TS (M)-[10 -> 11]A Heat of formation = -8.079939 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.445437	1	0.000000	0	0.000000	0	1	0	0
N	1.588245	1	107.869378	1	0.000000	0	1	2	0
C	1.565479	1	112.687681	1	-136.118035	1	1	2	3
O	1.639740	1	98.082584	1	111.469933	1	1	2	3
C	1.438119	1	111.450272	1	13.839935	1	2	1	3
C	1.511354	1	103.281067	1	-17.018733	1	3	1	2
C	1.482600	1	115.789924	1	-134.121865	1	3	1	2
B	1.594888	1	111.314806	1	96.825275	1	3	1	2
C	1.293650	1	113.312477	1	176.203467	1	5	1	2
C	1.515157	1	108.246200	1	-124.827252	1	6	2	1
C	1.515815	1	108.059302	1	117.321157	1	6	2	1
C	1.535622	1	107.820535	1	-112.454797	1	7	3	1
C	1.521494	1	105.906367	1	-18.348854	1	13	7	3
O	1.913746	1	95.837739	1	77.023610	1	10	5	1
C	1.477582	1	121.479643	1	-167.795688	1	10	5	1
C	1.400020	1	121.725976	1	160.681398	1	11	6	2
C	1.401058	1	119.214648	1	-21.135187	1	11	6	2
C	1.400979	1	120.838882	1	173.323005	1	12	6	2
C	1.400550	1	120.260168	1	-5.275693	1	12	6	2
C	1.419865	1	114.756066	1	106.416617	1	15	10	5
C	1.384258	1	126.292091	1	-54.345539	1	16	10	5
C	1.427179	1	113.506898	1	126.700644	1	16	10	5
C	1.394186	1	120.439292	1	177.746379	1	17	11	6
C	1.393952	1	120.381995	1	-177.691728	1	18	11	6
C	1.393304	1	120.557799	1	-178.643560	1	19	12	6
C	1.394426	1	120.466329	1	178.623058	1	20	12	6
C	1.499438	1	112.363260	1	-57.653169	1	21	15	10
C	1.385186	1	121.005026	1	73.298218	1	28	21	15
C	1.437838	1	119.251881	1	-174.899821	1	22	16	10
C	1.366796	1	121.065855	1	178.188975	1	23	16	10
C	1.394152	1	120.258084	1	-0.195635	1	25	18	11
C	1.393707	1	120.268291	1	0.010911	1	27	20	12
C	1.418728	1	118.802536	1	-105.308860	1	28	21	15
C	1.431674	1	119.883673	1	-173.608401	1	29	28	21
C	1.417819	1	119.738821	1	-4.282927	1	30	22	16
C	1.423336	1	122.040296	1	174.220109	1	30	22	16
C	1.370544	1	120.705532	1	176.803645	1	34	28	21
C	1.418632	1	119.144539	1	-4.707393	1	35	29	28
C	1.423353	1	122.343376	1	173.922818	1	35	29	28
C	1.420999	1	119.778099	1	-179.584512	1	36	30	22
C	1.373970	1	121.008597	1	-179.790356	1	37	30	22
C	1.422115	1	119.458395	1	-179.614971	1	39	35	29
C	1.373007	1	120.911274	1	-179.667259	1	40	35	29
C	1.373357	1	120.553379	1	-1.195786	1	41	36	30
C	1.372603	1	120.653471	1	-1.191506	1	43	39	35
H	1.128791	1	107.107409	1	130.760310	1	7	3	1
H	1.119008	1	111.556394	1	101.334479	1	13	7	3
H	1.117104	1	109.840125	1	-139.143445	1	13	7	3
H	1.118253	1	110.865268	1	-100.598167	1	14	13	7
H	1.116744	1	111.356818	1	139.234940	1	14	13	7
H	1.125196	1	108.447406	1	-122.827359	1	8	3	1
H	1.122564	1	110.439137	1	-4.730568	1	8	3	1
H	1.102522	1	119.337826	1	3.112062	1	18	11	6
H	1.099734	1	119.656480	1	180.033837	1	25	18	11
H	1.099156	1	120.216992	1	179.815408	1	32	25	18
H	1.099446	1	119.729170	1	-179.971610	1	24	17	11
H	1.100505	1	120.661694	1	-2.318292	1	17	11	6
H	1.102983	1	119.426503	1	-0.944862	1	20	12	6
H	1.099770	1	119.686400	1	-179.716717	1	27	20	12
H	1.099333	1	120.239455	1	-179.774905	1	33	27	20
H	1.099643	1	119.770701	1	179.750215	1	26	19	12
H	1.100214	1	119.932655	1	1.005149	1	19	12	6
H	1.116849	1	120.523243	1	-11.232946	1	10	5	1
H	1.205698	1	108.075193	1	-61.348678	1	9	3	1
H	1.209945	1	108.981499	1	168.497229	1	9	3	1
H	1.107421	1	112.842613	1	-173.761470	1	4	1	2
H	1.109594	1	107.292827	1	64.239406	1	4	1	2
H	1.110234	1	105.632460	1	-53.046917	1	4	1	2
H	1.101702	1	118.714112	1	-2.271000	1	23	16	10
H	1.100589	1	120.969475	1	178.813351	1	31	23	16
H	1.100411	1	118.552596	1	179.110135	1	41	36	30
H	1.100130	1	120.753654	1	-179.878340	1	45	41	36
H	1.100305	1	120.397503	1	179.935903	1	42	37	30
H	1.102278	1	118.808015	1	0.256989	1	37	30	22
H	1.101342	1	118.567736	1	-0.044705	1	40	35	29
H	1.099971	1	120.503912	1	179.579440	1	44	40	35
H	1.099743	1	120.777749	1	-179.702509	1	46	43	39
H	1.100373	1	118.452960	1	179.380067	1	43	39	35
H	1.100454	1	120.848451	1	179.836378	1	38	34	28
H	1.101090	1	118.593765	1	-2.065353	1	34	28	21

TS (M)-[10 -> 11]B Heat of formation = -15.129378 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.456981	1	0.000000	0	0.000000	0	1	0	0
N	1.591476	1	107.275079	1	0.000000	0	1	2	0
C	1.560784	1	117.156864	1	-137.101116	1	1	2	3
O	1.615319	1	99.704151	1	114.752607	1	1	2	3
C	1.436945	1	112.152523	1	2.614130	1	2	1	3
C	1.503669	1	104.391505	1	8.551364	1	3	1	2
C	1.491489	1	113.018396	1	-105.807925	1	3	1	2
B	1.595487	1	113.501214	1	132.604905	1	3	1	2
C	1.301349	1	118.863157	1	48.842754	1	5	1	3
C	1.512848	1	107.995133	1	-131.014605	1	6	2	1
C	1.515656	1	108.334863	1	110.616508	1	6	2	1
C	1.533735	1	108.043114	1	-141.627453	1	7	3	1
C	1.534229	1	108.675594	1	134.707005	1	8	3	1
O	1.844915	1	92.197596	1	-77.765900	1	10	5	1
C	1.478750	1	117.462912	1	177.899922	1	10	5	1
C	1.400154	1	121.195539	1	155.114745	1	11	6	2
C	1.400444	1	119.465424	1	-27.487113	1	11	6	2
C	1.401478	1	121.248941	1	156.735902	1	12	6	2
C	1.400619	1	120.054113	1	-21.223173	1	12	6	2
C	1.417361	1	117.374514	1	-167.231800	1	15	10	5
C	1.389339	1	120.683558	1	167.878056	1	16	10	5
C	1.419868	1	118.583073	1	-11.604949	1	16	10	5
C	1.393808	1	120.281139	1	176.846468	1	17	11	6
C	1.394108	1	120.262737	1	-177.135987	1	18	11	6
C	1.393690	1	120.621151	1	-179.130726	1	19	12	6
C	1.394091	1	120.659015	1	179.071526	1	20	12	6
C	1.498508	1	112.923868	1	-34.343090	1	21	15	10
C	1.470163	1	120.153530	1	1.014517	1	22	16	10
C	1.431775	1	119.282069	1	-176.421425	1	22	16	10
C	1.369836	1	120.492839	1	178.882274	1	23	16	10
C	1.394634	1	120.188507	1	0.309338	1	24	17	11
C	1.394328	1	120.254987	1	0.484328	1	26	19	12
C	1.418201	1	118.447186	1	-113.166692	1	28	21	15
C	1.431375	1	120.709060	1	121.514479	1	29	22	16
C	1.419515	1	119.388768	1	-3.257615	1	30	22	16
C	1.424036	1	122.200436	1	175.069298	1	30	22	16
C	1.370655	1	120.726499	1	-177.564300	1	34	28	21
C	1.419077	1	119.218573	1	177.285815	1	35	29	22
C	1.423699	1	122.354595	1	-3.454513	1	35	29	22
C	1.422520	1	119.499293	1	-179.941729	1	36	30	22
C	1.372735	1	120.978757	1	-179.425779	1	37	30	22
C	1.422346	1	119.514308	1	-178.893516	1	39	35	29
C	1.372899	1	120.934880	1	179.422758	1	40	35	29
C	1.372351	1	120.655174	1	-1.133275	1	41	36	30
C	1.372433	1	120.635332	1	-1.084590	1	43	39	35
H	1.127804	1	107.450327	1	100.268658	1	7	3	1
H	1.116416	1	111.722560	1	136.780599	1	13	7	3
H	1.119668	1	109.136902	1	-104.307561	1	13	7	3
H	1.117784	1	110.413035	1	108.179716	1	14	8	3
H	1.117315	1	110.133582	1	-132.668361	1	14	8	3
H	1.123439	1	109.144743	1	-103.832558	1	8	3	1
H	1.124095	1	109.388891	1	14.737213	1	8	3	1
H	1.102298	1	119.261591	1	2.719006	1	18	11	6
H	1.099852	1	119.744920	1	179.930199	1	25	18	11
H	1.099484	1	120.057967	1	180.071363	1	32	24	17
H	1.099589	1	119.796964	1	-179.762362	1	24	17	11
H	1.101279	1	120.043161	1	-2.634311	1	17	11	6
H	1.102254	1	119.370993	1	0.291305	1	20	12	6
H	1.099830	1	119.702762	1	-179.887792	1	27	20	12
H	1.099368	1	120.186812	1	179.833011	1	33	26	19
H	1.099749	1	119.711652	1	180.033297	1	26	19	12
H	1.101206	1	120.133907	1	0.157095	1	19	12	6
H	1.112374	1	120.991949	1	19.972403	1	10	5	1
H	1.209206	1	107.821179	1	-160.500731	1	9	3	1
H	1.207418	1	107.647463	1	69.494420	1	9	3	1
H	1.108252	1	108.901345	1	176.615378	1	4	1	2
H	1.107984	1	109.363985	1	54.902293	1	4	1	2
H	1.109749	1	106.505043	1	-64.157265	1	4	1	2
H	1.103106	1	118.123325	1	-0.601404	1	23	16	10
H	1.100557	1	120.818864	1	179.381054	1	31	23	16
H	1.100545	1	118.441927	1	179.257608	1	41	36	30
H	1.100113	1	120.769494	1	-179.769286	1	45	41	36
H	1.100156	1	120.497102	1	179.813181	1	42	37	30
H	1.101945	1	118.609092	1	0.531637	1	37	30	22
H	1.101835	1	118.564034	1	-0.465220	1	40	35	29
H	1.100196	1	120.484131	1	179.981215	1	44	40	35
H	1.099949	1	120.780328	1	179.988884	1	46	43	39
H	1.100426	1	118.481600	1	179.098954	1	43	39	35
H	1.100632	1	120.870264	1	179.096690	1	38	34	28
H	1.101485	1	118.605124	1	2.217611	1	34	28	21

TS (P)-[10 -> 11]A Heat of formation = -14.147196 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.440153	1	0.000000	0	0.000000	0	1	0	0	
N	1.590596	1	108.224462	1	0.000000	0	1	2	0	
C	1.505809	1	104.580060	1	3.890296	1	3	1	2	
C	1.438573	1	112.268505	1	-1.755787	1	2	1	3	
C	1.483443	1	114.017532	1	-112.832095	1	3	1	2	
C	1.532633	1	108.602063	1	132.340444	1	6	3	1	
C	1.522711	1	106.111315	1	-17.203466	1	7	6	3	
B	1.597517	1	110.178490	1	121.029730	1	3	1	2	
C	1.560685	1	114.830467	1	-137.268191	1	1	2	3	
C	1.515430	1	107.228174	1	121.518411	1	5	2	1	
C	1.401166	1	119.973537	1	-19.629646	1	11	5	2	
C	1.401045	1	121.239286	1	159.077526	1	11	5	2	
C	1.393742	1	120.563664	1	-179.289989	1	13	11	5	
C	1.394023	1	120.578486	1	179.224347	1	12	11	5	
C	1.393892	1	120.234960	1	-0.106362	1	15	12	11	
C	1.515044	1	108.240162	1	-120.084141	1	5	2	1	
C	1.400706	1	119.355571	1	-22.727600	1	17	5	2	
C	1.400396	1	121.578259	1	158.074068	1	17	5	2	
C	1.394062	1	120.425059	1	179.179052	1	19	17	5	
C	1.394042	1	120.379364	1	-179.140298	1	18	17	5	
C	1.394197	1	120.244734	1	-0.045683	1	21	18	17	
O	1.642442	1	104.536513	1	-98.381968	1	1	3	4	
C	1.299612	1	117.523017	1	160.776535	1	23	1	2	
O	1.873604	1	94.956548	1	59.563285	1	24	23	1	
C	1.479582	1	116.581879	1	172.130871	1	24	23	1	
C	1.388576	1	121.475901	1	-167.082513	1	26	24	23	
C	1.420544	1	114.892000	1	144.424706	1	25	24	23	
C	1.500547	1	107.253480	1	57.564992	1	28	25	24	
C	1.386856	1	120.744552	1	-76.327967	1	29	28	25	
C	1.430661	1	119.753756	1	174.110324	1	30	29	28	
C	1.432410	1	119.398886	1	178.353709	1	27	26	24	
C	1.421329	1	117.976883	1	13.308544	1	26	24	23	
C	1.369432	1	120.615204	1	179.666146	1	33	26	24	
C	1.420832	1	120.379206	1	1.442064	1	34	33	26	
C	1.422382	1	120.882507	1	178.097948	1	35	34	33	
C	1.372429	1	120.642227	1	-177.980954	1	36	35	34	
C	1.423983	1	122.180185	1	-175.957985	1	32	27	26	
C	1.415208	1	120.052466	1	0.053461	1	37	36	35	
C	1.417346	1	118.829169	1	101.819350	1	29	28	25	
C	1.371074	1	120.582161	1	-176.331879	1	40	29	28	
C	1.420967	1	120.430932	1	1.195041	1	41	40	29	
C	1.423572	1	122.280897	1	-175.288494	1	31	30	29	
C	1.422354	1	121.019814	1	177.365544	1	42	41	40	
C	1.372456	1	120.638210	1	-178.490217	1	44	42	41	
C	1.415449	1	120.081401	1	-0.090199	1	45	44	42	
H	1.129649	1	106.870482	1	111.091524	1	4	3	1	
H	1.117545	1	110.541289	1	-111.668996	1	8	7	6	
H	1.118850	1	110.808592	1	129.334380	1	8	7	6	
H	1.116888	1	110.372735	1	-138.030800	1	7	6	3	
H	1.118288	1	110.265480	1	102.791393	1	7	6	3	
H	1.123218	1	108.861093	1	-106.160116	1	6	3	1	
H	1.124160	1	109.969636	1	12.316057	1	6	3	1	
H	1.208431	1	109.617576	1	155.099181	1	9	3	1	
H	1.205169	1	109.892935	1	-73.252367	1	9	3	1	
H	1.112437	1	121.827842	1	-30.786105	1	24	23	1	
H	1.108360	1	110.264723	1	173.664235	1	10	1	2	
H	1.109431	1	107.031345	1	-65.536143	1	10	1	2	
H	1.109507	1	107.812417	1	52.470459	1	10	1	2	
H	1.102433	1	119.423624	1	0.200313	1	12	11	5	
H	1.099748	1	119.718342	1	-179.775954	1	15	12	11	
H	1.099339	1	120.237979	1	-179.874559	1	16	15	12	
H	1.099732	1	119.712212	1	179.899072	1	14	13	11	
H	1.100727	1	120.109724	1	0.163152	1	13	11	5	
H	1.101079	1	120.340523	1	-0.788724	1	19	17	5	
H	1.099578	1	119.759944	1	179.857342	1	20	19	17	
H	1.099301	1	120.210745	1	179.990975	1	22	21	18	
H	1.099685	1	119.727163	1	179.910286	1	21	18	17	
H	1.102258	1	119.203369	1	1.566470	1	18	17	5	
H	1.103861	1	118.105009	1	-0.956031	1	33	26	24	
H	1.100614	1	120.792433	1	-179.521914	1	34	33	26	
H	1.100538	1	118.445178	1	1.665314	1	36	35	34	
H	1.100119	1	120.769216	1	179.802457	1	37	36	35	
H	1.100161	1	119.107694	1	179.313286	1	39	37	36	
H	1.101953	1	118.650860	1	-0.456501	1	38	32	27	
H	1.101813	1	118.510812	1	-1.113749	1	43	31	30	
H	1.100239	1	119.087352	1	179.542039	1	46	45	44	
H	1.099997	1	120.766881	1	179.762350	1	45	44	42	
H	1.100502	1	118.481498	1	1.201324	1	44	42	41	
H	1.100659	1	120.854758	1	-179.651133	1	41	40	29	
H	1.101025	1	118.698206	1	3.243836	1	40	29	28	

TS (P)-[10 -> 11]B Heat of formation = 2.637785 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.437706	1	0.000000	0	0.000000	0	1	0	0	0
N	1.586944	1	108.536509	1	0.000000	0	1	2	0	0
C	1.513190	1	102.625248	1	-12.573261	1	3	1	2	0
C	1.439563	1	111.475877	1	-1.462234	1	2	1	3	0
C	1.479831	1	113.811333	1	-127.323857	1	3	1	2	0
C	1.531435	1	109.679561	1	97.331820	1	6	3	1	0
C	1.520886	1	106.366054	1	7.898103	1	7	6	3	0
B	1.623947	1	113.495778	1	102.170804	1	3	1	2	0
C	1.555176	1	113.907045	1	-140.703717	1	1	2	3	0
C	1.512016	1	107.846370	1	137.158904	1	5	2	1	0
C	1.400321	1	119.939361	1	17.004675	1	11	5	2	0
C	1.400950	1	120.961189	1	-165.418502	1	11	5	2	0
C	1.393289	1	120.468498	1	-177.488579	1	13	11	5	0
C	1.394578	1	120.344540	1	177.665917	1	12	11	5	0
C	1.393771	1	120.273626	1	-0.192082	1	15	12	11	0
C	1.516115	1	109.976436	1	-104.945797	1	5	2	1	0
C	1.400124	1	119.983704	1	-10.868406	1	17	5	2	0
C	1.400114	1	120.975988	1	170.829507	1	17	5	2	0
C	1.393818	1	120.465404	1	178.112897	1	19	17	5	0
C	1.394036	1	120.412153	1	-178.003277	1	18	17	5	0
C	1.394005	1	120.249634	1	-0.154085	1	21	18	17	0
O	1.683158	1	94.208325	1	107.417239	1	1	2	3	0
C	1.276020	1	126.756888	1	173.946908	1	23	1	2	0
O	1.914007	1	93.138861	1	67.978099	1	24	23	1	0
C	1.486753	1	129.466732	1	-52.537765	1	24	23	1	0
C	1.380957	1	131.558674	1	96.634691	1	26	24	23	0
C	1.412987	1	118.070560	1	-152.904960	1	25	24	23	0
C	1.495053	1	111.807149	1	74.558895	1	28	25	24	0
C	1.382883	1	121.204655	1	-63.562960	1	29	28	25	0
C	1.437967	1	119.115237	1	169.313994	1	30	29	28	0
C	1.446276	1	118.700117	1	160.987340	1	27	26	24	0
C	1.436282	1	108.694681	1	-90.580430	1	26	24	23	0
C	1.363636	1	121.798039	1	-169.185740	1	33	26	24	0
C	1.422510	1	119.873947	1	3.583819	1	34	33	26	0
C	1.419773	1	120.909962	1	173.957372	1	35	34	33	0
C	1.374020	1	120.495822	1	-176.918931	1	36	35	34	0
C	1.423058	1	121.793053	1	-167.920485	1	32	27	26	0
C	1.412856	1	119.851042	1	0.177802	1	37	36	35	0
C	1.420522	1	118.286081	1	114.258097	1	29	28	25	0
C	1.369579	1	120.813594	1	-174.557299	1	40	29	28	0
C	1.421876	1	120.148884	1	2.938411	1	41	40	29	0
C	1.423531	1	122.300463	1	-171.186689	1	31	30	29	0
C	1.421637	1	120.897304	1	175.503635	1	42	41	40	0
C	1.372875	1	120.633895	1	-177.868003	1	44	42	41	0
C	1.414524	1	119.985330	1	0.063361	1	45	44	42	0
H	1.126372	1	108.202179	1	138.196620	1	4	3	1	0
H	1.118845	1	109.970560	1	-118.570749	1	8	7	6	0
H	1.117714	1	111.287393	1	122.013532	1	8	7	6	0
H	1.118225	1	110.403286	1	-112.379625	1	7	6	3	0
H	1.117379	1	110.203449	1	128.708336	1	7	6	3	0
H	1.127874	1	108.400088	1	-142.824737	1	6	3	1	0
H	1.123941	1	110.261949	1	-25.640848	1	6	3	1	0
H	1.124512	1	113.913621	1	157.392440	1	24	23	1	0
H	1.208808	1	107.690266	1	161.646935	1	9	3	1	0
H	1.207922	1	106.347468	1	-68.891364	1	9	3	1	0
H	1.108692	1	110.916021	1	-165.025982	1	10	1	2	0
H	1.109645	1	106.222573	1	-44.720611	1	10	1	2	0
H	1.109453	1	107.499545	1	73.377353	1	10	1	2	0
H	1.102060	1	119.471769	1	-2.317213	1	12	11	5	0
H	1.099781	1	119.685727	1	-179.969574	1	15	12	11	0
H	1.099351	1	120.217400	1	-179.712788	1	16	15	12	0
H	1.099585	1	119.796125	1	179.768992	1	14	13	11	0
H	1.100270	1	119.905230	1	2.807297	1	13	11	5	0
H	1.099874	1	120.387519	1	-1.682294	1	19	17	5	0
H	1.099427	1	119.762449	1	179.883691	1	20	19	17	0
H	1.099174	1	120.230538	1	179.991408	1	22	21	18	0
H	1.099455	1	119.723356	1	179.962854	1	21	18	17	0
H	1.102898	1	119.087554	1	3.326595	1	18	17	5	0
H	1.102948	1	118.070223	1	11.477767	1	33	26	24	0
H	1.100667	1	121.140855	1	-177.973350	1	34	33	26	0
H	1.100436	1	118.591226	1	2.514276	1	36	35	34	0
H	1.100007	1	120.787300	1	179.770692	1	37	36	35	0
H	1.100362	1	119.176512	1	178.693693	1	39	37	36	0
H	1.101894	1	119.119970	1	0.170393	1	38	32	27	0
H	1.101849	1	118.714680	1	0.262678	1	43	31	30	0
H	1.100260	1	119.127284	1	179.031631	1	46	45	44	0
H	1.099949	1	120.786448	1	179.789571	1	45	44	42	0
H	1.100475	1	118.490541	1	1.724620	1	44	42	41	0
H	1.100473	1	121.049396	1	-178.352609	1	41	40	29	0
H	1.101570	1	118.472596	1	5.276045	1	40	29	28	0

(M)-11 Heat of formation = -10.359292 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.419531	1	0.000000	0	0.000000	0	1	0	0
N	1.563724	1	109.766573	1	0.000000	0	1	2	0
C	1.560497	1	114.354360	1	-142.962251	1	1	2	3
O	1.766393	1	94.553973	1	110.560858	1	1	2	3
C	1.445695	1	111.660839	1	3.603725	1	2	1	3
C	1.513837	1	103.284297	1	-10.648454	1	3	1	2
C	1.485457	1	114.465387	1	-127.022286	1	3	1	2
B	1.622427	1	114.364922	1	104.405292	1	3	1	2
C	1.258613	1	114.627989	1	162.291328	1	5	1	2
C	1.513950	1	108.973244	1	-114.920075	1	6	2	1
C	1.513464	1	107.594532	1	127.482167	1	6	2	1
C	1.535985	1	107.742598	1	-112.947715	1	7	3	1
C	1.521518	1	105.799594	1	-18.602701	1	13	7	3
O	2.334923	1	90.261563	1	69.342789	1	10	5	1
C	1.471590	1	125.509765	1	-175.596170	1	10	5	1
C	1.400118	1	121.124787	1	165.962769	1	11	6	2
C	1.400164	1	119.736030	1	-16.023416	1	11	6	2
C	1.401311	1	120.690697	1	-173.985670	1	12	6	2
C	1.400201	1	120.328750	1	8.372497	1	12	6	2
C	1.409761	1	106.986360	1	115.675894	1	15	10	5
C	1.382286	1	125.715824	1	-63.393775	1	16	10	5
C	1.427689	1	113.483030	1	122.805179	1	16	10	5
C	1.393785	1	120.399860	1	177.277068	1	17	11	6
C	1.394089	1	120.351357	1	-177.217874	1	18	11	6
C	1.393141	1	120.539936	1	-177.869285	1	19	12	6
C	1.394729	1	120.413998	1	177.960379	1	20	12	6
C	1.504708	1	113.114785	1	-60.063022	1	21	15	10
C	1.383258	1	123.034460	1	78.281618	1	28	21	15
C	1.440181	1	118.830150	1	-167.966596	1	22	16	10
C	1.366002	1	120.997304	1	172.481391	1	23	16	10
C	1.393972	1	120.240097	1	-0.257460	1	25	18	11
C	1.393556	1	120.286134	1	-0.203488	1	27	20	12
C	1.422628	1	117.134274	1	-100.639413	1	28	21	15
C	1.436108	1	119.804857	1	-174.622516	1	29	28	21
C	1.417275	1	119.915185	1	-5.166936	1	30	22	16
C	1.422975	1	121.777836	1	173.667685	1	30	22	16
C	1.368649	1	121.184808	1	177.708394	1	34	28	21
C	1.417607	1	119.442321	1	-4.484003	1	35	29	28
C	1.423260	1	122.222634	1	174.690611	1	35	29	28
C	1.420428	1	119.752190	1	-179.673814	1	36	30	22
C	1.374305	1	120.950660	1	-179.747911	1	37	30	22
C	1.421429	1	119.617151	1	-178.981821	1	39	35	29
C	1.373493	1	120.988462	1	179.524869	1	40	35	29
C	1.373814	1	120.538553	1	-1.013144	1	41	36	30
C	1.372973	1	120.646311	1	-1.089553	1	43	39	35
H	1.128677	1	107.315165	1	129.885339	1	7	3	1
H	1.118944	1	111.451166	1	100.970575	1	13	7	3
H	1.117000	1	109.977451	1	-139.280819	1	13	7	3
H	1.118385	1	110.804216	1	-98.014123	1	14	13	7
H	1.116466	1	111.489607	1	141.623405	1	14	13	7
H	1.124988	1	108.098385	1	-119.859711	1	8	3	1
H	1.122769	1	110.734353	1	-1.569636	1	8	3	1
H	1.102294	1	119.387822	1	3.849188	1	18	11	6
H	1.099670	1	119.684727	1	-179.857154	1	25	18	11
H	1.099223	1	120.181452	1	179.917722	1	32	25	18
H	1.099436	1	119.745915	1	-179.961714	1	24	17	11
H	1.100052	1	120.527453	1	-2.830504	1	17	11	6
H	1.101938	1	119.657980	1	-1.664375	1	20	12	6
H	1.099849	1	119.658493	1	-179.894637	1	27	20	12
H	1.099444	1	120.239477	1	-179.750671	1	33	27	20
H	1.099715	1	119.786966	1	179.807711	1	26	19	12
H	1.100202	1	119.882232	1	2.068804	1	19	12	6
H	1.115752	1	121.396627	1	-0.253147	1	10	5	1
H	3.197000	-1	49.895658	1	89.305910	1	10	5	1
H	1.211315	1	106.745660	1	174.095408	1	9	3	1
H	1.107872	1	112.098277	1	179.709193	1	4	1	2
H	1.110689	1	105.965743	1	59.124333	1	4	1	2
H	1.109374	1	107.418160	1	-58.247345	1	4	1	2
H	1.101347	1	118.554559	1	-7.897614	1	23	16	10
H	1.100499	1	121.046281	1	178.587907	1	31	23	16
H	1.100359	1	118.585746	1	179.286062	1	41	36	30
H	1.100084	1	120.723548	1	-179.854022	1	45	41	36
H	1.100292	1	120.398778	1	179.884420	1	42	37	30
H	1.102378	1	118.757512	1	0.370184	1	37	30	22
H	1.101211	1	118.770494	1	-0.655115	1	40	35	29
H	1.099921	1	120.460765	1	179.877968	1	44	40	35
H	1.099594	1	120.801228	1	-179.932744	1	46	43	39
H	1.100336	1	118.475053	1	179.367123	1	43	39	35
H	1.100334	1	120.981440	1	179.611928	1	38	34	28
H	1.101660	1	118.179299	1	-1.139025	1	34	28	21

(M)-11 HEAT OF FORMATION = -18.639012 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.432892	1	.000000	0	.000000	0	1	0	0
N	1.566116	1	108.881102	1	.000000	0	1	2	0
C	1.554739	1	119.052786	1	-145.215828	1	1	2	3
O	1.742150	1	96.198255	1	113.230638	1	1	2	3
C	1.445924	1	111.424542	1	4.029948	1	2	1	3
C	1.501514	1	104.048201	1	8.302523	1	3	1	2
C	1.490992	1	112.410470	1	-105.544454	1	3	1	2
B	1.647704	1	114.544622	1	134.145823	1	3	1	2
C	1.263791	1	121.124317	1	56.153779	1	5	1	3
C	1.509502	1	107.995089	1	-133.302096	1	6	2	1
C	1.514842	1	107.901031	1	108.160184	1	6	2	1
C	1.533366	1	107.991504	1	-141.724941	1	7	3	1
C	1.534853	1	108.360893	1	135.414412	1	8	3	1
O	2.267303	1	87.071606	1	-74.001627	1	10	5	1
C	1.468338	1	119.934560	1	-168.325611	1	10	5	1
C	1.400090	1	120.961896	1	155.052038	1	11	6	2
C	1.400438	1	119.646240	1	-27.823734	1	11	6	2
C	1.401304	1	121.127020	1	156.256550	1	12	6	2
C	1.400909	1	120.133008	1	-21.965572	1	12	6	2
C	1.407958	1	120.426157	1	-175.389831	1	15	10	5
C	1.388416	1	120.156368	1	150.171061	1	16	10	5
C	1.420768	1	118.832706	1	-25.238027	1	16	10	5
C	1.393824	1	120.236676	1	176.535157	1	17	11	6
C	1.394048	1	120.254978	1	-176.957062	1	18	11	6
C	1.393774	1	120.593539	1	-179.210309	1	19	12	6
C	1.394038	1	120.623921	1	179.092438	1	20	12	6
C	1.504817	1	111.435935	1	-22.728665	1	21	15	10
C	1.473097	1	121.926879	1	7.332093	1	22	16	10
C	1.433433	1	119.045628	1	-172.733473	1	22	16	10
C	1.368940	1	120.573363	1	175.004484	1	23	16	10
C	1.394705	1	120.205026	1	.456775	1	24	17	11
C	1.394298	1	120.251437	1	.467101	1	26	19	12
C	1.422223	1	116.721417	1	-122.783802	1	28	21	15
C	1.435321	1	117.773690	1	110.961529	1	29	22	16
C	1.419024	1	119.572503	1	-2.743672	1	30	22	16
C	1.423826	1	121.917523	1	176.220196	1	30	22	16
C	1.369171	1	121.293666	1	-176.842629	1	34	28	21
C	1.417700	1	119.563875	1	175.585881	1	35	29	22
C	1.423747	1	122.108816	1	-4.535549	1	35	29	22
C	1.421971	1	119.463798	1	180.000111	1	36	30	22
C	1.372965	1	120.911741	1	-179.576405	1	37	30	22
C	1.421758	1	119.646675	1	-178.611449	1	39	35	29
C	1.373202	1	120.966801	1	179.003909	1	40	35	29
C	1.372800	1	120.630086	1	-.735648	1	41	36	30
C	1.372720	1	120.610393	1	-.880968	1	43	39	35
H	1.127907	1	107.337558	1	99.439751	1	7	3	1
H	1.116484	1	111.668910	1	136.791261	1	13	7	3
H	1.119406	1	109.185108	1	-104.210541	1	13	7	3
H	1.117873	1	110.240258	1	106.583931	1	14	8	3
H	1.117008	1	110.224035	1	-134.150752	1	14	8	3
H	1.123392	1	108.832994	1	-103.404227	1	8	3	1
H	1.124363	1	109.789019	1	15.331164	1	8	3	1
H	1.101999	1	119.347266	1	2.728004	1	18	11	6
H	1.099878	1	119.755889	1	180.028791	1	25	18	11
H	1.099588	1	120.060563	1	179.907137	1	32	24	17
H	1.099667	1	119.790724	1	-179.725614	1	24	17	11
H	1.101342	1	119.943534	1	-3.094268	1	17	11	6
H	1.102430	1	119.541004	1	.179835	1	20	12	6
H	1.099861	1	119.702533	1	-179.821138	1	27	20	12
H	1.099475	1	120.182350	1	179.794814	1	33	26	19
H	1.099854	1	119.708023	1	180.044540	1	26	19	12
H	1.101317	1	120.097318	1	.119956	1	19	12	6
H	1.111557	1	121.624170	1	11.210435	1	10	5	1
H	1.210538	1	105.420199	1	-179.010277	1	9	3	1
H	3.611000	-1	52.792797	1	-74.156879	1	10	5	1
H	1.108658	1	108.527720	1	-170.558837	1	4	1	2
H	1.108772	1	108.248639	1	68.452654	1	4	1	2
H	1.109161	1	107.303973	1	-50.816153	1	4	1	2
H	1.102178	1	118.127296	1	-4.048565	1	23	16	10
H	1.100398	1	120.916654	1	179.461599	1	31	23	16
H	1.100458	1	118.479262	1	179.618735	1	41	36	30
H	1.100138	1	120.728688	1	-179.772272	1	45	41	36
H	1.100124	1	120.514950	1	179.838786	1	42	37	30
H	1.102013	1	118.561938	1	.517100	1	37	30	22
H	1.101601	1	118.730249	1	-.687141	1	40	35	29
H	1.100159	1	120.461997	1	-179.895325	1	44	40	35
H	1.099826	1	120.800645	1	179.896115	1	46	43	39
H	1.100392	1	118.506392	1	179.215919	1	43	39	35
H	1.100600	1	120.961825	1	178.844683	1	38	34	28
H	1.101693	1	118.421011	1	2.500343	1	34	28	21

(P)-11 Heat of formation = -18.406140 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.413373	1	0.000000	0	0.000000	0	1	0	0
N	1.564876	1	109.911890	1	0.000000	0	1	2	0
C	1.507312	1	103.853861	1	7.445446	1	3	1	2
C	1.448478	1	111.804617	1	-3.562372	1	2	1	3
C	1.489388	1	111.621666	1	-107.307864	1	3	1	2
C	1.532987	1	108.794556	1	129.283678	1	6	3	1
C	1.523361	1	106.636732	1	-9.680826	1	7	6	3
B	1.632885	1	117.872332	1	125.975539	1	3	1	2
C	1.555137	1	117.579862	1	-145.254386	1	1	2	3
C	1.513292	1	106.976392	1	120.555101	1	5	2	1
C	1.401065	1	120.099700	1	-22.059032	1	11	5	2
C	1.401090	1	121.056275	1	156.706268	1	11	5	2
C	1.393773	1	120.519440	1	-179.351329	1	13	11	5
C	1.394032	1	120.554831	1	179.217566	1	12	11	5
C	1.393949	1	120.217869	1	-0.044254	1	15	12	11
C	1.512025	1	108.165671	1	-120.579234	1	5	2	1
C	1.400351	1	119.590851	1	-23.939545	1	17	5	2
C	1.400589	1	121.241011	1	156.794058	1	17	5	2
C	1.393919	1	120.358658	1	179.384510	1	19	17	5
C	1.394208	1	120.321709	1	-179.358254	1	18	17	5
C	1.394126	1	120.235284	1	0.018420	1	21	18	17
O	1.781679	1	106.589062	1	-91.023515	1	1	3	4
C	1.261100	1	115.084128	1	172.255900	1	23	1	2
O	2.833486	1	102.923383	1	39.078741	1	24	23	1
C	1.461388	1	121.948486	1	164.853501	1	24	23	1
C	1.392152	1	119.812616	1	-170.344747	1	26	24	23
C	1.412711	1	86.293430	1	145.324015	1	25	24	23
C	1.505870	1	108.405319	1	68.423652	1	28	25	24
C	1.385234	1	123.287556	1	-105.776934	1	29	28	25
C	1.434409	1	119.770125	1	177.018504	1	30	29	28
C	1.431105	1	119.112329	1	172.509887	1	27	26	24
C	1.420865	1	119.331491	1	5.444021	1	26	24	23
C	1.369221	1	120.575896	1	-174.482591	1	33	26	24
C	1.421530	1	120.308804	1	1.198756	1	34	33	26
C	1.422087	1	120.962704	1	177.765622	1	35	34	33
C	1.372778	1	120.609743	1	-178.728131	1	36	35	34
C	1.424206	1	121.839497	1	-176.175902	1	32	27	26
C	1.415397	1	120.183088	1	-0.102629	1	37	36	35
C	1.420976	1	116.689389	1	73.293800	1	29	28	25
C	1.369228	1	121.061291	1	-178.331516	1	40	29	28
C	1.421257	1	120.296868	1	0.738817	1	41	40	29
C	1.423502	1	122.212745	1	-177.000964	1	31	30	29
C	1.421770	1	121.011829	1	178.421958	1	42	41	40
C	1.372664	1	120.655380	1	-178.727935	1	44	42	41
C	1.414820	1	119.988192	1	-0.066528	1	45	44	42
H	1.129145	1	106.728108	1	107.374842	1	4	3	1
H	1.116794	1	111.287122	1	-123.273067	1	8	7	6
H	1.119910	1	110.278539	1	117.423744	1	8	7	6
H	1.117381	1	110.247849	1	-130.503182	1	7	6	3
H	1.118081	1	110.148484	1	110.453819	1	7	6	3
H	1.124743	1	108.147229	1	-109.547724	1	6	3	1
H	1.124235	1	109.996307	1	8.744899	1	6	3	1
H	1.210043	1	104.927247	1	-177.567298	1	9	3	1
H	2.480000	-1	74.213000	1	79.633000	1	24	23	1
H	1.116383	1	120.587045	1	-12.229830	1	24	23	1
H	1.109066	1	110.005764	1	172.616550	1	10	1	2
H	1.108913	1	108.190919	1	-65.754155	1	10	1	2
H	1.110503	1	106.534579	1	52.379414	1	10	1	2
H	1.102049	1	119.562777	1	0.092643	1	12	11	5
H	1.099791	1	119.720583	1	-179.744300	1	15	12	11
H	1.099486	1	120.218428	1	-179.912554	1	16	15	12
H	1.099855	1	119.705213	1	179.972158	1	14	13	11
H	1.101048	1	120.066679	1	0.130228	1	13	11	5
H	1.101199	1	120.234314	1	-0.604392	1	19	17	5
H	1.099688	1	119.763289	1	179.805416	1	20	19	17
H	1.099438	1	120.194057	1	180.021050	1	22	21	18
H	1.099745	1	119.712854	1	179.957006	1	21	18	17
H	1.102057	1	119.308083	1	1.378377	1	18	17	5
H	1.103068	1	118.038092	1	4.646428	1	33	26	24
H	1.100510	1	120.889117	1	-179.778680	1	34	33	26
H	1.100512	1	118.493932	1	0.942748	1	36	35	34
H	1.100375	1	120.690197	1	179.756920	1	37	36	35
H	1.100180	1	119.121793	1	179.622970	1	39	37	36
H	1.102242	1	118.504000	1	-0.765826	1	38	32	27
H	1.101526	1	118.745496	1	-0.912124	1	43	31	30
H	1.100176	1	119.095487	1	179.684143	1	46	45	44
H	1.099817	1	120.805780	1	179.830790	1	45	44	42
H	1.100529	1	118.473969	1	1.059173	1	44	42	41
H	1.100620	1	120.972957	1	-179.844890	1	41	40	29
H	1.101747	1	117.869709	1	0.781749	1	40	29	28

(P)-11 Heat of formation = -13.361039 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.446833	1	0.000000	0	0.000000	0	1	0	0
N	1.583978	1	107.740826	1	0.000000	0	1	2	0
C	1.510922	1	100.915981	1	-26.576613	1	3	1	2
C	1.442281	1	110.629585	1	16.176741	1	2	1	3
C	1.481307	1	112.526573	1	-139.644865	1	3	1	2
C	1.534851	1	109.460710	1	94.704585	1	6	3	1
C	1.522520	1	106.421353	1	4.132538	1	7	6	3
B	1.668500	1	119.252810	1	88.093834	1	3	1	2
C	1.561469	1	115.590015	1	-139.413481	1	1	2	3
C	1.512008	1	108.958168	1	122.484461	1	5	2	1
C	1.399303	1	120.739220	1	1.337802	1	11	5	2
C	1.401263	1	120.022594	1	179.842932	1	11	5	2
C	1.392905	1	120.392287	1	-178.617216	1	13	11	5
C	1.394866	1	120.243138	1	178.601700	1	12	11	5
C	1.393767	1	120.266835	1	-0.048795	1	15	12	11
C	1.516238	1	108.022393	1	-120.108096	1	5	2	1
C	1.402421	1	118.722313	1	-26.558579	1	17	5	2
C	1.399247	1	122.399512	1	156.128042	1	17	5	2
C	1.395016	1	120.436303	1	178.406917	1	19	17	5
C	1.393199	1	120.635710	1	-178.359356	1	18	17	5
C	1.394431	1	120.149166	1	0.216973	1	21	18	17
O	1.679015	1	100.124256	1	116.415989	1	1	2	3
C	1.267607	1	121.029671	1	-51.801042	1	23	1	2
O	2.266925	1	88.705758	1	-74.675127	1	24	23	1
C	1.466696	1	121.227879	1	-167.914191	1	24	23	1
C	1.388383	1	122.930937	1	33.987130	1	26	24	23
C	1.410923	1	124.516106	1	-66.941720	1	25	24	23
C	1.503275	1	111.640209	1	19.813401	1	28	25	24
C	1.385433	1	123.412168	1	-54.877330	1	29	28	25
C	1.435088	1	119.863869	1	177.556050	1	30	29	28
C	1.435472	1	119.030815	1	170.545423	1	27	26	24
C	1.423870	1	116.176858	1	-152.108969	1	26	24	23
C	1.367682	1	120.772267	1	-173.318932	1	33	26	24
C	1.422432	1	120.261812	1	1.737385	1	34	33	26
C	1.421164	1	120.943956	1	177.591261	1	35	34	33
C	1.373410	1	120.569629	1	-178.708951	1	36	35	34
C	1.423397	1	121.771472	1	-176.114499	1	32	27	26
C	1.414428	1	120.118310	1	-0.070402	1	37	36	35
C	1.421931	1	116.903805	1	125.867136	1	29	28	25
C	1.369214	1	121.292820	1	-179.354493	1	40	29	28
C	1.420663	1	120.295582	1	0.976725	1	41	40	29
C	1.423795	1	122.141202	1	-176.374974	1	31	30	29
C	1.421725	1	121.099388	1	178.143607	1	42	41	40
C	1.372618	1	120.625509	1	-178.922812	1	44	42	41
C	1.414910	1	119.990411	1	-0.034883	1	45	44	42
H	1.125030	1	108.009942	1	145.082895	1	4	3	1
H	1.119128	1	110.072687	1	-112.385440	1	8	7	6
H	1.116969	1	111.662529	1	127.852722	1	8	7	6
H	1.117827	1	110.492642	1	-116.247759	1	7	6	3
H	1.117443	1	110.138260	1	124.743927	1	7	6	3
H	1.126301	1	108.618172	1	-145.480348	1	6	3	1
H	1.122447	1	110.232085	1	-28.064892	1	6	3	1
H	1.114808	1	121.062812	1	12.280567	1	24	23	1
H	1.209231	1	105.291105	1	159.809921	1	9	3	1
H	1.213977	1	104.020957	1	-75.417417	1	9	3	1
H	1.107977	1	110.041570	1	-155.023872	1	10	1	2
H	1.109388	1	106.380729	1	-35.502332	1	10	1	2
H	1.109352	1	107.767506	1	83.256130	1	10	1	2
H	1.102217	1	119.492093	1	-1.258018	1	12	11	5
H	1.099845	1	119.676104	1	-179.887931	1	15	12	11
H	1.099496	1	120.185991	1	-179.836382	1	16	15	12
H	1.099686	1	119.836393	1	179.846889	1	14	13	11
H	1.100531	1	119.647116	1	1.070920	1	13	11	5
H	1.100250	1	120.903955	1	-1.469009	1	19	17	5
H	1.099906	1	119.639507	1	179.436044	1	20	19	17
H	1.099376	1	120.222241	1	-179.808711	1	22	21	18
H	1.099669	1	119.816589	1	179.815555	1	21	18	17
H	1.101917	1	119.232699	1	0.908269	1	18	17	5
H	1.101581	1	118.601348	1	6.355353	1	33	26	24
H	1.100472	1	120.977433	1	-179.290004	1	34	33	26
H	1.100427	1	118.559760	1	0.979447	1	36	35	34
H	1.100222	1	120.690539	1	179.798140	1	37	36	35
H	1.100174	1	119.145626	1	179.652492	1	39	37	36
H	1.102183	1	118.624105	1	-0.529772	1	38	32	27
H	1.101385	1	118.726373	1	-0.266964	1	43	31	30
H	1.100072	1	119.075411	1	179.565002	1	46	45	44
H	1.099728	1	120.810081	1	179.800967	1	45	44	42
H	1.100370	1	118.496892	1	0.816660	1	44	42	41
H	1.100500	1	120.969469	1	-179.580984	1	41	40	29
H	1.101423	1	118.464964	1	0.532127	1	40	29	28

TSa (P)-11 <--> (M)-11 Heat of formation = 14.016494 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.480671	1	0.000000	0	0.000000	0	1	0	0
N	1.637696	1	104.868820	1	0.000000	0	1	2	0
C	1.564532	1	114.828790	1	-129.499764	1	1	2	3
O	1.505777	1	104.683455	1	115.270046	1	1	2	3
C	1.428127	1	113.467436	1	1.917390	1	2	1	3
C	1.501387	1	105.002156	1	7.328892	1	3	1	2
C	1.487934	1	114.867972	1	-109.299073	1	3	1	2
B	1.545678	1	109.530793	1	129.239881	1	3	1	2
C	1.367736	1	116.113532	1	52.759744	1	5	1	3
C	1.518095	1	108.006804	1	-128.069613	1	6	2	1
C	1.515930	1	108.575096	1	113.810261	1	6	2	1
C	1.534369	1	108.241306	1	-140.381726	1	7	3	1
C	1.533796	1	108.804278	1	134.115182	1	8	3	1
O	1.484368	1	104.571901	1	-78.540959	1	10	5	1
C	1.502808	1	115.234430	1	163.309561	1	10	5	1
C	1.400341	1	121.524092	1	155.079213	1	11	6	2
C	1.400762	1	119.288224	1	-26.133159	1	11	6	2
C	1.401582	1	121.367120	1	158.382312	1	12	6	2
C	1.400529	1	119.916352	1	-19.202170	1	12	6	2
C	1.449371	1	112.578687	1	-94.552441	1	15	10	5
C	1.394732	1	125.364232	1	32.191813	1	16	10	5
C	1.429223	1	112.740179	1	-155.280771	1	16	10	5
C	1.394023	1	120.378239	1	178.822047	1	17	11	6
C	1.394271	1	120.300526	1	-178.786362	1	18	11	6
C	1.393622	1	120.632404	1	-179.009303	1	19	12	6
C	1.394182	1	120.632542	1	179.008909	1	20	12	6
C	1.497037	1	112.063152	1	53.762630	1	21	15	10
C	1.487914	1	116.866330	1	23.967886	1	22	16	10
C	1.454050	1	114.194257	1	-168.354858	1	22	16	10
C	1.363773	1	120.311348	1	-168.784160	1	23	16	10
C	1.394511	1	120.170834	1	-0.090758	1	24	17	11
C	1.394381	1	120.236569	1	0.533741	1	26	19	12
C	1.421730	1	112.700578	1	100.792894	1	28	21	15
C	1.445093	1	129.109953	1	-141.549721	1	29	22	16
C	1.425830	1	117.954568	1	-32.844046	1	30	22	16
C	1.417585	1	109.699451	1	-2.434157	1	30	29	35
C	1.363019	1	120.829733	1	-168.491887	1	34	28	21
C	1.427070	1	119.748907	1	167.334901	1	35	29	22
C	1.420352	1	100.664781	1	31.002015	1	35	22	30
C	1.418841	1	120.263724	1	-164.610265	1	36	30	22
C	1.377975	1	121.953568	1	168.233997	1	37	30	22
C	1.422832	1	121.274700	1	-169.164766	1	39	35	29
C	1.374210	1	123.276932	1	169.968186	1	40	35	29
C	1.375353	1	120.366327	1	-10.628847	1	41	36	30
C	1.370893	1	120.977118	1	-4.894623	1	43	39	35
H	1.129792	1	106.837029	1	102.113847	1	7	3	1
H	1.116607	1	111.875933	1	132.760096	1	13	7	3
H	1.119640	1	109.199131	1	-108.417279	1	13	7	3
H	1.117835	1	110.523545	1	108.948003	1	14	8	3
H	1.117538	1	110.063043	1	-132.042561	1	14	8	3
H	1.123819	1	109.301152	1	-104.239138	1	8	3	1
H	1.123563	1	109.371148	1	14.128647	1	8	3	1
H	1.102962	1	119.131306	1	1.491177	1	18	11	6
H	1.099990	1	119.708281	1	179.808584	1	25	18	11
H	1.099476	1	120.083129	1	-179.731393	1	32	24	17
H	1.099656	1	119.793406	1	-179.907582	1	24	17	11
H	1.101380	1	120.130491	1	-0.764739	1	17	11	6
H	1.102651	1	119.239876	1	0.398100	1	20	12	6
H	1.099801	1	119.686867	1	-179.962485	1	27	20	12
H	1.099304	1	120.173537	1	179.869110	1	33	26	19
H	1.099662	1	119.729886	1	180.045062	1	26	19	12
H	1.101016	1	120.120327	1	0.254852	1	19	12	6
H	1.132355	1	113.718402	1	32.567341	1	10	5	1
H	1.204385	1	113.766315	1	-152.983412	1	9	3	1
H	1.199807	1	111.600410	1	62.861666	1	9	3	1
H	1.107949	1	109.244401	1	173.618557	1	4	1	2
H	1.107549	1	110.393615	1	51.112574	1	4	1	2
H	1.110048	1	105.349332	1	-67.795885	1	4	1	2
H	1.101567	1	118.729771	1	6.187818	1	23	16	10
H	1.099323	1	121.897690	1	169.260103	1	31	23	16
H	1.100163	1	118.557907	1	171.750514	1	41	36	30
H	1.098967	1	121.260876	1	178.415972	1	45	41	36
H	1.099975	1	120.243897	1	-178.152380	1	42	37	30
H	1.100917	1	119.075502	1	-22.040010	1	37	30	22
H	1.088708	1	119.441354	1	-16.196752	1	40	35	29
H	1.100188	1	120.166267	1	-178.398425	1	44	40	35
H	1.098867	1	121.501018	1	178.357284	1	46	43	39
H	1.100755	1	118.187468	1	175.502788	1	43	39	35
H	1.099985	1	121.547615	1	174.483646	1	38	34	28
H	1.101999	1	118.925009	1	8.305432	1	34	28	21

TSb (P)-11 <--> (M)-11 Heat of formation = 14.786412 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.474051	1	0.000000	0	0.000000	0	1	0	0
N	1.637365	1	105.182219	1	0.000000	0	1	2	0
C	1.567287	1	114.757156	1	-128.667424	1	1	2	3
O	1.508148	1	102.857584	1	118.302507	1	1	2	3
C	1.427258	1	113.475342	1	-2.086881	1	2	1	3
C	1.506053	1	104.273193	1	11.458849	1	3	1	2
C	1.492560	1	112.827838	1	-102.217730	1	3	1	2
B	1.550835	1	113.876397	1	134.806473	1	3	1	2
C	1.368171	1	118.571481	1	32.310666	1	5	1	3
C	1.515729	1	108.153236	1	-126.281857	1	6	2	1
C	1.517478	1	108.275635	1	115.358991	1	6	2	1
C	1.535227	1	107.871090	1	-142.541144	1	7	3	1
C	1.534403	1	108.498261	1	136.933388	1	8	3	1
O	1.708135	1	48.346260	1	37.150649	1	9	5	10
C	1.508287	1	112.886652	1	174.292492	1	10	5	1
C	1.400051	1	121.418217	1	157.354619	1	11	6	2
C	1.400500	1	119.316841	1	-24.503186	1	11	6	2
C	1.401342	1	121.586200	1	157.024600	1	12	6	2
C	1.400913	1	119.789785	1	-20.731137	1	12	6	2
C	1.444847	1	111.944799	1	-161.660738	1	15	10	5
C	1.398348	1	122.580242	1	-165.928576	1	16	10	5
C	1.424019	1	114.388438	1	22.855066	1	16	10	5
C	1.393776	1	120.330894	1	177.426974	1	17	11	6
C	1.394206	1	120.266445	1	-177.728041	1	18	11	6
C	1.393854	1	120.661578	1	-179.072296	1	19	12	6
C	1.393992	1	120.709333	1	179.050661	1	20	12	6
C	1.495961	1	110.663259	1	-41.548188	1	21	15	10
C	1.491413	1	115.890599	1	-13.632427	1	22	16	10
C	1.449037	1	114.954414	1	177.176205	1	22	16	10
C	1.364554	1	119.921159	1	163.640606	1	23	16	10
C	1.394523	1	120.182237	1	0.406971	1	24	17	11
C	1.394173	1	120.269652	1	0.511563	1	26	19	12
C	1.420299	1	113.434635	1	-95.575492	1	28	21	15
C	1.445132	1	129.486428	1	134.247683	1	29	22	16
C	1.427287	1	118.287428	1	26.614992	1	30	22	16
C	1.419757	1	107.130308	1	-9.849433	1	30	29	35
C	1.363790	1	120.509859	1	170.107709	1	34	28	21
C	1.427633	1	119.430451	1	-158.883397	1	35	29	22
C	1.420328	1	102.278731	1	-26.918180	1	35	22	30
C	1.421291	1	120.437577	1	163.667470	1	36	30	22
C	1.375893	1	122.371101	1	-166.427141	1	37	30	22
C	1.422927	1	121.076759	1	168.671306	1	39	35	29
C	1.374312	1	123.122563	1	-169.909985	1	40	35	29
C	1.373138	1	120.596985	1	9.675409	1	41	36	30
C	1.371169	1	120.933631	1	5.945993	1	43	39	35
H	1.128254	1	107.684999	1	99.651812	1	7	3	1
H	1.116530	1	111.712595	1	136.286352	1	13	7	3
H	1.119549	1	109.231128	1	-104.892528	1	13	7	3
H	1.117722	1	110.631639	1	105.321421	1	14	8	3
H	1.117325	1	110.053936	1	-135.536144	1	14	8	3
H	1.122545	1	109.759445	1	-100.898717	1	8	3	1
H	1.124547	1	108.966575	1	17.772583	1	8	3	1
H	1.102869	1	119.181058	1	2.601227	1	18	11	6
H	1.099833	1	119.714030	1	-179.972230	1	25	18	11
H	1.099331	1	120.071874	1	180.019036	1	32	24	17
H	1.099445	1	119.808728	1	-179.763795	1	24	17	11
H	1.101122	1	120.065498	1	-2.158583	1	17	11	6
H	1.102346	1	119.235916	1	0.499837	1	20	12	6
H	1.099784	1	119.705504	1	-179.864521	1	27	20	12
H	1.099276	1	120.200218	1	179.823685	1	33	26	19
H	1.099687	1	119.702756	1	179.996384	1	26	19	12
H	1.100940	1	120.228055	1	0.123305	1	19	12	6
H	1.122332	1	115.378451	1	40.649504	1	10	5	1
H	1.204339	1	112.661428	1	-138.517252	1	9	3	1
H	1.202871	1	112.773830	1	78.355292	1	9	3	1
H	1.107982	1	109.543990	1	166.468247	1	4	1	2
H	1.107470	1	110.118659	1	44.003833	1	4	1	2
H	1.110362	1	105.629177	1	-74.670399	1	4	1	2
H	1.103984	1	118.203582	1	-11.303677	1	23	16	10
H	1.099699	1	121.674515	1	-169.900046	1	31	23	16
H	1.100463	1	118.345216	1	-172.158761	1	41	36	30
H	1.098889	1	121.419593	1	-178.131588	1	45	41	36
H	1.099993	1	120.293525	1	178.101904	1	42	37	30
H	1.097589	1	119.132161	1	24.307583	1	37	30	22
H	1.090397	1	119.297396	1	17.985160	1	40	35	29
H	1.100332	1	120.189722	1	178.508350	1	44	40	35
H	1.099042	1	121.479789	1	-178.495167	1	46	43	39
H	1.100757	1	118.208483	1	-174.913442	1	43	39	35
H	1.100083	1	121.585710	1	-173.887480	1	38	34	28
H	1.102140	1	118.885081	1	-6.736713	1	34	28	21

TS (M,Si)-[11 -> 12] Heat of formation = -3.437683 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.421092	1	0.000000	0	0.000000	0	1	0	0
N	1.592949	1	109.056270	1	0.000000	0	1	2	0
C	1.558016	1	117.086155	1	-140.118941	1	1	2	3
O	1.714143	1	94.795940	1	110.811462	1	1	2	3
C	1.444394	1	112.054785	1	-6.173574	1	2	1	3
C	1.509214	1	103.205456	1	10.947289	1	3	1	2
C	1.489747	1	111.815632	1	-103.032268	1	3	1	2
B	1.606579	1	116.797553	1	129.110080	1	3	1	2
C	1.283903	1	110.057613	1	-167.551517	1	5	1	2
C	1.512388	1	108.331066	1	-119.690206	1	6	2	1
C	1.514060	1	106.932349	1	121.108164	1	6	2	1
C	1.533495	1	107.813399	1	-137.712405	1	7	3	1
C	1.523267	1	106.666523	1	14.199451	1	13	7	3
O	2.911086	1	116.618037	1	22.498346	1	10	5	1
C	1.471894	1	123.643230	1	-179.659071	1	10	5	1
C	1.400774	1	121.131676	1	157.863351	1	11	6	2
C	1.400036	1	119.668090	1	-22.577722	1	11	6	2
C	1.400833	1	121.290355	1	154.953720	1	12	6	2
C	1.401374	1	119.905673	1	-23.723820	1	12	6	2
C	1.419038	1	83.894376	1	167.793521	1	15	10	5
C	1.385876	1	124.322251	1	-136.941879	1	16	10	5
C	1.425804	1	114.423204	1	52.085388	1	16	10	5
C	1.393649	1	120.361646	1	179.465173	1	17	11	6
C	1.394421	1	120.280242	1	-179.459011	1	18	11	6
C	1.393929	1	120.529227	1	-179.318658	1	19	12	6
C	1.393851	1	120.594100	1	179.207895	1	20	12	6
C	1.500791	1	114.200014	1	-77.325442	1	21	15	10
C	1.384228	1	123.792773	1	99.496332	1	28	21	15
C	1.440051	1	118.339979	1	-160.831675	1	22	16	10
C	1.367116	1	120.878178	1	165.543451	1	23	16	10
C	1.394001	1	120.249128	1	-0.025329	1	25	18	11
C	1.394014	1	120.206834	1	-0.075723	1	27	20	12
C	1.422978	1	115.957057	1	-77.594844	1	28	21	15
C	1.439770	1	119.110105	1	-171.013860	1	29	28	21
C	1.417616	1	120.049870	1	-6.600383	1	30	22	16
C	1.423573	1	121.592957	1	171.949998	1	30	22	16
C	1.367948	1	121.236785	1	174.832014	1	34	28	21
C	1.417735	1	119.722897	1	-5.384563	1	35	29	28
C	1.423806	1	122.124327	1	172.982570	1	35	29	28
C	1.421080	1	119.684066	1	179.521709	1	36	30	22
C	1.373802	1	120.938142	1	-178.907254	1	37	30	22
C	1.421497	1	119.757033	1	-179.729407	1	39	35	29
C	1.373528	1	121.077121	1	-179.586016	1	40	35	29
C	1.373321	1	120.568893	1	-0.828954	1	41	36	30
C	1.372758	1	120.641929	1	-1.223116	1	43	39	35
H	1.129134	1	107.054946	1	104.303363	1	7	3	1
H	1.116802	1	111.812922	1	136.330375	1	13	7	3
H	1.120077	1	108.935354	1	-104.862583	1	13	7	3
H	1.117833	1	110.796391	1	-123.169339	1	14	13	7
H	1.117533	1	111.162083	1	116.833318	1	14	13	7
H	1.124209	1	108.956017	1	-108.593025	1	8	3	1
H	1.124548	1	109.541618	1	9.888423	1	8	3	1
H	1.102173	1	119.310411	1	1.466536	1	18	11	6
H	1.099748	1	119.695834	1	-179.867355	1	25	18	11
H	1.099414	1	120.190966	1	-179.917605	1	32	25	18
H	1.099595	1	119.780768	1	179.807497	1	24	17	11
H	1.101138	1	120.184729	1	-0.539733	1	17	11	6
H	1.102226	1	119.472650	1	0.164576	1	20	12	6
H	1.099782	1	119.740365	1	-179.735051	1	27	20	12
H	1.099424	1	120.220823	1	-179.890047	1	33	27	20
H	1.099826	1	119.689325	1	179.935388	1	26	19	12
H	1.101038	1	120.148414	1	0.077798	1	19	12	6
H	1.121504	1	118.740066	1	-24.886045	1	10	5	1
H	1.697434	1	96.081639	1	69.590195	1	10	5	1
H	1.206990	1	108.819202	1	-153.373119	1	9	3	1
H	1.108469	1	110.419045	1	168.382633	1	4	1	2
H	1.109931	1	107.202868	1	47.561451	1	4	1	2
H	1.109248	1	107.363003	1	-70.532840	1	4	1	2
H	1.102301	1	117.977975	1	-14.701713	1	23	16	10
H	1.100478	1	121.008889	1	179.366409	1	31	23	16
H	1.100424	1	118.533254	1	179.478481	1	41	36	30
H	1.100103	1	120.738754	1	-179.784101	1	45	41	36
H	1.100252	1	120.426091	1	179.651492	1	42	37	30
H	1.102073	1	118.735541	1	1.006282	1	37	30	22
H	1.101539	1	118.930665	1	-0.051491	1	40	35	29
H	1.100091	1	120.417050	1	179.665826	1	44	40	35
H	1.099711	1	120.825760	1	-179.763070	1	46	43	39
H	1.100358	1	118.473761	1	179.242803	1	43	39	35
H	1.100321	1	121.073067	1	179.310508	1	38	34	28
H	1.101509	1	117.999577	1	-4.192815	1	34	28	21

TS (M,Re)-[11 -> 12] Heat of formation = -8.191711 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.414369	1	0.000000	0	0.000000	0	1	0	0
N	1.576100	1	109.061148	1	0.000000	0	1	2	0
C	1.549389	1	118.124232	1	-144.584386	1	1	2	3
O	1.776805	1	90.385374	1	107.651907	1	1	2	3
C	1.447422	1	112.088433	1	-7.862229	1	2	1	3
C	1.508940	1	103.533687	1	13.385934	1	3	1	2
C	1.492660	1	111.626683	1	-100.232775	1	3	1	2
B	1.598737	1	116.373390	1	133.051497	1	3	1	2
C	1.273957	1	123.882142	1	-51.917145	1	5	1	3
C	1.511024	1	108.564583	1	-119.430109	1	6	2	1
C	1.513607	1	106.825978	1	121.156470	1	6	2	1
C	1.533223	1	107.772093	1	-139.338767	1	7	3	1
C	1.534133	1	108.537098	1	132.305368	1	8	3	1
O	3.264582	1	99.125583	1	8.145154	1	10	5	1
C	1.474904	1	124.438189	1	-64.143738	1	10	5	1
C	1.400827	1	121.015710	1	157.565597	1	11	6	2
C	1.399964	1	119.753275	1	-22.869937	1	11	6	2
C	1.400763	1	121.258843	1	154.949002	1	12	6	2
C	1.401484	1	119.920429	1	-23.754052	1	12	6	2
C	1.409679	1	110.122239	1	166.531327	1	15	10	5
C	1.386129	1	122.835951	1	153.892132	1	16	10	5
C	1.423752	1	117.056667	1	-30.407585	1	16	10	5
C	1.393635	1	120.345187	1	179.374391	1	17	11	6
C	1.394464	1	120.260217	1	-179.366899	1	18	11	6
C	1.393945	1	120.520907	1	-179.324637	1	19	12	6
C	1.393838	1	120.579953	1	179.199260	1	20	12	6
C	1.503674	1	114.902095	1	-15.557056	1	21	15	10
C	1.471861	1	121.868904	1	-2.578374	1	22	16	10
C	1.432996	1	119.728046	1	177.215374	1	22	16	10
C	1.368735	1	121.001921	1	-176.403972	1	23	16	10
C	1.394700	1	120.166161	1	0.028502	1	24	17	11
C	1.394250	1	120.272928	1	0.339633	1	26	19	12
C	1.421375	1	117.618131	1	-124.492425	1	28	21	15
C	1.431655	1	118.494520	1	89.731959	1	29	22	16
C	1.417916	1	119.593547	1	-1.431443	1	30	22	16
C	1.423474	1	121.799853	1	178.656043	1	30	22	16
C	1.370128	1	121.131138	1	179.965279	1	34	28	21
C	1.417937	1	119.361640	1	178.380756	1	35	29	22
C	1.423577	1	122.091689	1	-1.556244	1	35	29	22
C	1.421615	1	119.484639	1	-179.772601	1	36	30	22
C	1.373217	1	120.814939	1	179.827005	1	37	30	22
C	1.421905	1	119.488326	1	179.927029	1	39	35	29
C	1.372902	1	120.859992	1	180.065765	1	40	35	29
C	1.373065	1	120.561336	1	-0.120973	1	41	36	30
C	1.372656	1	120.618083	1	0.032054	1	43	39	35
H	1.127910	1	107.185966	1	102.260596	1	7	3	1
H	1.116824	1	111.712629	1	137.031681	1	13	7	3
H	1.119927	1	108.997159	1	-104.104379	1	13	7	3
H	1.117817	1	110.319027	1	109.217859	1	14	8	3
H	1.117419	1	110.105804	1	-131.722851	1	14	8	3
H	1.124128	1	108.855048	1	-106.082504	1	8	3	1
H	1.124383	1	109.449365	1	12.455016	1	8	3	1
H	1.102225	1	119.257796	1	1.694024	1	18	11	6
H	1.099795	1	119.698385	1	-179.953794	1	25	18	11
H	1.099464	1	120.064954	1	180.009983	1	32	24	17
H	1.099611	1	119.790480	1	179.921797	1	24	17	11
H	1.101150	1	120.135129	1	-0.563432	1	17	11	6
H	1.102246	1	119.519987	1	0.141392	1	20	12	6
H	1.099821	1	119.737676	1	-179.718281	1	27	20	12
H	1.099460	1	120.176071	1	179.751801	1	33	26	19
H	1.099849	1	119.689432	1	179.938790	1	26	19	12
H	1.101082	1	120.141676	1	0.066776	1	19	12	6
H	1.117615	1	117.273860	1	137.211974	1	10	5	1
H	1.733929	1	97.327499	1	46.840865	1	10	5	1
H	3.734595	1	90.685078	1	44.005207	1	10	5	1
H	1.109148	1	109.169028	1	-169.195471	1	4	1	2
H	1.109742	1	107.610526	1	69.995148	1	4	1	2
H	1.109183	1	106.997585	1	-48.318648	1	4	1	2
H	1.102665	1	118.072329	1	3.111355	1	23	16	10
H	1.100453	1	120.833950	1	179.569204	1	31	23	16
H	1.100350	1	118.533264	1	180.014846	1	41	36	30
H	1.100101	1	120.707008	1	-179.916560	1	45	41	36
H	1.100078	1	120.517561	1	179.977019	1	42	37	30
H	1.101859	1	118.560523	1	-0.180843	1	37	30	22
H	1.101360	1	118.633377	1	0.380972	1	40	35	29
H	1.100119	1	120.527425	1	-179.962232	1	44	40	35
H	1.099815	1	120.775021	1	180.042085	1	46	43	39
H	1.100425	1	118.498964	1	-179.912938	1	43	39	35
H	1.100538	1	120.874232	1	-179.886300	1	38	34	28
H	1.101387	1	118.535728	1	0.555189	1	34	28	21

TS (P,Si)-[11 -> 12] Heat of formation = -13.100837 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.429913	1	0.000000	0	0.000000	0	1	0	0	0
N	1.611628	1	108.108943	1	0.000000	0	1	2	0	0
C	1.508568	1	103.167829	1	12.468109	1	3	1	2	0
C	1.440728	1	112.350959	1	-7.681224	1	2	1	3	0
C	1.490044	1	111.678473	1	-101.110062	1	3	1	2	0
C	1.534274	1	108.613307	1	131.865553	1	6	3	1	0
C	1.523500	1	106.433129	1	-11.357248	1	7	6	3	0
B	1.591870	1	116.246810	1	131.147542	1	3	1	2	0
C	1.559254	1	116.571403	1	-136.589986	1	1	2	3	0
C	1.514691	1	106.959108	1	122.095706	1	5	2	1	0
C	1.401450	1	119.795340	1	-23.802315	1	11	5	2	0
C	1.400759	1	121.401160	1	154.801629	1	11	5	2	0
C	1.393964	1	120.533915	1	-179.279575	1	13	11	5	0
C	1.393844	1	120.590793	1	179.179298	1	12	11	5	0
C	1.394031	1	120.210389	1	-0.095114	1	15	12	11	0
C	1.513436	1	108.372534	1	-118.817944	1	5	2	1	0
C	1.400239	1	119.571722	1	-22.421589	1	17	5	2	0
C	1.400680	1	121.246480	1	158.068319	1	17	5	2	0
C	1.393763	1	120.379523	1	179.414911	1	19	17	5	0
C	1.394389	1	120.284967	1	-179.392633	1	18	17	5	0
C	1.394103	1	120.254969	1	-0.044849	1	21	18	17	0
O	1.667864	1	108.248914	1	-90.457723	1	1	3	4	0
C	1.301049	1	109.701368	1	-167.149945	1	23	1	2	0
O	2.945037	1	116.449456	1	23.223350	1	24	23	1	0
C	1.466859	1	122.720881	1	167.643172	1	24	23	1	0
C	1.392017	1	119.065518	1	169.561702	1	26	24	23	0
C	1.421170	1	86.521007	1	163.075680	1	25	24	23	0
C	1.504663	1	109.895857	1	64.783456	1	28	25	24	0
C	1.385055	1	124.253479	1	-105.116086	1	29	28	25	0
C	1.436890	1	119.527566	1	178.371468	1	30	29	28	0
C	1.431005	1	118.993154	1	170.033085	1	27	26	24	0
C	1.419114	1	119.761712	1	-15.944863	1	26	24	23	0
C	1.369790	1	120.394309	1	-172.125424	1	33	26	24	0
C	1.421687	1	120.344767	1	1.181878	1	34	33	26	0
C	1.422199	1	120.989995	1	177.316654	1	35	34	33	0
C	1.372729	1	120.634581	1	-179.179030	1	36	35	34	0
C	1.423985	1	121.828723	1	-175.849808	1	32	27	26	0
C	1.415461	1	120.171087	1	-0.145174	1	37	36	35	0
C	1.422291	1	115.746541	1	74.735514	1	29	28	25	0
C	1.368465	1	121.266606	1	-179.546162	1	40	29	28	0
C	1.420980	1	120.183403	1	0.738641	1	41	40	29	0
C	1.423827	1	122.114302	1	-177.246166	1	31	30	29	0
C	1.421735	1	120.940425	1	178.746527	1	42	41	40	0
C	1.372659	1	120.631681	1	-178.649124	1	44	42	41	0
C	1.414624	1	119.950512	1	0.022738	1	45	44	42	0
H	1.128658	1	107.204961	1	103.277132	1	4	3	1	0
H	1.116795	1	111.482113	1	-124.115394	1	8	7	6	0
H	1.119932	1	110.356532	1	116.399164	1	8	7	6	0
H	1.117419	1	110.085503	1	-131.994719	1	7	6	3	0
H	1.117840	1	110.386650	1	108.960130	1	7	6	3	0
H	1.123668	1	109.285240	1	-106.393821	1	6	3	1	0
H	1.124825	1	109.307158	1	12.178589	1	6	3	1	0
H	1.206736	1	111.026659	1	-146.076717	1	9	3	1	0
H	1.598533	1	97.995737	1	68.848186	1	24	23	1	0
H	1.119999	1	118.189298	1	-32.223413	1	24	23	1	0
H	1.108443	1	110.543769	1	164.208430	1	10	1	2	0
H	1.109515	1	106.975047	1	-75.052595	1	10	1	2	0
H	1.109640	1	107.561527	1	43.073594	1	10	1	2	0
H	1.102427	1	119.422975	1	0.188378	1	12	11	5	0
H	1.099791	1	119.736283	1	-179.728400	1	15	12	11	0
H	1.099411	1	120.223543	1	-179.881056	1	16	15	12	0
H	1.099798	1	119.691852	1	179.931019	1	14	13	11	0
H	1.100947	1	120.176563	1	0.105815	1	13	11	5	0
H	1.101167	1	120.174663	1	-0.425440	1	19	17	5	0
H	1.099602	1	119.787696	1	179.957012	1	20	19	17	0
H	1.099419	1	120.194458	1	179.937429	1	22	21	18	0
H	1.099816	1	119.691986	1	179.940719	1	21	18	17	0
H	1.102542	1	119.246945	1	1.449299	1	18	17	5	0
H	1.102917	1	117.955532	1	7.411047	1	33	26	24	0
H	1.100512	1	120.858795	1	-179.667331	1	34	33	26	0
H	1.100511	1	118.474344	1	0.571172	1	36	35	34	0
H	1.100237	1	120.705753	1	179.796059	1	37	36	35	0
H	1.100163	1	119.103989	1	179.776924	1	39	37	36	0
H	1.101974	1	118.473377	1	-0.991330	1	38	32	27	0
H	1.101681	1	118.846406	1	-0.536135	1	43	31	30	0
H	1.100231	1	119.105963	1	179.542247	1	46	45	44	0
H	1.099861	1	120.814252	1	179.849375	1	45	44	42	0
H	1.100470	1	118.478385	1	1.102899	1	44	42	41	0
H	1.100558	1	121.021119	1	-179.820620	1	41	40	29	0
H	1.101749	1	117.906811	1	-0.297443	1	40	29	28	0

TS (P,Re)-[11 -> 12] Heat of formation = -1.280491 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.441809	1	0.000000	0	0.000000	0	1	0	0	0
N	1.595531	1	108.247947	1	0.000000	0	1	2	0	0
C	1.514951	1	103.460875	1	-9.786206	1	3	1	2	0
C	1.437366	1	112.102547	1	11.611466	1	2	1	3	0
C	1.484516	1	114.593109	1	-125.752286	1	3	1	2	0
C	1.531617	1	109.557046	1	104.553212	1	6	3	1	0
C	1.519859	1	105.734122	1	16.287940	1	7	6	3	0
B	1.616276	1	114.764096	1	105.117622	1	3	1	2	0
C	1.559201	1	116.027041	1	-139.816086	1	1	2	3	0
C	1.514493	1	107.834501	1	114.708213	1	5	2	1	0
C	1.400800	1	120.020828	1	-18.931541	1	11	5	2	0
C	1.401226	1	121.077858	1	159.434088	1	11	5	2	0
C	1.393547	1	120.515175	1	-179.026705	1	13	11	5	0
C	1.394215	1	120.496802	1	178.956638	1	12	11	5	0
C	1.393840	1	120.244985	1	-0.140235	1	15	12	11	0
C	1.516700	1	107.577904	1	-127.406782	1	5	2	1	0
C	1.401525	1	119.160395	1	-25.342906	1	17	5	2	0
C	1.400165	1	121.804576	1	156.239056	1	17	5	2	0
C	1.394395	1	120.402443	1	179.060830	1	19	17	5	0
C	1.393892	1	120.446576	1	-178.991231	1	18	17	5	0
C	1.394390	1	120.199300	1	0.098727	1	21	18	17	0
O	1.651081	1	99.946931	1	113.206769	1	1	2	3	0
C	1.289995	1	118.130300	1	-57.805048	1	23	1	2	0
O	3.049938	1	78.068113	1	-81.765276	1	24	23	1	0
C	1.462344	1	120.404430	1	-148.235280	1	24	23	1	0
C	1.390484	1	123.185119	1	13.176341	1	26	24	23	0
C	1.394666	1	105.182338	1	-28.242423	1	25	24	23	0
C	1.505376	1	117.452847	1	-31.697230	1	28	25	24	0
C	1.381460	1	127.898769	1	-17.155374	1	29	28	25	0
C	1.440637	1	119.895903	1	179.549470	1	30	29	28	0
C	1.434999	1	119.210263	1	167.502922	1	27	26	24	0
C	1.426154	1	116.131945	1	-174.465948	1	26	24	23	0
C	1.366808	1	120.913256	1	-170.334481	1	33	26	24	0
C	1.423264	1	120.306758	1	1.306007	1	34	33	26	0
C	1.420535	1	121.068792	1	177.334193	1	35	34	33	0
C	1.373968	1	120.549130	1	-179.333534	1	36	35	34	0
C	1.422925	1	121.648422	1	-175.856472	1	32	27	26	0
C	1.414056	1	120.166003	1	-0.132515	1	37	36	35	0
C	1.429864	1	112.985770	1	164.913939	1	29	28	25	0
C	1.366064	1	121.910949	1	179.333097	1	40	29	28	0
C	1.421476	1	120.133872	1	0.682118	1	41	40	29	0
C	1.423563	1	121.989480	1	-177.316247	1	31	30	29	0
C	1.420594	1	121.096227	1	178.636495	1	42	41	40	0
C	1.373289	1	120.590211	1	-179.334354	1	44	42	41	0
C	1.413800	1	119.888498	1	-0.013374	1	45	44	42	0
H	1.130033	1	106.777765	1	120.744085	1	4	3	1	0
H	1.116410	1	111.229756	1	-139.248889	1	8	7	6	0
H	1.120327	1	110.306105	1	101.575268	1	8	7	6	0
H	1.118667	1	110.375854	1	-103.551207	1	7	6	3	0
H	1.116843	1	110.480262	1	137.123764	1	7	6	3	0
H	1.127501	1	107.786342	1	-136.293016	1	6	3	1	0
H	1.122079	1	110.764311	1	-17.965711	1	6	3	1	0
H	1.115415	1	119.698676	1	42.999594	1	24	23	1	0
H	1.212178	1	107.303948	1	-165.309520	1	9	3	1	0
H	1.770443	1	103.277470	1	-46.186428	1	24	23	1	0
H	1.109820	1	109.436626	1	-164.016931	1	10	1	2	0
H	1.109721	1	105.950801	1	-45.036043	1	10	1	2	0
H	1.108704	1	108.593626	1	73.734614	1	10	1	2	0
H	1.103159	1	119.446612	1	-0.142484	1	12	11	5	0
H	1.099869	1	119.693239	1	-179.802355	1	15	12	11	0
H	1.099476	1	120.227557	1	-179.874248	1	16	15	12	0
H	1.099783	1	119.731573	1	179.943497	1	14	13	11	0
H	1.100794	1	120.072920	1	0.471350	1	13	11	5	0
H	1.101169	1	120.472466	1	-0.633694	1	19	17	5	0
H	1.099939	1	119.710782	1	179.760051	1	20	19	17	0
H	1.099576	1	120.195329	1	179.977629	1	22	21	18	0
H	1.100003	1	119.744988	1	179.754196	1	21	18	17	0
H	1.102564	1	119.295276	1	0.579486	1	18	17	5	0
H	1.101493	1	118.526219	1	8.837711	1	33	26	24	0
H	1.100291	1	120.982292	1	-179.706260	1	34	33	26	0
H	1.100287	1	118.584831	1	0.292276	1	36	35	34	0
H	1.100184	1	120.651770	1	179.733295	1	37	36	35	0
H	1.100023	1	119.152837	1	179.697732	1	39	37	36	0
H	1.101933	1	118.588266	1	-0.414753	1	38	32	27	0
H	1.101405	1	118.980778	1	-0.113077	1	43	31	30	0
H	1.100069	1	119.109955	1	179.747361	1	46	45	44	0
H	1.099599	1	120.824193	1	179.872193	1	45	44	42	0
H	1.100323	1	118.536387	1	0.451356	1	44	42	41	0
H	1.100427	1	121.093068	1	-179.804157	1	41	40	29	0
H	1.101724	1	118.137741	1	-0.652103	1	40	29	28	0

(M)-12 HEAT OF FORMATION = -62.184020 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.442143	1	.000000	0	.000000	0	1	0	0
N	1.592176	1	107.569184	1	.000000	0	1	2	0
C	1.554938	1	116.749091	1	-141.271274	1	1	2	3
O	1.626977	1	107.976192	1	98.818816	1	1	2	3
C	1.443085	1	111.833011	1	8.257428	1	2	1	3
C	1.496109	1	105.394779	1	-.423561	1	3	1	2
C	1.471432	1	120.130140	1	-123.769674	1	3	1	2
B	1.582290	1	88.105880	1	117.683617	1	3	1	2
C	1.434354	1	118.163460	1	113.532066	1	5	1	3
C	1.513407	1	107.784442	1	-131.012156	1	6	2	1
C	1.514294	1	107.901427	1	110.514994	1	6	2	1
C	1.534031	1	108.086324	1	-133.716072	1	7	3	1
C	1.533817	1	108.973626	1	121.967955	1	8	3	1
O	2.803604	1	62.376170	1	-103.270229	1	10	5	1
C	1.499949	1	106.767651	1	157.693809	1	10	5	1
C	1.400442	1	121.285225	1	155.370763	1	11	6	2
C	1.400367	1	119.540565	1	-25.759271	1	11	6	2
C	1.401605	1	121.016532	1	158.096082	1	12	6	2
C	1.400547	1	120.192073	1	-20.101728	1	12	6	2
C	1.427022	1	91.366747	1	-113.208907	1	15	10	5
C	1.383973	1	122.968530	1	115.938207	1	16	10	5
C	1.421173	1	116.753774	1	-62.886981	1	16	10	5
C	1.393879	1	120.349589	1	179.118949	1	17	11	6
C	1.394169	1	120.340731	1	-179.136822	1	18	11	6
C	1.393566	1	120.574387	1	-179.160393	1	19	12	6
C	1.394204	1	120.581204	1	179.091708	1	20	12	6
C	1.501336	1	107.302163	1	-68.610384	1	21	15	10
C	1.472075	1	121.781963	1	3.311293	1	22	16	10
C	1.434540	1	119.501571	1	-176.545615	1	22	16	10
C	1.369054	1	120.994629	1	177.948838	1	23	16	10
C	1.394473	1	120.204698	1	-.092273	1	24	17	11
C	1.394510	1	120.234255	1	.416897	1	26	19	12
C	1.419891	1	117.243302	1	-77.552758	1	28	21	15
C	1.433625	1	118.974486	1	111.224383	1	29	22	16
C	1.418252	1	119.569715	1	-1.929851	1	30	22	16
C	1.423645	1	122.036895	1	176.966124	1	30	22	16
C	1.369833	1	120.933619	1	177.391129	1	34	28	21
C	1.418366	1	119.504439	1	177.392717	1	35	29	22
C	1.423674	1	122.046627	1	-3.582430	1	35	29	22
C	1.421820	1	119.569968	1	179.738518	1	36	30	22
C	1.373055	1	120.965537	1	-179.356226	1	37	30	22
C	1.422073	1	119.525432	1	179.973993	1	39	35	29
C	1.372954	1	120.934241	1	-179.577076	1	40	35	29
C	1.372663	1	120.639155	1	-.612133	1	41	36	30
C	1.372550	1	120.634384	1	-.667469	1	43	39	35
H	1.130189	1	107.521855	1	108.460456	1	7	3	1
H	1.117110	1	112.023827	1	127.009448	1	13	7	3
H	1.119675	1	109.018899	1	-114.214320	1	13	7	3
H	1.117471	1	110.285646	1	123.701665	1	14	8	3
H	1.118057	1	110.151032	1	-117.430301	1	14	8	3
H	1.124937	1	108.948134	1	-117.263374	1	8	3	1
H	1.124383	1	109.298261	1	.668225	1	8	3	1
H	1.101968	1	119.361847	1	1.208100	1	18	11	6
H	1.099852	1	119.747827	1	-179.737265	1	25	18	11
H	1.099486	1	120.110051	1	179.719845	1	32	24	17
H	1.099628	1	119.768027	1	179.708392	1	24	17	11
H	1.101157	1	120.210728	1	-.934135	1	17	11	6
H	1.102573	1	119.462499	1	.205788	1	20	12	6
H	1.099813	1	119.695598	1	-179.835244	1	27	20	12
H	1.099451	1	120.161291	1	179.790425	1	33	26	19
H	1.099824	1	119.727530	1	179.967042	1	26	19	12
H	1.101132	1	120.019026	1	.192762	1	19	12	6
H	1.124425	1	107.004683	1	39.185335	1	10	5	1
H	1.201727	1	113.844222	1	99.017707	1	9	3	1
H	1.121639	1	110.091050	1	-79.825946	1	10	5	1
H	1.108212	1	109.138550	1	-166.824177	1	4	1	2
H	1.108696	1	108.939622	1	71.727139	1	4	1	2
H	1.109192	1	106.314653	1	-47.451308	1	4	1	2
H	1.101513	1	117.928396	1	-1.068037	1	23	16	10
H	1.100260	1	120.991740	1	179.851016	1	31	23	16
H	1.100341	1	118.481509	1	179.597723	1	41	36	30
H	1.099740	1	120.781643	1	-179.860474	1	45	41	36
H	1.100013	1	120.493147	1	179.910647	1	42	37	30
H	1.101827	1	118.583244	1	.851114	1	37	30	22
H	1.101784	1	118.550113	1	.617394	1	40	35	29
H	1.099982	1	120.495806	1	179.918414	1	44	40	35
H	1.099778	1	120.775937	1	-179.912283	1	46	43	39
H	1.100295	1	118.484092	1	179.549565	1	43	39	35
H	1.100224	1	120.970174	1	179.742521	1	38	34	28
H	1.101005	1	118.216134	1	-1.908568	1	34	28	21

(M)-12 HEAT OF FORMATION = -54.747862 kcal/mol

C	.000000	0	.000000	0	.000000	0	0	0	0
C	1.372570	1	.000000	0	.000000	0	1	0	0
C	1.415502	1	120.088888	1	.000000	0	2	1	0
C	1.372869	1	120.403552	1	-.209720	1	3	2	1
C	1.423749	1	120.852194	1	.066643	1	4	3	2
C	1.417787	1	118.551342	1	.185759	1	5	4	3
C	1.420144	1	119.174770	1	179.348820	1	6	5	4
C	1.370323	1	120.430789	1	.842870	1	7	6	5
C	1.420877	1	121.232299	1	.637453	1	8	7	6
C	1.385869	1	119.455830	1	-2.204929	1	9	8	7
C	1.496402	1	121.927749	1	176.085507	1	9	10	5
O	1.423534	1	119.900064	1	87.792143	1	11	9	10
B	1.611712	1	122.147812	1	82.611358	1	12	11	9
O	1.445718	1	102.172883	1	108.699732	1	13	12	11
N	1.590184	1	90.761437	1	-143.034937	1	13	12	11
O	2.505842	1	96.395126	1	142.134725	1	15	13	14
B	1.590111	1	89.903328	1	111.185109	1	15	13	14
C	1.420279	1	113.945399	1	145.436205	1	16	17	15
C	1.498385	1	113.782866	1	66.583834	1	18	16	17
C	1.472549	1	121.168807	1	-4.342585	1	10	9	11
C	1.431025	1	119.365198	1	94.495038	1	20	10	9
C	1.423321	1	122.035679	1	-.959010	1	21	20	10
C	1.373002	1	120.800792	1	-179.881639	1	22	21	20
C	1.415380	1	120.401013	1	-.011779	1	23	22	21
C	1.372757	1	120.126372	1	-.024942	1	24	23	22
C	1.418312	1	119.321358	1	179.138132	1	21	20	10
C	1.421049	1	119.315899	1	.031213	1	26	21	20
C	1.419914	1	118.216914	1	-131.158784	1	19	18	16
C	1.553414	1	121.433081	1	-113.978602	1	13	15	17
C	2.699905	1	135.848270	1	-76.119913	1	14	13	15
C	1.394089	1	169.490412	1	-21.159570	1	30	14	13
C	1.394156	1	120.237955	1	101.974697	1	31	30	14
C	1.394182	1	119.670928	1	-.006564	1	32	31	30
C	1.393987	1	120.211000	1	-.035575	1	33	32	31
C	1.400426	1	120.458617	1	-.001506	1	34	33	32
C	1.439454	1	112.108976	1	3.216048	1	14	13	15
C	1.496180	1	105.522559	1	-2.908401	1	15	13	14
C	1.535994	1	107.887580	1	-125.355575	1	37	15	13
C	1.523241	1	106.516730	1	-10.426831	1	38	37	15
C	1.471630	1	119.649885	1	-125.974314	1	15	13	14
C	2.540881	1	133.895168	1	131.439613	1	36	14	13
C	1.514926	1	107.466514	1	119.994007	1	36	14	13
C	1.401182	1	119.982186	1	-16.502414	1	42	36	14
C	1.394052	1	120.548570	1	179.171902	1	43	42	36
C	1.393864	1	120.242358	1	-.014693	1	44	43	42
C	1.393680	1	120.555544	1	-179.261666	1	41	42	36
H	1.101015	1	118.717088	1	1.087767	1	28	19	18
H	1.100485	1	120.864536	1	-179.866674	1	27	28	19
H	1.100378	1	118.516129	1	180.059153	1	25	26	21
H	1.099901	1	120.737465	1	-179.937125	1	24	25	26
H	1.100036	1	120.523318	1	180.007833	1	23	22	21
H	1.101526	1	118.508833	1	.326099	1	22	21	20
H	1.101619	1	118.535509	1	.442770	1	4	5	10
H	1.099973	1	120.535564	1	180.036776	1	3	4	5
H	1.099809	1	120.758670	1	-179.958754	1	2	1	6
H	1.100289	1	118.502626	1	-179.807844	1	1	6	5
H	1.100350	1	120.833044	1	-179.591201	1	7	8	9
H	1.101808	1	118.665290	1	3.158726	1	8	9	11
H	1.124021	1	109.743357	1	-57.506070	1	18	16	17
H	1.126832	1	103.677507	1	-174.355233	1	18	16	17
H	1.130112	1	103.414912	1	-156.082158	1	11	12	13
H	1.126855	1	105.221666	1	-41.209516	1	11	12	13
H	1.128715	1	107.394471	1	117.562087	1	37	15	13
H	1.117953	1	109.574396	1	-130.833938	1	38	37	15
H	1.118417	1	111.765093	1	109.974510	1	38	37	15
H	1.118068	1	110.213571	1	110.288382	1	39	40	15
H	1.117097	1	110.385746	1	-130.764831	1	39	40	15
H	1.102118	1	119.270001	1	1.368471	1	30	35	36
H	1.099787	1	119.719590	1	-179.822914	1	31	30	35
H	1.099387	1	120.120423	1	179.913364	1	32	33	34
H	1.099583	1	119.752562	1	179.940358	1	33	34	35
H	1.100940	1	120.464097	1	-.628537	1	34	35	36
H	1.100501	1	120.126930	1	.141590	1	41	42	36
H	1.099723	1	119.726829	1	179.865345	1	46	41	42
H	1.099366	1	120.164007	1	179.755628	1	45	46	41
H	1.099773	1	119.709274	1	-179.734430	1	44	43	42
H	1.102753	1	119.430407	1	-.006273	1	43	42	36
H	1.109706	1	107.463108	1	62.111028	1	29	13	14
H	1.109334	1	107.122549	1	-56.029835	1	29	13	14
H	1.108369	1	109.882360	1	-177.086028	1	29	13	14
H	1.124896	1	108.957645	1	-113.678065	1	40	15	13
H	1.124535	1	109.296958	1	4.211710	1	40	15	13

(P)-12 Heat of formation = -61.313813 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.438975	1	0.000000	0	0.000000	0	1	0	0
N	1.590587	1	107.874617	1	0.000000	0	1	2	0
C	1.495556	1	105.490720	1	-0.321930	1	3	1	2
C	1.441301	1	112.100867	1	2.591264	1	2	1	3
C	1.471714	1	119.816823	1	-123.661832	1	3	1	2
C	1.533537	1	108.829844	1	124.648994	1	6	3	1
C	1.523270	1	106.760373	1	-5.899695	1	7	6	3
B	1.584041	1	89.327156	1	113.940840	1	3	1	2
C	1.554082	1	115.686562	1	-140.018169	1	1	2	3
C	1.514476	1	107.342288	1	118.611443	1	5	2	1
C	1.401196	1	119.949647	1	-19.175645	1	11	5	2
C	1.400962	1	121.214422	1	159.574936	1	11	5	2
C	1.393765	1	120.541723	1	-179.278955	1	13	11	5
C	1.394062	1	120.541513	1	179.185771	1	12	11	5
C	1.393943	1	120.235856	1	-0.059910	1	15	12	11
C	1.514236	1	108.103128	1	-122.697507	1	5	2	1
C	1.400638	1	119.361078	1	-22.646403	1	17	5	2
C	1.400511	1	121.578148	1	158.145459	1	17	5	2
C	1.393985	1	120.431520	1	179.395669	1	19	17	5
C	1.394128	1	120.378227	1	-179.373127	1	18	17	5
C	1.394119	1	120.249079	1	0.027018	1	21	18	17
O	1.633072	1	91.208681	1	-103.723953	1	1	3	4
C	1.431237	1	116.608282	1	120.997365	1	23	1	2
O	2.782469	1	62.726767	1	92.277403	1	24	23	1
C	1.499545	1	107.903820	1	-173.331835	1	24	23	1
C	1.384047	1	122.590037	1	-120.428891	1	26	24	23
C	1.425935	1	95.275930	1	122.944810	1	25	24	23
C	1.501372	1	107.803664	1	63.759838	1	28	25	24
C	1.384787	1	122.253071	1	-96.995467	1	29	28	25
C	1.432647	1	119.693245	1	176.508648	1	30	29	28
C	1.433556	1	119.570506	1	178.310044	1	27	26	24
C	1.420669	1	117.069911	1	59.109999	1	26	24	23
C	1.369450	1	120.868182	1	-179.151946	1	33	26	24
C	1.421238	1	120.288664	1	0.516629	1	34	33	26
C	1.421977	1	121.061130	1	178.859641	1	35	34	33
C	1.372616	1	120.636895	1	-178.941796	1	36	35	34
C	1.423513	1	122.033217	1	-177.892749	1	32	27	26
C	1.415011	1	120.060451	1	-0.067863	1	37	36	35
C	1.419549	1	117.515114	1	81.577611	1	29	28	25
C	1.370099	1	120.899494	1	-177.729766	1	40	29	28
C	1.420871	1	120.316699	1	0.686660	1	41	40	29
C	1.423623	1	122.054126	1	-177.413162	1	31	30	29
C	1.422052	1	121.107182	1	178.481959	1	42	41	40
C	1.372541	1	120.627443	1	-179.017528	1	44	42	41
C	1.415233	1	120.075431	1	-0.125316	1	45	44	42
H	1.129166	1	107.334594	1	113.756704	1	4	3	1
H	1.118058	1	110.402855	1	-115.569741	1	8	7	6
H	1.118714	1	110.919093	1	125.427333	1	8	7	6
H	1.117528	1	110.281591	1	-126.594998	1	7	6	3
H	1.117998	1	110.175295	1	114.594008	1	7	6	3
H	1.125046	1	108.926685	1	-114.098947	1	6	3	1
H	1.124549	1	109.171488	1	3.707396	1	6	3	1
H	1.200716	1	116.117237	1	-118.710785	1	9	3	1
H	1.122040	1	110.411461	1	63.881680	1	24	23	1
H	1.124444	1	106.270027	1	-55.379244	1	24	23	1
H	1.108281	1	109.894026	1	-173.123412	1	10	1	2
H	1.109272	1	107.057053	1	-52.521364	1	10	1	2
H	1.109528	1	107.786748	1	65.838814	1	10	1	2
H	1.102662	1	119.451121	1	0.117105	1	12	11	5
H	1.099817	1	119.704312	1	-179.719744	1	15	12	11
H	1.099465	1	120.230258	1	-179.856832	1	16	15	12
H	1.099806	1	119.718036	1	179.873458	1	14	13	11
H	1.100680	1	120.116266	1	0.087134	1	13	11	5
H	1.101042	1	120.377443	1	-0.465956	1	19	17	5
H	1.099641	1	119.773337	1	179.838495	1	20	19	17
H	1.099420	1	120.211433	1	-179.904298	1	22	21	18
H	1.099775	1	119.719841	1	180.029191	1	21	18	17
H	1.102124	1	119.295406	1	1.229806	1	18	17	5
H	1.101957	1	117.909692	1	-0.405022	1	33	26	24
H	1.100309	1	120.938611	1	179.922446	1	34	33	26
H	1.100361	1	118.482842	1	0.857025	1	36	35	34
H	1.099830	1	120.766848	1	179.861866	1	37	36	35
H	1.099978	1	119.100824	1	179.788791	1	39	37	36
H	1.101791	1	118.562105	1	-0.875060	1	38	32	27
H	1.101832	1	118.507124	1	-0.943705	1	43	31	30
H	1.100034	1	119.083567	1	179.814483	1	46	45	44
H	1.099822	1	120.765583	1	179.825738	1	45	44	42
H	1.100356	1	118.491257	1	0.792679	1	44	42	41
H	1.100345	1	120.940208	1	-179.866451	1	41	40	29
H	1.101018	1	118.333388	1	1.602280	1	40	29	28
H	1.122423	1	111.378087	1	-58.429456	1	30	29	28

(P)-12 Heat of formation = -55.203354 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0
O	1.440325	1	0.000000	0	0.000000	0	1	0	0
N	1.580436	1	107.677207	1	0.000000	0	1	2	0
C	1.495420	1	105.404994	1	-10.116407	1	3	1	2
C	1.444280	1	111.484662	1	12.638751	1	2	1	3
C	1.467556	1	120.457561	1	-133.617827	1	3	1	2
C	1.534380	1	109.031266	1	118.322460	1	6	3	1
C	1.523560	1	106.682268	1	-2.088937	1	7	6	3
B	1.614080	1	88.882949	1	102.986831	1	3	1	2
C	1.553914	1	116.670533	1	-143.093718	1	1	2	3
C	1.513524	1	107.938521	1	112.629603	1	5	2	1
C	1.400549	1	120.231245	1	-16.355070	1	11	5	2
C	1.401280	1	120.831571	1	162.294431	1	11	5	2
C	1.393413	1	120.508262	1	-179.089783	1	13	11	5
C	1.394336	1	120.463405	1	178.997377	1	12	11	5
C	1.393835	1	120.247888	1	-0.048392	1	15	12	11
C	1.514352	1	107.604200	1	-129.263638	1	5	2	1
C	1.401223	1	119.212937	1	-25.769478	1	17	5	2
C	1.400166	1	121.725737	1	155.798221	1	17	5	2
C	1.394300	1	120.402243	1	179.140106	1	19	17	5
C	1.393976	1	120.417850	1	-179.131849	1	18	17	5
C	1.394332	1	120.210985	1	0.195269	1	21	18	17
O	1.587904	1	91.723341	1	6.913119	1	9	3	1
C	1.433949	1	122.248777	1	14.119621	1	23	1	2
O	3.330683	1	39.592469	1	-140.258753	1	24	23	1
C	1.498800	1	108.348035	1	-153.764811	1	24	23	1
C	1.386046	1	121.994173	1	-50.133398	1	26	24	23
C	1.409004	1	98.519175	1	-61.653413	1	25	24	23
C	1.503334	1	118.375560	1	-34.302125	1	28	25	24
C	1.381906	1	128.637589	1	-12.473263	1	29	28	25
C	1.440779	1	119.720736	1	178.933651	1	30	29	28
C	1.433289	1	119.575082	1	174.691053	1	27	26	24
C	1.420023	1	117.722834	1	127.527560	1	26	24	23
C	1.369980	1	120.872683	1	-176.521463	1	33	26	24
C	1.420981	1	120.352253	1	1.104547	1	34	33	26
C	1.421910	1	121.161882	1	178.231529	1	35	34	33
C	1.372694	1	120.605663	1	-179.493689	1	36	35	34
C	1.423454	1	121.916373	1	-177.207086	1	32	27	26
C	1.415055	1	120.113697	1	-0.065620	1	37	36	35
C	1.430535	1	112.220866	1	168.378855	1	29	28	25
C	1.365616	1	121.959690	1	-179.563704	1	40	29	28
C	1.421434	1	120.101069	1	0.253081	1	41	40	29
C	1.423684	1	121.815010	1	-178.332950	1	31	30	29
C	1.420517	1	121.115492	1	179.015682	1	42	41	40
C	1.373308	1	120.562792	1	-179.780482	1	44	42	41
C	1.413830	1	119.902402	1	-0.038007	1	45	44	42
H	1.129075	1	107.350226	1	120.130618	1	4	3	1
H	1.118142	1	110.259909	1	-115.090023	1	8	7	6
H	1.118360	1	111.064590	1	125.770683	1	8	7	6
H	1.117490	1	110.373720	1	-122.711927	1	7	6	3
H	1.117864	1	110.111085	1	118.411863	1	7	6	3
H	1.126274	1	108.361993	1	-121.278015	1	6	3	1
H	1.124462	1	109.507422	1	-3.211133	1	6	3	1
H	1.123799	1	104.978709	1	87.000946	1	24	23	1
H	1.203172	1	111.867672	1	-110.139946	1	9	3	1
H	1.123530	1	109.748316	1	-31.307637	1	24	23	1
H	1.108593	1	109.363569	1	-163.913251	1	10	1	2
H	1.109105	1	106.589377	1	-44.347571	1	10	1	2
H	1.108904	1	108.270219	1	74.725052	1	10	1	2
H	1.103020	1	119.488601	1	-0.241872	1	12	11	5
H	1.099878	1	119.684850	1	-179.738051	1	15	12	11
H	1.099533	1	120.220976	1	-179.841188	1	16	15	12
H	1.099824	1	119.752113	1	179.877117	1	14	13	11
H	1.100765	1	119.972665	1	0.356578	1	13	11	5
H	1.101090	1	120.480897	1	-0.561311	1	19	17	5
H	1.099857	1	119.732590	1	179.745445	1	20	19	17
H	1.099572	1	120.193066	1	180.057938	1	22	21	18
H	1.099969	1	119.738788	1	179.962268	1	21	18	17
H	1.102339	1	119.367218	1	0.646577	1	18	17	5
H	1.101174	1	118.673921	1	3.022722	1	33	26	24
H	1.100195	1	120.891340	1	-179.672391	1	34	33	26
H	1.100216	1	118.515293	1	0.269813	1	36	35	34
H	1.099766	1	120.739535	1	179.860883	1	37	36	35
H	1.099841	1	119.082859	1	179.776970	1	39	37	36
H	1.101496	1	118.521319	1	-0.125105	1	38	32	27
H	1.101816	1	118.859282	1	-0.462670	1	43	31	30
H	1.100040	1	119.110129	1	180.036825	1	46	45	44
H	1.099596	1	120.810355	1	179.964787	1	45	44	42
H	1.100234	1	118.556777	1	0.169786	1	44	42	41
H	1.100321	1	121.106672	1	180.002683	1	41	40	29
H	1.101761	1	118.122452	1	0.297245	1	40	29	28

TSa (P)-12 <--> (M)-12 Heat of formation = -27.192198 kcal/mol

B	0.000000	0	0.000000	0	0.000000	0	0	0	0	0
O	1.435903	1	0.000000	0	0.000000	0	1	0	0	
N	1.589826	1	107.878405	1	0.000000	0	1	2	0	
C	1.497513	1	105.293544	1	-3.956773	1	3	1	2	
C	1.441906	1	112.202682	1	0.113045	1	2	1	3	
C	1.472432	1	119.913022	1	-126.926240	1	3	1	2	
C	1.534313	1	108.643949	1	121.450240	1	6	3	1	
C	1.523344	1	106.284709	1	-9.964155	1	7	6	3	
B	1.577592	1	89.275666	1	110.268599	1	3	1	2	
C	1.553596	1	115.394815	1	-140.235463	1	1	2	3	
C	1.513554	1	107.679442	1	125.864018	1	5	2	1	
C	1.400488	1	120.339959	1	-5.344314	1	11	5	2	
C	1.401216	1	120.739835	1	173.242364	1	11	5	2	
C	1.393184	1	120.551749	1	-178.725142	1	13	11	5	
C	1.394610	1	120.439043	1	178.717758	1	12	11	5	
C	1.393614	1	120.282854	1	-0.041161	1	15	12	11	
C	1.515646	1	108.403080	1	-115.971590	1	5	2	1	
C	1.401156	1	119.265025	1	-20.440887	1	17	5	2	
C	1.400112	1	121.764791	1	160.831025	1	17	5	2	
C	1.394223	1	120.468890	1	178.610051	1	19	17	5	
C	1.393893	1	120.453283	1	-178.577995	1	18	17	5	
C	1.394164	1	120.242778	1	-0.079481	1	21	18	17	
O	1.650862	1	91.434158	1	-107.269277	1	1	3	4	
C	1.428467	1	115.750421	1	125.546938	1	23	1	2	
O	2.721746	1	64.000618	1	94.013713	1	24	23	1	
C	1.498443	1	110.609826	1	-168.628881	1	24	23	1	
C	1.399450	1	123.923337	1	-143.063368	1	26	24	23	
C	1.422683	1	82.171039	1	122.075251	1	25	24	23	
C	1.499391	1	110.843921	1	67.836435	1	28	25	24	
C	1.398144	1	124.044170	1	-127.535919	1	29	28	25	
C	1.447346	1	114.374569	1	-144.267464	1	30	29	28	
C	1.447479	1	114.299118	1	-142.221859	1	27	26	24	
C	1.424870	1	115.668078	1	45.554809	1	26	24	23	
C	1.367000	1	120.925395	1	163.469405	1	33	26	24	
C	1.424639	1	118.667643	1	-11.895775	1	34	33	26	
C	1.418991	1	120.644121	1	-163.696549	1	35	34	33	
C	1.374814	1	120.421471	1	165.406870	1	36	35	34	
C	1.420454	1	100.492676	1	-22.191986	1	32	30	31	
C	1.411507	1	119.529182	1	-1.929095	1	37	36	35	
C	1.423598	1	115.621523	1	59.394606	1	29	28	25	
C	1.367180	1	120.925185	1	165.184245	1	40	29	28	
C	1.424577	1	118.642330	1	-11.644261	1	41	40	29	
C	1.420517	1	100.552208	1	-21.501385	1	31	27	32	
C	1.419144	1	120.573215	1	-164.138520	1	42	41	40	
C	1.374693	1	120.430469	1	165.454281	1	44	42	41	
C	1.411566	1	119.510877	1	-2.004965	1	45	44	42	
H	1.127772	1	107.676438	1	122.617551	1	4	3	1	
H	1.118831	1	110.028787	1	-105.393474	1	8	7	6	
H	1.117275	1	111.535169	1	135.026211	1	8	7	6	
H	1.116982	1	110.487836	1	-130.694101	1	7	6	3	
H	1.118100	1	110.162802	1	110.240891	1	7	6	3	
H	1.124886	1	108.924537	1	-117.374250	1	6	3	1	
H	1.124412	1	109.190077	1	0.597920	1	6	3	1	
H	1.201279	1	115.494642	1	-116.004573	1	9	3	1	
H	1.119872	1	111.184363	1	64.176480	1	24	23	1	
H	1.129829	1	105.675073	1	-53.739737	1	24	23	1	
H	1.107980	1	110.257830	1	-171.641839	1	10	1	2	
H	1.109472	1	107.078189	1	-50.804743	1	10	1	2	
H	1.109564	1	107.431601	1	67.309290	1	10	1	2	
H	1.102403	1	119.592224	1	-0.744610	1	12	11	5	
H	1.099898	1	119.662203	1	-179.775665	1	15	12	11	
H	1.099468	1	120.241204	1	-179.789420	1	16	15	12	
H	1.099729	1	119.769196	1	179.772568	1	14	13	11	
H	1.100140	1	119.978229	1	0.937992	1	13	11	5	
H	1.100631	1	120.662735	1	-1.379623	1	19	17	5	
H	1.099682	1	119.734847	1	179.949990	1	20	19	17	
H	1.099411	1	120.229177	1	179.952666	1	22	21	18	
H	1.099816	1	119.718234	1	179.862904	1	21	18	17	
H	1.102336	1	119.303751	1	2.046681	1	18	17	5	
H	1.103620	1	117.470613	1	-18.289907	1	33	26	24	
H	1.099076	1	121.782952	1	173.095663	1	34	33	26	
H	1.100152	1	118.592351	1	-12.341338	1	36	35	34	
H	1.099409	1	120.896883	1	-179.646647	1	37	36	35	
H	1.099943	1	119.266051	1	-173.185048	1	39	37	36	
H	1.102315	1	118.984367	1	-5.463182	1	38	32	27	
H	1.102362	1	118.993028	1	-5.757627	1	43	31	30	
H	1.099965	1	119.263074	1	-173.115393	1	46	45	44	
H	1.099404	1	120.907404	1	-179.697184	1	45	44	42	
H	1.100141	1	118.591310	1	-12.309633	1	44	42	41	
H	1.099036	1	121.847446	1	173.218313	1	41	40	29	
H	1.101516	1	117.418825	1	-16.721504	1	40	29	28	

TSb (P)-12 <--> (M)-12 HEAT OF FORMATION = -24.182848 kcal/mol

B	.000000	0	.000000	0	.000000	0	0	0	0
O	1.437619	1	.000000	0	.000000	0	1	0	0
N	1.591831	1	107.904758	1	.000000	0	1	2	0
C	1.495278	1	105.444024	1	.940558	1	3	1	2
C	1.441576	1	112.125861	1	1.479979	1	2	1	3
C	1.471851	1	119.646298	1	-122.233599	1	3	1	2
C	1.533525	1	108.812760	1	125.311261	1	6	3	1
C	1.523275	1	106.765150	1	-6.104288	1	7	6	3
B	1.584353	1	89.319151	1	115.348625	1	3	1	2
C	1.553432	1	116.034071	1	-140.571531	1	1	2	3
C	1.514346	1	107.324780	1	119.143092	1	5	2	1
C	1.401169	1	119.973860	1	-19.507718	1	11	5	2
C	1.400987	1	121.199147	1	159.261772	1	11	5	2
C	1.393715	1	120.543812	1	-179.325748	1	13	11	5
C	1.394058	1	120.548760	1	179.258900	1	12	11	5
C	1.393911	1	120.235332	1	-.096678	1	15	12	11
C	1.514207	1	108.121417	1	-122.163891	1	5	2	1
C	1.400680	1	119.377852	1	-22.789572	1	17	5	2
C	1.400539	1	121.553365	1	158.071410	1	17	5	2
C	1.393967	1	120.425555	1	179.264594	1	19	17	5
C	1.394180	1	120.377075	1	-179.262295	1	18	17	5
C	1.394158	1	120.241501	1	.035739	1	21	18	17
O	1.633109	1	90.797969	1	-102.189263	1	1	3	4
C	1.430568	1	117.981609	1	117.567948	1	23	1	2
O	2.857576	1	61.030629	1	92.195887	1	24	23	1
C	1.503108	1	108.466605	1	178.581055	1	24	23	1
C	1.397719	1	124.654017	1	-140.851330	1	26	24	23
C	1.424967	1	82.855905	1	132.515600	1	25	24	23
C	1.504908	1	107.819253	1	61.802965	1	28	25	24
C	1.396077	1	125.162889	1	-125.716600	1	29	28	25
C	1.444578	1	115.732082	1	-167.561066	1	30	29	28
C	1.444417	1	115.723695	1	-165.244315	1	27	26	24
C	1.425484	1	114.344643	1	37.641931	1	26	24	23
C	1.365506	1	120.726657	1	-175.207803	1	33	26	24
C	1.421245	1	119.033318	1	-12.654018	1	34	33	26
C	1.420615	1	120.148884	1	-172.786845	1	35	34	33
C	1.373541	1	120.554271	1	165.616295	1	36	35	34
C	1.419193	1	104.847563	1	13.626204	1	32	30	31
C	1.412042	1	118.852458	1	-4.760375	1	37	36	35
C	1.424981	1	113.575165	1	50.390222	1	29	28	25
C	1.365263	1	120.702239	1	-173.634659	1	40	29	28
C	1.421633	1	118.990630	1	-12.064748	1	41	40	29
C	1.419147	1	104.919819	1	14.697963	1	31	27	32
C	1.420586	1	120.013858	1	-173.137104	1	42	41	40
C	1.373524	1	120.584362	1	166.101207	1	44	42	41
C	1.411857	1	118.836544	1	-4.741145	1	45	44	42
H	1.129125	1	107.308676	1	112.792633	1	4	3	1
H	1.117965	1	110.444089	1	-116.134009	1	8	7	6
H	1.118813	1	110.871145	1	124.889068	1	8	7	6
H	1.117537	1	110.270517	1	-126.804346	1	7	6	3
H	1.118032	1	110.186182	1	114.375980	1	7	6	3
H	1.124933	1	108.998429	1	-113.436064	1	6	3	1
H	1.124684	1	109.097591	1	4.472904	1	6	3	1
H	1.200771	1	116.456401	1	-119.929542	1	9	3	1
H	1.119202	1	110.499449	1	52.926437	1	24	23	1
H	1.127012	1	105.481744	1	-65.200079	1	24	23	1
H	1.108493	1	109.888036	1	-178.669839	1	10	1	2
H	1.109322	1	106.941528	1	-58.245169	1	10	1	2
H	1.109291	1	107.769081	1	60.321927	1	10	1	2
H	1.102567	1	119.462168	1	.225543	1	12	11	5
H	1.099834	1	119.710570	1	-179.756140	1	15	12	11
H	1.099446	1	120.231426	1	-179.855967	1	16	15	12
H	1.099789	1	119.715243	1	179.867279	1	14	13	11
H	1.100687	1	120.131606	1	.061667	1	13	11	5
H	1.101056	1	120.374962	1	-.511597	1	19	17	5
H	1.099662	1	119.765376	1	179.933524	1	20	19	17
H	1.099445	1	120.203155	1	179.971787	1	22	21	18
H	1.099903	1	119.711532	1	179.999615	1	21	18	17
H	1.102244	1	119.298910	1	1.236073	1	18	17	5
H	1.103409	1	118.043024	1	.102582	1	33	26	24
H	1.099645	1	121.572638	1	170.755740	1	34	33	26
H	1.100310	1	118.426705	1	-12.609461	1	36	35	34
H	1.098979	1	121.237071	1	178.632890	1	37	36	35
H	1.099907	1	119.264175	1	-170.235794	1	39	37	36
H	1.098159	1	118.759952	1	-19.184511	1	38	32	27
H	1.097965	1	118.827076	1	-19.077776	1	43	31	30
H	1.099942	1	119.267254	1	-170.377579	1	46	45	44
H	1.098983	1	121.240491	1	178.600212	1	45	44	42
H	1.100319	1	118.432015	1	-12.188447	1	44	42	41
H	1.099511	1	121.697848	1	171.059307	1	41	40	29
H	1.101897	1	117.781707	1	1.335241	1	40	29	28
H	1.119244	1	111.910841	1	-62.500508	1	28	25	24