H	1.124405	1	108.233600	1	-112.114963	1	8	3	1
H	1.124171	1	109.723138	1	6.191095	1	8	3	1
H	1.101899	1	119.385552	1	2.781224	1	18	11	6
H	1.099709	1	119.663415	1	-179.905070	1	25	18	11
H	1.099386	1	120.040589	1	-179.845334	1	32	24	17
H	1.099581	1	119.768743	1	179.902704	1	24	17	11
H	1.101124	1	120.127575	1	-1.617429	1	17	11	6
H	1.101660	1	119.711404	1	0.141691	1	20	12	6
H	1.099867	1	119.725596	1	-179.711166	1	27	20	12
H	1.099516	1	120.176200	1	179.747726	1	33	26	19
H	1.099919	1	119.700571	1	179.980039	1	26	19	12
H	1.101477	1	120.004802	1	0.045929	1	19	12	6
H	1.212848	1	104.787113	1	65.065774	1	9	3	1
H	1.209860	1	106.814343	1	-55.153242	1	9	3	1
H	1.209170	1	105.955486	1	-175.598103	1	9	3	1
H	1.109253	1	108.511091	1	-151.532314	1	4	1	2
H	1.109992	1	106.878110	1	88.282299	1	4	1	2
H	1.109001	1	107.651188	1	-31.256965	1	4	1	2
H	1.108342	1	118.297849	1	-1.435631	1	23	16	10
H	1.100840	1	120.622695	1	179.705694	1	31	23	16
H	1.100638	1	118.396365	1	178.988518	1	41	36	30
H	1.100099	1	120.808138	1	-179.784654	1	45	41	36
H	1.100198	1	120.473788	1	179.764187	1	42	37	30
H	1.101841	1	118.742500	1	0.307658	1	37	30	22
H	1.101908	1	118.545087	1	0.595281	1	40	35	29
H	1.100261	1	120.487902	1	179.600442	1	44	40	35
H	1.100044	1	120.776504	1	-179.667575	1	46	43	39
H	1.100511	1	118.460692	1	179.120354	1	43	39	35
H	1.100695	1	120.817060	1	179.230136	1	38	34	28
H	1.100873	1	118.890165	1	-5.158267	1	34	28	21
H	1.123871	1	102.896955	1	176.943216	1	21	15	10

TS (M)-[13 -> 8]B Heat of formation = 9.357162 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.371817	1	0.000000	0	0.000000	0	1	0	0
N	1.526577	1	111.524764	1	0.000000	0	1	2	0
C	1.539089	1	122.248654	1	-170.267212	1	1	2	3
O	2.267887	1	79.692021	1	111.340595	1	1	2	3
C	1.463894	1	111.689553	1	2.077390	1	2	1	3
C	1.506434	1	104.390583	1	3.642613	1	3	1	2
C	1.488020	1	114.201952	1	-113.428121	1	3	1	2
B	1.603748	1	108.195990	1	123.140099	1	3	1	2
C	1.234054	1	156.488764	1	175.099918	1	5	1	2
C	1.507390	1	108.350603	1	-125.202518	1	6	2	1
C	1.511884	1	106.900960	1	115.391700	1	6	2	1
C	1.531564	1	108.198275	1	-133.257205	1	7	3	1
C	1.522717	1	106.548383	1	14.640148	1	13	7	3
O	1.375363	1	111.904130	1	159.984117	1	10	5	1
C	1.477179	1	127.452360	1	-16.669759	1	10	5	1
C	1.401224	1	120.619296	1	157.224510	1	11	6	2
C	1.399417	1	120.047207	1	-23.728172	1	11	6	2
C	1.401443	1	120.771282	1	157.857986	1	12	6	2
C	1.400998	1	120.470019	1	-20.901300	1	12	6	2
C	1.431474	1	117.577388	1	169.600055	1	15	10	5
C	1.388129	1	123.113424	1	-131.430669	1	16	10	5
C	1.420267	1	115.967272	1	48.985043	1	16	10	5
C	1.393274	1	120.295854	1	178.358230	1	17	11	6
C	1.394860	1	120.170007	1	-178.262282	1	18	11	6
C	1.393631	1	120.560900	1	-179.494460	1	19	12	6
C	1.394089	1	120.608688	1	179.356236	1	20	12	6
C	1.494085	1	110.097133	1	-63.725481	1	21	15	10
C	1.387938	1	119.650460	1	69.871184	1	28	21	15
C	1.432580	1	119.083469	1	-173.652542	1	22	16	10
C	1.370217	1	120.279039	1	176.715270	1	23	16	10
C	1.393694	1	120.277430	1	-0.305668	1	25	18	11
C	1.393788	1	120.225722	1	-0.088516	1	27	20	12
C	1.415533	1	119.536418	1	-107.141180	1	28	21	15
C	1.430266	1	119.457912	1	-170.820146	1	29	28	21
C	1.419566	1	119.384526	1	-4.905710	1	30	22	16
C	1.424261	1	122.294333	1	172.852018	1	30	22	16
C	1.371439	1	120.351665	1	174.498867	1	34	28	21
C	1.419809	1	119.095857	1	-5.399711	1	35	29	28
C	1.423795	1	122.441338	1	172.560853	1	35	29	28
C	1.422860	1	119.555976	1	179.984542	1	36	30	22
C	1.372669	1	121.027331	1	-179.183440	1	37	30	22
C	1.422629	1	119.473107	1	179.975875	1	39	35	29
C	1.372752	1	120.934629	1	-179.141744	1	40	35	29
C	1.372035	1	120.667082	1	-1.406831	1	41	36	30
C	1.372245	1	120.650482	1	-1.365259	1	43	39	35
H	1.128790	1	106.867738	1	108.121897	1	7	3	1
H	1.116723	1	111.935285	1	136.814842	1	13	7	3
H	1.120202	1	108.893129	1	-104.274743	1	13	7	3
H	1.117348	1	111.045641	1	-131.976881	1	14	13	7
H	1.118220	1	110.822830	1	108.135783	1	14	13	7
H	1.125557	1	107.906485	1	-120.255023	1	8	3	1
H	1.123320	1	109.877635	1	-2.296191	1	8	3	1
H	1.102293	1	119.441764	1	3.532350	1	18	11	6
H	1.099658	1	119.597439	1	-179.809025	1	25	18	11
H	1.099428	1	120.199476	1	-179.947555	1	32	25	18
H	1.099561	1	119.783719	1	179.847795	1	24	17	11
H	1.101073	1	120.189135	1	-1.803865	1	17	11	6
H	1.101332	1	119.825718	1	0.431748	1	20	12	6
H	1.099902	1	119.702405	1	-179.744504	1	27	20	12
H	1.099535	1	120.228226	1	-179.915587	1	33	27	20
H	1.099957	1	119.686540	1	179.975512	1	26	19	12
H	1.101270	1	120.082837	1	-0.096372	1	19	12	6
H	1.209497	1	105.749851	1	-51.480250	1	9	3	1
H	1.209073	1	106.194393	1	-171.946796	1	9	3	1
H	1.212353	1	104.848365	1	68.704108	1	9	3	1
H	1.111364	1	107.252224	1	-134.169195	1	4	1	2
H	1.109281	1	107.896198	1	105.863055	1	4	1	2
H	1.108876	1	107.819392	1	-14.629448	1	4	1	2
H	1.109794	1	118.431495	1	-3.233269	1	23	16	10
H	1.100942	1	120.581345	1	179.620185	1	31	23	16
H	1.100642	1	118.392840	1	179.042134	1	41	36	30
H	1.100067	1	120.805839	1	-179.774740	1	45	41	36
H	1.100169	1	120.474568	1	179.725931	1	42	37	30
H	1.101823	1	118.727261	1	0.461299	1	37	30	22
H	1.101903	1	118.551657	1	0.610684	1	40	35	29
H	1.100237	1	120.485505	1	179.647050	1	44	40	35
H	1.100019	1	120.776705	1	-179.695965	1	46	43	39
H	1.100508	1	118.464553	1	179.135450	1	43	39	35
H	1.100637	1	120.848552	1	179.316314	1	38	34	28
H	1.100816	1	118.898680	1	-5.036576	1	34	28	21

TS (P)-[13 -> 8]A HEAT OF FORMATION = 9.235479 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.373018	1	.000000	0	.000000	0	1	0	0
N	1.525091	1	111.437119	1	.000000	0	1	2	0
C	1.506274	1	104.603583	1	2.170787	1	3	1	2
C	1.462615	1	111.835164	1	1.349827	1	2	1	3
C	1.486981	1	114.278845	1	-115.297351	1	3	1	2
C	1.532588	1	109.277153	1	116.725972	1	6	3	1
C	1.522464	1	106.491535	1	7.058203	1	7	6	3
B	1.607758	1	107.752107	1	121.549858	1	3	1	2
C	1.538195	1	122.193028	1	-171.086721	1	1	2	3
C	1.511385	1	106.950257	1	118.188662	1	5	2	1
C	1.400984	1	120.457372	1	-19.139079	1	11	5	2
C	1.401490	1	120.769061	1	159.583940	1	11	5	2
C	1.393555	1	120.563440	1	-179.466484	1	13	11	5
C	1.394185	1	120.583129	1	179.345725	1	12	11	5
C	1.393734	1	120.241800	1	-.110746	1	15	12	11
C	1.508853	1	108.131945	1	-122.602555	1	5	2	1
C	1.399922	1	119.895590	1	-22.781444	1	17	5	2
C	1.400945	1	120.841567	1	157.977569	1	17	5	2
C	1.393557	1	120.315116	1	178.599427	1	19	17	5
C	1.394606	1	120.235638	1	-178.559203	1	18	17	5
C	1.393880	1	120.255730	1	-.221357	1	21	18	17
O	2.308078	1	79.079030	1	110.641864	1	1	2	3
C	1.233954	1	143.222807	1	166.585990	1	23	1	2
O	1.376036	1	112.150327	1	-37.363029	1	24	23	1
C	1.476357	1	126.986931	1	138.986930	1	24	23	1
C	1.387775	1	123.305684	1	132.508384	1	26	24	23
C	1.431780	1	117.563454	1	-170.794862	1	25	24	23
C	1.494053	1	110.055516	1	64.142203	1	28	25	24
C	1.387938	1	119.717008	1	-69.798675	1	29	28	25
C	1.430411	1	119.442978	1	170.780201	1	30	29	28
C	1.432776	1	119.051453	1	173.622233	1	27	26	24
C	1.420655	1	115.762544	1	-47.823768	1	26	24	23
C	1.370042	1	120.299052	1	-176.790803	1	33	26	24
C	1.420385	1	120.394155	1	1.320594	1	34	33	26
C	1.422786	1	120.773464	1	176.819800	1	35	34	33
C	1.372100	1	120.667204	1	-177.595157	1	36	35	34
C	1.424188	1	122.285077	1	-172.721498	1	32	27	26
C	1.415298	1	120.006490	1	.127230	1	37	36	35
C	1.415627	1	119.472795	1	107.234599	1	29	28	25
C	1.371389	1	120.360716	1	-174.519351	1	40	29	28
C	1.420807	1	120.384107	1	2.011499	1	41	40	29
C	1.423803	1	122.438961	1	-172.457515	1	31	30	29
C	1.422619	1	120.852262	1	176.240241	1	42	41	40
C	1.372250	1	120.649745	1	-177.491237	1	44	42	41
C	1.415446	1	120.054369	1	.035362	1	45	44	42
H	1.128508	1	106.789884	1	111.062214	1	4	3	1
H	1.116655	1	111.412711	1	-134.740866	1	8	7	6
H	1.120174	1	110.245534	1	105.876931	1	8	7	6
H	1.118263	1	110.352217	1	-113.261937	1	7	6	3
H	1.117331	1	110.292778	1	127.694540	1	7	6	3
H	1.125902	1	107.810243	1	-122.999386	1	6	3	1
H	1.123151	1	109.908641	1	-5.155735	1	6	3	1
H	1.209857	1	105.429346	1	-52.242553	1	9	3	1
H	1.209318	1	105.071516	1	67.709562	1	9	3	1
H	1.209625	1	105.979076	1	-172.045165	1	9	3	1
H	1.112167	1	107.096881	1	-133.276882	1	10	1	2
H	1.109067	1	107.736037	1	-14.546586	1	10	1	2
H	1.108813	1	108.181223	1	106.388331	1	10	1	2
H	1.101381	1	119.840064	1	.426973	1	12	11	5
H	1.099925	1	119.685961	1	-179.775612	1	15	12	11
H	1.099531	1	120.233811	1	-179.920008	1	16	15	12
H	1.099928	1	119.693927	1	179.976705	1	14	13	11
H	1.101036	1	120.099812	1	-.044507	1	13	11	5
H	1.101051	1	120.263186	1	-1.553778	1	19	17	5
H	1.099605	1	119.764766	1	179.973525	1	20	19	17
H	1.099468	1	120.188164	1	179.957645	1	22	21	18
H	1.099811	1	119.646427	1	-179.963469	1	21	18	17
H	1.102604	1	119.374130	1	3.095835	1	18	17	5
H	1.105606	1	118.309231	1	3.024109	1	33	26	24
H	1.100735	1	120.682745	1	-179.559152	1	34	33	26
H	1.100608	1	118.404951	1	1.944664	1	36	35	34
H	1.100072	1	120.802392	1	179.765374	1	37	36	35
H	1.100178	1	119.103323	1	178.925887	1	39	37	36
H	1.101837	1	118.724331	1	-.431509	1	38	32	27
H	1.101924	1	118.554912	1	-.563272	1	43	31	30
H	1.100233	1	119.086705	1	179.015757	1	46	45	44
H	1.100024	1	120.777868	1	179.694427	1	45	44	42
H	1.100513	1	118.464874	1	2.000948	1	44	42	41
H	1.100645	1	120.849661	1	-179.294439	1	41	40	29
H	1.100846	1	118.900392	1	5.024250	1	40	29	28

TS (P)-[13 -> 8]B Heat of formation = 10.228426 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.382007	1	0.000000	0	0.000000	0	1	0	0
N	1.533925	1	111.089258	1	0.000000	0	1	2	0
C	1.505946	1	104.214435	1	7.225607	1	3	1	2
C	1.460314	1	111.683653	1	-1.004711	1	2	1	3
C	1.490830	1	112.869254	1	-108.523858	1	3	1	2
C	1.533394	1	109.199194	1	123.301812	1	6	3	1
C	1.523028	1	106.574854	1	0.876435	1	7	6	3
B	1.602651	1	111.020755	1	128.028450	1	3	1	2
C	1.543622	1	121.382422	1	-161.638504	1	1	2	3
C	1.512274	1	106.883469	1	116.526060	1	5	2	1
C	1.401063	1	120.351606	1	-22.282675	1	11	5	2
C	1.401247	1	120.854136	1	156.532843	1	11	5	2
C	1.393697	1	120.538409	1	-179.449958	1	13	11	5
C	1.394016	1	120.592260	1	179.300091	1	12	11	5
C	1.393878	1	120.215038	1	-0.040721	1	15	12	11
C	1.507855	1	108.328905	1	-124.200468	1	5	2	1
C	1.399760	1	119.918409	1	-24.569436	1	17	5	2
C	1.400919	1	120.740854	1	156.534213	1	17	5	2
C	1.393469	1	120.286075	1	178.379218	1	19	17	5
C	1.394557	1	120.178838	1	-178.269425	1	18	17	5
C	1.393902	1	120.262462	1	-0.254159	1	21	18	17
O	2.022313	1	112.424361	1	-83.722681	1	1	3	4
C	1.237775	1	158.484284	1	-164.981229	1	23	1	2
O	1.376950	1	110.319109	1	-156.635339	1	24	23	1
C	1.474392	1	129.085225	1	18.006373	1	24	23	1
C	1.387985	1	123.118073	1	134.134316	1	26	24	23
C	1.432134	1	117.976712	1	-170.732028	1	25	24	23
C	1.492634	1	110.469564	1	62.994149	1	28	25	24
C	1.387602	1	119.511420	1	-69.382276	1	29	28	25
C	1.429982	1	119.491254	1	171.054262	1	30	29	28
C	1.433010	1	119.139637	1	172.799814	1	27	26	24
C	1.421095	1	116.161472	1	-46.583108	1	26	24	23
C	1.369829	1	120.447843	1	-175.798759	1	33	26	24
C	1.420385	1	120.362910	1	1.042118	1	34	33	26
C	1.422618	1	120.800685	1	177.002345	1	35	34	33
C	1.372210	1	120.656107	1	-178.100291	1	36	35	34
C	1.424055	1	122.266342	1	-172.931924	1	32	27	26
C	1.415149	1	120.004884	1	0.131178	1	37	36	35
C	1.415434	1	119.695973	1	108.066965	1	29	28	25
C	1.371540	1	120.311280	1	-175.084694	1	40	29	28
C	1.420894	1	120.418020	1	2.224307	1	41	40	29
C	1.423777	1	122.360380	1	-172.093714	1	31	30	29
C	1.422490	1	120.927409	1	176.222085	1	42	41	40
C	1.372373	1	120.622622	1	-177.300565	1	44	42	41
C	1.415461	1	120.107607	1	0.088025	1	45	44	42
H	1.128191	1	106.924127	1	105.663361	1	4	3	1
H	1.116636	1	111.643434	1	-132.780442	1	8	7	6
H	1.120178	1	110.235865	1	107.519669	1	8	7	6
H	1.118065	1	110.219771	1	-119.528271	1	7	6	3
H	1.117414	1	110.293953	1	121.385566	1	7	6	3
H	1.125006	1	108.009705	1	-116.165213	1	6	3	1
H	1.123743	1	109.825693	1	1.919029	1	6	3	1
H	1.212429	1	104.810719	1	64.466434	1	9	3	1
H	1.209619	1	106.011345	1	-175.985263	1	9	3	1
H	1.209131	1	106.158541	1	-55.336952	1	9	3	1
H	1.108664	1	108.965156	1	-158.541846	1	10	1	2
H	1.109359	1	107.911783	1	-37.567352	1	10	1	2
H	1.110460	1	106.417153	1	81.373141	1	10	1	2
H	1.101608	1	119.725064	1	0.265205	1	12	11	5
H	1.099862	1	119.719710	1	-179.718530	1	15	12	11
H	1.099503	1	120.218166	1	-179.912880	1	16	15	12
H	1.099911	1	119.692282	1	179.971646	1	14	13	11
H	1.101296	1	120.058766	1	-0.017890	1	13	11	5
H	1.101116	1	120.160132	1	-1.676716	1	19	17	5
H	1.099578	1	119.781773	1	179.768401	1	20	19	17
H	1.099373	1	120.187420	1	180.061104	1	22	21	18
H	1.099679	1	119.634003	1	-179.973984	1	21	18	17
H	1.102504	1	119.396444	1	3.062628	1	18	17	5
H	1.103307	1	118.411867	1	6.208512	1	33	26	24
H	1.100584	1	120.675555	1	-178.780552	1	34	33	26
H	1.100574	1	118.406766	1	1.740666	1	36	35	34
H	1.100022	1	120.799087	1	179.918649	1	37	36	35
H	1.100118	1	119.108894	1	179.077627	1	39	37	36
H	1.101763	1	118.760103	1	-0.553429	1	38	32	27
H	1.102454	1	118.542886	1	-0.023734	1	43	31	30
H	1.100259	1	119.123787	1	178.759633	1	46	45	44
H	1.100016	1	120.744975	1	179.695021	1	45	44	42
H	1.100340	1	118.481096	1	2.169356	1	44	42	41
H	1.100539	1	120.829403	1	-179.098393	1	41	40	29
H	1.100655	1	118.931542	1	4.558725	1	40	29	28

(M)-8 HEAT OF FORMATION = 7.813336 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.411757	1	.000000	0	.000000	0	1	0	0
N	1.549857	1	110.054123	1	.000000	0	1	2	0
C	1.550138	1	118.510483	1	-149.279767	1	1	2	3
O	1.832181	1	87.979164	1	107.638949	1	1	2	3
C	1.450723	1	111.574489	1	-4.594530	1	2	1	3
C	1.505290	1	104.062321	1	10.065668	1	3	1	2
C	1.490236	1	112.133106	1	-104.888917	1	3	1	2
B	1.603634	1	113.052221	1	131.289067	1	3	1	2
C	1.252854	1	129.713189	1	-85.380928	1	5	1	3
C	1.510684	1	108.378284	1	-121.661881	1	6	2	1
C	1.513485	1	106.937550	1	119.434299	1	6	2	1
C	1.532511	1	107.992495	1	-137.152803	1	7	3	1
C	1.533706	1	108.998225	1	127.633852	1	8	3	1
O	1.357372	1	114.466857	1	-6.835627	1	10	5	1
C	1.475633	1	123.138824	1	-179.287801	1	10	5	1
C	1.400624	1	121.098851	1	155.806898	1	11	6	2
C	1.400178	1	119.721467	1	-25.020012	1	11	6	2
C	1.401082	1	121.047056	1	156.029949	1	12	6	2
C	1.401112	1	120.124515	1	-22.776463	1	12	6	2
C	1.438315	1	118.016924	1	173.892994	1	15	10	5
C	1.387637	1	123.431872	1	-138.911260	1	16	10	5
C	1.422038	1	115.628120	1	41.661806	1	16	10	5
C	1.393906	1	120.349226	1	179.207558	1	17	11	6
C	1.394131	1	120.320990	1	-179.120266	1	18	11	6
C	1.393787	1	120.530221	1	-179.365278	1	19	12	6
C	1.394002	1	120.563721	1	179.218274	1	20	12	6
C	1.491066	1	110.899120	1	-62.029035	1	21	15	10
C	1.468328	1	120.523517	1	6.724412	1	22	16	10
C	1.434046	1	118.793956	1	-171.679283	1	22	16	10
C	1.368815	1	120.389407	1	175.173948	1	23	16	10
C	1.394464	1	120.197153	1	-.113730	1	24	17	11
C	1.394363	1	120.251869	1	.339590	1	26	19	12
C	1.415557	1	119.208105	1	-108.265411	1	28	21	15
C	1.430466	1	121.484830	1	126.821437	1	29	22	16
C	1.419273	1	119.541185	1	-5.854759	1	30	22	16
C	1.423766	1	122.097502	1	171.987930	1	30	22	16
C	1.371481	1	120.294800	1	175.698725	1	34	28	21
C	1.419889	1	119.031885	1	176.303784	1	35	29	22
C	1.423892	1	122.545933	1	-5.909852	1	35	29	22
C	1.421991	1	119.587854	1	179.898817	1	36	30	22
C	1.373237	1	120.979763	1	-179.100837	1	37	30	22
C	1.422763	1	119.488072	1	-179.746398	1	39	35	29
C	1.372673	1	120.954041	1	-179.400291	1	40	35	29
C	1.372735	1	120.618485	1	-1.347901	1	41	36	30
C	1.372103	1	120.660624	1	-1.516932	1	43	39	35
H	1.128206	1	106.677026	1	104.474076	1	7	3	1
H	1.116470	1	111.949735	1	137.697357	1	13	7	3
H	1.120045	1	108.878404	1	-103.357468	1	13	7	3
H	1.117590	1	110.243536	1	115.589130	1	14	8	3
H	1.117655	1	110.206365	1	-125.321513	1	14	8	3
H	1.124217	1	108.153506	1	-111.592429	1	8	3	1
H	1.124088	1	109.877481	1	6.657963	1	8	3	1
H	1.101706	1	119.219401	1	1.704747	1	18	11	6
H	1.099525	1	119.756411	1	179.899175	1	25	18	11
H	1.099333	1	120.085244	1	179.997388	1	32	24	17
H	1.099634	1	119.764870	1	179.722854	1	24	17	11
H	1.101228	1	120.143019	1	-.876769	1	17	11	6
H	1.102055	1	119.536411	1	.017898	1	20	12	6
H	1.099737	1	119.726240	1	-179.753980	1	27	20	12
H	1.099415	1	120.165327	1	179.775084	1	33	26	19
H	1.099810	1	119.709186	1	179.999821	1	26	19	12
H	1.101211	1	120.014467	1	.154425	1	19	12	6
H	1.210416	1	106.603374	1	-61.114744	1	9	3	1
H	1.209846	1	106.008475	1	178.699579	1	9	3	1
H	1.210945	1	104.932913	1	58.466042	1	9	3	1
H	1.109227	1	109.022386	1	-177.922658	1	4	1	2
H	1.109842	1	107.056856	1	61.227961	1	4	1	2
H	1.108626	1	107.835582	1	-57.694428	1	4	1	2
H	1.102861	1	118.244687	1	-5.584178	1	23	16	10
H	1.100640	1	120.846341	1	179.404018	1	31	23	16
H	1.100580	1	118.482851	1	179.011690	1	41	36	30
H	1.100269	1	120.759824	1	-179.827737	1	45	41	36
H	1.100330	1	120.443270	1	179.755459	1	42	37	30
H	1.102189	1	118.719781	1	.697062	1	37	30	22
H	1.101530	1	118.669733	1	-.134583	1	40	35	29
H	1.100199	1	120.476514	1	179.499022	1	44	40	35
H	1.099939	1	120.793715	1	-179.588933	1	46	43	39
H	1.100549	1	118.436103	1	179.261451	1	43	39	35
H	1.100764	1	120.774543	1	179.719518	1	38	34	28
H	1.100733	1	118.978931	1	-3.116447	1	34	28	21

(M)-8 HEAT OF FORMATION = 8.003103 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.394043	1	.000000	0	.000000	0	1	0	0
N	1.543289	1	110.582728	1	.000000	0	1	2	0
C	1.544657	1	120.431980	1	203.865093	1	1	2	3
O	1.924264	1	84.762779	1	105.671557	1	1	2	3
C	1.457334	1	111.595678	1	355.537259	1	2	1	3
C	1.506539	1	103.714424	1	11.820227	1	3	1	2
C	1.491885	1	112.510165	1	257.305172	1	3	1	2
B	1.600517	1	112.842862	1	133.211421	1	3	1	2
C	1.242457	1	139.889007	1	136.367814	1	5	1	2
C	1.508436	1	108.473405	1	236.547157	1	6	2	1
C	1.512735	1	106.921365	1	117.330438	1	6	2	1
C	1.531633	1	107.874925	1	220.659661	1	7	3	1
C	1.523897	1	106.400185	1	16.946379	1	13	7	3
O	1.373936	1	110.014564	1	191.663580	1	10	5	1
C	1.474735	1	129.808678	1	15.444169	1	10	5	1
C	1.400853	1	120.808685	1	155.169223	1	11	6	2
C	1.399740	1	119.901715	1	334.297466	1	11	6	2
C	1.401211	1	120.866665	1	155.757707	1	12	6	2
C	1.400990	1	120.312488	1	337.007888	1	12	6	2
C	1.434234	1	117.395992	1	166.371559	1	15	10	5
C	1.389299	1	122.485170	1	230.979173	1	16	10	5
C	1.419657	1	116.505799	1	53.102279	1	16	10	5
C	1.393620	1	120.298948	1	179.049236	1	17	11	6
C	1.394437	1	120.236052	1	180.959177	1	18	11	6
C	1.393761	1	120.524376	1	180.642817	1	19	12	6
C	1.394011	1	120.582225	1	179.179312	1	20	12	6
C	1.493822	1	110.066630	1	298.132478	1	21	15	10
C	1.388395	1	119.616612	1	70.204004	1	28	21	15
C	1.431733	1	119.131705	1	186.560682	1	22	16	10
C	1.370469	1	120.224370	1	176.129047	1	23	16	10
C	1.393983	1	120.242983	1	.000000	1	25	18	11
C	1.393937	1	120.205980	1	.000000	1	27	20	12
C	1.415256	1	119.580155	1	253.046513	1	28	21	15
C	1.429589	1	119.525181	1	188.675927	1	29	28	21
C	1.419852	1	119.367554	1	356.046553	1	30	22	16
C	1.424409	1	122.312109	1	173.788715	1	30	22	16
C	1.371691	1	120.311757	1	174.757734	1	34	28	21
C	1.419894	1	119.059806	1	354.935150	1	35	29	28
C	1.423804	1	122.445218	1	173.050423	1	35	29	28
C	1.422991	1	119.553564	1	180.034830	1	36	30	22
C	1.372515	1	121.018788	1	180.708801	1	37	30	22
C	1.422729	1	119.452301	1	179.988396	1	39	35	29
C	1.372705	1	120.910791	1	180.779648	1	40	35	29
C	1.371929	1	120.662008	1	358.626380	1	41	36	30
C	1.372215	1	120.644393	1	358.743298	1	43	39	35
H	1.127873	1	106.856038	1	101.669465	1	7	3	1
H	1.116579	1	111.763078	1	139.102107	1	13	7	3
H	1.120062	1	108.925873	1	258.115360	1	13	7	3
H	1.117605	1	110.783278	1	233.235976	1	14	13	7
H	1.117637	1	111.075166	1	113.171313	1	14	13	7
H	1.124026	1	108.315438	1	249.863434	1	8	3	1
H	1.124197	1	109.774469	1	8.333802	1	8	3	1
H	1.101622	1	119.358152	1	2.135680	1	18	11	6
H	1.099562	1	119.679045	1	180.251025	1	25	18	11
H	1.099384	1	120.183775	1	180.133992	1	32	25	18
H	1.099606	1	119.777166	1	179.741711	1	24	17	11
H	1.101177	1	120.120661	1	358.945327	1	17	11	6
H	1.101682	1	119.645193	1	.039657	1	20	12	6
H	1.099785	1	119.728139	1	180.293675	1	27	20	12
H	1.099484	1	120.210345	1	180.069158	1	33	27	20
H	1.099904	1	119.698585	1	179.995925	1	26	19	12
H	1.101445	1	120.000498	1	.074868	1	19	12	6
H	1.209503	1	106.751936	1	307.482754	1	9	3	1
H	1.209454	1	105.996839	1	186.975395	1	9	3	1
H	1.213276	1	104.903030	1	68.006936	1	9	3	1
H	1.109860	1	108.627328	1	204.257822	1	4	1	2
H	1.109850	1	107.072842	1	84.111122	1	4	1	2
H	1.108677	1	107.903878	1	324.873574	1	4	1	2
H	1.110326	1	118.496178	1	355.978735	1	23	16	10
H	1.101140	1	120.501529	1	179.556676	1	31	23	16
H	1.100729	1	118.393905	1	179.018247	1	41	36	30
H	1.100161	1	120.804295	1	180.159751	1	45	41	36
H	1.100237	1	120.469649	1	179.813088	1	42	37	30
H	1.101839	1	118.764781	1	.367631	1	37	30	22
H	1.101920	1	118.550549	1	.615930	1	40	35	29
H	1.100314	1	120.489726	1	179.689850	1	44	40	35
H	1.100128	1	120.767918	1	180.277762	1	46	43	39
H	1.100559	1	118.469242	1	179.199041	1	43	39	35
H	1.100772	1	120.815404	1	179.414429	1	38	34	28
H	1.100895	1	118.927432	1	355.240821	1	34	28	21

(M)-8 HEAT OF FORMATION = 7.533095 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.409480	1	.000000	0	.000000	0	1	0	0
N	1.553800	1	109.984039	1	.000000	0	1	2	0
C	1.552455	1	119.729715	1	-150.356789	1	1	2	3
O	1.842434	1	97.215392	1	113.471479	1	1	2	3
C	1.452417	1	111.213919	1	5.150752	1	2	1	3
C	1.505927	1	103.759861	1	7.169445	1	3	1	2
C	1.492216	1	112.438271	1	-106.740982	1	3	1	2
B	1.601312	1	113.701649	1	129.994126	1	3	1	2
C	1.252292	1	135.109692	1	-73.857763	1	5	1	2
C	1.508243	1	108.404014	1	-134.438620	1	6	2	1
C	1.515007	1	107.723389	1	107.211853	1	6	2	1
C	1.532027	1	107.883520	1	-141.098337	1	7	3	1
C	1.534526	1	108.307279	1	134.494938	1	8	3	1
O	1.357461	1	114.554300	1	33.688085	1	10	5	1
C	1.476164	1	123.388902	1	-144.550169	1	10	5	1
C	1.400400	1	121.008629	1	151.505136	1	11	6	2
C	1.400501	1	119.616875	1	-30.550777	1	11	6	2
C	1.401564	1	120.747647	1	156.684286	1	12	6	2
C	1.400507	1	120.461117	1	-21.730127	1	12	6	2
C	1.439409	1	117.326085	1	171.966272	1	15	10	5
C	1.387649	1	123.641745	1	-132.807257	1	16	10	5
C	1.421457	1	115.178311	1	48.635117	1	16	10	5
C	1.394095	1	120.267495	1	177.974593	1	17	11	6
C	1.394263	1	120.194997	1	-177.846485	1	18	11	6
C	1.393552	1	120.573495	1	-179.312273	1	19	12	6
C	1.394191	1	120.583967	1	179.163444	1	20	12	6
C	1.493280	1	109.869079	1	-65.552092	1	21	15	10
C	1.468409	1	120.277324	1	4.615453	1	22	16	10
C	1.432627	1	118.899589	1	-173.013051	1	22	16	10
C	1.369774	1	120.170277	1	176.349935	1	23	16	10
C	1.394590	1	120.171339	1	-.154287	1	24	17	11
C	1.394484	1	120.228874	1	.448509	1	26	19	12
C	1.415796	1	119.291313	1	-107.818724	1	28	21	15
C	1.430358	1	121.675497	1	127.486763	1	29	22	16
C	1.419893	1	119.415532	1	-4.969716	1	30	22	16
C	1.424305	1	122.263674	1	172.751779	1	30	22	16
C	1.371460	1	120.363835	1	174.820363	1	34	28	21
C	1.419760	1	119.098943	1	175.353185	1	35	29	22
C	1.423808	1	122.438726	1	-6.766414	1	35	29	22
C	1.422811	1	119.543263	1	-179.848255	1	36	30	22
C	1.372636	1	121.027921	1	-179.286406	1	37	30	22
C	1.422641	1	119.476847	1	-179.873121	1	39	35	29
C	1.372747	1	120.931174	1	-179.188949	1	40	35	29
C	1.372087	1	120.670969	1	-1.538242	1	41	36	30
C	1.372215	1	120.645317	1	-1.532217	1	43	39	35
H	1.127943	1	107.141544	1	99.462879	1	7	3	1
H	1.116498	1	111.691823	1	136.528421	1	13	7	3
H	1.119587	1	109.080445	1	-104.442804	1	13	7	3
H	1.117956	1	110.136629	1	107.024673	1	14	8	3
H	1.116984	1	110.236544	1	-133.723187	1	14	8	3
H	1.123200	1	108.539839	1	-104.476892	1	8	3	1
H	1.124497	1	109.805816	1	14.296509	1	8	3	1
H	1.101949	1	119.299925	1	2.743005	1	18	11	6
H	1.099834	1	119.685712	1	179.745106	1	25	18	11
H	1.099427	1	120.057772	1	-179.536911	1	32	24	17
H	1.099695	1	119.776442	1	-179.831435	1	24	17	11
H	1.101388	1	120.032674	1	-1.688476	1	17	11	6
H	1.102294	1	119.625490	1	.183463	1	20	12	6
H	1.099852	1	119.703202	1	-179.803128	1	27	20	12
H	1.099472	1	120.168863	1	179.795134	1	33	26	19
H	1.099863	1	119.729221	1	180.065170	1	26	19	12
H	1.101586	1	119.939079	1	.099330	1	19	12	6
H	1.211075	1	105.050471	1	51.843540	1	9	3	1
H	1.212820	1	107.453750	1	-67.778192	1	9	3	1
H	1.209398	1	106.331039	1	172.526650	1	9	3	1
H	1.108354	1	108.887203	1	-166.674768	1	4	1	2
H	1.109594	1	106.972921	1	72.733035	1	4	1	2
H	1.109096	1	107.655265	1	-46.373676	1	4	1	2
H	1.106967	1	118.073576	1	-2.363068	1	23	16	10
H	1.100844	1	120.674493	1	179.631149	1	31	23	16
H	1.100703	1	118.403814	1	178.957030	1	41	36	30
H	1.100144	1	120.797564	1	-179.756916	1	45	41	36
H	1.100244	1	120.475691	1	179.714038	1	42	37	30
H	1.101859	1	118.751303	1	.332554	1	37	30	22
H	1.101914	1	118.597829	1	.452281	1	40	35	29
H	1.100287	1	120.479831	1	179.559082	1	44	40	35
H	1.100087	1	120.784819	1	-179.644009	1	46	43	39
H	1.100526	1	118.465583	1	179.017140	1	43	39	35
H	1.100687	1	120.822592	1	179.116384	1	38	34	28
H	1.101653	1	118.868992	1	-4.271773	1	34	28	21

(P)-8 Heat of formation = 5.376319 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.410202	1	0.000000	0	0.000000	0	1	0	0
N	1.555810	1	109.931127	1	0.000000	0	1	2	0
C	1.505839	1	104.167429	1	7.973807	1	3	1	2
C	1.449845	1	111.827027	1	-3.856065	1	2	1	3
C	1.490144	1	111.915194	1	-107.148610	1	3	1	2
C	1.533160	1	109.149820	1	125.839141	1	6	3	1
C	1.522866	1	106.654112	1	-3.658058	1	7	6	3
B	1.601694	1	113.513901	1	128.946997	1	3	1	2
C	1.550381	1	118.361859	1	-148.753378	1	1	2	3
C	1.513424	1	106.862227	1	120.439170	1	5	2	1
C	1.401285	1	120.053884	1	-22.111780	1	11	5	2
C	1.401013	1	121.135691	1	156.673852	1	11	5	2
C	1.393837	1	120.537953	1	-179.386851	1	13	11	5
C	1.393977	1	120.571926	1	179.253016	1	12	11	5
C	1.393958	1	120.221953	1	-0.046072	1	15	12	11
C	1.511308	1	108.342576	1	-120.565062	1	5	2	1
C	1.400259	1	119.712649	1	-23.273796	1	17	5	2
C	1.400734	1	121.110271	1	157.317769	1	17	5	2
C	1.393852	1	120.360393	1	179.288066	1	19	17	5
C	1.394293	1	120.306379	1	-179.296770	1	18	17	5
C	1.394108	1	120.241955	1	-0.008164	1	21	18	17
O	1.826486	1	88.815367	1	107.454170	1	1	2	3
C	1.254675	1	128.129712	1	170.184240	1	23	1	2
O	1.356829	1	114.258187	1	-16.951115	1	24	23	1
C	1.475110	1	123.280179	1	161.397864	1	24	23	1
C	1.388530	1	123.588997	1	136.033701	1	26	24	23
C	1.439009	1	117.665652	1	-175.995577	1	25	24	23
C	1.492754	1	109.268734	1	68.279238	1	28	25	24
C	1.388012	1	119.700945	1	-68.860297	1	29	28	25
C	1.430655	1	119.383921	1	170.124659	1	30	29	28
C	1.432955	1	118.867502	1	172.480069	1	27	26	24
C	1.421541	1	115.379936	1	-45.000603	1	26	24	23
C	1.369851	1	120.279309	1	-175.911443	1	33	26	24
C	1.420235	1	120.352548	1	1.415613	1	34	33	26
C	1.422817	1	120.731864	1	176.642536	1	35	34	33
C	1.372043	1	120.654729	1	-177.531476	1	36	35	34
C	1.424400	1	122.211306	1	-172.374325	1	32	27	26
C	1.415384	1	120.017120	1	0.128602	1	37	36	35
C	1.415554	1	119.411877	1	107.835139	1	29	28	25
C	1.371378	1	120.321337	1	-174.040794	1	40	29	28
C	1.420823	1	120.381024	1	2.111665	1	41	40	29
C	1.423795	1	122.451929	1	-172.220123	1	31	30	29
C	1.422584	1	120.821291	1	176.108918	1	42	41	40
C	1.372278	1	120.639245	1	-177.517058	1	44	42	41
C	1.415464	1	120.056076	1	0.072915	1	45	44	42
H	1.128280	1	106.674923	1	106.973613	1	4	3	1
H	1.116610	1	111.480980	1	-128.900838	1	8	7	6
H	1.120052	1	110.223680	1	111.668630	1	8	7	6
H	1.117774	1	110.217130	1	-124.256665	1	7	6	3
H	1.117671	1	110.244086	1	116.721533	1	7	6	3
H	1.124480	1	108.144649	1	-113.361769	1	6	3	1
H	1.123983	1	109.902590	1	4.768025	1	6	3	1
H	1.213028	1	106.826885	1	-62.355800	1	9	3	1
H	1.210392	1	105.340720	1	56.991887	1	9	3	1
H	1.209311	1	106.325450	1	177.847840	1	9	3	1
H	1.108977	1	109.254524	1	179.923385	1	10	1	2
H	1.108914	1	107.579773	1	-59.906111	1	10	1	2
H	1.109909	1	107.082743	1	58.908709	1	10	1	2
H	1.102107	1	119.558057	1	0.136186	1	12	11	5
H	1.099759	1	119.718297	1	-179.744781	1	15	12	11
H	1.099424	1	120.223464	1	-179.920918	1	16	15	12
H	1.099816	1	119.700526	1	179.981234	1	14	13	11
H	1.101014	1	120.086530	1	0.089422	1	13	11	5
H	1.101209	1	120.165976	1	-0.719843	1	19	17	5
H	1.099601	1	119.769178	1	179.966822	1	20	19	17
H	1.099367	1	120.185900	1	179.939396	1	22	21	18
H	1.099717	1	119.698220	1	-179.942565	1	21	18	17
H	1.102205	1	119.266137	1	1.725635	1	18	17	5
H	1.104973	1	118.228932	1	3.547127	1	33	26	24
H	1.100853	1	120.687618	1	-179.551483	1	34	33	26
H	1.100709	1	118.412531	1	1.990172	1	36	35	34
H	1.100250	1	120.794923	1	179.755992	1	37	36	35
H	1.100249	1	119.105754	1	178.882768	1	39	37	36
H	1.101854	1	118.776827	1	-0.370465	1	38	32	27
H	1.101885	1	118.620032	1	-0.458173	1	43	31	30
H	1.100370	1	119.093385	1	178.959965	1	46	45	44
H	1.100144	1	120.769869	1	179.703313	1	45	44	42
H	1.100579	1	118.475824	1	1.983996	1	44	42	41
H	1.100801	1	120.844578	1	-179.208370	1	41	40	29
H	1.100954	1	118.914598	1	5.579029	1	40	29	28

(P)-8 Heat of formation = 9.831858 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.392107	1	0.000000	0	0.000000	0	1	0	0
N	1.539647	1	110.712348	1	0.000000	0	1	2	0
C	1.505966	1	104.298486	1	7.556158	1	3	1	2
C	1.457031	1	111.725132	1	-2.892675	1	2	1	3
C	1.491404	1	112.035546	1	-107.856423	1	3	1	2
C	1.533061	1	109.190242	1	123.395258	1	6	3	1
C	1.522907	1	106.600992	1	0.177338	1	7	6	3
B	1.599635	1	111.914818	1	128.895449	1	3	1	2
C	1.547289	1	119.877541	1	-154.942613	1	1	2	3
C	1.512788	1	106.721480	1	119.173718	1	5	2	1
C	1.401189	1	120.249740	1	-21.646369	1	11	5	2
C	1.401200	1	120.961669	1	157.113665	1	11	5	2
C	1.393779	1	120.544547	1	-179.405341	1	13	11	5
C	1.394024	1	120.590505	1	179.243280	1	12	11	5
C	1.393892	1	120.220481	1	-0.030051	1	15	12	11
C	1.509147	1	108.432647	1	-121.620686	1	5	2	1
C	1.399864	1	119.870518	1	-23.240827	1	17	5	2
C	1.400932	1	120.865183	1	157.509006	1	17	5	2
C	1.393560	1	120.322795	1	178.806453	1	19	17	5
C	1.394552	1	120.232113	1	-178.758900	1	18	17	5
C	1.393873	1	120.257800	1	-0.164289	1	21	18	17
O	1.929670	1	111.023059	1	-84.686804	1	1	3	4
C	1.243403	1	145.880010	1	-162.620300	1	23	1	2
O	1.374728	1	109.624621	1	178.122470	1	24	23	1
C	1.473632	1	129.993426	1	-8.219652	1	24	23	1
C	1.388121	1	122.729400	1	133.137555	1	26	24	23
C	1.434296	1	117.860898	1	-169.511035	1	25	24	23
C	1.492111	1	110.464145	1	61.948199	1	28	25	24
C	1.387882	1	119.523206	1	-69.269763	1	29	28	25
C	1.429480	1	119.512846	1	170.830445	1	30	29	28
C	1.432959	1	119.155186	1	173.340284	1	27	26	24
C	1.420773	1	116.511768	1	-48.043805	1	26	24	23
C	1.369469	1	120.479218	1	-175.924292	1	33	26	24
C	1.420672	1	120.350841	1	0.826937	1	34	33	26
C	1.422380	1	120.769040	1	177.430482	1	35	34	33
C	1.372343	1	120.640798	1	-178.043607	1	36	35	34
C	1.423928	1	122.260671	1	-173.652074	1	32	27	26
C	1.415012	1	120.011238	1	0.141787	1	37	36	35
C	1.415398	1	119.714401	1	108.174051	1	29	28	25
C	1.371653	1	120.303374	1	-175.222003	1	40	29	28
C	1.420894	1	120.428539	1	2.409138	1	41	40	29
C	1.423792	1	122.284245	1	-171.366709	1	31	30	29
C	1.422378	1	120.980235	1	176.207331	1	42	41	40
C	1.372500	1	120.594093	1	-176.954963	1	44	42	41
C	1.415439	1	120.150199	1	0.275481	1	45	44	42
H	1.128359	1	106.870805	1	106.883765	1	4	3	1
H	1.116620	1	111.587990	1	-132.195330	1	8	7	6
H	1.120145	1	110.222511	1	108.222199	1	8	7	6
H	1.118041	1	110.217888	1	-120.260485	1	7	6	3
H	1.117464	1	110.279988	1	120.679420	1	7	6	3
H	1.124834	1	108.038696	1	-115.955063	1	6	3	1
H	1.124031	1	109.791596	1	2.062785	1	6	3	1
H	1.211866	1	104.753059	1	56.553514	1	9	3	1
H	1.209679	1	106.374653	1	176.784684	1	9	3	1
H	1.210700	1	106.414829	1	-62.997556	1	9	3	1
H	1.108542	1	109.619292	1	179.386094	1	10	1	2
H	1.109095	1	108.295352	1	-58.849594	1	10	1	2
H	1.111098	1	105.921979	1	59.414820	1	10	1	2
H	1.101755	1	119.683714	1	0.202567	1	12	11	5
H	1.099805	1	119.715714	1	-179.700871	1	15	12	11
H	1.099494	1	120.223544	1	-179.916025	1	16	15	12
H	1.099902	1	119.691878	1	179.979100	1	14	13	11
H	1.101166	1	120.080501	1	0.013713	1	13	11	5
H	1.101108	1	120.184104	1	-1.381021	1	19	17	5
H	1.099533	1	119.771071	1	179.807865	1	20	19	17
H	1.099347	1	120.193562	1	180.014495	1	22	21	18
H	1.099671	1	119.630838	1	-179.855589	1	21	18	17
H	1.102384	1	119.354425	1	2.774919	1	18	17	5
H	1.102086	1	118.391156	1	4.863795	1	33	26	24
H	1.100402	1	120.789682	1	-179.251278	1	34	33	26
H	1.100472	1	118.456057	1	1.808112	1	36	35	34
H	1.100036	1	120.786812	1	179.963440	1	37	36	35
H	1.100150	1	119.114836	1	179.148494	1	39	37	36
H	1.101890	1	118.762137	1	-0.660114	1	38	32	27
H	1.102856	1	118.485640	1	1.014193	1	43	31	30
H	1.100231	1	119.153628	1	178.263685	1	46	45	44
H	1.100013	1	120.708564	1	179.703276	1	45	44	42
H	1.100251	1	118.492859	1	2.450799	1	44	42	41
H	1.100537	1	120.813040	1	-179.018914	1	41	40	29
H	1.100569	1	118.940081	1	4.366158	1	40	29	28

(P)-8 HEAT OF FORMATION = 9.321930 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.414308	1	.000000	0	.000000	0	1	0	0
N	1.545040	1	110.136818	1	.000000	0	1	2	0
C	1.505363	1	103.798250	1	8.543715	1	3	1	2
C	1.451952	1	111.066849	1	3.708901	1	2	1	3
C	1.492531	1	112.672556	1	-105.381732	1	3	1	2
C	1.534676	1	108.322019	1	134.710829	1	6	3	1
C	1.525142	1	106.400927	1	-12.719680	1	7	6	3
B	1.607622	1	113.254728	1	131.712283	1	3	1	2
C	1.551942	1	119.790332	1	-150.934600	1	1	2	3
C	1.514435	1	107.665907	1	108.165981	1	5	2	1
C	1.400732	1	120.356776	1	-22.204621	1	11	5	2
C	1.401374	1	120.841671	1	156.313600	1	11	5	2
C	1.393649	1	120.563778	1	-179.336897	1	13	11	5
C	1.394101	1	120.577861	1	179.195148	1	12	11	5
C	1.393906	1	120.224725	1	-.120366	1	15	12	11
C	1.508552	1	108.349455	1	-133.305047	1	5	2	1
C	1.400424	1	119.744513	1	-29.605947	1	17	5	2
C	1.400509	1	120.947501	1	152.045446	1	17	5	2
C	1.394058	1	120.281651	1	178.481218	1	19	17	5
C	1.394176	1	120.253185	1	-178.566790	1	18	17	5
C	1.394454	1	120.217158	1	.154450	1	21	18	17
O	1.843735	0	93.609705	1	114.796391	1	1	2	3
C	1.249898	1	137.536889	1	47.944735	0	23	1	3
O	1.356941	1	115.042261	1	2.265834	-1	24	23	1
C	1.477075	1	122.987384	1	176.330098	1	24	23	1
C	1.387485	1	123.238825	1	135.620355	1	26	24	23
C	1.438776	1	117.715079	1	-171.388121	1	25	24	23
C	1.491911	1	110.601493	1	61.999626	1	28	25	24
C	1.387994	1	119.885467	1	-69.819562	1	29	28	25
C	1.430214	1	119.521780	1	171.710936	1	30	29	28
C	1.433640	1	118.848278	1	172.299079	1	27	26	24
C	1.421450	1	115.782868	1	-44.857163	1	26	24	23
C	1.369020	1	120.361315	1	-175.672864	1	33	26	24
C	1.421446	1	120.290386	1	1.229302	1	34	33	26
C	1.422012	1	120.763257	1	176.493582	1	35	34	33
C	1.372713	1	120.618371	1	-177.863457	1	36	35	34
C	1.423761	1	122.128811	1	-172.307627	1	32	27	26
C	1.414876	1	120.041959	1	.044946	1	37	36	35
C	1.415444	1	119.320437	1	107.709911	1	29	28	25
C	1.371534	1	120.312763	1	-175.350296	1	40	29	28
C	1.420500	1	120.429281	1	1.929349	1	41	40	29
C	1.423796	1	122.535009	1	-172.335499	1	31	30	29
C	1.422757	1	120.807047	1	176.280939	1	42	41	40
C	1.372079	1	120.656778	1	-177.091597	1	44	42	41
C	1.415483	1	120.038435	1	.082561	1	45	44	42
H	1.127964	1	107.034080	1	98.707621	1	4	3	1
H	1.116495	1	111.574859	1	-123.519061	1	8	7	6
H	1.119529	1	110.312024	1	116.652815	1	8	7	6
H	1.116945	1	110.258820	1	-133.556549	1	7	6	3
H	1.117907	1	110.119261	1	107.171345	1	7	6	3
H	1.123373	1	108.421364	1	-104.364380	1	6	3	1
H	1.124422	1	109.930924	1	14.469141	1	6	3	1
H	1.209374	1	104.705086	1	56.555301	1	9	3	1
H	1.210827	1	105.522054	1	176.620208	1	9	3	1
H	1.209218	1	107.035001	1	-63.788217	1	9	3	1
H	1.108828	1	108.534609	1	-163.062658	1	10	1	2
H	1.108685	1	108.018554	1	-42.683470	1	10	1	2
H	1.109585	1	106.908415	1	76.541789	1	10	1	2
H	1.102411	1	119.598395	1	.112380	1	12	11	5
H	1.099831	1	119.711363	1	-179.833163	1	15	12	11
H	1.099463	1	120.219534	1	-179.961052	1	16	15	12
H	1.099838	1	119.728053	1	-179.933475	1	14	13	11
H	1.101490	1	119.956469	1	.111499	1	13	11	5
H	1.101441	1	119.944596	1	-1.245718	1	19	17	5
H	1.099709	1	119.790452	1	-179.774585	1	20	19	17
H	1.099492	1	120.147933	1	179.750223	1	22	21	18
H	1.099815	1	119.756055	1	179.903295	1	21	18	17
H	1.101693	1	119.268348	1	1.706502	1	18	17	5
H	1.102469	1	118.298591	1	4.785421	1	33	26	24
H	1.100707	1	120.844539	1	-179.415087	1	34	33	26
H	1.100614	1	118.484746	1	1.790770	1	36	35	34
H	1.100255	1	120.755386	1	179.802944	1	37	36	35
H	1.100351	1	119.125108	1	179.105379	1	39	37	36
H	1.102164	1	118.694068	1	-.731655	1	38	32	27
H	1.101545	1	118.673148	1	-.217087	1	43	31	30
H	1.100180	1	119.087860	1	178.667271	1	46	45	44
H	1.099969	1	120.792512	1	179.479464	1	45	44	42
H	1.100540	1	118.448798	1	2.081742	1	44	42	41
H	1.100756	1	120.787672	1	-179.838228	1	41	40	29
H	1.100689	1	118.965032	1	3.509014	1	40	29	28

TSa (P)-8 <--> (M)-8 Heat of formation = 45.075857 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.409653	1	0.000000	0	0.000000	0	1	0	0
N	1.551668	1	109.972763	1	0.000000	0	1	2	0
C	1.552300	1	120.050118	1	-151.385531	1	1	2	3
O	1.863096	1	97.524239	1	113.693126	1	1	2	3
C	1.453636	1	110.968421	1	7.925079	1	2	1	3
C	1.505941	1	103.884723	1	4.994334	1	3	1	2
C	1.491358	1	112.814934	1	-109.427658	1	3	1	2
B	1.600240	1	113.402404	1	126.733856	1	3	1	2
C	1.245715	1	137.940908	1	-65.743790	1	5	1	2
C	1.507874	1	108.704179	1	-136.889488	1	6	2	1
C	1.515565	1	107.841875	1	104.953195	1	6	2	1
C	1.531874	1	107.956214	1	-140.525072	1	7	3	1
C	1.534376	1	108.396591	1	133.860976	1	8	3	1
O	1.363953	1	116.122680	1	25.153595	1	10	5	1
C	1.485773	1	124.871608	1	-148.746821	1	10	5	1
C	1.400523	1	121.038489	1	149.369948	1	11	6	2
C	1.400197	1	119.603865	1	-33.551075	1	11	6	2
C	1.401825	1	120.583717	1	157.020209	1	12	6	2
C	1.400107	1	120.618050	1	-21.410229	1	12	6	2
C	1.444702	1	112.059803	1	155.577610	1	15	10	5
C	1.401409	1	127.213677	1	-118.540750	1	16	10	5
C	1.424179	1	109.596617	1	66.261899	1	16	10	5
C	1.394092	1	120.295980	1	177.132081	1	17	11	6
C	1.394605	1	120.216929	1	-176.798914	1	18	11	6
C	1.393384	1	120.572683	1	-179.340102	1	19	12	6
C	1.394349	1	120.582290	1	179.190279	1	20	12	6
C	1.495757	1	106.856158	1	-51.791116	1	21	15	10
C	1.486781	1	115.961497	1	-2.842634	1	22	16	10
C	1.443043	1	115.448111	1	179.782581	1	22	16	10
C	1.364326	1	120.060000	1	168.452637	1	23	16	10
C	1.394487	1	120.190452	1	-0.377941	1	24	17	11
C	1.394613	1	120.219296	1	0.454036	1	26	19	12
C	1.424778	1	114.847984	1	-79.498088	1	28	21	15
C	1.449469	1	127.426328	1	132.660053	1	29	22	16
C	1.427272	1	119.466087	1	17.063543	1	30	22	16
C	1.421910	1	100.986296	1	-24.983065	1	30	29	35
C	1.365285	1	120.211812	1	165.302552	1	34	28	21
C	1.424405	1	118.450598	1	-136.204250	1	35	29	22
C	1.418588	1	108.327141	1	4.000291	1	35	22	30
C	1.423782	1	120.918072	1	165.285203	1	36	30	22
C	1.372967	1	123.012639	1	-165.696380	1	37	30	22
C	1.419746	1	119.982420	1	166.693688	1	39	35	29
C	1.377178	1	121.751148	1	-170.641615	1	40	35	29
C	1.370697	1	120.947980	1	4.984064	1	41	36	30
C	1.374991	1	120.354299	1	11.003230	1	43	39	35
H	1.128409	1	107.017484	1	100.238014	1	7	3	1
H	1.116419	1	111.730922	1	135.755997	1	13	7	3
H	1.119733	1	109.044149	1	-105.237770	1	13	7	3
H	1.117995	1	110.125560	1	107.679005	1	14	8	3
H	1.117023	1	110.237807	1	-133.113788	1	14	8	3
H	1.123353	1	108.463655	1	-105.156339	1	8	3	1
H	1.124338	1	109.871353	1	13.578987	1	8	3	1
H	1.101756	1	119.219441	1	3.466365	1	18	11	6
H	1.099918	1	119.747377	1	179.062062	1	25	18	11
H	1.099596	1	120.078155	1	-179.470035	1	32	24	17
H	1.099781	1	119.770584	1	179.882364	1	24	17	11
H	1.101469	1	120.117862	1	-2.457114	1	17	11	6
H	1.102271	1	119.653879	1	0.162512	1	20	12	6
H	1.099885	1	119.699510	1	-179.833741	1	27	20	12
H	1.099493	1	120.162125	1	179.809394	1	33	26	19
H	1.099880	1	119.738884	1	-179.911073	1	26	19	12
H	1.101697	1	119.893776	1	0.103452	1	19	12	6
H	1.211008	1	105.116509	1	53.660989	1	9	3	1
H	1.212462	1	106.839610	1	-66.332574	1	9	3	1
H	1.209564	1	106.312804	1	174.047388	1	9	3	1
H	1.108630	1	108.811110	1	-163.648267	1	4	1	2
H	1.109580	1	107.049547	1	75.814901	1	4	1	2
H	1.109026	1	107.701814	1	-43.394494	1	4	1	2
H	1.109812	1	118.495043	1	-7.993284	1	23	16	10
H	1.100497	1	121.278046	1	-173.245980	1	31	23	16
H	1.100982	1	118.119152	1	-175.420004	1	41	36	30
H	1.099157	1	121.466886	1	-177.852707	1	45	41	36
H	1.100206	1	120.271618	1	178.644245	1	42	37	30
H	1.095402	1	118.581178	1	24.658933	1	37	30	22
H	1.101641	1	118.746282	1	18.390007	1	40	35	29
H	1.099925	1	120.356228	1	178.296124	1	44	40	35
H	1.099182	1	121.209373	1	-178.625190	1	46	43	39
H	1.100288	1	118.541913	1	-171.318812	1	43	39	35
H	1.099671	1	121.782774	1	-169.019305	1	38	34	28
H	1.103634	1	118.360135	1	-8.002153	1	34	28	21

TSb (P)-8 <--> (M)-8 Heat of formation = 44.392175 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.404783	1	0.000000	0	0.000000	0	1	0	0
N	1.550027	1	110.174198	1	0.000000	0	1	2	0
C	1.551008	1	120.231801	1	-152.550278	1	1	2	3
O	1.877811	1	96.189301	1	113.522923	1	1	2	3
C	1.454287	1	111.158091	1	6.530022	1	2	1	3
C	1.506097	1	103.896465	1	5.409694	1	3	1	2
C	1.491426	1	112.586372	1	-108.990684	1	3	1	2
B	1.600662	1	113.347326	1	127.359370	1	3	1	2
C	1.243329	1	138.195610	1	-72.149173	1	5	1	2
C	1.507739	1	108.511798	1	-134.778448	1	6	2	1
C	1.514748	1	107.634209	1	106.748363	1	6	2	1
C	1.531867	1	108.004825	1	-139.833225	1	7	3	1
C	1.534178	1	108.459075	1	133.197155	1	8	3	1
O	1.363437	1	116.672551	1	29.274081	1	10	5	1
C	1.483003	1	126.058883	1	-145.606622	1	10	5	1
C	1.400583	1	120.953038	1	151.204986	1	11	6	2
C	1.400155	1	119.677270	1	-30.879162	1	11	6	2
C	1.401644	1	120.693822	1	156.410475	1	12	6	2
C	1.400436	1	120.505386	1	-22.161494	1	12	6	2
C	1.444857	1	112.291303	1	163.036945	1	15	10	5
C	1.394726	1	125.782093	1	-112.430931	1	16	10	5
C	1.428451	1	110.880964	1	75.936432	1	16	10	5
C	1.394107	1	120.283768	1	178.118722	1	17	11	6
C	1.394579	1	120.171974	1	-178.086135	1	18	11	6
C	1.393550	1	120.560958	1	-179.402985	1	19	12	6
C	1.394205	1	120.579096	1	179.216982	1	20	12	6
C	1.498422	1	107.368507	1	-60.184480	1	21	15	10
C	1.488514	1	117.200149	1	-14.217388	1	22	16	10
C	1.448386	1	114.534126	1	176.853148	1	22	16	10
C	1.364522	1	119.596102	1	164.205542	1	23	16	10
C	1.394459	1	120.171511	1	-0.187127	1	24	17	11
C	1.394426	1	120.229369	1	0.465022	1	26	19	12
C	1.420690	1	113.315789	1	-89.927622	1	28	21	15
C	1.443784	1	128.282464	1	139.158485	1	29	22	16
C	1.425464	1	118.764401	1	26.580098	1	30	22	16
C	1.419368	1	106.120052	1	-4.980617	1	30	29	35
C	1.364848	1	120.439847	1	166.179454	1	34	28	21
C	1.426812	1	119.036995	1	-152.929842	1	35	29	22
C	1.421082	1	102.816190	1	-19.951070	1	35	22	30
C	1.421108	1	120.138771	1	164.958190	1	36	30	22
C	1.375834	1	122.082908	1	-168.121563	1	37	30	22
C	1.422804	1	120.780133	1	164.501910	1	39	35	29
C	1.373835	1	122.798948	1	-165.715363	1	40	35	29
C	1.373713	1	120.506766	1	10.065344	1	41	36	30
C	1.371464	1	120.814243	1	6.764501	1	43	39	35
H	1.128405	1	107.054881	1	100.937128	1	7	3	1
H	1.116618	1	111.719110	1	135.591163	1	13	7	3
H	1.119630	1	109.047886	1	-105.433986	1	13	7	3
H	1.117864	1	110.131556	1	108.239792	1	14	8	3
H	1.117096	1	110.227378	1	-132.578290	1	14	8	3
H	1.123441	1	108.450189	1	-105.816107	1	8	3	1
H	1.124436	1	109.844764	1	12.868809	1	8	3	1
H	1.101914	1	119.310252	1	2.582616	1	18	11	6
H	1.099926	1	119.661253	1	179.922127	1	25	18	11
H	1.099518	1	120.062377	1	-179.639728	1	32	24	17
H	1.099704	1	119.790169	1	179.964207	1	24	17	11
H	1.101357	1	120.069070	1	-1.652346	1	17	11	6
H	1.102242	1	119.655035	1	0.175091	1	20	12	6
H	1.099894	1	119.704982	1	-179.773011	1	27	20	12
H	1.099483	1	120.163749	1	179.753653	1	33	26	19
H	1.099869	1	119.729597	1	-179.909363	1	26	19	12
H	1.101565	1	119.931657	1	0.054063	1	19	12	6
H	1.210538	1	105.240777	1	51.564536	1	9	3	1
H	1.212436	1	106.897700	1	-68.337887	1	9	3	1
H	1.209606	1	106.371297	1	172.193827	1	9	3	1
H	1.108497	1	108.873250	1	-163.728320	1	4	1	2
H	1.109758	1	106.797078	1	75.709864	1	4	1	2
H	1.109113	1	107.748608	1	-43.391989	1	4	1	2
H	1.108598	1	118.377675	1	-10.784115	1	23	16	10
H	1.100092	1	121.487458	1	-169.797066	1	31	23	16
H	1.100472	1	118.413266	1	-172.042177	1	41	36	30
H	1.099148	1	121.307454	1	-178.478704	1	45	41	36
H	1.099925	1	120.360738	1	178.380593	1	42	37	30
H	1.100770	1	118.441964	1	21.964815	1	37	30	22
H	1.097225	1	118.503307	1	25.004813	1	40	35	29
H	1.100251	1	120.302363	1	178.384900	1	44	40	35
H	1.099048	1	121.468083	1	-177.773704	1	46	43	39
H	1.100716	1	118.225698	1	-173.987329	1	43	39	35
H	1.100103	1	121.529269	1	-171.856859	1	38	34	28
H	1.103535	1	118.848275	1	-8.217932	1	34	28	21

TS (M,Re)-[8 -> 9] Heat of formation = 13.807345 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.440465	1	0.000000	0	0.000000	0	1	0	0
N	1.595778	1	107.821797	1	0.000000	0	1	2	0
C	1.561727	1	117.148907	1	-137.537277	1	1	2	3
O	1.649606	1	100.965418	1	116.188163	1	1	2	3
C	1.439784	1	112.167669	1	1.708536	1	2	1	3
C	1.507401	1	103.626098	1	10.139418	1	3	1	2
C	1.493422	1	112.603768	1	-103.310385	1	3	1	2
B	1.562793	1	113.910521	1	133.071227	1	3	1	2
C	1.301214	1	123.992913	1	-92.032289	1	5	1	2
C	1.511949	1	108.443367	1	-131.593604	1	6	2	1
C	1.516834	1	108.193328	1	110.218196	1	6	2	1
C	1.532719	1	107.618039	1	-143.035389	1	7	3	1
C	1.534967	1	108.342962	1	135.263772	1	8	3	1
O	1.370003	1	112.466390	1	61.028359	1	10	5	1
C	1.489906	1	118.951217	1	-144.932414	1	10	5	1
C	1.400353	1	121.162521	1	153.703132	1	11	6	2
C	1.400462	1	119.513485	1	-28.073347	1	11	6	2
C	1.401629	1	121.078865	1	157.575373	1	12	6	2
C	1.400488	1	120.245357	1	-20.288775	1	12	6	2
C	1.435411	1	117.413695	1	159.778850	1	15	10	5
C	1.387148	1	124.358945	1	-115.395256	1	16	10	5
C	1.423430	1	115.214218	1	64.180169	1	16	10	5
C	1.394020	1	120.317889	1	177.785858	1	17	11	6
C	1.394312	1	120.198882	1	-177.745342	1	18	11	6
C	1.393619	1	120.639860	1	-179.166458	1	19	12	6
C	1.394158	1	120.671395	1	179.079075	1	20	12	6
C	1.492518	1	108.774410	1	-75.482578	1	21	15	10
C	1.468550	1	121.845690	1	7.027744	1	22	16	10
C	1.436657	1	118.847893	1	-171.656491	1	22	16	10
C	1.368032	1	120.824633	1	176.060842	1	23	16	10
C	1.394500	1	120.150765	1	0.034408	1	24	17	11
C	1.394363	1	120.248328	1	0.539545	1	26	19	12
C	1.415759	1	119.447955	1	-108.551711	1	28	21	15
C	1.431729	1	121.249016	1	127.492247	1	29	22	16
C	1.418383	1	119.686568	1	-7.225469	1	30	22	16
C	1.423904	1	122.104435	1	170.536403	1	30	22	16
C	1.371186	1	120.304485	1	172.811101	1	34	28	21
C	1.419736	1	119.104751	1	173.944105	1	35	29	22
C	1.423710	1	122.455751	1	-8.294219	1	35	29	22
C	1.421783	1	119.725868	1	-179.779341	1	36	30	22
C	1.373443	1	121.043835	1	-179.309667	1	37	30	22
C	1.422476	1	119.496548	1	-179.896172	1	39	35	29
C	1.372912	1	120.941519	1	-179.145945	1	40	35	29
C	1.372719	1	120.606920	1	-1.585536	1	41	36	30
C	1.372329	1	120.647900	1	-1.572431	1	43	39	35
H	1.128282	1	107.248176	1	97.868957	1	7	3	1
H	1.116312	1	111.668503	1	138.695453	1	13	7	3
H	1.119728	1	109.142459	1	-102.307286	1	13	7	3
H	1.117677	1	110.437616	1	107.588277	1	14	8	3
H	1.117260	1	110.066111	1	-133.234564	1	14	8	3
H	1.122719	1	109.230077	1	-103.246797	1	8	3	1
H	1.124379	1	109.320264	1	15.503562	1	8	3	1
H	1.102347	1	119.219367	1	2.940470	1	18	11	6
H	1.099824	1	119.684520	1	179.779338	1	25	18	11
H	1.099333	1	120.061575	1	-179.475114	1	32	24	17
H	1.099533	1	119.797080	1	-179.639456	1	24	17	11
H	1.101211	1	120.052481	1	-1.795607	1	17	11	6
H	1.102175	1	119.411346	1	0.431292	1	20	12	6
H	1.099816	1	119.704798	1	-179.864287	1	27	20	12
H	1.099342	1	120.189337	1	179.827841	1	33	26	19
H	1.099752	1	119.718786	1	-179.938266	1	26	19	12
H	1.101407	1	120.076892	1	0.049358	1	19	12	6
H	1.205768	1	109.527334	1	72.444528	1	9	3	1
H	1.557606	1	103.003248	1	-38.781230	1	10	5	1
H	1.204371	1	110.709365	1	-154.513245	1	9	3	1
H	1.107854	1	109.240271	1	176.259846	1	4	1	2
H	1.108263	1	108.896750	1	54.688162	1	4	1	2
H	1.109978	1	106.497224	1	-64.229058	1	4	1	2
H	1.104565	1	118.136284	1	-3.616276	1	23	16	10
H	1.100600	1	120.842775	1	179.229654	1	31	23	16
H	1.100552	1	118.464280	1	178.903931	1	41	36	30
H	1.100094	1	120.795963	1	-179.771325	1	45	41	36
H	1.100254	1	120.416955	1	179.687424	1	42	37	30
H	1.101826	1	118.866044	1	0.275245	1	37	30	22
H	1.101761	1	118.630008	1	0.327097	1	40	35	29
H	1.100247	1	120.465654	1	179.499580	1	44	40	35
H	1.100012	1	120.779221	1	-179.613389	1	46	43	39
H	1.100476	1	118.466081	1	179.053392	1	43	39	35
H	1.100581	1	120.859133	1	179.124614	1	38	34	28
H	1.100971	1	118.898610	1	-6.415907	1	34	28	21

TS (M,Si)-[8 -> 9] Heat of formation = 11.720262 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.428859	1	0.000000	0	0.000000	0	1	0	0
N	1.581955	1	108.469738	1	0.000000	0	1	2	0
C	1.553176	1	117.390265	1	-141.640974	1	1	2	3
O	1.711340	1	92.431244	1	108.569194	1	1	2	3
C	1.443704	1	111.826811	1	-10.163017	1	2	1	3
C	1.506707	1	103.448527	1	15.789970	1	3	1	2
C	1.492861	1	111.695614	1	-97.680000	1	3	1	2
B	1.576648	1	114.580472	1	138.279591	1	3	1	2
C	1.288587	1	120.961811	1	-56.323910	1	5	1	3
C	1.512089	1	108.595580	1	-118.498361	1	6	2	1
C	1.514567	1	106.925860	1	122.529785	1	6	2	1
C	1.533143	1	107.631385	1	-140.667990	1	7	3	1
C	1.534638	1	108.735727	1	131.011893	1	8	3	1
O	1.365031	1	112.126724	1	-50.669708	1	10	5	1
C	1.481377	1	120.655237	1	155.694743	1	10	5	1
C	1.400521	1	121.221097	1	156.829545	1	11	6	2
C	1.400369	1	119.592806	1	-23.830988	1	11	6	2
C	1.400818	1	121.316668	1	155.623429	1	12	6	2
C	1.401441	1	119.865873	1	-22.951471	1	12	6	2
C	1.435424	1	118.229287	1	-168.580955	1	15	10	5
C	1.388362	1	123.620103	1	-159.712097	1	16	10	5
C	1.422745	1	115.641771	1	21.129679	1	16	10	5
C	1.393944	1	120.364210	1	179.233061	1	17	11	6
C	1.394205	1	120.295906	1	-179.138567	1	18	11	6
C	1.393948	1	120.540807	1	-179.260294	1	19	12	6
C	1.393927	1	120.568644	1	179.115234	1	20	12	6
C	1.490676	1	111.864475	1	-60.327637	1	21	15	10
C	1.468478	1	120.726321	1	7.444974	1	22	16	10
C	1.434118	1	118.867416	1	-170.962667	1	22	16	10
C	1.368849	1	120.478958	1	174.847147	1	23	16	10
C	1.394453	1	120.180783	1	-0.080274	1	24	17	11
C	1.394244	1	120.255438	1	0.386381	1	26	19	12
C	1.415851	1	119.234747	1	-109.273325	1	28	21	15
C	1.431042	1	121.490144	1	127.185331	1	29	22	16
C	1.419110	1	119.560092	1	-6.376366	1	30	22	16
C	1.423976	1	122.119242	1	171.439365	1	30	22	16
C	1.371262	1	120.336506	1	176.683604	1	34	28	21
C	1.419843	1	119.074015	1	175.923609	1	35	29	22
C	1.423887	1	122.520779	1	-6.188256	1	35	29	22
C	1.422118	1	119.608655	1	180.020971	1	36	30	22
C	1.373129	1	121.004590	1	-179.163697	1	37	30	22
C	1.422650	1	119.502434	1	-179.587193	1	39	35	29
C	1.372751	1	120.957879	1	-179.541551	1	40	35	29
C	1.372584	1	120.626596	1	-1.455394	1	41	36	30
C	1.372174	1	120.655532	1	-1.559381	1	43	39	35
H	1.127082	1	107.074274	1	100.826614	1	7	3	1
H	1.116399	1	111.814258	1	140.434150	1	13	7	3
H	1.120022	1	108.975853	1	-100.558154	1	13	7	3
H	1.117473	1	110.399648	1	112.543789	1	14	8	3
H	1.117612	1	110.065257	1	-128.294811	1	14	8	3
H	1.123253	1	108.934467	1	-107.773799	1	8	3	1
H	1.124357	1	109.315164	1	10.684824	1	8	3	1
H	1.102317	1	119.160065	1	1.685970	1	18	11	6
H	1.099682	1	119.718863	1	179.747382	1	25	18	11
H	1.099325	1	120.074399	1	-179.845397	1	32	24	17
H	1.099581	1	119.784265	1	179.874871	1	24	17	11
H	1.101177	1	120.122184	1	-0.705546	1	17	11	6
H	1.102433	1	119.428874	1	0.075384	1	20	12	6
H	1.099740	1	119.728574	1	-179.702893	1	27	20	12
H	1.099396	1	120.168587	1	179.746389	1	33	26	19
H	1.099766	1	119.704404	1	179.983055	1	26	19	12
H	1.101097	1	120.086921	1	0.160252	1	19	12	6
H	1.695107	1	97.881491	1	52.165759	1	10	5	1
H	1.205650	1	108.942367	1	-156.616096	1	9	3	1
H	1.207426	1	107.994443	1	74.802068	1	9	3	1
H	1.108670	1	109.212755	1	176.822266	1	4	1	2
H	1.109053	1	107.993266	1	55.316939	1	4	1	2
H	1.109071	1	106.748242	1	-63.602779	1	4	1	2
H	1.104129	1	118.153256	1	-5.642082	1	23	16	10
H	1.100616	1	120.791404	1	179.315177	1	31	23	16
H	1.100547	1	118.462536	1	178.955710	1	41	36	30
H	1.100182	1	120.776040	1	-179.788641	1	45	41	36
H	1.100251	1	120.447216	1	179.710443	1	42	37	30
H	1.102047	1	118.743706	1	0.574212	1	37	30	22
H	1.101602	1	118.645246	1	-0.191258	1	40	35	29
H	1.100162	1	120.470322	1	179.580991	1	44	40	35
H	1.099906	1	120.787777	1	-179.658514	1	46	43	39
H	1.100467	1	118.452741	1	179.111809	1	43	39	35
H	1.100624	1	120.820001	1	179.407897	1	38	34	28
H	1.100653	1	118.946264	1	-2.591194	1	34	28	21

TS (P,Re)-[8 -> 9]B Heat of formation = 13.152107 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.430291	1	0.000000	0	0.000000	0	1	0	0
N	1.574796	1	108.829059	1	0.000000	0	1	2	0
C	1.506297	1	103.732375	1	9.003863	1	3	1	2
C	1.444073	1	111.689643	1	2.639811	1	2	1	3
C	1.492668	1	112.684832	1	-104.907880	1	3	1	2
C	1.534686	1	108.473818	1	133.857271	1	6	3	1
C	1.524526	1	106.405340	1	-11.220214	1	7	6	3
B	1.581474	1	113.619746	1	132.075118	1	3	1	2
C	1.557907	1	117.992195	1	-142.463982	1	1	2	3
C	1.515850	1	107.982058	1	109.640276	1	5	2	1
C	1.400612	1	120.265785	1	-21.458965	1	11	5	2
C	1.401489	1	121.017261	1	156.728527	1	11	5	2
C	1.393635	1	120.611349	1	-179.229662	1	13	11	5
C	1.394106	1	120.641351	1	179.130127	1	12	11	5
C	1.393797	1	120.229291	1	-0.233212	1	15	12	11
C	1.510839	1	108.366126	1	-131.983986	1	5	2	1
C	1.400607	1	119.611786	1	-28.037322	1	17	5	2
C	1.400416	1	121.095841	1	153.395589	1	17	5	2
C	1.394088	1	120.308123	1	178.510325	1	19	17	5
C	1.394272	1	120.232778	1	-178.518551	1	18	17	5
C	1.394480	1	120.241304	1	0.012879	1	21	18	17
O	1.716518	1	99.476084	1	114.404962	1	1	2	3
C	1.285428	1	125.449546	1	-87.237335	1	23	1	2
O	1.363847	1	112.590227	1	58.423175	1	24	23	1
C	1.482071	1	120.506540	1	-147.097405	1	24	23	1
C	1.388182	1	123.673677	1	159.160847	1	26	24	23
C	1.436120	1	118.162340	1	167.096316	1	25	24	23
C	1.490961	1	111.439096	1	62.220060	1	28	25	24
C	1.387544	1	119.954294	1	-68.939995	1	29	28	25
C	1.431034	1	119.420761	1	171.900508	1	30	29	28
C	1.434357	1	118.912434	1	171.724946	1	27	26	24
C	1.422750	1	115.620221	1	-21.389754	1	26	24	23
C	1.368731	1	120.530797	1	-175.463529	1	33	26	24
C	1.421071	1	120.295894	1	1.394924	1	34	33	26
C	1.422084	1	120.784591	1	176.314110	1	35	34	33
C	1.372600	1	120.625270	1	-177.702605	1	36	35	34
C	1.423965	1	122.158756	1	-171.703717	1	32	27	26
C	1.414840	1	120.004876	1	0.112335	1	37	36	35
C	1.415882	1	119.271532	1	109.444365	1	29	28	25
C	1.371240	1	120.352716	1	-175.996842	1	40	29	28
C	1.420724	1	120.387749	1	2.206666	1	41	40	29
C	1.423775	1	122.475584	1	-171.770126	1	31	30	29
C	1.422530	1	120.827376	1	176.145449	1	42	41	40
C	1.372268	1	120.637790	1	-177.091730	1	44	42	41
C	1.415328	1	120.052071	1	0.117574	1	45	44	42
H	1.128010	1	107.155133	1	98.924810	1	4	3	1
H	1.116380	1	111.577991	1	-125.141194	1	8	7	6
H	1.119738	1	110.325931	1	115.074330	1	8	7	6
H	1.117228	1	110.133706	1	-131.897167	1	7	6	3
H	1.117737	1	110.310559	1	108.919878	1	7	6	3
H	1.123287	1	108.814537	1	-104.979291	1	6	3	1
H	1.124191	1	109.562875	1	13.688469	1	6	3	1
H	1.206119	1	107.539677	1	66.160874	1	9	3	1
H	1.205980	1	108.324880	1	-165.994533	1	9	3	1
H	1.699046	1	100.994550	1	-39.937444	1	24	23	1
H	1.107964	1	109.025201	1	-178.673684	1	10	1	2
H	1.109454	1	106.999967	1	-58.841108	1	10	1	2
H	1.108826	1	108.147653	1	60.114741	1	10	1	2
H	1.102285	1	119.462552	1	0.259306	1	12	11	5
H	1.099815	1	119.712511	1	-179.849738	1	15	12	11
H	1.099362	1	120.243728	1	-179.932796	1	16	15	12
H	1.099759	1	119.720611	1	-179.958730	1	14	13	11
H	1.101366	1	120.046147	1	0.105838	1	13	11	5
H	1.101304	1	119.990341	1	-1.198147	1	19	17	5
H	1.099558	1	119.796253	1	-179.656284	1	20	19	17
H	1.099420	1	120.156286	1	179.678541	1	22	21	18
H	1.099829	1	119.731406	1	179.876748	1	21	18	17
H	1.102142	1	119.207172	1	2.177522	1	18	17	5
H	1.103513	1	118.135973	1	4.833244	1	33	26	24
H	1.100639	1	120.819422	1	-179.364986	1	34	33	26
H	1.100575	1	118.462056	1	1.917460	1	36	35	34
H	1.100180	1	120.778871	1	179.816017	1	37	36	35
H	1.100276	1	119.125768	1	178.983580	1	39	37	36
H	1.101984	1	118.766040	1	-0.482877	1	38	32	27
H	1.101723	1	118.617988	1	0.160770	1	43	31	30
H	1.100198	1	119.099174	1	178.544194	1	46	45	44
H	1.099977	1	120.774805	1	179.546373	1	45	44	42
H	1.100392	1	118.472430	1	2.188063	1	44	42	41
H	1.100590	1	120.843870	1	-179.211040	1	41	40	29
H	1.100705	1	118.905538	1	3.675110	1	40	29	28

TS (P,Re)-[8 -> 9]A Heat of formation = 13.661790 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.420483	1	0.000000	0	0.000000	0	1	0	0
N	1.570962	1	108.905597	1	0.000000	0	1	2	0
C	1.507398	1	103.630472	1	14.904056	1	3	1	2
C	1.446476	1	111.859704	1	-8.651008	1	2	1	3
C	1.493270	1	112.281767	1	-99.009224	1	3	1	2
C	1.534408	1	108.651508	1	131.801218	1	6	3	1
C	1.523914	1	106.498096	1	-9.035221	1	7	6	3
B	1.571436	1	113.620944	1	137.332775	1	3	1	2
C	1.552364	1	117.478993	1	-143.505359	1	1	2	3
C	1.514400	1	106.816844	1	120.847232	1	5	2	1
C	1.401580	1	119.900677	1	-23.527082	1	11	5	2
C	1.400774	1	121.326610	1	155.101791	1	11	5	2
C	1.393987	1	120.547928	1	-179.305192	1	13	11	5
C	1.393793	1	120.612149	1	179.180530	1	12	11	5
C	1.394042	1	120.207725	1	-0.067129	1	15	12	11
C	1.510595	1	108.739567	1	-119.770047	1	5	2	1
C	1.399900	1	119.799978	1	-22.736463	1	17	5	2
C	1.400806	1	120.950905	1	157.719170	1	17	5	2
C	1.393597	1	120.344872	1	179.111916	1	19	17	5
C	1.394509	1	120.236163	1	-179.119484	1	18	17	5
C	1.394018	1	120.257747	1	-0.109735	1	21	18	17
O	1.745960	1	108.534572	1	-83.343656	1	1	3	4
C	1.285806	1	125.308102	1	-149.609448	1	23	1	2
O	1.372406	1	107.583155	1	134.029189	1	24	23	1
C	1.482713	1	125.656120	1	-74.831708	1	24	23	1
C	1.388950	1	123.874940	1	161.454181	1	26	24	23
C	1.432992	1	118.286906	1	168.182061	1	25	24	23
C	1.491260	1	111.517143	1	61.221454	1	28	25	24
C	1.387793	1	119.785533	1	-69.807008	1	29	28	25
C	1.430531	1	119.461880	1	172.676035	1	30	29	28
C	1.434173	1	119.108989	1	171.418833	1	27	26	24
C	1.422347	1	115.540948	1	-21.169861	1	26	24	23
C	1.368709	1	120.690867	1	-174.966394	1	33	26	24
C	1.420750	1	120.313387	1	1.506390	1	34	33	26
C	1.422119	1	120.769142	1	176.867951	1	35	34	33
C	1.372521	1	120.619385	1	-177.381631	1	36	35	34
C	1.424087	1	122.222262	1	-172.573462	1	32	27	26
C	1.414833	1	119.983683	1	0.181936	1	37	36	35
C	1.415594	1	119.419769	1	108.652832	1	29	28	25
C	1.371405	1	120.327229	1	-176.578316	1	40	29	28
C	1.420702	1	120.411148	1	2.154014	1	41	40	29
C	1.423864	1	122.445117	1	-172.172996	1	31	30	29
C	1.422609	1	120.858393	1	176.553226	1	42	41	40
C	1.372233	1	120.638787	1	-177.096631	1	44	42	41
C	1.415413	1	120.072612	1	0.221375	1	45	44	42
H	1.127581	1	107.109877	1	100.714086	1	4	3	1
H	1.116703	1	111.655885	1	-126.858976	1	8	7	6
H	1.119933	1	110.292700	1	113.404289	1	8	7	6
H	1.117527	1	110.068015	1	-129.616879	1	7	6	3
H	1.117657	1	110.336648	1	111.263992	1	7	6	3
H	1.123342	1	108.802474	1	-107.040891	1	6	3	1
H	1.124125	1	109.462344	1	11.564345	1	6	3	1
H	1.207468	1	107.973605	1	68.654066	1	9	3	1
H	1.205542	1	108.981629	1	-163.178141	1	9	3	1
H	1.674063	1	101.471729	1	33.081760	1	24	23	1
H	1.108213	1	109.479196	1	-172.749457	1	10	1	2
H	1.109618	1	106.776478	1	-52.181600	1	10	1	2
H	1.109546	1	107.730646	1	66.150932	1	10	1	2
H	1.102279	1	119.469900	1	0.185779	1	12	11	5
H	1.099751	1	119.745362	1	-179.705171	1	15	12	11
H	1.099371	1	120.222162	1	-179.892995	1	16	15	12
H	1.099801	1	119.687440	1	179.944100	1	14	13	11
H	1.101125	1	120.131684	1	0.061222	1	13	11	5
H	1.101096	1	120.088507	1	-0.941212	1	19	17	5
H	1.099445	1	119.793151	1	179.982955	1	20	19	17
H	1.099316	1	120.180253	1	179.959074	1	22	21	18
H	1.099681	1	119.684395	1	-179.874812	1	21	18	17
H	1.102223	1	119.241861	1	2.141331	1	18	17	5
H	1.103810	1	118.141851	1	4.836665	1	33	26	24
H	1.100636	1	120.807316	1	-179.408516	1	34	33	26
H	1.100533	1	118.466840	1	2.240949	1	36	35	34
H	1.100138	1	120.791424	1	179.853933	1	37	36	35
H	1.100273	1	119.121174	1	178.925952	1	39	37	36
H	1.102019	1	118.792481	1	-0.328003	1	38	32	27
H	1.101850	1	118.503247	1	0.673551	1	43	31	30
H	1.100076	1	119.096652	1	178.463628	1	46	45	44
H	1.099932	1	120.762961	1	179.635269	1	45	44	42
H	1.100355	1	118.466511	1	2.232576	1	44	42	41
H	1.100576	1	120.820914	1	-179.215833	1	41	40	29
H	1.100712	1	118.933455	1	2.971800	1	40	29	28

TS (P,Si)-[8 -> 9] HEAT OF FORMATION = 12.326833 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.437441	1	.000000	0	.000000	0	1	0	0
N	1.603253	1	107.596299	1	.000000	0	1	2	0
C	1.507008	1	103.373103	1	15.905217	1	3	1	2
C	1.439625	1	112.213657	1	-10.709473	1	2	1	3
C	1.492907	1	111.485425	1	-97.194698	1	3	1	2
C	1.534658	1	108.640624	1	132.362909	1	6	3	1
C	1.523842	1	106.376501	1	-10.057068	1	7	6	3
B	1.563879	1	114.771136	1	138.344627	1	3	1	2
C	1.555938	1	116.473412	1	-137.173586	1	1	2	3
C	1.515159	1	106.837359	1	123.351436	1	5	2	1
C	1.401793	1	119.671136	1	-23.518659	1	11	5	2
C	1.400593	1	121.552371	1	155.002339	1	11	5	2
C	1.394078	1	120.551365	1	-179.251074	1	13	11	5
C	1.393762	1	120.602035	1	179.147749	1	12	11	5
C	1.394082	1	120.215261	1	-.101148	1	15	12	11
C	1.512862	1	108.750120	1	-117.389546	1	5	2	1
C	1.400174	1	119.643973	1	-21.783133	1	17	5	2
C	1.400783	1	121.160985	1	158.610328	1	17	5	2
C	1.393721	1	120.384207	1	179.266400	1	19	17	5
C	1.394464	1	120.264001	1	-179.293867	1	18	17	5
C	1.394121	1	120.263301	1	-.064454	1	21	18	17
O	1.655233	1	94.380114	1	110.031527	1	1	2	3
C	1.302092	1	119.154821	1	-164.808245	1	23	1	2
O	1.370035	1	111.973707	1	-50.028705	1	24	23	1
C	1.487666	1	119.537928	1	155.201731	1	24	23	1
C	1.387300	1	124.471760	1	119.259989	1	26	24	23
C	1.435257	1	117.382051	1	-164.434109	1	25	24	23
C	1.492670	1	108.290000	1	77.559043	1	28	25	24
C	1.386642	1	119.481183	1	-66.662132	1	29	28	25
C	1.432021	1	119.218755	1	167.835614	1	30	29	28
C	1.436946	1	118.782988	1	170.952398	1	27	26	24
C	1.423670	1	115.111849	1	-60.699014	1	26	24	23
C	1.367839	1	120.868604	1	-175.542733	1	33	26	24
C	1.421160	1	120.156652	1	1.993692	1	34	33	26
C	1.421706	1	120.818092	1	175.480696	1	35	34	33
C	1.372778	1	120.605032	1	-177.456770	1	36	35	34
C	1.423885	1	122.073750	1	-170.328595	1	32	27	26
C	1.414477	1	119.957929	1	.128371	1	37	36	35
C	1.415748	1	119.440662	1	108.670877	1	29	28	25
C	1.371104	1	120.302838	1	-172.329128	1	40	29	28
C	1.421047	1	120.326436	1	2.474424	1	41	40	29
C	1.423688	1	122.449962	1	-171.176524	1	31	30	29
C	1.422442	1	120.800016	1	175.540975	1	42	41	40
C	1.372364	1	120.645332	1	-177.181305	1	44	42	41
C	1.415236	1	120.038001	1	.063636	1	45	44	42
H	1.127467	1	107.191517	1	100.921561	1	4	3	1
H	1.116638	1	111.656170	1	-126.617743	1	8	7	6
H	1.119871	1	110.338979	1	113.684246	1	8	7	6
H	1.117538	1	110.029962	1	-130.549362	1	7	6	3
H	1.117569	1	110.472992	1	110.323541	1	7	6	3
H	1.122851	1	109.284087	1	-106.081481	1	6	3	1
H	1.124613	1	109.132190	1	12.404810	1	6	3	1
H	1.572603	1	100.495819	1	51.600354	1	24	23	1
H	1.205422	1	109.868650	1	80.052253	1	9	3	1
H	1.204797	1	110.839551	1	-146.422612	1	9	3	1
H	1.108487	1	109.517999	1	170.566662	1	10	1	2
H	1.109434	1	106.372221	1	-70.063645	1	10	1	2
H	1.108898	1	108.332858	1	48.721912	1	10	1	2
H	1.102675	1	119.382736	1	.227005	1	12	11	5
H	1.099765	1	119.737150	1	-179.706161	1	15	12	11
H	1.099352	1	120.227270	1	-179.883122	1	16	15	12
H	1.099754	1	119.687574	1	179.937534	1	14	13	11
H	1.100893	1	120.205015	1	.090908	1	13	11	5
H	1.101169	1	120.098774	1	-.484260	1	19	17	5
H	1.099502	1	119.802450	1	-179.822620	1	20	19	17
H	1.099360	1	120.184409	1	179.864058	1	22	21	18
H	1.099812	1	119.681695	1	-179.960292	1	21	18	17
H	1.102742	1	119.174116	1	1.787479	1	18	17	5
H	1.103466	1	118.108587	1	4.594448	1	33	26	24
H	1.100581	1	120.873623	1	-179.019040	1	34	33	26
H	1.100556	1	118.466949	1	2.053854	1	36	35	34
H	1.100110	1	120.793922	1	179.760382	1	37	36	35
H	1.100275	1	119.133443	1	178.827382	1	39	37	36
H	1.101816	1	118.873120	1	-.276393	1	38	32	27
H	1.101791	1	118.644741	1	-.354643	1	43	31	30
H	1.100286	1	119.102499	1	178.774795	1	46	45	44
H	1.100042	1	120.777558	1	179.624416	1	45	44	42
H	1.100514	1	118.469487	1	2.200166	1	44	42	41
H	1.100661	1	120.881901	1	-179.094422	1	41	40	29
H	1.100773	1	118.908253	1	7.168556	1	40	29	28

(R,M)-9 HEAT OF FORMATION = -31.344789 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.441731	1	.000000	0	.000000	0	1	0	0
N	1.580316	1	107.625252	1	.000000	0	1	2	0
C	1.554796	1	116.850975	1	-142.273189	1	1	2	3
O	1.660661	1	108.509569	1	98.623326	1	1	2	3
C	1.444561	1	111.498370	1	11.367160	1	2	1	3
C	1.494377	1	105.642302	1	-3.549433	1	3	1	2
C	1.471583	1	119.814780	1	-126.761634	1	3	1	2
B	1.628908	1	42.501338	1	84.432044	1	5	3	8
C	1.426503	1	119.422714	1	117.897653	1	5	1	3
C	1.512489	1	107.939171	1	-132.997877	1	6	2	1
C	1.514389	1	108.021195	1	108.729658	1	6	2	1
C	1.534013	1	108.278907	1	-132.010181	1	7	3	1
C	1.533771	1	109.032897	1	120.884307	1	8	3	1
O	1.422068	1	100.743729	1	-133.856633	1	10	5	1
C	1.512032	1	109.558043	1	104.704487	1	10	5	1
C	1.400607	1	121.241060	1	154.265338	1	11	6	2
C	1.400092	1	119.514594	1	-27.620199	1	11	6	2
C	1.401836	1	120.851284	1	159.331491	1	12	6	2
C	1.400279	1	120.336947	1	-18.719396	1	12	6	2
C	1.422126	1	116.669014	1	-146.825472	1	15	10	5
C	1.389322	1	120.731268	1	178.234342	1	16	10	5
C	1.417885	1	119.184830	1	-2.713191	1	16	10	5
C	1.393737	1	120.349054	1	178.380248	1	17	11	6
C	1.394370	1	120.274066	1	-178.191623	1	18	11	6
C	1.393411	1	120.573198	1	-179.075747	1	19	12	6
C	1.394340	1	120.561964	1	179.003362	1	20	12	6
C	1.495462	1	111.803811	1	-54.252225	1	21	15	10
C	1.468960	1	119.861058	1	-.680567	1	22	16	10
C	1.432632	1	119.644357	1	-176.478854	1	22	16	10
C	1.370371	1	120.913973	1	179.802739	1	23	16	10
C	1.394459	1	120.168756	1	-.273759	1	24	17	11
C	1.394624	1	120.222596	1	.438043	1	26	19	12
C	1.415402	1	119.802411	1	-107.059837	1	28	21	15
C	1.429528	1	122.285294	1	128.066502	1	29	22	16
C	1.418951	1	119.371711	1	-4.822732	1	30	22	16
C	1.424331	1	122.479641	1	172.984791	1	30	22	16
C	1.371693	1	120.382632	1	176.824606	1	34	28	21
C	1.419823	1	119.080762	1	175.416912	1	35	29	22
C	1.423942	1	122.428350	1	-6.134029	1	35	29	22
C	1.422548	1	119.703049	1	-179.454855	1	36	30	22
C	1.372757	1	121.093377	1	-179.706948	1	37	30	22
C	1.422752	1	119.421400	1	-179.451638	1	39	35	29
C	1.372648	1	120.931212	1	-179.731314	1	40	35	29
C	1.371972	1	120.650417	1	-1.637469	1	41	36	30
C	1.372215	1	120.668980	1	-1.382055	1	43	39	35
H	1.129997	1	107.209056	1	110.319754	1	7	3	1
H	1.117120	1	112.072444	1	125.699206	1	13	7	3
H	1.119551	1	109.084273	1	-115.481621	1	13	7	3
H	1.117488	1	110.282561	1	124.056520	1	14	8	3
H	1.118049	1	110.207278	1	-117.078663	1	14	8	3
H	1.125303	1	108.689230	1	-118.505893	1	8	3	1
H	1.124031	1	109.584332	1	-.628556	1	8	3	1
H	1.102142	1	119.438768	1	1.725710	1	18	11	6
H	1.100135	1	119.692172	1	-179.940419	1	25	18	11
H	1.099444	1	120.099082	1	180.031307	1	32	24	17
H	1.099663	1	119.775768	1	179.743364	1	24	17	11
H	1.101117	1	120.282869	1	-1.295022	1	17	11	6
H	1.102661	1	119.508418	1	.131784	1	20	12	6
H	1.099840	1	119.681347	1	-179.851234	1	27	20	12
H	1.099471	1	120.154751	1	179.795155	1	33	26	19
H	1.099829	1	119.737298	1	179.982524	1	26	19	12
H	1.101195	1	119.974188	1	.275096	1	19	12	6
H	1.129518	1	110.928364	1	-18.604060	1	10	5	1
H	1.198766	1	112.555533	1	-117.570182	1	9	3	1
H	1.202229	1	111.104779	1	101.372408	1	9	3	1
H	1.108588	1	109.192823	1	-163.582473	1	4	1	2
H	1.109166	1	108.617632	1	75.326375	1	4	1	2
H	1.109430	1	106.649941	1	-43.742535	1	4	1	2
H	1.103704	1	118.533768	1	.068996	1	23	16	10
H	1.100440	1	120.763348	1	179.247238	1	31	23	16
H	1.100387	1	118.433127	1	178.833469	1	41	36	30
H	1.099757	1	120.849179	1	-179.830336	1	45	41	36
H	1.100062	1	120.456582	1	179.822653	1	42	37	30
H	1.101744	1	118.767493	1	-.106906	1	37	30	22
H	1.102049	1	118.426891	1	.224912	1	40	35	29
H	1.100125	1	120.510461	1	179.792560	1	44	40	35
H	1.099899	1	120.781062	1	-179.873689	1	46	43	39
H	1.100421	1	118.451422	1	178.905453	1	43	39	35
H	1.100412	1	120.840986	1	179.122531	1	38	34	28
H	1.100787	1	118.869241	1	-2.880981	1	34	28	21

(S,M)-9 Heat of formation = -32.316800 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.441763	1	0.000000	0	0.000000	0	1	0	0
N	1.585745	1	107.268480	1	0.000000	0	1	2	0
C	1.552293	1	117.155612	1	-142.952077	1	1	2	3
O	1.663431	1	108.078754	1	97.953705	1	1	2	3
C	1.442884	1	111.895633	1	10.555332	1	2	1	3
C	1.493693	1	105.854821	1	-4.315989	1	3	1	2
C	1.470960	1	119.595615	1	-127.665327	1	3	1	2
B	1.576915	1	88.569315	1	112.204904	1	3	1	2
C	1.430480	1	118.538952	1	4.304293	1	5	1	2
C	1.514097	1	107.742030	1	-131.011970	1	6	2	1
C	1.513866	1	107.950943	1	110.704953	1	6	2	1
C	1.534575	1	108.290910	1	-130.073509	1	7	3	1
C	1.523268	1	106.907809	1	0.858198	1	13	7	3
O	3.725940	-1	15.783000	1	-6.658000	1	9	5	10
C	1.506594	1	111.576468	1	-158.305045	1	10	5	1
C	1.400396	1	121.423546	1	155.579223	1	11	6	2
C	1.401084	1	119.398110	1	-25.954813	1	11	6	2
C	1.401533	1	121.001143	1	159.797416	1	12	6	2
C	1.400592	1	120.144441	1	-18.446163	1	12	6	2
C	1.423986	1	118.266872	1	94.841593	1	15	10	5
C	1.387125	1	123.601025	1	-58.585751	1	16	10	5
C	1.420123	1	116.086777	1	122.839127	1	16	10	5
C	1.394076	1	120.369701	1	178.802885	1	17	11	6
C	1.394290	1	120.302863	1	-178.782346	1	18	11	6
C	1.393487	1	120.552709	1	-179.095085	1	19	12	6
C	1.394296	1	120.520507	1	179.030335	1	20	12	6
C	1.492376	1	113.795140	1	-52.326261	1	21	15	10
C	1.387527	1	119.815547	1	70.350512	1	28	21	15
C	1.433844	1	119.394503	1	-172.547588	1	22	16	10
C	1.369768	1	120.830774	1	176.016787	1	23	16	10
C	1.394309	1	120.241272	1	0.085288	1	25	18	11
C	1.393775	1	120.255572	1	-0.216801	1	27	20	12
C	1.415916	1	119.551909	1	-108.973609	1	28	21	15
C	1.430208	1	119.577257	1	-173.825625	1	29	28	21
C	1.418818	1	119.438659	1	-5.243084	1	30	22	16
C	1.423858	1	122.321511	1	172.677001	1	30	22	16
C	1.371365	1	120.428027	1	177.325615	1	34	28	21
C	1.419776	1	119.083159	1	-5.178774	1	35	29	28
C	1.423885	1	122.493918	1	172.946388	1	35	29	28
C	1.422252	1	119.663273	1	-179.849396	1	36	30	22
C	1.373066	1	121.051460	1	-179.372330	1	37	30	22
C	1.422648	1	119.474538	1	-179.619558	1	39	35	29
C	1.372709	1	120.963485	1	-179.562975	1	40	35	29
C	1.372322	1	120.633477	1	-1.399545	1	41	36	30
C	1.372119	1	120.671070	1	-1.419418	1	43	39	35
H	1.129432	1	107.292508	1	112.487338	1	7	3	1
H	1.117427	1	112.054514	1	122.224857	1	13	7	3
H	1.119264	1	109.154350	1	-118.922991	1	13	7	3
H	1.117647	1	111.009552	1	-121.323355	1	14	13	7
H	1.117933	1	110.835376	1	118.974061	1	14	13	7
H	1.125133	1	108.827996	1	-117.855664	1	8	3	1
H	1.124497	1	109.336408	1	-0.009734	1	8	3	1
H	1.103522	1	119.336399	1	1.610543	1	18	11	6
H	1.100064	1	119.671577	1	179.995702	1	25	18	11
H	1.099586	1	120.178183	1	179.942274	1	32	25	18
H	1.099756	1	119.766346	1	179.934992	1	24	17	11
H	1.101220	1	120.290114	1	-0.860065	1	17	11	6
H	1.103011	1	119.475656	1	0.094800	1	20	12	6
H	1.099862	1	119.673176	1	-179.815392	1	27	20	12
H	1.099477	1	120.237780	1	-179.860404	1	33	27	20
H	1.099791	1	119.739439	1	179.948503	1	26	19	12
H	1.100886	1	120.025667	1	0.306293	1	19	12	6
H	1.133876	1	109.851977	1	-33.648636	1	10	5	1
H	1.202932	1	112.889879	1	-115.523842	1	9	3	1
H	1.201426	1	111.577820	1	104.570502	1	9	3	1
H	1.108074	1	109.225300	1	-166.911252	1	4	1	2
H	1.108727	1	108.752757	1	71.498626	1	4	1	2
H	1.109565	1	105.890350	1	-47.705882	1	4	1	2
H	1.101643	1	118.807139	1	-4.200318	1	23	16	10
H	1.100374	1	120.884816	1	179.285834	1	31	23	16
H	1.100390	1	118.469818	1	178.994361	1	41	36	30
H	1.099858	1	120.810759	1	-179.808334	1	45	41	36
H	1.100050	1	120.455373	1	179.805381	1	42	37	30
H	1.101953	1	118.699434	1	0.372601	1	37	30	22
H	1.101869	1	118.476641	1	-0.109124	1	40	35	29
H	1.099927	1	120.498841	1	179.666051	1	44	40	35
H	1.099758	1	120.787802	1	-179.781962	1	46	43	39
H	1.100302	1	118.449447	1	179.026642	1	43	39	35
H	1.100310	1	120.854574	1	179.316093	1	38	34	28
H	1.100710	1	118.875346	1	-2.228670	1	34	28	21

(R,P)-9 HEAT OF FORMATION = -28.848574 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.435775	1	.000000	0	.000000	0	1	0	0
N	1.585756	1	107.837046	1	.000000	0	1	2	0
C	1.496016	1	105.449904	1	-2.493348	1	3	1	2
C	1.443189	1	111.842676	1	8.419626	1	2	1	3
C	1.470958	1	119.894747	1	-125.588071	1	3	1	2
C	1.533620	1	108.872037	1	127.346264	1	6	3	1
C	1.523308	1	106.621653	1	-8.136410	1	7	6	3
B	1.569753	1	88.951612	1	113.343905	1	3	1	2
C	1.554410	1	115.897221	1	-140.666517	1	1	2	3
C	1.516158	1	107.865599	1	112.429273	1	5	2	1
C	1.400135	1	120.434381	1	-14.298536	1	11	5	2
C	1.402071	1	120.803813	1	163.479574	1	11	5	2
C	1.393254	1	120.621742	1	-178.874295	1	13	11	5
C	1.394520	1	120.582937	1	178.820174	1	12	11	5
C	1.393537	1	120.267691	1	-.319276	1	15	12	11
C	1.513098	1	108.260263	1	-129.939747	1	5	2	1
C	1.400143	1	119.338539	1	-26.233837	1	17	5	2
C	1.400368	1	121.419088	1	155.935844	1	17	5	2
C	1.393857	1	120.373752	1	177.535618	1	19	17	5
C	1.394205	1	120.244907	1	-177.398144	1	18	17	5
C	1.394074	1	120.288467	1	-.237229	1	21	18	17
O	1.679993	1	102.902313	1	95.378101	1	1	2	3
C	1.430339	1	116.406485	1	129.893124	1	23	1	2
O	1.410760	1	103.213854	1	-77.134030	1	24	23	1
C	1.506851	1	112.406743	1	156.188862	1	24	23	1
C	1.385889	1	124.599341	1	64.560891	1	26	24	23
C	1.423129	1	118.604195	1	-101.969152	1	25	24	23
C	1.491723	1	113.883393	1	55.514651	1	28	25	24
C	1.386766	1	119.873346	1	-70.033211	1	29	28	25
C	1.430341	1	119.615999	1	174.341635	1	30	29	28
C	1.435598	1	119.372236	1	171.747842	1	27	26	24
C	1.422230	1	115.306394	1	-116.806360	1	26	24	23
C	1.368830	1	121.041324	1	-175.792874	1	33	26	24
C	1.420609	1	120.220566	1	1.861126	1	34	33	26
C	1.421849	1	120.837013	1	176.397630	1	35	34	33
C	1.372553	1	120.610934	1	-177.341697	1	36	35	34
C	1.423828	1	122.321254	1	-171.720698	1	32	27	26
C	1.414570	1	119.936294	1	.185356	1	37	36	35
C	1.415994	1	119.531869	1	110.062691	1	29	28	25
C	1.371437	1	120.405759	1	-178.616353	1	40	29	28
C	1.420719	1	120.435093	1	2.370910	1	41	40	29
C	1.423784	1	122.494216	1	-172.309971	1	31	30	29
C	1.422641	1	120.959611	1	176.995643	1	42	41	40
C	1.372160	1	120.671600	1	-177.061040	1	44	42	41
C	1.415354	1	120.053069	1	.170202	1	45	44	42
H	1.129902	1	107.091023	1	111.289428	1	4	3	1
H	1.117638	1	110.242970	1	-114.900637	1	8	7	6
H	1.118785	1	110.916984	1	126.166178	1	8	7	6
H	1.117416	1	110.284247	1	-128.848385	1	7	6	3
H	1.118026	1	110.202989	1	112.262194	1	7	6	3
H	1.124486	1	109.087386	1	-111.641364	1	6	3	1
H	1.124905	1	109.311358	1	6.562245	1	6	3	1
H	1.133590	1	109.979824	1	33.587813	1	24	23	1
H	1.204836	1	111.143064	1	101.829233	1	9	3	1
H	1.200414	1	113.952798	1	-118.176748	1	9	3	1
H	1.108354	1	111.129268	1	175.165748	1	10	1	2
H	1.110809	1	106.454594	1	-63.849613	1	10	1	2
H	1.109464	1	107.343979	1	54.591475	1	10	1	2
H	1.102282	1	119.530322	1	.060211	1	12	11	5
H	1.099818	1	119.666404	1	-179.877591	1	15	12	11
H	1.099400	1	120.261083	1	-179.875690	1	16	15	12
H	1.099772	1	119.748756	1	179.982742	1	14	13	11
H	1.100983	1	119.937530	1	.525815	1	13	11	5
H	1.101002	1	120.366342	1	-2.267276	1	19	17	5
H	1.099489	1	119.789459	1	179.813535	1	20	19	17
H	1.099263	1	120.213539	1	180.015439	1	22	21	18
H	1.099728	1	119.655904	1	-179.893198	1	21	18	17
H	1.102127	1	119.281194	1	3.299535	1	18	17	5
H	1.101654	1	118.812112	1	4.756263	1	33	26	24
H	1.100360	1	120.940930	1	-179.050158	1	34	33	26
H	1.100373	1	118.486074	1	2.237554	1	36	35	34
H	1.099850	1	120.816755	1	179.829475	1	37	36	35
H	1.100141	1	119.111414	1	178.865991	1	39	37	36
H	1.101956	1	118.778852	1	-.193312	1	38	32	27
H	1.101716	1	118.499246	1	.820008	1	43	31	30
H	1.099888	1	119.099238	1	178.618529	1	46	45	44
H	1.099719	1	120.783573	1	179.696854	1	45	44	42
H	1.100221	1	118.450801	1	2.282560	1	44	42	41
H	1.100373	1	120.837750	1	-179.131030	1	41	40	29
H	1.100658	1	118.875070	1	1.073943	1	40	29	28

(S,P)-9 HEAT OF FORMATION = -31.459310 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0	
O	1.434600	1	.000000	0	.000000	0	1	0	0	
N	1.583147	1	108.115540	1	.000000	0	1	2	0	
C	1.497362	1	105.333362	1	-4.835499	1	3	1	2	
C	1.442559	1	112.083731	1	4.371552	1	2	1	3	
C	1.471547	1	119.472052	1	-127.496620	1	3	1	2	
C	1.533822	1	108.952265	1	120.735363	1	6	3	1	
C	1.523205	1	106.672562	1	-5.608857	1	7	6	3	
C	1.552431	1	115.427794	1	-142.024969	1	1	2	3	
C	1.514239	1	107.359415	1	119.944035	1	5	2	1	
C	1.401276	1	120.013117	1	-16.774721	1	10	5	2	
C	1.400804	1	121.125757	1	162.138828	1	10	5	2	
C	1.393740	1	120.533459	1	-179.297016	1	12	10	5	
C	1.394082	1	120.515084	1	179.187233	1	11	10	5	
C	1.393955	1	120.241878	1	.007221	1	14	11	10	
C	1.514211	1	108.136603	1	-121.435883	1	5	2	1	
C	1.400913	1	119.285822	1	-22.135264	1	16	5	2	
C	1.400414	1	121.686652	1	158.750120	1	16	5	2	
C	1.394089	1	120.441191	1	179.303381	1	18	16	5	
C	1.394066	1	120.404395	1	-179.336179	1	17	16	5	
C	1.394130	1	120.244251	1	.102502	1	20	17	16	
O	1.669592	1	90.482562	1	-107.227832	1	1	3	4	
C	1.416872	1	118.436783	1	120.248215	1	22	1	2	
O	1.421389	1	104.279781	1	68.762139	1	23	22	1	
C	1.509440	1	110.918688	1	-167.147158	1	23	22	1	
C	1.389457	1	119.871530	1	174.224131	1	25	23	22	
C	1.423735	1	116.182152	1	154.867376	1	24	23	22	
C	1.495562	1	111.804880	1	51.298396	1	27	24	23	
C	1.388290	1	119.634074	1	-71.742814	1	28	27	24	
C	1.429673	1	119.557169	1	172.998530	1	29	28	27	
C	1.431112	1	119.558836	1	176.653940	1	26	25	23	
C	1.416683	1	119.693467	1	-3.894335	1	25	23	22	
C	1.371118	1	120.586120	1	-179.790761	1	32	25	23	
C	1.419698	1	120.475149	1	1.519035	1	33	32	25	
C	1.422777	1	120.919446	1	177.092220	1	34	33	32	
C	1.371904	1	120.667869	1	-177.597507	1	35	34	33	
C	1.424133	1	122.444462	1	-173.241041	1	31	26	25	
C	1.415405	1	119.995366	1	.138340	1	36	35	34	
C	1.415378	1	119.678788	1	106.742640	1	28	27	24	
C	1.371580	1	120.392781	1	-176.207160	1	39	28	27	
C	1.420703	1	120.407814	1	1.651807	1	40	39	28	
C	1.423812	1	122.430373	1	-173.384554	1	30	29	28	
C	1.422657	1	120.889024	1	176.780170	1	41	40	39	
C	1.372180	1	120.651552	1	-177.803663	1	43	41	40	
C	1.415544	1	120.071288	1	.041018	1	44	43	41	
H	1.128537	1	107.230692	1	119.492237	1	4	3	1	
H	1.118390	1	110.225157	1	-112.611378	1	8	7	6	
H	1.118200	1	111.107618	1	128.258436	1	8	7	6	
H	1.117415	1	110.359674	1	-126.312949	1	7	6	3	
H	1.118010	1	110.142082	1	114.834708	1	7	6	3	
H	1.124914	1	108.870276	1	-118.376618	1	6	3	1	
H	1.124489	1	109.340966	1	-.509535	1	6	3	1	
H	1.130901	1	107.279665	1	-46.578339	1	23	22	1	
H	1.108493	1	110.064695	1	-168.825669	1	9	1	2	
H	1.109466	1	106.952193	1	-48.298857	1	9	1	2	
H	1.109635	1	107.423681	1	69.883826	1	9	1	2	
H	1.102755	1	119.474759	1	.008918	1	11	10	5	
H	1.099816	1	119.697952	1	-179.674494	1	14	11	10	
H	1.099453	1	120.227899	1	-179.848464	1	15	14	11	
H	1.099788	1	119.721503	1	179.844465	1	13	12	10	
H	1.100546	1	120.111034	1	.061111	1	12	10	5	
H	1.100933	1	120.486361	1	-.629857	1	18	16	5	
H	1.099616	1	119.752276	1	179.872615	1	19	18	16	
H	1.099390	1	120.211598	1	180.036961	1	21	20	17	
H	1.099833	1	119.692607	1	-179.823773	1	20	17	16	
H	1.102277	1	119.332515	1	1.363649	1	17	16	5	
H	1.104048	1	118.567022	1	.168774	1	32	25	23	
H	1.100558	1	120.690526	1	-179.369493	1	33	32	25	
H	1.100476	1	118.420257	1	2.002250	1	35	34	33	
H	1.099837	1	120.821929	1	179.807036	1	36	35	34	
H	1.100000	1	119.084926	1	178.991182	1	38	36	35	
H	1.101741	1	118.660071	1	-.228799	1	37	31	26	
H	1.102087	1	118.475804	1	-.587174	1	42	30	29	
H	1.100139	1	119.086541	1	179.157969	1	45	44	43	
H	1.099957	1	120.771340	1	179.762684	1	44	43	41	
H	1.100408	1	118.469102	1	1.807682	1	43	41	40	
H	1.100481	1	120.856049	1	-179.394961	1	40	39	28	
H	1.100766	1	118.889520	1	3.462717	1	39	28	27	
H	1.124018	1	109.419569	1	-71.650459	1	27	24	23	
H	1.124341	1	103.212254	1	171.643080	1	27	24	23	
B	1.624259	1	120.756305	1	90.235199	1	22	23	25	

TSa (P)-9 <--> (M)-9 Heat of formation = 4.611430 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.441407	1	0.000000	0	0.000000	0	1	0	0
N	1.584359	1	107.341645	1	0.000000	0	1	2	0
C	1.552066	1	117.162168	1	-143.189134	1	1	2	3
O	1.670332	1	108.093420	1	97.951102	1	1	2	3
C	1.443199	1	111.859973	1	10.357642	1	2	1	3
C	1.493920	1	105.834045	1	-3.623279	1	3	1	2
C	1.471201	1	119.589393	1	-126.919865	1	3	1	2
B	1.576898	1	88.719967	1	112.919438	1	3	1	2
C	1.424308	1	118.092150	1	3.114781	1	5	1	2
C	1.513869	1	107.758870	1	-131.396249	1	6	2	1
C	1.513818	1	107.988560	1	110.306686	1	6	2	1
C	1.534337	1	108.281160	1	-130.932862	1	7	3	1
C	1.533624	1	109.023378	1	121.012269	1	8	3	1
O	1.416538	1	103.967426	1	81.599118	1	10	5	1
C	1.510277	1	113.828917	1	-157.840114	1	10	5	1
C	1.400359	1	121.404843	1	155.068927	1	11	6	2
C	1.401082	1	119.407259	1	-26.562151	1	11	6	2
C	1.401548	1	120.961407	1	159.258356	1	12	6	2
C	1.400528	1	120.188188	1	-19.006095	1	12	6	2
C	1.429705	1	113.395021	1	95.532629	1	15	10	5
C	1.395860	1	125.813368	1	-38.693273	1	16	10	5
C	1.428216	1	111.585727	1	151.735238	1	16	10	5
C	1.394073	1	120.363902	1	178.700557	1	17	11	6
C	1.394261	1	120.300838	1	-178.668166	1	18	11	6
C	1.393446	1	120.552025	1	-179.163562	1	19	12	6
C	1.394290	1	120.525697	1	179.119201	1	20	12	6
C	1.498470	1	110.449478	1	-55.829061	1	21	15	10
C	1.491856	1	116.792780	1	-15.743562	1	22	16	10
C	1.452412	1	114.625784	1	175.736336	1	22	16	10
C	1.363639	1	120.338091	1	163.783406	1	23	16	10
C	1.394430	1	120.199415	1	-0.209857	1	24	17	11
C	1.394604	1	120.221910	1	0.371031	1	26	19	12
C	1.419946	1	113.111915	1	-95.137976	1	28	21	15
C	1.444950	1	129.520798	1	136.737527	1	29	22	16
C	1.426220	1	118.255421	1	29.790630	1	30	22	16
C	1.418709	1	108.061047	1	-4.650787	1	30	29	35
C	1.363582	1	120.555638	1	166.925934	1	34	28	21
C	1.427872	1	119.503151	1	-162.519274	1	35	29	22
C	1.420667	1	101.732635	1	-29.635569	1	35	22	30
C	1.419968	1	120.421471	1	163.825150	1	36	30	22
C	1.376914	1	122.205953	1	-166.966050	1	37	30	22
C	1.423028	1	121.169420	1	168.460951	1	39	35	29
C	1.374138	1	123.255888	1	-169.413810	1	40	35	29
C	1.374239	1	120.461285	1	10.182680	1	41	36	30
C	1.370818	1	121.004284	1	5.476027	1	43	39	35
H	1.129538	1	107.296213	1	111.548867	1	7	3	1
H	1.117266	1	112.065709	1	124.084259	1	13	7	3
H	1.119424	1	109.119179	1	-117.085021	1	13	7	3
H	1.117568	1	110.274793	1	123.088305	1	14	8	3
H	1.118003	1	110.220216	1	-118.063131	1	14	8	3
H	1.125197	1	108.786287	1	-118.253060	1	8	3	1
H	1.124402	1	109.366928	1	-0.403675	1	8	3	1
H	1.103339	1	119.328122	1	1.600516	1	18	11	6
H	1.100050	1	119.678332	1	179.864370	1	25	18	11
H	1.099578	1	120.087340	1	-179.832362	1	32	24	17
H	1.099782	1	119.761491	1	179.871084	1	24	17	11
H	1.101218	1	120.293792	1	-0.945310	1	17	11	6
H	1.102973	1	119.474225	1	0.205935	1	20	12	6
H	1.099874	1	119.681607	1	-179.856588	1	27	20	12
H	1.099461	1	120.149062	1	179.812691	1	33	26	19
H	1.099766	1	119.737423	1	179.952385	1	26	19	12
H	1.100965	1	120.025645	1	0.257523	1	19	12	6
H	1.201387	1	111.441357	1	103.574342	1	9	3	1
H	1.131859	1	109.769998	1	-30.927997	1	10	5	1
H	1.202117	1	112.913437	1	-116.396479	1	9	3	1
H	1.108089	1	109.173219	1	-166.501030	1	4	1	2
H	1.108758	1	108.733706	1	71.971590	1	4	1	2
H	1.109535	1	105.964599	1	-47.250772	1	4	1	2
H	1.101747	1	118.767952	1	-10.759507	1	23	16	10
H	1.099360	1	121.846593	1	-169.379491	1	31	23	16
H	1.100198	1	118.462960	1	-171.840526	1	41	36	30
H	1.098815	1	121.354823	1	-178.173063	1	45	41	36
H	1.099894	1	120.270398	1	178.000909	1	42	37	30
H	1.099053	1	119.023614	1	23.552605	1	37	30	22
H	1.089292	1	119.390560	1	17.711005	1	40	35	29
H	1.100056	1	120.190048	1	178.404461	1	44	40	35
H	1.098669	1	121.524470	1	-178.365248	1	46	43	39
H	1.100719	1	118.165902	1	-175.163466	1	43	39	35
H	1.099875	1	121.586758	1	-173.925710	1	38	34	28
H	1.101456	1	118.786790	1	-9.082630	1	34	28	21

TSb (P)-9 <--> (M)-9 Heat of formation = 4.108602 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.441614	1	0.000000	0	0.000000	0	1	0	0
N	1.584348	1	107.367180	1	0.000000	0	1	2	0
C	1.552651	1	116.861354	1	-143.133353	1	1	2	3
O	1.667893	1	108.135737	1	98.042640	1	1	2	3
C	1.443157	1	111.816027	1	10.560866	1	2	1	3
C	1.494181	1	105.795849	1	-3.719369	1	3	1	2
C	1.471219	1	119.788568	1	-127.080832	1	3	1	2
B	1.577112	1	88.712431	1	112.785536	1	3	1	2
C	1.425018	1	118.253282	1	3.334399	1	5	1	2
C	1.513663	1	107.775712	1	-131.532225	1	6	2	1
C	1.513738	1	107.935140	1	110.005616	1	6	2	1
C	1.534350	1	108.284414	1	-130.935447	1	7	3	1
C	1.533672	1	109.028894	1	120.196582	1	8	3	1
O	1.414742	1	104.289304	1	80.587579	1	10	5	1
C	1.512585	1	113.611819	1	-157.538273	1	10	5	1
C	1.400418	1	121.401481	1	155.304037	1	11	6	2
C	1.401064	1	119.413545	1	-26.136077	1	11	6	2
C	1.401420	1	121.027110	1	158.609180	1	12	6	2
C	1.400722	1	120.114894	1	-19.692151	1	12	6	2
C	1.429618	1	113.531319	1	91.451885	1	15	10	5
C	1.399464	1	126.815206	1	-42.424390	1	16	10	5
C	1.425471	1	111.031071	1	144.901226	1	16	10	5
C	1.394051	1	120.372396	1	178.897062	1	17	11	6
C	1.394368	1	120.292316	1	-178.894316	1	18	11	6
C	1.393594	1	120.537353	1	-179.156917	1	19	12	6
C	1.394159	1	120.527062	1	179.090822	1	20	12	6
C	1.495540	1	110.074072	1	-51.084010	1	21	15	10
C	1.490033	1	117.030433	1	-11.724223	1	22	16	10
C	1.446492	1	115.374273	1	176.475231	1	22	16	10
C	1.364069	1	120.810859	1	167.365244	1	23	16	10
C	1.394510	1	120.187021	1	-0.178695	1	24	17	11
C	1.394580	1	120.230684	1	0.371835	1	26	19	12
C	1.423216	1	114.220874	1	-86.498672	1	28	21	15
C	1.446612	1	127.998765	1	134.852860	1	29	22	16
C	1.425534	1	119.147167	1	23.817488	1	30	22	16
C	1.420491	1	103.312547	1	-14.977967	1	30	29	35
C	1.365025	1	120.249022	1	164.509510	1	34	28	21
C	1.425925	1	118.846421	1	-144.989511	1	35	29	22
C	1.420486	1	105.455485	1	-9.991531	1	35	22	30
C	1.421842	1	120.720811	1	164.295664	1	36	30	22
C	1.374406	1	122.696251	1	-165.866789	1	37	30	22
C	1.421499	1	120.391227	1	165.609664	1	39	35	29
C	1.375324	1	122.403911	1	-168.249121	1	40	35	29
C	1.372306	1	120.725440	1	7.340549	1	41	36	30
C	1.373003	1	120.657340	1	9.198084	1	43	39	35
H	1.129569	1	107.330454	1	111.510705	1	7	3	1
H	1.117215	1	112.048554	1	124.689151	1	13	7	3
H	1.119440	1	109.095141	1	-116.472347	1	13	7	3
H	1.117420	1	110.270170	1	124.347134	1	14	8	3
H	1.118066	1	110.231621	1	-116.790263	1	14	8	3
H	1.125300	1	108.738620	1	-119.156961	1	8	3	1
H	1.124097	1	109.432862	1	-1.311777	1	8	3	1
H	1.103458	1	119.357322	1	1.397426	1	18	11	6
H	1.100044	1	119.643071	1	179.927340	1	25	18	11
H	1.099540	1	120.082088	1	-179.897585	1	32	24	17
H	1.099747	1	119.776253	1	179.870322	1	24	17	11
H	1.101273	1	120.260270	1	-0.775438	1	17	11	6
H	1.103172	1	119.459715	1	0.130361	1	20	12	6
H	1.099892	1	119.682409	1	-179.795785	1	27	20	12
H	1.099454	1	120.143992	1	179.790740	1	33	26	19
H	1.099771	1	119.730704	1	179.966822	1	26	19	12
H	1.100929	1	120.046135	1	0.239782	1	19	12	6
H	1.201320	1	111.438592	1	103.767722	1	9	3	1
H	1.133085	1	109.435000	1	-31.271408	1	10	5	1
H	1.202151	1	112.912058	1	-116.053201	1	9	3	1
H	1.109001	1	109.082201	1	-160.243105	1	4	1	2
H	1.108764	1	108.953200	1	77.973743	1	4	1	2
H	1.109810	1	105.946294	1	-41.223934	1	4	1	2
H	1.102327	1	118.825989	1	-8.319315	1	23	16	10
H	1.099611	1	121.675296	1	-171.367021	1	31	23	16
H	1.100379	1	118.247000	1	-174.938241	1	41	36	30
H	1.098886	1	121.454439	1	-178.062762	1	45	41	36
H	1.099935	1	120.292225	1	178.542067	1	42	37	30
H	1.098942	1	118.114409	1	25.522180	1	37	30	22
H	1.099333	1	118.518259	1	21.993063	1	40	35	29
H	1.099704	1	120.352699	1	178.225356	1	44	40	35
H	1.098613	1	121.413600	1	-178.138943	1	46	43	39
H	1.100279	1	118.343114	1	-172.423620	1	43	39	35
H	1.099359	1	121.705648	1	-170.294890	1	38	34	28
H	1.101036	1	118.563549	1	-9.566766	1	34	28	21

TS (R,M)-9 --> (R,M)-10 HEAT OF FORMATION = -17.048852 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.464569	1	.000000	0	.000000	0	1	0	0
N	1.605648	1	106.685826	1	.000000	0	1	2	0
C	1.561063	1	115.146252	1	-135.112553	1	1	2	3
O	1.532236	1	109.487848	1	104.012926	1	1	2	3
C	1.435757	1	111.983272	1	7.800844	1	2	1	3
C	1.497608	1	105.140819	1	2.057828	1	3	1	2
C	1.477047	1	119.344453	1	-119.646358	1	3	1	2
B	1.996200	1	41.014905	1	88.184950	1	5	3	8
C	1.397741	1	120.400476	1	92.024053	1	5	1	3
C	1.515221	1	107.827196	1	-132.436868	1	6	2	1
C	1.515379	1	108.486519	1	109.447555	1	6	2	1
C	1.533036	1	108.231213	1	-137.426848	1	7	3	1
C	1.533656	1	109.137085	1	125.175567	1	8	3	1
O	1.448055	1	94.473557	1	-93.936120	1	10	5	1
C	1.504012	1	110.931127	1	145.108003	1	10	5	1
C	1.400249	1	121.335759	1	154.487387	1	11	6	2
C	1.400525	1	119.452804	1	-26.948554	1	11	6	2
C	1.401768	1	121.116972	1	158.892241	1	12	6	2
C	1.400374	1	120.154674	1	-18.743869	1	12	6	2
C	1.428675	1	118.154762	1	-128.111042	1	15	10	5
C	1.387339	1	122.950211	1	160.708677	1	16	10	5
C	1.421159	1	116.806478	1	-21.841535	1	16	10	5
C	1.393891	1	120.350106	1	178.581830	1	17	11	6
C	1.394185	1	120.305978	1	-178.593986	1	18	11	6
C	1.393502	1	120.627956	1	-179.052015	1	19	12	6
C	1.394250	1	120.620294	1	179.038562	1	20	12	6
C	1.494547	1	108.961733	1	-65.896328	1	21	15	10
C	1.468816	1	120.798740	1	.140347	1	22	16	10
C	1.434789	1	119.373905	1	-176.631341	1	22	16	10
C	1.369212	1	120.913934	1	-179.840407	1	23	16	10
C	1.394442	1	120.186647	1	-.039187	1	24	17	11
C	1.394468	1	120.230029	1	.531766	1	26	19	12
C	1.415770	1	119.615674	1	-106.214634	1	28	21	15
C	1.430828	1	121.782323	1	127.311211	1	29	22	16
C	1.418603	1	119.499178	1	-5.637328	1	30	22	16
C	1.424051	1	122.359007	1	172.244179	1	30	22	16
C	1.371251	1	120.371720	1	174.366783	1	34	28	21
C	1.419613	1	119.151248	1	175.003752	1	35	29	22
C	1.423772	1	122.377792	1	-6.884939	1	35	29	22
C	1.422199	1	119.721575	1	-179.558697	1	36	30	22
C	1.373101	1	121.102445	1	-179.608169	1	37	30	22
C	1.422538	1	119.460510	1	-179.907673	1	39	35	29
C	1.372805	1	120.938873	1	-179.243497	1	40	35	29
C	1.372284	1	120.651180	1	-1.567043	1	41	36	30
C	1.372307	1	120.657899	1	-1.372732	1	43	39	35
H	1.130776	1	106.977101	1	104.548401	1	7	3	1
H	1.116761	1	111.961991	1	130.801667	1	13	7	3
H	1.119767	1	109.124067	1	-110.406117	1	13	7	3
H	1.117483	1	110.409242	1	121.401414	1	14	8	3
H	1.118081	1	110.089386	1	-119.702208	1	14	8	3
H	1.125455	1	108.808115	1	-113.995782	1	8	3	1
H	1.123679	1	109.500392	1	3.892971	1	8	3	1
H	1.102270	1	119.300785	1	1.364603	1	18	11	6
H	1.099901	1	119.755939	1	-179.880054	1	25	18	11
H	1.099414	1	120.114150	1	179.913326	1	32	24	17
H	1.099563	1	119.783903	1	179.935034	1	24	17	11
H	1.101171	1	120.146420	1	-1.183139	1	17	11	6
H	1.102798	1	119.336800	1	.313869	1	20	12	6
H	1.099805	1	119.686752	1	180.005860	1	27	20	12
H	1.099340	1	120.171382	1	179.875264	1	33	26	19
H	1.099701	1	119.734337	1	-179.955748	1	26	19	12
H	1.101187	1	120.046947	1	.196194	1	19	12	6
H	1.127186	1	114.366146	1	16.987754	1	10	5	1
H	1.210011	1	110.407530	1	-147.805003	1	9	3	1
H	1.198421	1	116.568211	1	71.122786	1	9	3	1
H	1.108326	1	108.876927	1	-169.038666	1	4	1	2
H	1.108018	1	110.161288	1	69.037036	1	4	1	2
H	1.109359	1	105.718359	1	-50.241621	1	4	1	2
H	1.103807	1	118.152125	1	.580202	1	23	16	10
H	1.100452	1	120.835402	1	179.236444	1	31	23	16
H	1.100439	1	118.436172	1	178.883861	1	41	36	30
H	1.099792	1	120.839362	1	-179.811365	1	45	41	36
H	1.100075	1	120.441683	1	179.802697	1	42	37	30
H	1.101671	1	118.806504	1	.030078	1	37	30	22
H	1.101971	1	118.479810	1	.622572	1	40	35	29
H	1.100111	1	120.496225	1	179.701864	1	44	40	35
H	1.099908	1	120.776064	1	-179.759123	1	46	43	39
H	1.100378	1	118.464333	1	179.059548	1	43	39	35
H	1.100368	1	120.881517	1	179.209390	1	38	34	28
H	1.100629	1	118.882906	1	-5.254940	1	34	28	21

TS (R,P)-9 --> (R,P)-10 HEAT OF FORMATION = -3.930133 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.471038	1	.000000	0	.000000	0	1	0	0
N	1.631527	1	105.709835	1	.000000	0	1	2	0
C	1.505647	1	104.570126	1	-3.777895	1	3	1	2
C	1.428318	1	112.512805	1	-7.804125	1	2	1	3
C	1.477948	1	117.440683	1	-123.177677	1	3	1	2
C	1.533190	1	109.259523	1	114.666229	1	6	3	1
C	1.521013	1	106.079539	1	-8.454128	1	7	6	3
C	1.557752	1	111.050068	1	-130.450787	1	1	2	3
C	1.514215	1	107.787222	1	138.652508	1	5	2	1
C	1.400994	1	119.643308	1	14.089182	1	10	5	2
C	1.400607	1	121.418339	1	-168.129294	1	10	5	2
C	1.393558	1	120.561294	1	-177.715273	1	12	10	5
C	1.394393	1	120.432972	1	177.878115	1	11	10	5
C	1.393798	1	120.286138	1	-.158949	1	14	11	10
C	1.519073	1	109.941025	1	-103.243469	1	5	2	1
C	1.400493	1	119.659547	1	-9.050249	1	16	5	2
C	1.399898	1	121.382063	1	172.093135	1	16	5	2
C	1.393976	1	120.518184	1	178.363907	1	18	16	5
C	1.394007	1	120.448954	1	-178.287205	1	17	16	5
C	1.394076	1	120.250680	1	-.224807	1	20	17	16
O	1.514952	1	100.313062	1	102.407847	1	1	2	3
C	1.385238	1	123.856167	1	151.608579	1	22	1	2
O	1.432807	1	96.579307	1	85.830863	1	23	22	1
C	1.504391	1	121.553058	1	-43.958187	1	23	22	1
C	1.384951	1	128.319804	1	114.025030	1	25	23	22
C	1.423700	1	118.266466	1	-166.974441	1	24	23	22
C	1.492131	1	109.340385	1	86.600033	1	27	24	23
C	1.384610	1	119.951359	1	-61.481915	1	28	27	24
C	1.435749	1	118.821955	1	167.191307	1	29	28	27
C	1.441662	1	118.775939	1	160.556842	1	26	25	23
C	1.429073	1	111.837058	1	-72.739305	1	25	23	22
C	1.365973	1	121.577055	1	-168.143576	1	32	25	23
C	1.421895	1	119.902583	1	3.119862	1	33	32	25
C	1.420691	1	120.920773	1	173.742695	1	34	33	32
C	1.373301	1	120.573593	1	-176.971013	1	35	34	33
C	1.423445	1	122.016380	1	-167.314721	1	31	26	25
C	1.413625	1	119.867026	1	.157048	1	36	35	34
C	1.417290	1	118.947860	1	114.421180	1	28	27	24
C	1.370065	1	120.489660	1	-172.633714	1	39	28	27
C	1.421361	1	120.149526	1	2.987305	1	40	39	28
C	1.423819	1	122.389897	1	-169.869971	1	30	29	28
C	1.422102	1	120.756007	1	175.229718	1	41	40	39
C	1.372518	1	120.651683	1	-176.939841	1	43	41	40
C	1.414799	1	119.982446	1	.225827	1	44	43	41
H	1.127362	1	108.330603	1	129.961931	1	4	3	1
H	1.119421	1	110.138912	1	-103.873688	1	8	7	6
H	1.117041	1	111.473498	1	136.185895	1	8	7	6
H	1.117142	1	110.496467	1	-129.098732	1	7	6	3
H	1.118091	1	110.270545	1	111.828060	1	7	6	3
H	1.125253	1	109.378166	1	-124.368754	1	6	3	1
H	1.123676	1	109.565407	1	-6.305096	1	6	3	1
H	1.139389	1	105.395500	1	-164.987862	1	23	22	1
H	1.108954	1	111.451999	1	178.479299	1	9	1	2
H	1.110571	1	105.440161	1	-61.775755	1	9	1	2
H	1.108607	1	108.168866	1	56.150103	1	9	1	2
H	1.102448	1	119.411125	1	-2.141341	1	11	10	5
H	1.099794	1	119.678521	1	-179.955270	1	14	11	10
H	1.099292	1	120.246460	1	-179.733240	1	15	14	11
H	1.099545	1	119.779180	1	179.762682	1	13	12	10
H	1.099863	1	120.104207	1	2.430043	1	12	10	5
H	1.099725	1	120.465854	1	-1.328870	1	18	16	5
H	1.099421	1	119.771924	1	-179.860900	1	19	18	16
H	1.099201	1	120.241325	1	179.863408	1	21	20	17
H	1.099554	1	119.717158	1	179.895501	1	20	17	16
H	1.103401	1	118.926583	1	3.217432	1	17	16	5
H	1.102946	1	117.704173	1	12.621698	1	32	25	23
H	1.100399	1	121.134318	1	-178.343416	1	33	32	25
H	1.100430	1	118.516667	1	2.464638	1	35	34	33
H	1.099814	1	120.818353	1	179.746555	1	36	35	34
H	1.100174	1	119.145589	1	178.649451	1	38	36	35
H	1.101605	1	118.960651	1	-.120406	1	37	31	26
H	1.102168	1	118.634916	1	.332886	1	42	30	29
H	1.100223	1	119.130277	1	178.611238	1	45	44	43
H	1.099936	1	120.795684	1	179.826910	1	44	43	41
H	1.100405	1	118.471429	1	2.591876	1	43	41	40
H	1.100333	1	121.023108	1	-178.453960	1	40	39	28
H	1.100871	1	118.779487	1	7.276239	1	39	28	27
H	1.122432	1	109.631113	1	-35.875723	1	27	24	23
H	1.123956	1	104.506878	1	-153.702723	1	27	24	23
B	2.116366	1	98.620296	1	-129.210773	1	22	23	25

TS (S,M)-9 --> (S,M)-10 HEAT OF FORMATION = -10.218933 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0	0
O	1.462456	1	.000000	0	.000000	0	1	0	0	
N	1.611816	1	106.774803	1	.000000	0	1	2	0	
C	1.563361	1	112.165222	1	-131.543311	1	1	2	3	
O	1.526367	1	101.883858	1	101.227563	1	1	2	3	
C	1.431494	1	112.679481	1	.857728	1	2	1	3	
C	1.503357	1	105.089762	1	1.771215	1	3	1	2	
C	1.477092	1	117.769647	1	-118.194813	1	3	1	2	
B	2.064599	1	40.616442	1	93.932257	1	5	3	8	
C	1.390798	1	117.039689	1	147.032464	1	5	1	2	
C	1.516626	1	108.385403	1	-122.058496	1	6	2	1	
C	1.517283	1	107.652632	1	119.941993	1	6	2	1	
C	1.535625	1	108.337268	1	-131.167832	1	7	3	1	
C	1.522053	1	106.662738	1	-5.003208	1	13	7	3	
O	1.945667	1	63.666198	1	-6.416466	1	9	5	10	
C	1.503533	1	113.842307	1	-141.740516	1	10	5	1	
C	1.400288	1	121.679415	1	158.853207	1	11	6	2	
C	1.400630	1	119.238171	1	-22.226222	1	11	6	2	
C	1.401329	1	121.303954	1	162.748113	1	12	6	2	
C	1.400947	1	119.978260	1	-15.482376	1	12	6	2	
C	1.429397	1	118.522903	1	117.589834	1	15	10	5	
C	1.385000	1	126.222564	1	-69.087023	1	16	10	5	
C	1.424732	1	113.944700	1	111.183210	1	16	10	5	
C	1.393965	1	120.445384	1	178.527438	1	17	11	6	
C	1.394080	1	120.343630	1	-178.484952	1	18	11	6	
C	1.393601	1	120.627809	1	-178.994140	1	19	12	6	
C	1.394183	1	120.612419	1	178.979159	1	20	12	6	
C	1.492672	1	111.525171	1	-68.046419	1	21	15	10	
C	1.386045	1	119.797551	1	68.904286	1	28	21	15	
C	1.437749	1	119.293910	1	-171.713345	1	22	16	10	
C	1.367842	1	121.272543	1	176.267818	1	23	16	10	
C	1.394149	1	120.266843	1	-.169138	1	25	18	11	
C	1.393726	1	120.256402	1	-.221226	1	27	20	12	
C	1.416836	1	119.464412	1	-108.816369	1	28	21	15	
C	1.431720	1	119.402878	1	-170.911073	1	29	28	21	
C	1.417848	1	119.667442	1	-7.076636	1	30	22	16	
C	1.423785	1	122.264452	1	170.785482	1	30	22	16	
C	1.370803	1	120.428980	1	175.180340	1	34	28	21	
C	1.419503	1	119.136809	1	-6.284891	1	35	29	28	
C	1.423546	1	122.405839	1	171.956358	1	35	29	28	
C	1.421549	1	119.849046	1	-179.494736	1	36	30	22	
C	1.373627	1	121.107246	1	-179.618497	1	37	30	22	
C	1.422241	1	119.485467	1	-179.393963	1	39	35	29	
C	1.373008	1	120.922561	1	-179.825673	1	40	35	29	
C	1.372731	1	120.591131	1	-1.637927	1	41	36	30	
C	1.372437	1	120.638998	1	-1.437008	1	43	39	35	
H	1.130031	1	106.975457	1	111.839729	1	7	3	1	
H	1.118027	1	111.932264	1	115.580128	1	13	7	3	
H	1.118442	1	109.501656	1	-125.324676	1	13	7	3	
H	1.118201	1	110.905707	1	-107.441149	1	14	13	7	
H	1.117050	1	111.344936	1	132.498622	1	14	13	7	
H	1.124073	1	109.715751	1	-107.087435	1	8	3	1	
H	1.124566	1	109.383344	1	11.303254	1	8	3	1	
H	1.102422	1	119.200357	1	2.388966	1	18	11	6	
H	1.099627	1	119.694589	1	-179.948206	1	25	18	11	
H	1.099163	1	120.209954	1	180.023210	1	32	25	18	
H	1.099383	1	119.781923	1	179.955562	1	24	17	11	
H	1.100934	1	120.393580	1	-1.408626	1	17	11	6	
H	1.102670	1	119.348375	1	.064377	1	20	12	6	
H	1.099729	1	119.700626	1	-179.830478	1	27	20	12	
H	1.099268	1	120.263355	1	-179.846399	1	33	27	20	
H	1.099661	1	119.727567	1	179.878832	1	26	19	12	
H	1.100519	1	120.094593	1	.423889	1	19	12	6	
H	1.130172	1	114.205748	1	-15.148327	1	10	5	1	
H	1.196731	1	117.602156	1	-86.071417	1	9	3	1	
H	1.209905	1	109.211848	1	127.871124	1	9	3	1	
H	1.108432	1	111.405549	1	173.046351	1	4	1	2	
H	1.109391	1	107.915398	1	51.860340	1	4	1	2	
H	1.109708	1	106.405134	1	-65.885849	1	4	1	2	
H	1.102140	1	118.651130	1	-4.491924	1	23	16	10	
H	1.100455	1	120.982547	1	178.787980	1	31	23	16	
H	1.100402	1	118.495748	1	178.766984	1	41	36	30	
H	1.099859	1	120.825355	1	-179.851779	1	45	41	36	
H	1.100177	1	120.402873	1	179.820098	1	42	37	30	
H	1.101820	1	118.881247	1	.060664	1	37	30	22	
H	1.101768	1	118.521965	1	-.451513	1	40	35	29	
H	1.099982	1	120.474038	1	179.593398	1	44	40	35	
H	1.099811	1	120.761226	1	-179.705612	1	46	43	39	
H	1.100259	1	118.480011	1	179.158221	1	43	39	35	
H	1.100299	1	120.900536	1	179.101210	1	38	34	28	
H	1.100579	1	118.845218	1	-4.396636	1	34	28	21	

TS (S,P)-9 --> (S,P)-10 HEAT OF FORMATION = -15.703023 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.459726	1	.000000	0	.000000	0	1	0	0
N	1.613015	1	106.827856	1	.000000	0	1	2	0
C	1.502216	1	105.058588	1	3.785526	1	3	1	2
C	1.432087	1	112.669306	1	-2.339702	1	2	1	3
C	1.476674	1	117.714691	1	-116.368756	1	3	1	2
C	1.532950	1	109.017701	1	129.322932	1	6	3	1
C	1.521972	1	106.377001	1	-12.428128	1	7	6	3
C	1.560482	1	112.901076	1	-132.726158	1	1	2	3
C	1.516280	1	107.325299	1	122.581279	1	5	2	1
C	1.401506	1	119.724113	1	-19.028733	1	10	5	2
C	1.400790	1	121.515194	1	159.632722	1	10	5	2
C	1.393886	1	120.581099	1	-179.250270	1	12	10	5
C	1.393932	1	120.591151	1	179.204752	1	11	10	5
C	1.393951	1	120.238465	1	-.120649	1	14	11	10
C	1.516655	1	108.391857	1	-118.857411	1	5	2	1
C	1.400817	1	119.285377	1	-21.071279	1	16	5	2
C	1.400423	1	121.703032	1	159.508367	1	16	5	2
C	1.394047	1	120.471923	1	179.181811	1	18	16	5
C	1.394068	1	120.395738	1	-179.096242	1	17	16	5
C	1.394194	1	120.260126	1	-.185356	1	20	17	16
O	1.531452	1	96.208640	1	-100.365754	1	1	3	4
C	1.392895	1	117.862311	1	143.022414	1	22	1	2
O	1.448835	1	95.032530	1	83.518869	1	23	22	1
C	1.504478	1	111.266866	1	-156.323630	1	23	22	1
C	1.387871	1	121.542184	1	-167.452415	1	25	23	22
C	1.428767	1	117.859460	1	138.021196	1	24	23	22
C	1.495011	1	109.524973	1	59.452671	1	27	24	23
C	1.387829	1	119.724615	1	-71.387244	1	28	27	24
C	1.430357	1	119.455494	1	171.611855	1	29	28	27
C	1.432712	1	119.407895	1	176.925123	1	26	25	23
C	1.419046	1	117.919439	1	14.679192	1	25	23	22
C	1.370291	1	120.586214	1	179.948010	1	32	25	23
C	1.420184	1	120.420034	1	1.579499	1	33	32	25
C	1.422572	1	120.867095	1	177.044813	1	34	33	32
C	1.372117	1	120.672557	1	-177.513509	1	35	34	33
C	1.424033	1	122.396510	1	-173.124626	1	31	26	25
C	1.415143	1	119.968635	1	.146489	1	36	35	34
C	1.415810	1	119.500823	1	106.054587	1	28	27	24
C	1.371339	1	120.389990	1	-175.022177	1	39	28	27
C	1.420881	1	120.383464	1	1.831624	1	40	39	28
C	1.423772	1	122.369447	1	-173.063771	1	30	29	28
C	1.422555	1	120.894576	1	176.468228	1	41	40	39
C	1.372302	1	120.647305	1	-177.720782	1	43	41	40
C	1.415449	1	120.072653	1	-.007719	1	44	43	41
H	1.129677	1	107.006703	1	111.712125	1	4	3	1
H	1.118062	1	110.375618	1	-112.719354	1	8	7	6
H	1.118759	1	110.958824	1	128.340358	1	8	7	6
H	1.117326	1	110.274046	1	-133.146171	1	7	6	3
H	1.118185	1	110.341095	1	107.924272	1	7	6	3
H	1.124435	1	109.591377	1	-109.185995	1	6	3	1
H	1.124501	1	109.322133	1	8.956282	1	6	3	1
H	1.123643	1	115.188992	1	-28.518771	1	23	22	1
H	1.108214	1	110.506490	1	177.854211	1	9	1	2
H	1.109736	1	106.437844	1	-61.547453	1	9	1	2
H	1.109203	1	108.304650	1	56.305688	1	9	1	2
H	1.102845	1	119.329464	1	.214818	1	11	10	5
H	1.099761	1	119.715411	1	-179.759441	1	14	11	10
H	1.099325	1	120.245630	1	-179.849485	1	15	14	11
H	1.099703	1	119.707320	1	179.856930	1	13	12	10
H	1.100469	1	120.204713	1	.125610	1	12	10	5
H	1.101039	1	120.357547	1	-.714392	1	18	16	5
H	1.099560	1	119.777513	1	179.960722	1	19	18	16
H	1.099304	1	120.220255	1	179.988063	1	21	20	17
H	1.099725	1	119.726832	1	179.788223	1	20	17	16
H	1.102539	1	119.163601	1	1.595592	1	17	16	5
H	1.104875	1	118.261398	1	-.474461	1	32	25	23
H	1.100513	1	120.751820	1	-179.435584	1	33	32	25
H	1.100481	1	118.418027	1	2.066317	1	35	34	33
H	1.099843	1	120.825554	1	179.806992	1	36	35	34
H	1.100069	1	119.094716	1	178.966642	1	38	36	35
H	1.101696	1	118.714445	1	-.209659	1	37	31	26
H	1.102056	1	118.485159	1	-.778828	1	42	30	29
H	1.100187	1	119.094527	1	179.158592	1	45	44	43
H	1.099984	1	120.769342	1	179.726561	1	44	43	41
H	1.100430	1	118.471791	1	1.852618	1	43	41	40
H	1.100490	1	120.867603	1	-179.323676	1	40	39	28
H	1.100729	1	118.886736	1	4.624523	1	39	28	27
H	1.123019	1	109.526671	1	-62.941302	1	27	24	23
H	1.123299	1	104.317078	1	179.429581	1	27	24	23
B	2.038344	1	99.370926	1	116.776448	1	22	23	25

(R,M)-10 Heat of formation = -21.424672 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.476565	1	0.000000	0	0.000000	0	1	0	0
N	1.636957	1	105.070679	1	0.000000	0	1	2	0
C	1.567076	1	114.615587	1	-128.719988	1	1	2	3
O	1.502942	1	103.351678	1	117.792399	1	1	2	3
C	1.427200	1	113.533812	1	-1.267999	1	2	1	3
C	1.505247	1	104.531239	1	10.201485	1	3	1	2
C	1.491791	1	113.259138	1	-104.206027	1	3	1	2
B	1.547791	1	113.066695	1	133.092545	1	3	1	2
C	1.370802	1	118.190509	1	37.990015	1	5	1	3
C	1.516462	1	108.149458	1	-126.275269	1	6	2	1
C	1.517035	1	108.353699	1	115.457518	1	6	2	1
C	1.535193	1	108.008662	1	-141.684023	1	7	3	1
C	1.534070	1	108.582714	1	136.350567	1	8	3	1
O	1.489450	1	98.624599	1	-78.786418	1	10	5	1
C	1.504086	1	112.383364	1	165.900896	1	10	5	1
C	1.400202	1	121.504416	1	156.218612	1	11	6	2
C	1.400480	1	119.251471	1	-25.618585	1	11	6	2
C	1.401468	1	121.474850	1	157.404595	1	12	6	2
C	1.400683	1	119.845024	1	-20.312676	1	12	6	2
C	1.440037	1	116.622893	1	-163.248198	1	15	10	5
C	1.389380	1	120.380922	1	179.923450	1	16	10	5
C	1.417088	1	118.897557	1	-0.943106	1	16	10	5
C	1.393849	1	120.355768	1	177.766494	1	17	11	6
C	1.394157	1	120.275304	1	-177.883021	1	18	11	6
C	1.393790	1	120.639088	1	-179.020977	1	19	12	6
C	1.394102	1	120.668426	1	178.982756	1	20	12	6
C	1.490549	1	113.502821	1	-38.783184	1	21	15	10
C	1.469083	1	119.246429	1	1.582178	1	22	16	10
C	1.430990	1	119.379963	1	-175.561619	1	22	16	10
C	1.371026	1	120.378554	1	178.934397	1	23	16	10
C	1.394514	1	120.160498	1	0.114676	1	24	17	11
C	1.394275	1	120.251887	1	0.524912	1	26	19	12
C	1.416628	1	119.049402	1	-110.802192	1	28	21	15
C	1.430519	1	121.973672	1	126.612794	1	29	22	16
C	1.419651	1	119.217674	1	-4.977715	1	30	22	16
C	1.424075	1	122.439245	1	172.915008	1	30	22	16
C	1.370903	1	120.423072	1	-178.878074	1	34	28	21
C	1.419840	1	119.149469	1	177.857790	1	35	29	22
C	1.423719	1	122.424857	1	-3.445379	1	35	29	22
C	1.422793	1	119.515419	1	-179.769778	1	36	30	22
C	1.372585	1	121.027770	1	-179.411536	1	37	30	22
C	1.422507	1	119.492866	1	-178.890461	1	39	35	29
C	1.372944	1	120.932997	1	179.490523	1	40	35	29
C	1.372022	1	120.692716	1	-1.471293	1	41	36	30
C	1.372378	1	120.632444	1	-1.317704	1	43	39	35
H	1.128687	1	107.449706	1	100.757181	1	7	3	1
H	1.116603	1	111.777297	1	134.914977	1	13	7	3
H	1.119589	1	109.196822	1	-106.287912	1	13	7	3
H	1.117792	1	110.597340	1	105.836817	1	14	8	3
H	1.117403	1	110.059041	1	-135.066353	1	14	8	3
H	1.122907	1	109.641716	1	-101.580558	1	8	3	1
H	1.124243	1	109.090102	1	17.018349	1	8	3	1
H	1.102694	1	119.172120	1	2.402964	1	18	11	6
H	1.099801	1	119.711456	1	179.942439	1	25	18	11
H	1.099349	1	120.055867	1	-179.894033	1	32	24	17
H	1.099482	1	119.817723	1	180.063394	1	24	17	11
H	1.101183	1	120.125760	1	-1.797094	1	17	11	6
H	1.102346	1	119.241302	1	0.379541	1	20	12	6
H	1.099766	1	119.696342	1	-179.858615	1	27	20	12
H	1.099324	1	120.182939	1	179.812960	1	33	26	19
H	1.099708	1	119.715645	1	180.011447	1	26	19	12
H	1.101041	1	120.150532	1	0.197990	1	19	12	6
H	1.125785	1	115.289732	1	35.586142	1	10	5	1
H	1.204667	1	112.609868	1	-140.832756	1	9	3	1
H	1.202132	1	112.899355	1	75.172251	1	9	3	1
H	1.107995	1	109.493010	1	167.768933	1	4	1	2
H	1.107530	1	110.160928	1	45.248477	1	4	1	2
H	1.110253	1	105.603679	1	-73.455121	1	4	1	2
H	1.103782	1	118.188638	1	-1.019745	1	23	16	10
H	1.100588	1	120.744506	1	179.189941	1	31	23	16
H	1.100568	1	118.408982	1	178.944599	1	41	36	30
H	1.099881	1	120.818106	1	-179.795319	1	45	41	36
H	1.100111	1	120.502104	1	179.783991	1	42	37	30
H	1.101709	1	118.644570	1	0.336919	1	37	30	22
H	1.102187	1	118.553777	1	-0.715402	1	40	35	29
H	1.100198	1	120.461149	1	179.985225	1	44	40	35
H	1.100077	1	120.761365	1	179.974969	1	46	43	39
H	1.100406	1	118.482207	1	178.954743	1	43	39	35
H	1.100560	1	120.853695	1	179.068205	1	38	34	28
H	1.101216	1	118.799240	1	1.174584	1	34	28	21

(S,M)-10 HEAT OF FORMATION = -16.854443 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0	.1574
O	1.469861	1	.000000	0	.000000	0	1	0	0	-.3113
N	1.645326	1	105.179724	1	.000000	0	1	2	0	-.1333
C	1.568859	1	111.883450	1	-127.468707	1	1	2	3	-.2769
O	1.508833	1	100.574763	1	112.564194	1	1	2	3	-.3088
C	1.428560	1	112.252838	1	16.968348	1	2	1	3	.1939
C	1.508896	1	103.330239	1	-18.431570	1	3	1	2	-.0551
C	1.482113	1	116.192452	1	-135.847967	1	3	1	2	-.0991
B	1.545707	1	108.587758	1	95.918538	1	3	1	2	.1405
C	1.373363	1	113.061961	1	-172.014326	1	5	1	2	.2182
C	1.518487	1	107.906158	1	-128.118979	1	6	2	1	-.0762
C	1.517097	1	108.584084	1	114.270768	1	6	2	1	-.0837
C	1.536070	1	107.765926	1	-112.795872	1	7	3	1	-.1714
C	1.520999	1	106.056608	1	-18.096659	1	13	7	3	-.1719
O	1.761757	1	57.501903	1	-17.036288	1	9	5	10	-.2624
C	1.503191	1	113.501109	1	-153.728619	1	10	5	1	-.0896
C	1.399933	1	121.951185	1	160.737266	1	11	6	2	-.1372
C	1.401299	1	119.029958	1	-20.846397	1	11	6	2	-.0814
C	1.400881	1	121.184592	1	172.193826	1	12	6	2	-.1272
C	1.400762	1	119.944400	1	-6.129420	1	12	6	2	-.1009
C	1.443726	1	117.580953	1	98.723644	1	15	10	5	.0269
C	1.385710	1	124.632819	1	-58.997968	1	16	10	5	.0132
C	1.422013	1	115.187170	1	120.245819	1	16	10	5	-.1143
C	1.394321	1	120.481362	1	178.167569	1	17	11	6	-.1398
C	1.393967	1	120.378030	1	-178.074943	1	18	11	6	-.1364
C	1.393429	1	120.586394	1	-178.364835	1	19	12	6	-.1393
C	1.394361	1	120.484359	1	178.343591	1	20	12	6	-.1399
C	1.489997	1	113.373233	1	-54.030113	1	21	15	10	-.1004
C	1.387166	1	120.011105	1	70.980684	1	28	21	15	.0080
C	1.434909	1	119.441998	1	-174.889786	1	22	16	10	-.0350
C	1.368959	1	120.929041	1	178.450012	1	23	16	10	-.1171
C	1.394227	1	120.285896	1	-.199688	1	25	18	11	-.1332
C	1.393777	1	120.271109	1	.017124	1	27	20	12	-.1301
C	1.416867	1	119.392052	1	-108.583929	1	28	21	15	-.1032
C	1.430197	1	119.621215	1	-174.040567	1	29	28	21	-.0200
C	1.418525	1	119.469109	1	-5.496416	1	30	22	16	-.0303
C	1.423738	1	122.340296	1	172.510798	1	30	22	16	-.1120
C	1.371094	1	120.399518	1	178.037660	1	34	28	21	-.1104
C	1.419455	1	119.059477	1	-5.691363	1	35	29	28	-.0272
C	1.423611	1	122.421283	1	172.439720	1	35	29	28	-.1067
C	1.421855	1	119.732085	1	-179.572460	1	36	30	22	-.1244
C	1.373302	1	121.052644	1	-179.616909	1	37	30	22	-.1302
C	1.422483	1	119.425574	1	-179.291150	1	39	35	29	-.1247
C	1.372846	1	120.906248	1	-179.746527	1	40	35	29	-.1312
C	1.372605	1	120.604198	1	-1.505642	1	41	36	30	-.1196
C	1.372402	1	120.647768	1	-1.670726	1	43	39	35	-.1223
H	1.129037	1	107.311965	1	130.575331	1	7	3	1	.1169
H	1.119352	1	111.394913	1	101.376598	1	13	7	3	.1174
H	1.117078	1	109.863977	1	-139.129426	1	13	7	3	.0954
H	1.118164	1	110.992918	1	-101.380839	1	14	13	7	.0887
H	1.116930	1	111.306867	1	138.473575	1	14	13	7	.0979
H	1.125366	1	109.176038	1	-122.923430	1	8	3	1	.1040
H	1.122757	1	110.008744	1	-4.999638	1	8	3	1	.1111
H	1.103177	1	119.244784	1	2.744066	1	18	11	6	.1678
H	1.099737	1	119.629737	1	179.884786	1	25	18	11	.1300
H	1.099164	1	120.238612	1	179.825023	1	32	25	18	.1245
H	1.099437	1	119.748990	1	-179.924264	1	24	17	11	.1243
H	1.100578	1	120.662000	1	-1.699105	1	17	11	6	.1192
H	1.103713	1	119.255649	1	-1.305870	1	20	12	6	.1620
H	1.099763	1	119.673812	1	-179.696885	1	27	20	12	.1294
H	1.099295	1	120.246923	1	-179.746015	1	33	27	20	.1274
H	1.099595	1	119.778833	1	179.734276	1	26	19	12	.1273
H	1.100020	1	119.977033	1	1.249526	1	19	12	6	.1291
H	1.134173	1	114.085890	1	-26.116447	1	10	5	1	.1040
H	1.199334	1	113.264834	1	-61.470904	1	9	3	1	-.0114
H	1.205260	1	113.652920	1	151.848601	1	9	3	1	-.0636
H	1.107811	1	112.299703	1	-170.761737	1	4	1	2	.0482
H	1.108559	1	109.334241	1	65.845762	1	4	1	2	.0679
H	1.110965	1	104.186077	1	-51.786573	1	4	1	2	.0926
H	1.101637	1	118.893797	1	-2.083138	1	23	16	10	.1369
H	1.100521	1	120.907857	1	178.967717	1	31	23	16	.1372
H	1.100421	1	118.497961	1	178.846165	1	41	36	30	.1342
H	1.099918	1	120.806726	1	-179.872183	1	45	41	36	.1342
H	1.100243	1	120.431077	1	179.870268	1	42	37	30	.1357
H	1.102004	1	118.778287	1	.222984	1	37	30	22	.1489
H	1.101723	1	118.509085	1	-.407523	1	40	35	29	.1465
H	1.100025	1	120.496892	1	179.478576	1	44	40	35	.1340
H	1.099872	1	120.769130	1	-179.650769	1	46	43	39	.1318
H	1.100361	1	118.454277	1	178.976635	1	43	39	35	.1322
H	1.100471	1	120.803858	1	179.372324	1	38	34	28	.1361
H	1.100708	1	118.925401	1	-1.283662	1	34	28	21	.1360

(R,P)-10 Heat of formation = -10.362621 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.478808	1	0.000000	0	0.000000	0	1	0	0
N	1.652420	1	105.476433	1	0.000000	0	1	2	0
C	1.512122	1	103.040238	1	-8.895966	1	3	1	2
C	1.425336	1	112.132962	1	-7.021764	1	2	1	3
C	1.481790	1	114.824672	1	-124.510436	1	3	1	2
C	1.530637	1	109.443666	1	97.658527	1	6	3	1
C	1.520779	1	106.359128	1	8.060324	1	7	6	3
B	1.535477	1	109.548615	1	106.800521	1	3	1	2
C	1.563608	1	110.742821	1	-126.706071	1	1	2	3
C	1.513635	1	107.982457	1	142.304652	1	5	2	1
C	1.400832	1	119.476147	1	19.155073	1	11	5	2
C	1.400474	1	121.448728	1	-163.053487	1	11	5	2
C	1.393648	1	120.481757	1	-177.594988	1	13	11	5
C	1.394375	1	120.352101	1	177.776375	1	12	11	5
C	1.393972	1	120.273230	1	-0.138435	1	15	12	11
C	1.519253	1	110.524158	1	-99.505366	1	5	2	1
C	1.400287	1	119.816949	1	-6.851895	1	17	5	2
C	1.399966	1	121.158625	1	174.637570	1	17	5	2
C	1.393883	1	120.508575	1	178.433977	1	19	17	5
C	1.394169	1	120.384513	1	-178.322418	1	18	17	5
C	1.394059	1	120.279002	1	-0.127639	1	21	18	17
O	1.501900	1	98.175059	1	112.234828	1	1	2	3
C	1.368287	1	121.999395	1	-177.655679	1	23	1	2
O	1.455715	1	103.312792	1	67.669646	1	24	23	1
C	1.511313	1	118.795431	1	-65.442672	1	24	23	1
C	1.383635	1	129.796518	1	112.397392	1	26	24	23
C	1.435715	1	117.023151	1	-160.223809	1	25	24	23
C	1.488878	1	110.509735	1	84.269818	1	28	25	24
C	1.384790	1	119.561968	1	-65.443719	1	29	28	25
C	1.434435	1	118.981263	1	168.901686	1	30	29	28
C	1.441384	1	119.057160	1	163.669616	1	27	26	24
C	1.430236	1	110.772137	1	-71.881727	1	26	24	23
C	1.365735	1	121.646761	1	-170.856965	1	33	26	24
C	1.421735	1	119.961761	1	3.103371	1	34	33	26
C	1.420605	1	120.931562	1	173.975937	1	35	34	33
C	1.373324	1	120.563288	1	-176.862316	1	36	35	34
C	1.423383	1	122.119133	1	-167.477295	1	32	27	26
C	1.413592	1	119.851445	1	0.178270	1	37	36	35
C	1.417310	1	119.372152	1	111.603063	1	29	28	25
C	1.370572	1	120.359098	1	-174.494307	1	40	29	28
C	1.421820	1	120.227946	1	3.275215	1	41	40	29
C	1.423531	1	122.374174	1	-170.235364	1	31	30	29
C	1.422035	1	120.819664	1	175.459268	1	42	41	40
C	1.372761	1	120.621276	1	-176.860467	1	44	42	41
C	1.414844	1	120.056336	1	0.196924	1	45	44	42
H	1.126577	1	108.732174	1	137.782507	1	4	3	1
H	1.119396	1	110.027518	1	-117.616116	1	8	7	6
H	1.117591	1	111.319889	1	122.739674	1	8	7	6
H	1.118491	1	110.257288	1	-112.031114	1	7	6	3
H	1.117367	1	110.268207	1	129.015127	1	7	6	3
H	1.127930	1	109.062654	1	-142.132365	1	6	3	1
H	1.123725	1	110.018134	1	-24.986836	1	6	3	1
H	1.142383	1	105.715808	1	175.346316	1	24	23	1
H	1.203615	1	114.199110	1	143.309368	1	9	3	1
H	1.199957	1	113.675661	1	-65.769851	1	9	3	1
H	1.109057	1	111.151615	1	-171.463581	1	10	1	2
H	1.110153	1	104.834455	1	-52.185667	1	10	1	2
H	1.108711	1	109.041797	1	65.759244	1	10	1	2
H	1.102419	1	119.314396	1	-2.380744	1	12	11	5
H	1.099782	1	119.687129	1	-179.965244	1	15	12	11
H	1.099310	1	120.219387	1	-179.730763	1	16	15	12
H	1.099514	1	119.800552	1	179.766343	1	14	13	11
H	1.100060	1	120.032904	1	2.737761	1	13	11	5
H	1.099864	1	120.344229	1	-0.945580	1	19	17	5
H	1.099358	1	119.792228	1	-179.925185	1	20	19	17
H	1.099174	1	120.239379	1	179.904017	1	22	21	18
H	1.099498	1	119.685176	1	179.912849	1	21	18	17
H	1.104527	1	118.925438	1	3.016552	1	18	17	5
H	1.103317	1	117.758874	1	10.245874	1	33	26	24
H	1.100565	1	121.091560	1	-178.265386	1	34	33	26
H	1.100488	1	118.526827	1	2.571053	1	36	35	34
H	1.099838	1	120.824210	1	179.746416	1	37	36	35
H	1.100253	1	119.141194	1	178.574995	1	39	37	36
H	1.101528	1	119.029035	1	0.005070	1	38	32	27
H	1.102293	1	118.613475	1	0.542538	1	43	31	30
H	1.100337	1	119.146991	1	178.627453	1	46	45	44
H	1.100130	1	120.747398	1	179.817812	1	45	44	42
H	1.100449	1	118.498285	1	2.685527	1	44	42	41
H	1.100458	1	120.974045	1	-178.145756	1	41	40	29
H	1.101019	1	118.793831	1	5.410082	1	40	29	28

(S,P)-10 Heat of formation = -21.326416 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.461535	1	0.000000	0	0.000000	0	1	0	0	0
N	1.640571	1	105.879794	1	0.000000	0	1	2	0	0
C	1.505212	1	104.066766	1	12.653564	1	3	1	2	0
C	1.430341	1	112.959443	1	-8.430723	1	2	1	3	0
C	1.482773	1	114.775451	1	-103.452097	1	3	1	2	0
C	1.534094	1	108.697042	1	134.371530	1	6	3	1	0
C	1.523016	1	106.201360	1	-14.308432	1	7	6	3	0
B	1.543353	1	107.379242	1	129.887842	1	3	1	2	0
C	1.564684	1	113.251761	1	-128.729919	1	1	2	3	0
C	1.516882	1	107.141236	1	123.439655	1	5	2	1	0
C	1.401537	1	119.582747	1	-23.086773	1	11	5	2	0
C	1.400766	1	121.670771	1	155.397454	1	11	5	2	0
C	1.394100	1	120.572994	1	-179.268574	1	13	11	5	0
C	1.393817	1	120.623183	1	179.191188	1	12	11	5	0
C	1.394055	1	120.218704	1	-0.150290	1	15	12	11	0
C	1.516218	1	108.540463	1	-117.719221	1	5	2	1	0
C	1.400517	1	119.345892	1	-21.408079	1	17	5	2	0
C	1.400505	1	121.564534	1	158.868894	1	17	5	2	0
C	1.393938	1	120.444621	1	179.590370	1	19	17	5	0
C	1.394216	1	120.332981	1	-179.542085	1	18	17	5	0
C	1.394204	1	120.266229	1	-0.092434	1	21	18	17	0
O	1.515480	1	104.959846	1	-92.814535	1	1	3	4	0
C	1.373386	1	115.922862	1	164.225283	1	23	1	2	0
O	1.764051	1	58.282746	1	10.963637	1	9	23	24	0
C	1.506285	1	110.944816	1	176.491621	1	24	23	1	0
C	1.388645	1	120.872046	1	178.927080	1	26	24	23	0
C	1.442144	1	115.894590	1	148.448972	1	25	24	23	0
C	1.493321	1	109.466120	1	55.119052	1	28	25	24	0
C	1.388187	1	119.959647	1	-74.337140	1	29	28	25	0
C	1.429631	1	119.580652	1	173.904979	1	30	29	28	0
C	1.431277	1	119.604793	1	177.716487	1	27	26	24	0
C	1.418335	1	118.626247	1	1.162964	1	26	24	23	0
C	1.370815	1	120.498440	1	179.431602	1	33	26	24	0
C	1.420087	1	120.507191	1	1.491791	1	34	33	26	0
C	1.422706	1	120.901111	1	177.292842	1	35	34	33	0
C	1.372040	1	120.663775	1	-177.588336	1	36	35	34	0
C	1.423937	1	122.448619	1	-173.675479	1	32	27	26	0
C	1.415336	1	120.012178	1	0.161773	1	37	36	35	0
C	1.416109	1	119.361492	1	104.651936	1	29	28	25	0
C	1.371290	1	120.376598	1	-177.008311	1	40	29	28	0
C	1.420975	1	120.423404	1	1.697664	1	41	40	29	0
C	1.423658	1	122.371985	1	-173.573402	1	31	30	29	0
C	1.422535	1	120.905029	1	176.788533	1	42	41	40	0
C	1.372356	1	120.631899	1	-177.697911	1	44	42	41	0
C	1.415508	1	120.095348	1	-0.024276	1	45	44	42	0
H	1.129352	1	107.354185	1	103.197788	1	4	3	1	0
H	1.117281	1	111.050348	1	-118.874282	1	8	7	6	0
H	1.119383	1	110.602385	1	122.069140	1	8	7	6	0
H	1.117255	1	110.160233	1	-134.946976	1	7	6	3	0
H	1.117898	1	110.490918	1	106.003425	1	7	6	3	0
H	1.122689	1	109.658719	1	-103.666990	1	6	3	1	0
H	1.124524	1	109.200017	1	14.807266	1	6	3	1	0
H	1.204360	1	113.292365	1	134.898423	1	9	3	1	0
H	1.199070	1	114.994330	1	-77.838927	1	9	3	1	0
H	1.128156	1	114.502459	1	-55.850181	1	24	23	1	0
H	1.108159	1	110.137008	1	169.386110	1	10	1	2	0
H	1.109962	1	105.905171	1	-70.834472	1	10	1	2	0
H	1.108562	1	109.296060	1	47.190678	1	10	1	2	0
H	1.102695	1	119.246282	1	0.325274	1	12	11	5	0
H	1.099698	1	119.731186	1	-179.713062	1	15	12	11	0
H	1.099321	1	120.241905	1	-179.860898	1	16	15	12	0
H	1.099718	1	119.694535	1	179.908497	1	14	13	11	0
H	1.100750	1	120.210782	1	0.054335	1	13	11	5	0
H	1.101093	1	120.188743	1	-0.282082	1	19	17	5	0
H	1.099489	1	119.806663	1	179.955389	1	20	19	17	0
H	1.099282	1	120.209963	1	179.989708	1	22	21	18	0
H	1.099740	1	119.699268	1	179.920954	1	21	18	17	0
H	1.102755	1	119.120582	1	1.349472	1	18	17	5	0
H	1.104540	1	118.311330	1	-0.576406	1	33	26	24	0
H	1.100694	1	120.689701	1	-179.387201	1	34	33	26	0
H	1.100555	1	118.425755	1	2.042149	1	36	35	34	0
H	1.099939	1	120.807084	1	179.832396	1	37	36	35	0
H	1.100067	1	119.093642	1	178.998932	1	39	37	36	0
H	1.101708	1	118.701176	1	-0.289664	1	38	32	27	0
H	1.102169	1	118.488408	1	-0.719450	1	43	31	30	0
H	1.100252	1	119.092018	1	179.159496	1	46	45	44	0
H	1.100090	1	120.758588	1	179.700766	1	45	44	42	0
H	1.100501	1	118.482303	1	1.878711	1	44	42	41	0
H	1.100618	1	120.835278	1	-179.354667	1	41	40	29	0
H	1.100848	1	118.946132	1	2.686913	1	40	29	28	0

TSa (P)-10 <--> (M)-10 Heat of formation = 20.189940 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.470469	1	0.000000	0	0.000000	0	1	0	0
N	1.648677	1	104.765725	1	0.000000	0	1	2	0
C	1.568631	1	112.494209	1	-127.317660	1	1	2	3
O	1.511809	1	100.643702	1	112.811058	1	1	2	3
C	1.428931	1	111.882787	1	20.803304	1	2	1	3
C	1.508544	1	103.212250	1	-20.117621	1	3	1	2
C	1.481964	1	116.229831	1	-137.501591	1	3	1	2
B	1.548455	1	108.851085	1	94.265012	1	3	1	2
C	1.371508	1	112.346068	1	-169.422397	1	5	1	2
C	1.518525	1	107.847980	1	-132.339479	1	6	2	1
C	1.517242	1	108.927699	1	110.395964	1	6	2	1
C	1.536000	1	107.795865	1	-113.913066	1	7	3	1
C	1.521142	1	106.010877	1	-17.943391	1	13	7	3
O	1.750413	1	57.298439	1	-17.824528	1	9	5	10
C	1.501763	1	115.772946	1	-159.143669	1	10	5	1
C	1.399995	1	121.813561	1	159.858916	1	11	6	2
C	1.401058	1	119.125853	1	-21.979787	1	11	6	2
C	1.401194	1	121.085230	1	173.018336	1	12	6	2
C	1.400432	1	120.061136	1	-4.893662	1	12	6	2
C	1.447713	1	112.547613	1	96.534429	1	15	10	5
C	1.394460	1	125.566864	1	-32.958971	1	16	10	5
C	1.430398	1	112.683156	1	154.699517	1	16	10	5
C	1.394250	1	120.474473	1	177.877087	1	17	11	6
C	1.394087	1	120.340620	1	-177.903884	1	18	11	6
C	1.393225	1	120.614149	1	-178.152434	1	19	12	6
C	1.394513	1	120.494754	1	178.170120	1	20	12	6
C	1.497165	1	112.425107	1	-54.281778	1	21	15	10
C	1.404193	1	125.210806	1	75.611660	1	28	21	15
C	1.455972	1	113.844138	1	167.002573	1	22	16	10
C	1.363386	1	120.395591	1	169.238701	1	23	16	10
C	1.394230	1	120.305675	1	-0.038430	1	25	18	11
C	1.393622	1	120.281039	1	-0.099447	1	27	20	12
C	1.421163	1	112.414122	1	-102.150535	1	28	21	15
C	1.445284	1	116.266586	1	-178.197209	1	29	28	21
C	1.425681	1	117.877498	1	34.355694	1	30	22	16
C	1.417109	1	110.461659	1	6.286461	1	30	29	35
C	1.362778	1	120.960835	1	171.683947	1	34	28	21
C	1.426933	1	119.904722	1	8.706885	1	35	29	28
C	1.420219	1	100.204291	1	-31.575446	1	35	22	30
C	1.418179	1	120.261352	1	164.613407	1	36	30	22
C	1.378618	1	121.876376	1	-168.439366	1	37	30	22
C	1.423126	1	121.382768	1	170.996603	1	39	35	29
C	1.374116	1	123.450354	1	-171.740854	1	40	35	29
C	1.375944	1	120.303158	1	10.910170	1	41	36	30
C	1.370642	1	121.056999	1	4.144582	1	43	39	35
H	1.129384	1	107.225765	1	129.537495	1	7	3	1
H	1.119227	1	111.482847	1	101.438270	1	13	7	3
H	1.117054	1	109.868088	1	-138.963069	1	13	7	3
H	1.118180	1	110.982152	1	-100.504938	1	14	13	7
H	1.116845	1	111.354344	1	139.292587	1	14	13	7
H	1.125217	1	109.157249	1	-121.309683	1	8	3	1
H	1.122849	1	110.043043	1	-3.295507	1	8	3	1
H	1.103133	1	119.231576	1	2.879745	1	18	11	6
H	1.100043	1	119.613397	1	-179.842099	1	25	18	11
H	1.099188	1	120.251798	1	179.651243	1	32	25	18
H	1.099456	1	119.759342	1	-179.846625	1	24	17	11
H	1.100659	1	120.610492	1	-1.900329	1	17	11	6
H	1.103711	1	119.265503	1	-1.450308	1	20	12	6
H	1.099778	1	119.664962	1	-179.809312	1	27	20	12
H	1.099274	1	120.256486	1	-179.765518	1	33	27	20
H	1.099545	1	119.789297	1	179.781414	1	26	19	12
H	1.100141	1	119.921218	1	1.539754	1	19	12	6
H	1.131782	1	113.842628	1	-28.684315	1	10	5	1
H	1.199019	1	112.705606	1	-61.040539	1	9	3	1
H	1.204961	1	113.893241	1	152.821450	1	9	3	1
H	1.107781	1	112.267047	1	-170.997042	1	4	1	2
H	1.108556	1	109.412839	1	65.562472	1	4	1	2
H	1.111047	1	104.153061	1	-52.178120	1	4	1	2
H	1.101112	1	118.721745	1	-5.400458	1	23	16	10
H	1.099232	1	121.990542	1	-168.996109	1	31	23	16
H	1.100118	1	118.612210	1	-171.597360	1	41	36	30
H	1.099006	1	121.234629	1	-178.440691	1	45	41	36
H	1.100015	1	120.216157	1	178.079013	1	42	37	30
H	1.101649	1	119.152153	1	21.686264	1	37	30	22
H	1.087596	1	119.544964	1	13.455088	1	40	35	29
H	1.100206	1	120.142712	1	178.700822	1	44	40	35
H	1.098840	1	121.527997	1	-178.645160	1	46	43	39
H	1.101085	1	118.108208	1	-175.861686	1	43	39	35
H	1.100276	1	121.474860	1	-175.240902	1	38	34	28
H	1.102072	1	118.940730	1	-5.340157	1	34	28	21

TSb (P)-10 <--> (M)-10 Heat of formation = 14.786424 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.474131	1	0.000000	0	0.000000	0	1	0	0
N	1.637212	1	105.187084	1	0.000000	0	1	2	0
C	1.567269	1	114.765752	1	-128.691033	1	1	2	3
O	1.508217	1	102.832929	1	118.298056	1	1	2	3
C	1.427253	1	113.469712	1	-2.019915	1	2	1	3
C	1.506054	1	104.274694	1	11.426061	1	3	1	2
C	1.492575	1	112.836095	1	-102.255662	1	3	1	2
B	1.550833	1	113.870230	1	134.778732	1	3	1	2
C	1.368160	1	118.572247	1	32.323616	1	5	1	3
C	1.515727	1	108.150831	1	-126.349335	1	6	2	1
C	1.517473	1	108.282958	1	115.292186	1	6	2	1
C	1.535215	1	107.871136	1	-142.551126	1	7	3	1
C	1.534402	1	108.498197	1	136.934574	1	8	3	1
O	1.708088	1	48.353178	1	37.132677	1	9	5	10
C	1.508313	1	112.884516	1	174.300716	1	10	5	1
C	1.400049	1	121.417303	1	157.342075	1	11	6	2
C	1.400499	1	119.317210	1	-24.515798	1	11	6	2
C	1.401344	1	121.585679	1	157.051265	1	12	6	2
C	1.400911	1	119.790581	1	-20.697502	1	12	6	2
C	1.444861	1	111.942625	1	-161.688613	1	15	10	5
C	1.398367	1	122.584368	1	-165.939247	1	16	10	5
C	1.424006	1	114.383864	1	22.838154	1	16	10	5
C	1.393776	1	120.330629	1	177.424588	1	17	11	6
C	1.394206	1	120.266068	1	-177.726074	1	18	11	6
C	1.393852	1	120.661976	1	-179.071118	1	19	12	6
C	1.393993	1	120.709514	1	179.049575	1	20	12	6
C	1.495954	1	110.659004	1	-41.520819	1	21	15	10
C	1.491419	1	115.886138	1	-13.595580	1	22	16	10
C	1.449016	1	114.957384	1	177.201119	1	22	16	10
C	1.364554	1	119.922208	1	163.637405	1	23	16	10
C	1.394523	1	120.182149	1	0.408034	1	24	17	11
C	1.394173	1	120.269487	1	0.513556	1	26	19	12
C	1.420302	1	113.438088	1	-95.548331	1	28	21	15
C	1.445143	1	129.486431	1	134.221475	1	29	22	16
C	1.427292	1	118.290646	1	26.585169	1	30	22	16
C	1.419771	1	107.115079	1	-9.913306	1	30	29	35
C	1.363788	1	120.508528	1	170.106827	1	34	28	21
C	1.427629	1	119.427759	1	-158.840518	1	35	29	22
C	1.420323	1	102.288797	1	-26.873884	1	35	22	30
C	1.421301	1	120.440590	1	163.660606	1	36	30	22
C	1.375881	1	122.374410	1	-166.410936	1	37	30	22
C	1.422924	1	121.074066	1	168.673704	1	39	35	29
C	1.374319	1	123.120188	1	-169.917632	1	40	35	29
C	1.373125	1	120.598160	1	9.663217	1	41	36	30
C	1.371175	1	120.933326	1	5.955532	1	43	39	35
H	1.128257	1	107.684435	1	99.639343	1	7	3	1
H	1.116527	1	111.712203	1	136.288979	1	13	7	3
H	1.119549	1	109.231550	1	-104.888855	1	13	7	3
H	1.117720	1	110.631900	1	105.330653	1	14	8	3
H	1.117327	1	110.053277	1	-135.527216	1	14	8	3
H	1.122548	1	109.758435	1	-100.898676	1	8	3	1
H	1.124537	1	108.969092	1	17.772514	1	8	3	1
H	1.102867	1	119.181173	1	2.601758	1	18	11	6
H	1.099833	1	119.714109	1	-179.972574	1	25	18	11
H	1.099331	1	120.071928	1	180.019309	1	32	24	17
H	1.099444	1	119.808820	1	-179.762566	1	24	17	11
H	1.101123	1	120.064951	1	-2.162260	1	17	11	6
H	1.102349	1	119.235584	1	0.500666	1	20	12	6
H	1.099784	1	119.705313	1	-179.865972	1	27	20	12
H	1.099275	1	120.200178	1	179.824190	1	33	26	19
H	1.099687	1	119.702869	1	179.997656	1	26	19	12
H	1.100942	1	120.227566	1	0.122222	1	19	12	6
H	1.122327	1	115.376462	1	40.658082	1	10	5	1
H	1.204336	1	112.658454	1	-138.550344	1	9	3	1
H	1.202878	1	112.770091	1	78.329353	1	9	3	1
H	1.107980	1	109.533376	1	166.662885	1	4	1	2
H	1.107467	1	110.133764	1	44.199152	1	4	1	2
H	1.110358	1	105.622069	1	-74.478614	1	4	1	2
H	1.103986	1	118.205270	1	-11.309430	1	23	16	10
H	1.099700	1	121.673714	1	-169.907396	1	31	23	16
H	1.100464	1	118.344138	1	-172.165566	1	41	36	30
H	1.098888	1	121.420682	1	-178.127599	1	45	41	36
H	1.099993	1	120.293551	1	178.100941	1	42	37	30
H	1.097576	1	119.130885	1	24.326515	1	37	30	22
H	1.090405	1	119.298194	1	17.985378	1	40	35	29
H	1.100332	1	120.189712	1	178.507815	1	44	40	35
H	1.099042	1	121.479076	1	-178.495154	1	46	43	39
H	1.100756	1	118.208666	1	-174.904662	1	43	39	35
H	1.100081	1	121.586544	1	-173.882522	1	38	34	28
H	1.102139	1	118.884795	1	-6.734420	1	34	28	21