

Table 6. Enthalpy of formation,  $\Delta_f H_{298}$  and  $\Delta_f H_0$ , heat capacity and entropy at 298 K, and  $H_{298}-H_0$  from the original calculation *February 2 2010*.

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Air (standard mixture)	28.96518	-0.126	-0.125		29.104	198.824	8.649	†
AL(cr) REFERENCE ELEMENT	26.98154	0	0		24.2	28.3	4.540	*‡
AL	26.98154	329.7		±4.2	21.391	164.555	6.919	†
ALBr	106.88554	14.325	21.554		35.618	239.635	9.571	†
ALBr2	186.78954	-140.662	-125.	±50.	53.256	312.236	13.398	†
ALBr3	266.69354	-410.477	-387.1	±5.1	75.372	348.026	17.943	†
ALCL	62.43424	-51.007	-51.2	±3.	34.661	227.961	9.323	†
ALCL+	62.43369	861.849	855.286	±42.	33.794	232.190	9.154	†
ALCL2	97.88694	-240.874	-240.	±40.	51.566	290.374	12.847	†
ALCL3	133.33964	-584.679	-582.768	±5.	71.537	313.089	16.401	†
ALF	45.97994	-264.060	-264.	±3.	31.937	215.162	8.892	†
ALF+	45.97939	692.234	686.176	±25.	31.155	220.068	8.813	†
ALF2	64.97834	-631.764	-630.	±30.	45.418	264.924	11.601	†
ALF2-	64.97889	-853.231	-845.	±20.	44.746	257.272	11.332	†
ALF3	83.97675	-1209.277	-1205.543	±3.1	62.199	276.674	14.044	†
ALH	27.98948	249.250	249.356	±20	29.371	187.863	8.668	†
ALH2	28.99742	276.774	279.691	±20.	35.773	213.316	10.091	†
ALH3	30.00536	128.896	135.728	±20.	40.057	206.579	10.411	†
ALO	42.98094	67.319	67.411	±8	30.884	218.389	8.788	†
ALO+	42.98039	992.993	986.586		33.135	230.978	9.090	†
ALO-	42.98149	-272.972	-266.589	±11	30.335	211.945	8.745	†
ALOH	43.98888	-192.762	-190.	±13	43.512	222.643	10.352	†
HALO	43.98888	1.821	5.	±50.	40.996	219.696	9.935	†
ALO2	58.98034	-38.658	-38.799	±32	51.661	269.637	13.362	†
ALO2-	58.98089	-452.572	-443.799	±60	46.063	229.783	10.645	†
ALO2H (HALO2)	59.98828	-355.472	-350.	±50	51.256	254.826	11.981	†
AL(OH)2	60.99622	-507.661	-500.	±50	62.980	284.406	14.028	†
AL(OH)3	78.00356	-1016.668	-1000.		87.249	301.541	17.596	†
AL2	53.96308	501.302	500.243	±20	37.055	243.842	10.139	†
AL2O	69.96248	-148.611	-147.968	±20	51.978	253.135	12.777	†
AL2O+	69.96193	648.97	643.212		52.898	260.663	12.981	†
AL2O2	85.96188	-403.096	-401.178	±40.	68.122	288.044	15.843	†
AL2O2+	85.96133	557.439	554.026		68.924	289.704	14.975	†
AL2O3(S)	101.96128	-1675.700	-1663.616		79.033	50.920	10.016	†
AL2O3(G)	101.96128	-546.891	-544.39	±100.	86.990	316.662	19.598	†
AR REFERENCE ELEMENT	39.948	0	0		20.786	154.847	6.197	*‡
Ar+	39.94745	1526.778	1520.6	±0.001	20.984	166.406	6.206	†
B(S) REFERENCE ELEMENT	10.81	0.	0.		11.315	5.834	1.214	†
B	10.811	565.	559.898	±12	20.797	153.438	6.316	†
BBr	90.715	240.952	245.429		32.787	224.992	8.997	†
BBr2	170.619	97.829	111.362	±25.	48.451	294.539	12.201	†
BBr3	250.523	-205.3	-183.	±3.0	67.777	324.505	15.703	†
BCL	46.2637	183.173	180.117	±20.	31.656	213.244	8.861	†
BCL+	46.26315	1234.28	1225.027	±42.	31.644	219.133	8.860	†
BCLF	65.26210	-279.,184	-280.	±10	42.820	264.941	11.033	†
BCLF2	84.26050	-888.	-885.694	±5.	54.473	275.115	12.324	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
BCL2	81.7164	-60.881	-62.	$\pm 10.$	45.746	271.202	11.514	†
BCL2+	81.71585	672.315	663.664	$\pm 20.$	52.975	257.809	12.849	†
BCL2F	100.71480	-643.	-641.423	$\pm 5.$	58.911	287.581	13.231	†
BCL3	117.1691	-404.5	-403.485	$\pm 1.3$	62.556	289.468	13.971	†
BF	29.80940	-106.932	-110.	$\pm 10.$	29.594	200.453	8.695	†
BF2	48.80781	-499.427	-500.	$\pm 10.$	40.055	247.133	10.612	†
BF2+	48.80726	322.6	315.816	$\pm 2.5$	44.291	225.151	10.612	†
BF2-	48.80355	-733.803	-728.	$\pm 14.$	39.436	240.589	10.434	†
BF3	67.80621	-1136.0	-1133.2	$\pm 0.8$	50.462	254.429	11.651	†
BF4-	86.80516	-1761.266	-1750.	$\pm 40.$	67.794	268.855	13.796	†
BH	11.81894	448.727	445.536	$\pm 2.$	29.181	171.836	8.639	†
BHF2	49.81575	-733.858		$\pm 3.3$	42.341	244.025		†
BH2	12.82688	328.909	328.568	$\pm 10$	34.975	193.675	10.024	†
BH3	13.83482	104.747	108.603		36.018	188.251	10.060	†
BH4	14.84276	255.210	262.560		44.277	211.994	10.771	†
BH5	15.85070	77.387	87.199		52.616	229.580	12.572	†
BI Mono Iodo Boron	137.71547	325.988	324.657	$\pm 12$	33.731	233.319	9.142	†
BI2	264.61994	238.036	239.810	$\pm 10$	50.294	311.115	12.688	†
BI3 BoronTrilodide	391.52441	21.400	25.475	$\pm 4.$	71.027	350.427	16.933	†
BO	26.81040	20.406	17.286	$\pm 10$	29.196	203.468	8.674	†
BO-	26.81095	-277.791	-274.714	$\pm 5.$	29.197	197.683	8.674	†
BOCL OBCl	62.2631	-318.537	-319.	$\pm 10$	45.079	237.306	10.608	†
BOCL2	97.7158	-361.566	-360	$\pm 60$	58.826	292.296	13.170	†
BOF OBF	45.80880	-592.978	-593.	$\pm 10$	41.653	224.981	9.988	†
BOF2 OBF2	64.80721	-832.768	-830.	$\pm 50$	50.491	268.239	11.611	†
BO2	42.80980	-309.122	-310.		43.285	230.138	10.772	†
BO2-	42.81035	-714.494	-708.	$\pm 20.$	39.147	215.734	9.598	†
B2	21.62200	857.371	850.993	$\pm 15.$	31.503	202.064	8.805	†
B2CL4	163.4328	-490.	-490.798	$\pm 10.$	97.997	371.268	21.588	†
B2F4	97.61561	-1438.	-1435.6	$\pm 7.$	80.629	326.206	17.681	†
B2H	22.62994	796.270	792.816		42.328	214.282	10.116	†
B2H2	23.63788	454.475	455.001	$\pm 8.4$	46.880	213.225	10.371	†
B2H6	27.66964	36.6	52.5	$\pm 2.$	56.643	232.027	11.932	†
B2O	37.6214	192.798	187.783	$\pm 100.$	47.247	226.244	11.783	†
B2O2 (BO)2	53.6208	-457.711	-460.	$\pm 10.$	60.269	249.669	13.397	†
B2O3(L)	69.6182	-1273.5	-1267.353	$\pm 1.4$	62.761	53.97	9.301	†
B2O3	69.6202	-835.382	-834.353	$\pm 8.$	64.917	285.902	14.419	†
B3O3CL3 (BOCl)3	186.7893	-1635.982	-1630.	$\pm 15$	124.123	380.039	24.452	†
B3O3F3 (BOF)3	137.42641	-2382.7	-2374.	$\pm 12$	110.653	343.946	21.201	†
B3O3H3 BOROXIN	83.45502	-1203.761	-1190.	$\pm 20$	80.615	286.152	15.603	†
H3B3O6 BORIC ACID	131.45322	-2263.688	-2245.	$\pm 20$	133.912	359.908	23.697	†
BaO	153.32640	-117.95	-		32.898	235.460		†
Bi(s) REFERENCE ELEMENT	208.98040	0.	0.		25.5	56.7	6.43	#
Bi	208.98040	207.			20.786	187.090	6.200	#
Bi-		116.2						X
BiCl	244.43308	74.30			36.134	255.753	9.767	#
BiCl2 BiChloroBismuth	279.88587	-93.692			56.839	322.337	14.850	#
BiCl3 TrichloroBismuth	315.33848	-265.266			81.609	373.383	20.878	#
BiF MonofluoroBismuth	227.97878	-29.384			34.309	250.982	9.255	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
BiF2 BiFluoroBismuth	246.97719	-200.359			48.723	289.057	12.176	#
BiF3 TrifluoroBismuth	265.97559	-707.933			67.996	312.818	15.565	#
BiH3 Bismuthine	212.00420	58.430			43.070	249.004	10.691	#
BiI MonolodoBismuth	335.88485	102.80			37.155	280.376	10.327	#
Bi(OH)3	260.00240	-198.234			99.223	351.516	18.607	#
BiO	244.97978	121.3		$\pm 12.6$	32.765	246.171	8.994	#
BiO-		-27.		$\pm 7.1$				X
BiO2-		-181.		$\pm 10.$				X
Bi2	417.96080	220.0			36.942	273.743	10.287	#
Bi2-		97.07		$\pm 0.88$				X
Bi2O3 $\begin{matrix} /O\backslash \\ \text{Bi-O-Bi} \\ \backslash O/ \end{matrix}$	465.95896	376.807			83.662	341.171	16.786	#
Bi2O3 O=Bi-O-Bi=O	465.95896	636.679			93.274	373.903	20.518	#
Br	79.904	111.86	117.93	$\pm 0.06$	20.789	175.017	6.167	†
Br+	79.90345	1257.917	1257.782	$\pm 0.055$	20.787	176.874	6.197	†
Br-	79.90455	-218.874	-206.614	$\pm 0.055$	20.786	163.493	6.197	†
BrCl	115.35670	14.789	22.233		35.011	240.049	9.407	†
DBr	81.91810	-37.036	-29.160		29.228	204.484	8.668	†
BrF	98.90240	-58.851	-51.200	$\pm 1.0$	32.959	228.988	9.021	†
BrF3	136.89921	-255.6	-244.81	$\pm 3.0$	67.354	295.775	14.712	†
BrF5	174.89602	-428.8	-413.65	$\pm 2.0$	101.335	323.253	19.175	†
HBr	80.91194	-36.29	-28.444	$\pm 0.16$	29.141	198.700	8.648	†
BrI Iodine Monobromide	206.80847	40.775	49.725	$\pm 0.076$	36.490	258.718	9.908	#
BRO	95.9034	125.8	133.333	$\pm 2.4$	34.17	232.921	9.061	#
BrO2 Br-O-O	111.9028	108	116.091	$\pm 40$	48.873	288.83	12.851	#
BrO2 O-Br-O	111.9028	152	161.545	$\pm 25$	45.364	271.112	11.395	#
BrO3	127.9022	221	233.180	$\pm 50$	59.995	284.507	13.101	#
Br2 (L) REFERENCE ELEMENT	159.8080	0	0		75.680	152.210	24.520	†
Br2 gas	159.8080	30.91	45.705	$\pm 0.11$	36.057	245.469	9.725	†
Br2O BrBrO	175.8074	168	183.722	$\pm 20$	51.385	312.704	13.137	†#
Br2O Br-O-Br	175.8074	107.6	124.061	$\pm 3.5$	50.168	290.823	12.399	†#
C(GR) REFERENCE ELEMENT	12.011	0	0		8.528	5.734	1.054	*†
C(diamond) solid	12.011	1.864		$\pm 0.043$	6.115	2.38	0.52	X
C	12.011	716.67	711.198	$\pm 0.45$	20.839	158.102	6.536	†
C+	12.01045	1809.444	1797.65	$\pm 0.8$	20.974	154.664	6.649	†
C-	12.01125	588.753	589.785	$\pm 0.146$	20.787	159.004	6.219	†
ALC	38.99224	682.28	678.815	$\pm 50.$	33.218	225.918	9.058	†
CBr	91.91470	495.85	500.2		32.370	230.888	8.946	#†
CBrClF2	165.36421	-435.	-423.8	$\pm 15$	74.650	318.724	15.528	†
CBrCl3 BromoTrichloroMethane	198.27280	-42.07	-32.92	$\pm 0.82$	85.307	320.288	17.934	#
CBrF3 Freon 1301	148.90991	-650.59	-638.48	$\pm 1.97$	69.270	297.695	14.444	†
CBr2	171.81870	343.51	356.89		49.273	288.706	12.192	#†
CBr2F2	209.81581	-380	-366.88	$\pm 15$	77.000	325.413	16.280	†
CBr3	251.72270	232.212	254.030	$\pm 4.2$	69.174	331.466	16.015	#†
CBr4	331.62670	119.20	148.90	$\pm 1.5$	91.162	358.185	20.396	#
CCL	47.46340	432.611	428.860		32.268	224.556	9.395	†
CCLF	66.46180	25.846	25.0	$\pm 30.$	42.962	259.150	10.902	†
COCIF Carbonic Chloride Fluoride	82.46120	-412.791	-410.054	$\pm 8.$	52.397	276.926	11.904	†#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CCLF2	85.46021	-275.	-272.96	$\pm 25.$	55.172	287.353	12.432	†
CCLF3 FC-13	104.45861	-710.02	-704.93	$\pm 2.19$	66.887	285.424	13.791	†
CLCN Cyanogen Chloride	61.47014	134.200	133.510	$\pm 2.0$	44.960	236.144	10.669	†
COCL Carbonyl Chloride	63.46280	-16.000	-17.567	$\pm 10.$	45.073	265.195	11.551	†
CCL2	82.91670	231.7	230.5	$\pm 1.7$	51.028	266.112	11.728	#
CCL2F	101.91450	-105.	-103.57	$\pm 20.$	59.121	298.917	13.217	†
CCL2F2 FREON-12	120.91291	-490.8	-486.62		72.477	300.908	14.881	†
COCL2 PHOSGEN	98.9158	-219.5	-217.80		57.761	283.752	12.879	†
CCL3	118.3697	71.128	71.553	$\pm 2.5$	63.500	303.100	14.400	†
CCL3F FC-11	137.36720	-283.700	-280.53		78.071	309.785	16.064	†
CCL3O	134.36850	-18.41	-16.48		83.245	322.749		#
CCL4 liquid	153.82150	-127.792		$\pm 0.55$				X
CCL4	153.82150	-95.6	-93.343	$\pm 2.5$	82.890	309.467	17.159	†
CD	14.0251	599.700	596.251		29.206	192.997	8.795	#
CD A $^4\Sigma^-$ (Excited state only)	14.02480	670.477	667.158		29.176	189.887	8.657	#
CDH3	17.04862	-78.45	-70.49		36.573	200.068	10.08	#
CDO Formyl – D Radical	30.0245	40.945	40.0		35.920	228.610		#
CD2	16.0389	382.59	382.063		36.262	204.294	10.150	#
CD2O Methanal-D2	32.0383	-114.893	-111.141		38.137	225.076	10.211	#
CD3	18.05301	138.69	141.841		41.807	207.024	10.756	#
CD3NO2	64.05885	-61.789	-48.423		63.166	291.669	13.556	#
CD4 RRHO	20.0671	-89.010	-81.166		40.536	199.014	10.348	
CD4 ANHARMONIC	20.0671	-89.010	-81.161		40.582	199.023	10.343	#
CD4O CD3OD	36.06651	-217.670	-207.07		49.478	249.248	11.932	#
CF	31.00910	246.932	243.333	$\pm 0.7$	30.056	213.034	9.065	†
CF+	31.00855	1131.292	1121.86	$\pm 0.92$	29.642	201.509	8.697	†
CF- <sup>a</sup>		208.94		$\pm 3.67$				X
FCN	45.01584	34.328	34.00	$\pm 20.$	42.359	224.607	10.129	†
COF	47.00850	-179.418	-180.	$\pm 40.$	38.980	248.992	10.388	†
CF2	50.00751	-191.26	-191.73	$\pm 1.35$	38.915	240.831	10.351	†
CF2+	50.00696	917.03	910.37	$\pm 1.6$	38.541	246.731	10.342	†
COF2	66.00721	-640	-636.92	$\pm 5.$	47.365	258.971	11.134	†
CF3	69.00591	-467.4	-464.6	$\pm 1.97$	49.642	264.521	11.491	†
CF3+	69.00536	411.627	408.179	$\pm 1.96$	49.339	254.540	11.541	†
CF3-	69.00645	-649.21	-641.079	$\pm 2.45$	56.614	263.934	12.358	#
CF3I	195.91068	-589.11		$\pm 3.3$	70.941	307.633		
CF3O Radical	85.00531	-630.696	-625.69	$\pm 8.$	64.550	283.750	13.622	#
CF3OO RADICAL	101.00471	-637.290	-630.602	$\pm 8.$	80.004	317.945	16.283	#
CF4 FC-14	88.00461	-933.4	-927.15	$\pm 0.53$	61.052	261.459	12.730	†
CH	13.01864	595.8	592.5	$\pm 0.6$	29.175	183.037	8.625	#
CH A $^4\Sigma^-$ (Excited state only)	13.01864	667.919	664.583		29.151	182.626	8.624	#
CH A $^2\Delta$ (Excited state only)	13.01864	876.167	872.829		29.156	177.109	8.626	#
CH B $^2\Sigma^-$ (Excited state only)	13.01864	909.012	905.656		29.298	178.364	8.643	#
CH+ ion	13.01809	1630.571	1621.033	$\pm 0.7$	29.159	171.673	8.628	†
CH- <sup>a</sup>		471.085		$\pm 0.729$				X
CHBr	92.92264	377.857	384.99	$\pm 2.$	39.789	252.872	10.416	#
CHBrCIF	137.37374	-230.000	-217.24	$\pm 15$	62.869	304.928	13.787	#
CHBrF2 HBFC-22B1	130.91975	-425.46	-412.26	$\pm 1.07$	58.767	295.230	13.170	†
CHBr2	172.82664	198.489	215.446		54.834	298.588	12.851	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CHBr3 Bromoform	252.73064	54.266	80.419		71.026	330.864	15.915	#
CHCL	48.47189	297.10	296.78		37.787	235.062	10.200	†
CHCLF	67.46974	-83.490	-80.0	±25.	43.662	266.544	10.801	†
CHCLF2 HCFC-22	86.46845	-490.72	-484.38	±2.28	55.851	280.895	12.362	†
CHCL2	83.92487	95.8	97.469		53.900	285.500	12.800	†
CHCL2F FC-21	102.9233	-284.934			61.077	293.204		†
CHCL2O CCl <sub>2</sub> OH	99.92374	-94.977	-91.0		69.410	307.164		#
CHCL3 liquid Chloroform	119.3779	-133.784		±0.72				X
CHCL3 CHLOROFORM	119.37674	-103.259	-98.353	±0.77	65.384	295.875	14.153	#†
CHCL3O CCl <sub>3</sub> OH	135.37644	-275.977	-270.06.	±3.2	86.644	323.540		#
CHD2NO2	63.05268	-57.716	-44.135		60.806	289.264	13.290	#
CHD3	19.06095	-85.290	-77.391		39.005	208.610	10.243	#
CHF RADICAL	32.01734	163.176			34.585	228.715		†
CHF2	51.01575	-254			45.279	258.506		†
CHF3 FLUOROFORM HFC-23	70.01385	-693.289	-686.34		51.139	259.375	11.573	†#
CHI2 DilodoMethyl Radical	266.82758	290.4	294.943	±6.	58.519	293.206	13.940	#
CHI3 IODOFORM	393.73205	210.874	218.799	±4.2	75.072	355.672	17.157	†
HCN anharmonic	27.02568	129.799	180.136	±0.38	35.857	201.824	9.235	†
HCN+	27.02483	1448.748	1442.676	±0.419	37.399	209.919	9.497	#
HNC	27.02568	191.908	191.530	±0.69	40.271	205.511	10.001	†
HNC+	27.02483	1353.40	1347.24	±1.94	38.160	208.755	9.584	#
HNCO Isocyanic acid	43.02478	-118.600	-115.60	±4.2	45.078	238.265	10.966	†
HOCN Cyanic acid	43.02478	-15.456	-12.76	±20.	46.047	241.244	11.268	#
HCNO Fulminic acid	43.02478	167.603	171.042	±12	48.395	225.025	10.623	#
HONC	43.02478	234.164	235.73	±17.	49.654	248.364	12.400	#
CHN2 HN*-CN Cyanamide Rad.	41.03242	319.796		±23.4	48.059	248.503		
CHN2 cy H(-C-N=N-) Diaziriny	41.03212	556.179	559.612	±8.	41.497	242.076	10.525	#
CH(NO2)3	151.03556	-13.389	+4.976		134.09	435.569	25.968	
CHO FORMYL RADICAL	29.01804	42.3	41.928	±0.3	34.680	224.28	10.000	#
CHO+	29.01749	833.940	827.4	±0.26	34.172	201.764	9.046	#†
CHO-	29.01859	5.958	11.747	±0.54	35.462	222.237	10.036	#
COH	29.01804	218.10	217.72	±0.83	34.970	225.030	10.008	#
COOH equilibrium HOCO	45.01744	-181.32	-178.16	±2.30	43.610	251.736	10.813	†
COOH+ <sup>a</sup>		603.208		±0.9				X
HCOO* Formyloxyl Radical	45.01744	-129.7	-126.955	±12.6	41.965	254.941	11.223	#
HCS	45.08494	300.47			37.059	236.148		
CSi see SiC Siliconcarbide								
CH2 Methylene Equilibrium	14.02658	391.2	390.7	±1.6	35.130	194.436	10.032	#
CH2 Methylene SINGLET	14.02658	428.8	428.3	±1.6	33.781	189.220	9.940	#
CH2 Methylene Triplet only	14.02658	391.2	390.7	±1.6	35.014	194.418	10.027	#
CH2+	14.02603	1399.825	1393.114	±0.276	35.109	191.690	10.036	#
CH2-	14.02713	322.326	328.113	±0.602	33.653	196.021	9.933	#
CH2BrCL HALON101	129.38358	-43.471	-29.305	±8.	52.663	287.768	12.206	†#
CH2BrI BromolodoMethane	220.83505	56.8	72.199	±6.	56.338	307.845	12.980	#
CH2Br2	173.83458	4.937	26.329	±2.	54.554	293.767	12.650	#
CH2CL	49.47928	119.2	122.332		43.173	242.634	10.980	†
CH2CLF GC-31	68.47768	-262.546	-255.274	±8.	47.046	264.426	11.252	†
CH2CL2 (liq) <sup>a</sup>	84.93198	-123.889		±0.692				X
CH2CL2	84.93198	-95.396	-88.547	±0.74	50.951	270.365	11.854	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CH2DNO2	62.04652	-52.532	-38.81		58.983	286.942	13.098	#
CH2D2	18.05478	-81.750	-73.81		37.663	207.948	10.152	#
CH2F	33.02498	-32.077	-28.572	$\pm 8.$	39.568	229.665	10.429	†
CH2F2 FC-32	52.02339	-452.709	-444.65	$\pm 1.0$	42.869	246.347	10.693	†
H2CN RADICAL	28.03332	240.162	243.822		37.768	224.307	10.167	#
HCNH trans	28.03332	298.738	302.384		38.072	229.017	10.211	#
HCNH cis	28.03332	319.658	323.236		38.892	229.734	10.278	#
H2NCO	44.03272	-13.493	-7.670	$\pm 8$	52.145	261.635	12.373	#
CH2NO CH2=N-O*	44.03272	154.574	161.568	$\pm 8.$	47.206	253.626	11.203	#
H2CNO H2C*N=O	44.03302	223.928		$\pm 8.4$	42.388	244.644		
CH2NO2 NITRO-METHYL RAD	60.03242	128.399	137.818	$\pm 8.$	58.673	288.583	13.118	#
CH2NO3 Methyl Nitrate Radical	76.03182	98.952	109.481		76.78	312.169	16.347	
CH2N2 CYANAMIDE H2N-CN	42.04006	134.553	140.881	$\pm 8$	51.224	242.169	11.864	#
H2CN2 HN=C=NH	42.04006	146.478	153.138	$\pm 8$	50.808	237.172	11.532	#
CH2N2 H2C=N=N	42.04006	268.425	274.647	$\pm 8$	51.781	242.272	11.969	#
H2CN2 Cy 3H-Diazirine	42.04006	315.365	323.136	$\pm 8.$	41.463	237.580	10.420	#
H2CN2 Cy 1H-Diazirine	42.04006	398.062	406.387	$\pm 8.$	45.208	246.252	10.866	#
CH2N2O H2C=N-N=O	58.03946	229.589	238.224	$\pm 8.$	61.025	275.259	13.897	#
CH2N2O2 H2C=N-NO2	74.03886	129.273	141.310	$\pm 8.$	70.391	293.002	14.835	#
CH2(NO2)2 H2C(NO2)2	106.03796	-52.421	-34.338	$\pm 8.$	84.334	356.676	17.469	#
CH2O FORMALDEHYDE	30.02598	-108.695	-104.853	$\pm 0.259$	35.388	218.764	10.020	†
CH2O CH*OH HydroxyMethylene	30.02598	125.578	129.365	$\pm 8.$	36.260	225.393	10.075	#
HCOOH (sol.liq) <sup>a</sup>	46.02568	-425.253		$\pm 0.250$				X
HCOOH FORMIC ACID	46.02568	-378.57	-371.296		41.305	247.148	10.928	†
H2CS	46.09258	114.951	118.676	$\pm 8.$	38.196	231.186	10.209	#
CH3	15.03452	146.7	150.0	$\pm 0.3$	38.417	194.008	10.366	#
CH3+	15.03397	1101.792	1099.37	$\pm 0.097$	34.749	186.827	9.983	#
CH3-	15.03507	135.50	145.454	$\pm 1.42$	34.935	193.515	9.999	#
CH3Br	94.93852	-36.443	-21.034	$\pm 2.$	42.312	245.954	10.607	#
CH3CL	50.48722	-81.87	-73.94	$\pm 0.6$	40.741	234.396	10.416	†
CH3F FC-41	34.03292	-239.55	-231.52	$\pm 2.65$	37.504	222.826	10.135	†
CH3F+ <sup>a</sup>		977.687		$\pm 3.98$				X
CH3Hg Methyl Mercury	215.62452	188.28	200.21	$\pm 8.4$	46.073	260.58	11.165	#
CH3I Methyl Iodide	141.93899	14.30	23.838	$\pm 1.4$	44.084	253.007	10.816	†#
CH3N (H2C=NH) Methaneimine	29.04126	84.015	91.93	$\pm 4.5$	38.084	221.567	10.176	#
CH3N Methyl-N Radical	29.04126	319.950	327.711	$\pm 4.5$	39.990	226.694	10.330	#
CH3NO NITROSOMETHYL	45.04096	70.760	80.677	$\pm 8.$	50.807	261.418	12.514	#
OCHNH2 FORMAMIDE	45.04066	-189.598	-178.241	$\pm 8.$	47.623	247.737	11.073	#
CH2=NOH Formaldehyde Oxime	45.04096	18.648	30.00	$\pm 8.$	47.876	253.486	11.072	#
NCH3O FORMIMIDIC ACID	45.04096	-121.537	-109.866	$\pm 8.$	45.004	257.645	10.760	#
H3CNO CH2-NH=O	45.04096	66.421	78.102	$\pm 8.$	45.193	251.503	10.750	#
CH3NO2 NITRO-METHANE	61.04036	-80.751	-66.85		55.528	282.863	12.610	#
CH3NO2 Methyl Nitrite CH3ONO	61.04036	-65.44	-54.015	$\pm 1.$	64.891	302.910	15.345	#
CH3NO3 METHYL-NITRATE	77.03976	-122.005	-107.13	$\pm 4.2$	76.597	305.793	16.234	#
CH3N2 CH3N=N*	43.04800	236.216	246.971	$\pm 8$	51.182	258.278	11.671	#
CH3N2 CH2*-N=NH	43.04800	332.448	343.709	$\pm 8.$	47.988	263.640	11.165	#
CH3N2 cy(-CH*-NH-NH-)	43.04800	461.257	472.900	$\pm 8.$	46.303	247.027	10.782	#
CH3N2 cy(-CH2-NH-N*-)	43.04800	383.158	394.889	$\pm 8.$	45.450	252.246	10.695	#
CH3N2O3 H2C(OH)-N*-NO2 rad	91.04620	40.715	58.170	$\pm 8.$	87.965	343.096	17.991	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CH3N3 CH <sub>3</sub> -N=N=N MethylAzide	57.05474	297.29	309.93	±8.	63.015	279.531	14.118	#
CH3O	31.03392	21.0	28.4	±2.1	42.541	234.278	10.719	#
CH3O <sup>+</sup> <sup>a</sup>		1063.23		±1.04				X
CH3O <sup>-</sup>	31.03446	-138.151	-123.924	±0.323	36.469	220.494	10.066	#
CH2OH	31.03392	-17.0	-10.7	± 0.7	47.401	244.170	11.781	†
CH2OH <sup>+</sup>	31.03337	716.400	718.149	± 0.3	37.835	228.047	10.149	†
CH3OD	33.04832	-205.331	-194.49		44.142	242.751	11.543	#
CH3O2 Peroxymethyl Radical	47.034	9.0		± 5.1	52.257	268.762		
CH3S Thiomethoxy Radical	47.10052	121.470	128.518	±8.	46.635	242.040	11.120	#
CH3SS	79.16652	80.00	88.839	±8.	62.225	291.673	13.743	#
CH4 RRHO	16.04276	-74.6	-66.633	±0.3	35.613	186.314	10.023	
CH4 ANHARMONIC	16.04276	-74.6	-66.626	±0.3	35.691	186.371	10.016	†
CH4 <sup>+</sup> Methane cation	16.04191	1149.992	1150.86	±0.260	44.371	196.529	10.925	#
CH4N CH <sub>3</sub> NH*	30.0492	187.569		±4.8	47.372	235.967		
CH4N *CH <sub>2</sub> NH <sub>2</sub>	30.0492	153.49	164.62	±8.	48.597	244.694		#
CH4N2 Diaziridine -H2CNHNH-	44.05594	239.505	255.450	±8.	46.098	242.397	10.714	#
(NH2)2C=O Urea	60.05534	-231.999	-215.617	±8.	77.445	299.707	14.618	#
CH4N4O2 Nitroguanidine, Picrite	104.06822	89.295	113.750	±8.	106.201	358.208	19.555	
CH4N4O2 NG (NH <sub>2</sub> ) <sub>2</sub> C=N-NO <sub>2</sub>	104.06822	48.162	73.401	±8.	106.906	348.642	18.762	#
CH3OH(L)	32.04216	-238.91	-235.57		81.080	127.269	18.995	†
CH3OH	32.04216	-200.94	-190.11		44.039	239.81	11.444	#†
CH4O2 (CH <sub>3</sub> OOH)	48.04126	-126.733	-114.22	±4.2	66.753	275.904	14.160	#
CH4S (CH <sub>3</sub> SH) MethylMercaptan	48.10846	-20.426	-9.927	±8.	50.185	253.190	11.903	#
CH5N CH <sub>3</sub> -NH <sub>2</sub> MethylAmine	31.05714	-19.380	-4.378	±8.	48.495	231.900	11.556	#
CH5N2 CH <sub>3</sub> N*NH <sub>2</sub>	45.06388	211.300	228.491	±8.	64.884	276.081	13.703	#
CH5N2 CH <sub>2</sub> *NHNH <sub>2</sub>	45.06388	269.236	236.059	±8.	68.327	287.002	14.071	#
CH5N3 GUANIDINE	59.07062	27.952	48.939	±8.	75.796	297.900	14.223	#
CH6N2 MethylHydrazine	46.07182	109.41	130.443	±8.	68.911	274.188		#
CH6Sn CH <sub>3</sub> SnH <sub>3</sub>	136.76834	118.407	136.091	±4.2	73.750	285.712	15.907	#
Cl Carbon Iodide	138.91517	570.201	568.358	±60.	36.908	241.318	9.494	†
Cl2 DilodoCarbene	265.81964	468.394	470.	±60.	50.945	304.324	12.643	†
Cl3 Triiodomethyl Radical	392.72411	405.984	410.000	±60.	70.550	361.033	16.831	#
Cl4 TetralodoMethane	519.62858	260.41	265.53		95.819	391.347	22.327	#
CN	26.01774	438.68	435.4	±2	29.156	202.643	8.672	†#
CN <sup>+</sup>	26.01689	1798.483	1788.992	±0.926	29.463	196.935	8.682	†
CN <sup>-</sup>	26.01799	59.98	62.895	±0.629	29.151	196.576	8.671	†
CNO (NCO)	42.01684	128.040	127.57	±4.2	39.989	232.229	10.198	†#
CNN	40.02418	591.87	591.216	±3.19.	42.656	232.398	10.378	†#
NCN (NCN)	40.02418	465.89	465.433	±1.78	41.946	225.814	10.180	†#
C(NO2)4 TetraNitroMethane	196.03316	82.383	101.856		176.119	503.723	33.993	
CO	28.0104	-110.53	-113.813	±0.17	29.141	197.657	8.671	†
CO <sup>+</sup>	28.00955	1247.812	1238.337	±0.034	19.137	203.230	8.671	†
COS Anharmonic	60.07610	-141.700	-141.836	±2.	41.549	231.650	9.942	†
CO2	44.0098	-393.51	-393.142	±0.13	37.135	213.787	9.365	†
CO2 <sup>+</sup>	44.00895	943.137	936.107	±0.023	41.799	228.017	10.566	†
CP	42.98446	520.162	517.860	±10.	29.910	216.257	8.715	†
CS	44.0767	278.550	275.307	±3.8	29.799	210.559	8.708	†
CS2 Anharmonic	76.143	116.70	115.913	±1.	45.482	237.889	10.664	†
CW Tungsten Carbide	195.8507	-40.54	---		35.378	32.374	----	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
ZrC Zirconium Carbide	103.23470	-196.648	-195.960	$\pm 13.$	37.899	33.321	5.862	†
C2 singlet $^1\Sigma_g^+$	24.0214	826.799	820.231	$\pm 1.6$	29.214	190.673	8.675	#†
C2 triplet $^3\Pi_u$	24.0214	842.402	827.260	$\pm 8.$	29.326	200.552	17.248	#
C2+ cation	24.02085	1980.05	1967.274	$\pm 9.$	29.400	204.179	8.685	†
C2- anion	24.02195	501.09	500.718	$\pm 1.67$	29.241	196.599	8.676	†
ALC2	51.00294	675.616	670.	$\pm 35.$	47.818	252.941	12.263	†
C2Br	103.9260	623.667	626.39	$\pm 2.$	45.103	295.017	11.648	#
C2Br2	183.8300	335.31	346.51	$\pm 2.$	68.067	294.448	15.427	#
C2Br2F4 HALON 2402	259.82301	-823.076	-802.65	$\pm 8.$	119.972	386.278	23.851	#
C2Br3	263.7340	385.388	405.674		83.269	369.892	18.602	#
C2Br4	343.638	215.584	218.816		102.196	387.413	22.410	#
C2Br5	423.54200	283.257	318.915		126.162	444.694	27.749	#
C2Br6	503.44600	165.480	209.480		146.665	459.134	31.667	#
C2CL	59.47410	534.083	530.	$\pm 50.$	45.046	241.948	10.781	†
C2CL2	94.92680	226.6	223.295	$\pm 14$	65.374	272.114	14.593	†
C2CL2F2 CCLF=CFCL E(trans)	132.92361	-341.486	-339.3	$\pm 8.$	87.333	327.192	17.925	#
C2CL2F2 CCLF=CCLF Z(cis)	132.92361	-339.548	-337.37	$\pm 8.$	87.632	327.213	17.934	#
C2CL2F4 FC-114	170.92101	-900.4			116.6	364.2		
C2CL3	130.3801	190.28	190.		76.033	328.166	16.150	†
CCl2F-CCLF2 FC-113	187.37531	-705.8			121	386.9		
C2CL3F3 FC-113A	187.37531	-740.6			120.3	369.3		
C2CL4	165.8322	-21.064	-20.159	$\pm 8.0$	94.781	341.211	19.564	#†
C2CL5	201.2855	39.			118.832	397.906		
C2CL6	236.7376	-162.110	-159.69	$\pm 8$	136.326	407.696	27.235	†#
C2D2	28.04960	222.672	222.470		49.378	208.869	10.879	#
C2D2O	44.04900	39.915	42.544		55.516	249.581	12.387	#
C2D4	32.07780	30.270	38.111		52.950	230.655	11.404	#
C2OD4	48.07721	-180.581	-170.731		66.931	270.623	13.735	#
C2D6	36.10601	-110.60	-94.786		59.774	236.691	12.001	#
C2D6N2 Azomethane-D6	64.11949	119.248	138.518		92.278	296.225	17.210	#
C2D6O DimethylEther-D6	52.10541	-208.406	-192.046		77.652	282.381	15.794	#
C2F	43.01980	353.847	350.00	$\pm 50.$	42.6	231.036	10.367	†
C2F2	62.01821	-144.666	-147.	$\pm 20$	60.114	249.570	13.266	†
C2F3	81.01661	-228.175	-227.0	$\pm 20.$	66.178	297.643	14.164	†
C2F4 FC-1114	100.01501	-675.34	-671.91	$\pm 2.0$	80.459	300.128	16.331	†#
C2F5	119.01402	-891.192			94.111	341.49		
C2F6 FC-116	138.01182	-1347.38	-1339.0	$\pm 0.31$	106.294	341.033	20.229	†#
CF3-O-O-CF3	170.01062	-1464.6	-1452.16	$\pm 8$	130.515	425.082	24.822	#
C2H ETHYNYL	25.02994	568.522		$\pm 4$	41.999	213.304		†
C2H+	25.02879	1697.10	1687.566	$\pm 0.317$	38.746	203.063	9.677	#
C2H -	25.02989	274.776	277.476	$\pm 0.493$	39.587	204.389	9.838	#
C2HBr	104.93394	282.43	289.073	$\pm 2$	55.087	252.719	11.948	#
C2HBr2	184.83794	333.590	348.909		68.272	326.691		#
C2HBr3	264.74194	144.13	168.884		85.590	359.979		#
C2HBr4 1,1,2,2-CHBr <sub>2</sub> CBr <sub>2</sub>	344.64534	218.823	250.685	$\pm 8.4$	107.701	425.045	23.519	#
C2HBr4 1,1,1,2-CBr <sub>3</sub> CHBr	344.64534	243.634	274.593	$\pm 8.4$	113.967	417.090	24.422	#
C2HBr5	424.54994	113.09	153.50		126.586	439.181		#
C2HCL	60.48204	227.292	226.246	$\pm 8.$	55.019	243.235	11.977	#†
C2HCLF 1,1-CLF Radical	79.48074	101.87	103.90	$\pm 8.$	63.592	289.422	13.317	#



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2HCLF2-1,1 FC-1122	98.47885	-333.654	-329.16		76.650	304.242	15.263	†
C2HCLF2 cis FC-1131	98.47885	-323.569			75.394	305.096		
C2HCLF2 trans	98.47885	-323.103			75.149	304.318		
CF2H-CCLF2 FC-124A	136.47625	-903.3			100.4	351.1		
CF3-CHCLF HCFC124	136.47625	-924.7			99.06	349.6		
C2HCL2F-1,1+cis+trans	114.93314	-168.648	-164.97		77.324	320.190	16.259	†
CF3-CHCL2 HCFC123	152.93055	-743.9			102.6	352.6		
CF2CL-CHFCL FC123A	152.93055	-710.			104.5	368.1		
CFCL2-CHF2	152.93055	-702.1			104.5	361.7		
C2HCL3	165.83220	-11.226	-7.316	±8	79.750	327.774	16.560	#†
C2HCL4	166.84014	21.824	26.108	±8.	100.608	375.159	20.419	#
C2HCL5	202.29284	-160.410	-153.83	±8.	113.348	379.920	22.716	#
C2HF	44.02774	41.692	41.	±25	52.268	231.573	11.446	†
C2HF2	63.02615	-42.5	-40.52	±17.9	59.249	279.393		#
C2HF3	82.02455	-490.78	-485.53	±8.24	69.191	292.665	14.328	†
C2HF5 FC-125	120.02136	-1120.00	-1110.4	±8.	95.808	334.635	18.776	#
HCCN singlet HC*-CN	39.03608	526.552	524.380	±8.	50.901	252.653	12.848	#
HCCN triplet HC*=C=N*	39.03608	476.541	475.094	±8.	51.486	247.916	12.848	#
C2HNO NC-CHO	55.03548	44.120	46.152	±8.	55.793	270.935	12.123	#
C2HNO2 HCC-NO <sub>2</sub>	71.03488	278.654	283.597	±8.	69.580	289.604	14.414	#
C2H(NO <sub>2</sub> ) <sub>2</sub> NO <sub>2</sub> -CH=C*NO <sub>2</sub>	117.04042	328.398	339.383	±8.	107.603	339.383	21.386	#
HCCO Ketyl Radical	41.02874	178.3	177.258	±1.5	49.975	246.408	11.665	#†
H2C2 VINYLIDENE	26.03728	414.788	414.489		42.614	221.021	10.874	†
C2H2 ACETYLENE	26.03728	228.20	228.769	±0.8	44.001	200.917	10.006	†
C2H2Br2 1,2-DiBromoEthylene	185.84528	99.286	119.008	±8.	69.704	313.877	15.373	#
C2H2Br4 CHBr <sub>2</sub> CHBr <sub>2</sub>	345.6532	32.719	69.245	±8.	107.898	398.858	23.089	#
C2H2CL CHCL=CH* Radical	61.48998	274.767	277.937	±8	53.700	270.153	11.996	#
C2H2CLF	80.48868	-165.393	-159.0	±15	64.216	283.339		†
C2H2CL2 CCL <sub>2</sub> =CH <sub>2</sub>	96.94328	2.2	8.084	±1.4	67.722	288.285		#
C2H2CL3 CH2-CCL3	132.39538	71.864	77.770	±8.	95.682	331.217	18.441	#
C2H2F2-1,1+cis+trans equilib.	64.03409	-336.4	-329.48	±4.	60.237	266.054	12.480	†
C2H2F2-1,1 FC-1132A	64.03409	-336.4	-329.48	±4.	60.123	266.041	12.476	#
H2C2F2 cis	64.03409	-306.5	-299.80	±5.	58.349	268.723	12.701	#
F2C2H2 trans FC-1132	64.03409	-303.73	-297.15	±5.	60.074	267.847	12.955	#
C2F3H2	83.03309	-517.142			79.499	303.093		
CF3-CFH2	102.03089	-913.3	-902.01	±17.5	86.273	315.752	16.937	#
CHF2-CHF2 HFC-134	102.03089	-883.3	-872.21	±5.5	84.129	313.143	17.130	#
C2H2N CH2CN Methyl-Cyanide	40.04402	257.78	260.54		54.345	255.826	12.356	#
C2H2N CH2NC Methyl Isocyanate	40.04402	358.23	360.59	±8.	53.971	256.71	12.550	#
C2H2NO NC-CH <sub>2</sub> -O*	56.04342	175.619	181.426	±8.	61.512	281.028	13.444	#
C2H2NO2 NC-CH <sub>2</sub> -O-O*	72.04282	177.987	185.371	±8.	74.150	312.514	16.207	#
1,2-C2H2(NO <sub>2</sub> ) <sub>2</sub> trans	118.04896	40.953	56.131	±8.	108.234	360.962	21.428	#
CH2CO Ketene	42.03668	-48.579	-45.460	±0.28	51.740	251.442	11.796	†
HCCOH ETHYNOL	42.03668	93.3	95.408	±18.3	57.592	249.544	12.810	#
C2H2O2 HOCH=C=O	58.03608	-155.159	-149.807	±8.	61.975	288.151	13.902	#
C2H2O2 HOCCOH Ethyndiol	58.03608	-27.953	-24.487	±8.	69.504	325.406	15.789	#
C2H2O2 trans & cis GLYOXAL	58.03608	-212.082	-206.51	±0.8	60.409	272.483	13.682	†
C2H2O2 cis GLYOXAL	58.03668	-193.35		±0.8				X
C2H2O2 Oxiranone	58.03608	-177.916	-170.37	±8.	53.635	263.960	11.713	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2H2O4 Oxalic Acid	90.03488	-731.8	-721.2	$\pm 2.0$	86.149	320.662		#
C2H3 VINYL RADICAL	27.04522	296.580	300.867	$\pm 0.92$	42.071	233.663	10.522	†#
C2H3+ Vinylum Ion	27.04467	1122.34	1119.2	$\pm 1.17$	50.714	225.350	11.780	#
C2H3-	27.04577	226.583	237.256	$\pm 1.00$	40.011	227.870	10.334	#
C2H3Br Bromoethylene	106.94922	74.070	89.049	$\pm 1.18$	54.824	275.474	12.090	#
C2H3BrO2 Bromoacetic Acid	138.94802	-383.5	-364.61	$\pm 3.1$	80.542	337.015		#
CH3CBr3 1,1,1-Tribromoethane	266.75722	3.18	34.718	$\pm 8.$	97.982	355.210	20.051	#
C2H3CL	62.49792	37.872	45.452	$\pm 8.$	53.681	264.024	11.820	#
C2H3CLO3	94.49672	-427.6	-416.0	$\pm 1.0$	78.839	325.918		#
C2H3CL3 CH <sub>3</sub> -CCL <sub>3</sub>	133.40332	-144.6	-133.98	$\pm 2.0$	92.410	320.413	18.025	#
C2H3F	46.04362	-140.1	-132.21	$\pm 2.5$	50.407	252.674	11.336	#
C2H3F2	65.04263	-302.503			67.256	288.291		
CH3CF3 FC-143A	84.04043	-755.655	-742.91	$\pm 1.0$	78.074	287.652	15.298	#
CH3CD3 1,1,1-Ethane-D3	33.08753	-107.57	-92.313	$\pm 3.3$	57.385	241.997	12.406	#
C2H3I Ethyl-Iodide	153.94969	128.867	137.906		56.071	299.640	12.368	#
C2H3N CH <sub>3</sub> CN Methylcyanide	41.05196	74.04	81.09	$\pm 0.37$	52.249	243.267	12.094	#
C2H3N CH <sub>3</sub> NC Methylcyanate	41.05196	163.5	169.982	$\pm 7.2$	52.947	246.658	12.660	#
C2H3NO NCCH <sub>2</sub> OH	57.05136	-49.910	-39.97	$\pm 8.$	64.965	280.796		#
C2H3NO2 NCCH <sub>2</sub> -O-OH	73.05136	29.476	39.641	$\pm 8.$	82.503	323.081	17.659	#
C2H3NO2 Nitroethylene	73.05136	33.284	46.001	$\pm 8.6$	73.68	300.503	15.108	
C2H3NO4 CH <sub>3</sub> C(O)-O-NO <sub>2</sub>	105.04956	-303.654	-287.915	$\pm 8.0$	101.794	351.943	20.765	#
C2H3NO5 CH <sub>3</sub> C(O)-OO-NO <sub>2</sub>	121.04896	-254.642	-237.021	$\pm 8.0$	116.800	373.968	23.223	#
C2H3O (CH <sub>3</sub> CO) RADICAL	43.04462	-10.3	-3.6	$\pm 1.8$	50.785	267.448	12.385	#
C2H3O+ (CH <sub>3</sub> CO+) ion	43.04471	669.952	670.921	$\pm 0.85$	52.589	243.392	11.977	#
C2H3O (CH <sub>2</sub> =CHO*) Radical	43.04462	12.753	20.189	$\pm 8.$	52.398	258.818	11.713	#
OH3C2 (*CH <sub>2</sub> CHO) RADICAL	43.04462	25.102			54.974	267.919	12.910	*
C2H3O OXYRANE RADICAL	43.04462	164.473	172.900	$\pm 8.0$	45.741	252.528	10.723	#
C2H3O2 HOCH <sub>2</sub> C*=O	59.04402	-145.423	-136.978	$\pm 8.$	66.163	304.877	15.044	#
C2H3O2 HOC*HCHOH	59.04402	-176.050	-167.064	$\pm 8.$	63.064	325.723	14.503	#
C2H3O2 *COOCH3 RADICAL	59.04402	-163.385	-154.616	$\pm 8.0$	66.197	288.777	14.720	#
C2H3O2 CH <sub>3</sub> (O)O* Acetic Rad	59.04402	-192.79	-183.115	$\pm 8.$	65.149	284.722	13.814	#
C2H4 ETHYLENE	28.0536	52.500	61.025		42.887	219.322	10.519	†
C2H4+	28.05261	1074.461	1074.912	$\pm 0.207$	48.804	246.866	12.395	#
C2H4Br2 liq. CH <sub>2</sub> Br-CH <sub>2</sub> Br liquid	187.8611	-79.26		$\pm 1.24$				X
C2H4Br2 CH <sub>2</sub> Br-CH <sub>2</sub> Br	187.8611	-37.5	-10.491		75.948	329.088	16.422	#
C2H4Br2 CH <sub>3</sub> -CHBr <sub>2</sub>	187.8611	-41.	-13.725		79.452	327.355	16.288	#
C2H4CL RADICAL	63.50646	90.12			58.635	281.459		
C2H4CIF ClFHC-CH3	82.50426	-310.700	-296.966	$\pm 8.$	70.860	291.429	14.313	#
C2H4CL2 CH <sub>2</sub> CL-CH <sub>2</sub> CL	98.95856	-130.069	-117.37	$\pm 0.6$	72.544	303.542	15.531	#
C2H4CL2 CH <sub>3</sub> -CHCL <sub>2</sub>	98.95856	-127.6		$\pm 1.1$				X
C2H4O2CL2 Cl <sub>2</sub> -Peroxyethane	130.95796	-231.375	-215.17		109.993	362.046	20.697	#
C2H4F RADICAL	47.05216	-72.216			58.857	273.845		
C2H4F2 CH <sub>2</sub> F-CH <sub>2</sub> F HFC-152	66.04997	-447.55	-433.78		64.238	279.918		#
C2H4F2 CH <sub>3</sub> -CHF <sub>2</sub> HFC-152a	66.04997	-497.0	-473.07	$\pm 8.0$	87.266	282.502		#
C2H4O VINYL-ALCOHOL	44.05316	-124.683			61.	289.996		
C2H4O OXYRANE	44.05316	-52.635	-40.082	$\pm 0.63$	47.624	242.870	10.831	†
CH3CHO ACETALDEHYDE	44.05316	-166.19	-155.70		55.319	263.952	12.897	†
HOCH2CHO Acetaldehyde-1-ol	60.05196	-306.553	-294.036	$\pm 8.$	66.391	309.242	15.206	#
CH3COOH liquid Acetic Acid	60.05196	-484.216		$\pm 0.17$				X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CH <sub>3</sub> COOH ACETIC ACID	60.05196	-432.253	-418.12		63.439	283.473	13.597	†
(HCOOH) <sub>2</sub> Formic Acid dimer	92.0512	-820.951			96.177	332.671		*
HCOOCH <sub>3</sub> (liq) Methyl Formate <sup>a</sup>	60.05196	-385.970		±0.578				X
HCOOCH <sub>3</sub> MethylFormate	60.05196	-363.619	-350.219	±8.	62.436	286.254	14.323	#
C <sub>2</sub> H <sub>5</sub> ETHYL RADICAL	29.06110	119.7	130.773	±0.7	50.679	242.984	12.204	#†
C <sub>2</sub> H <sub>5</sub> Br BROMOETHANE	108.9651	-61.60	-39.65	±1.01	64.206	287.668	13.584	#†
C <sub>2</sub> H <sub>5</sub> Cl CHLOROETHANE	64.5138	-106.827	-92.25	±0.41	62.738	276.274	13.294	#
C <sub>2</sub> H <sub>5</sub> ClO <sub>2</sub> Chloroperoxyethane	96.5132	-212.966	-194.27		92.223	336.239	17.853	#
C <sub>2</sub> H <sub>5</sub> F FLUOROETHANE	48.0595	-275.21	-260.41	±4.9	59.575	270.530	12.888	#
C <sub>2</sub> H <sub>5</sub> I IODOETHANE	155.96557	-7.047	8.253	±0.56	71.670	298.362	14.575	#
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> NITROETHANE	75.06724	-103.784	-83.506	±5.	79.018	320.512	16.015	
C <sub>2</sub> H <sub>5</sub> ONO <sub>2</sub> ETHYLNITRATE	91.06664	-154.975	-132.82	±8.	95.103	328.863	18.480	
C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> Ethyl Azide	71.08132	266.872	287.394	±8.	80.026	303.042	15.761	#
C <sub>2</sub> H <sub>5</sub> O* ETHOXY RADICAL	45.0609	-13.6	-0.2	±8.0	66.321	277.642	14.325	#
C*H <sub>2</sub> CH <sub>2</sub> OH RADICAL	45.0609	-23.849	-11.640	±8.0	68.668	291.708	15.564	
CH <sub>3</sub> C*HOH RADICAL	45.0609	-54.030	-40.776	±8.0	64.038	288.991	14.263	#
C <sub>2</sub> H <sub>5</sub> O Dimethylether Radical	45.0609	0.960	14.079	±8.0	66.124	281.519		#
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> HOCH <sub>2</sub> CH <sub>2</sub> O*	61.05990	-159.636	-143.869	±8	71.493	329.555	16.190	#
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> HOCH <sub>2</sub> C*HOH	61.05990	-207.443	-192.194	±8.	75.813	336.908	16.709	#
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> EthylPeroxy Radical	61.06050	-28.70	-12.450	±8.4	73.721	299.991		#
C <sub>2</sub> H <sub>5</sub> S* EthylThio Radical	61.12710	97.6	111.4	±8.	64.353	284.751	13.877	#
C <sub>2</sub> H <sub>6</sub> ETHANE	30.0694	-83.852	-68.232	±0.2	52.501	229.221	11.892	†
C <sub>2</sub> H <sub>6</sub> Bi Bi(CH <sub>3</sub> ) <sub>2</sub> Radical	239.04942	265.000		±22.	87.130	330.692	17.416	#
C <sub>2</sub> H <sub>6</sub> N (CH <sub>3</sub> ) <sub>2</sub> N* Dimethylazide R	44.07578	159.854	177.58	±8.	66.912	270.641.		#
C <sub>2</sub> H <sub>6</sub> N *CH <sub>2</sub> -NH-CH <sub>3</sub>	44.07578	156.58	174.07	±8.	70.233	279.671		#
C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> AZOMETHANE	58.08252	148.699	168.358		78.035	318.533	16.523	#
C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> N-NO <sub>2</sub>	90.08192	-4.8	20.279		103.204	328.138	19.783	#
C <sub>2</sub> H <sub>5</sub> OH(L) ETHANOL LIQUID	46.06904	-277.51	-269.74		112.250	160.100	24.082	†
C <sub>2</sub> H <sub>5</sub> OH ETHANOL	46.06904	-234.95	-217.641		65.309	280.593	14.542	†
CH <sub>3</sub> OCH <sub>3</sub> DIMETHYLETHER	46.06904	-184.054			65.823	267.381		
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> liq HO-CH <sub>2</sub> -CH <sub>2</sub> -OH liq	62.06784	-455.169		±0.375				X
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> 1,2-Ethane DiOl	62.06784	-389.362	-369.547	±0.614	74.572	323.647	16.376	#
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> PEROXYETHANE	62.06844	-173.636			82.969	314.534		
CH <sub>3</sub> OOCH <sub>3</sub> Dimethylperoxyde	62.0682	-125.5	-106.5	±5.0	80.717	308.409		#
C <sub>2</sub> H <sub>6</sub> S C <sub>2</sub> H <sub>5</sub> SH Ethanethiol	62.13504	-43.514	-27.099	±8.	71.312	300.135	15.509	#
C <sub>2</sub> H <sub>6</sub> S (CH <sub>3</sub> SCH <sub>3</sub> )Methylsulfide	62.13504	-35.376	-19.028	±8.	71.824	285.936	15.576	#
C <sub>2</sub> H <sub>6</sub> S <sub>2</sub> CH <sub>3</sub> -SS-CH <sub>3</sub>	94.20164	-17.732	-1.486	±8.	90.588	359.431	20.089	#
C <sub>2</sub> H <sub>6</sub> Sb Sb(CH <sub>3</sub> ) <sub>2</sub>	151.82904	143.93		±4.5	78.064	326.197	17.351	#
C <sub>2</sub> H <sub>7</sub> N CH <sub>3</sub> -NH-CH <sub>3</sub>	45.08372	-15.259	+6.501	±8.	68.541	267.185		#
C <sub>2</sub> H <sub>7</sub> N <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> N-NH*	59.09046	207.685	232.276	±8.	81.384	284.772		#
C <sub>2</sub> H <sub>7</sub> N <sub>2</sub> *CH <sub>2</sub> (CH <sub>3</sub> )N-NH <sub>2</sub>	59.09046	258.655	281.792	±8.	90.949	322.581	17.279	#
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> SYM Dimethylhydrazine	60.09840	106.173	133.504	±8.	86.934	310.941	17.319	#
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> UDMH	60.09840	93.487	121.271	±8.	90.405	305.644	16.866	#
CCN	38.02814	679.07	674.474	±6.23	44.231	237.159	11.089	#†
CNC	38.02814	675.85	670.935	±5.89	45.042	233.804	11.357	#†
C <sub>2</sub> NO O=C*-CN	54.02754	210.00	207.188	±10.	56.145	278.187	13.594	#†
C <sub>2</sub> N <sub>2</sub>	52.03488	309.28	307.342	±1.03	57.085	242.204	12.715	†
(CN) <sub>2</sub> Hg Hg(CN) <sub>2</sub> (solid)	252.62	263.6		±8.4				X
(CN) <sub>2</sub> Hg Hg(CN) <sub>2</sub> (gas)	252.62	372.4		±9.4				X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2N2O2Hg(s) Hg- Fulminate	284.6	386.						X
C2(NO2)2 Dinitroacetylene	116.03248	349.046	356.251	$\pm 8$	102.603	353.895	20.933	#
C2(NO2)4 Tetranitroethylene	208.04356	N/A	N/A		184.031	468.771	35.016	#
C2(NO2)6 Hexanitroethane	300.05524	179.		$\pm 5.9$	273.376	667.098		
C2O	40.02080	385.68	381.641	$\pm 1.9$	43.134	233.624	10.486	#
C2S2	88.15340	376.660	373.831		62.030	274.120	13.760	†
C2Si see SiC2								
C3 singlet $^1\Sigma_g^+$	36.03210	822.025	813.770	$\pm 8$	42.203	237.613	12.109	#†
C3Br2 BrC*=C=C*Br	195.84010	611.533	622.068	$\pm 8$	77.501	335.224	17.146	#
C3Br3 Br <sub>2</sub> C=C=C*Br	275.74410	449.906	468.756	$\pm 8$	96.993	393.290	21.090	#
C3Br3 1,2,3-triBrCyPropene-1-yl	275.74410	529.192	548.69	$\pm 8$	94.196	423.079	20.443	#
C3Br4 Br <sub>2</sub> C=C=CBr <sub>2</sub>	355.64810	316.394	343.175	$\pm 8$	117.375	420.589	25.420	#
C3Cl2 ClC*=C=C*Cl biradical	106.93750	519.876	514.996	$\pm 8$	77.130	319.091	17.220	#
C3Cl2 Cy (-ClC=C=CCl-)	106.93750	214.260	226.60	$\pm 120$	83.062	266.312	---	
C3Cl3 1,2,3-triClCyPropene-1-yl	142.3902	398.434	396.717	$\pm 8$	88.840	347.538	18.649	#
C3Cl3 Cl <sub>2</sub> C=C=CCl* radical	142.3902	311.296	307.497	$\pm 8$	95.298	372.338	20.731	#
C3Cl3O* Cl <sub>2</sub> C=C=CCl(O*) rad.	158.38960	95.571	94.555	$\pm 8$	105.684	397.707	22.288	#
C3Cl4 Cl <sub>2</sub> C=C=CCl <sub>2</sub>	177.8429	135.1	134.08	$\pm 8$	109.297	371.955	22.545	#
C3D4 Cyclopropene-D4	44.08851	263.592	271.241		63.845	254.235	12.650	#
C3D6 Cyclopropane-D6	48.11671	32.850	48.523		72.723	251.483	13.195	#
C3F Radical	55.030503	564.957	559.052	$\pm 8$	55.612	277.062	13.479	#
C3F3 FCC-CF <sub>2</sub> *	93.02731	-134.419	-135.23	$\pm 8$	81.990	326.463	17.210	#
C3F3 *CC-CF <sub>3</sub>	93.02731	-79.078	-79.609	$\pm 8$	80.749	313.306	16.929	#
C3F4 PerFluoroAllene	112.02571	-553.685	-551.89	$\pm 8$	92.135	336.733	19.021	#
C3F6 Hexafluoropropene	150.02252	-1157.253	-1150.95	$\pm 8$	121.759	373.675	23.337	#
C3F7 RADICAL	169.02182	-1347.122	-1339.5	$\pm 8$	135.964	416.386	26.401	#
C3F8 FC-218	188.02023	-1760.121			147.248	406.145		
C3H HC≡ C-C	37.04004	719.393	714.091	$\pm 8$	53.430	247.795	12.696	#
C3HBr2 1,3-DiBromoAllene Rad	196.84804	420.032	434.370	$\pm 8$	82.624	349.563	17.576	#
C3HBr2 1,1-DiBromoAllene Rad	196.84804	406.015	419.337	$\pm 8$	88.647	353.450	18.593	#
C3HBr2O BrHC=C=CBr(O*)	212.84744	195.142	210.448	$\pm 8$	97.345	394.220	20.949	#
C3HBr2O Br <sub>2</sub> C=C=CH(O*)	212.84744	239.032	254.141	$\pm 8$	97.059	384.601	21.145	#
C3HBr3 TriBromoAllene	276.75204	234.185	306.937	$\pm 8$	100.773	389.538	21.373	#
C3HCl2 DiChloroAllenyl Radical	107.94544	328.356	326.877	$\pm 8$	82.314	340.860	18.055	#
C3HCl2 1,1-DiChloroAllenyl Rad	107.94544	311.633	310.755	$\pm 8$	85.060	329.338	17.453	#
C3HCl2O* H(Cl)C=C=CCl(O*)	123.94484	104.792	105.885	$\pm 8$	93.127	365.659	19.823	#
C3HCl2O* Cl <sub>2</sub> C=C=CH(O*)	123.94484	151.578	152.696	$\pm 8$	92.814	359.360	19.797	#
C3HCl3 TriChloroAllene	143.39814	148.871	150.575	$\pm 8$	94.649	353.019	19.463	#
C3HF7 FC-227EA	169.02092	-1564.816	-1552.4	$\pm 8$	136.690	399.058	25.901	#
C3HN HC≡ CCN CyanoAcetylene	51.04678	368.414	367.225	$\pm 8$	62.633	247.991	12.918	#
C3H2(1) CyPropenylidene	38.04888	476.976	477.960		44.222	236.204	10.645	
C3H2(3) H2C*-C≡ C*	38.04888	651.030	650.361		54.719	254.549	12.298	
C3H2(3) *HC=C=CH*	38.04888	755.254	751.668	$\pm 62.7$	67.953	260.782	15.215	
C3H2(1) HC-C≡ CH*	38.04888	817.972	816.374	$\pm 62.7$	58.770	251.691	13.227	
C3H2Br2 HBrC=C=CHBr	197.85598	250.120	268.615	$\pm 8$	84.110	340.818	17.653	#
C3H2Cl HCIC=C=H*	73.50068	328.164	329.399	$\pm 8$	72.438	296.950	14.984	#
C3H2Cl2 HCIC=C=CClH	108.95338	161.440	165.569	$\pm 8$	80.178	316.701	16.680	#
C3H2Cl2O ClHC=C=CCl-OH	124.95278	-4.954	+0.493	$\pm 8$	96.536	355.053	19.703	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C3H2F3 CF <sub>3</sub> -CH=CH*	95.04319	-376.895	-369.47	±8	90.727	323.105	17.442	#
C3H2F3 CF <sub>3</sub> -C*=CH <sub>2</sub>	95.04319	-374.941	-367.82	±8	91.100	125.439	17.741	#
C3H2F4 CF <sub>3</sub> -CF=CH <sub>2</sub>	114.04159	-813.261	-803.168	±8	101.255	327.768	19.186	#
C3H2N HC*=CH-CN	52.05472	442.855	445.486	±8	59.531	272.030	13.333	#
C3H3 PROPARGYL RADICAL	39.05592	331.8	334.04	±8	64.891	256.659	13.620	†
C3H3 Propynyl Rad. H <sub>3</sub> C-C≡C*	39.05592	450.	453.46		53.	250.9	12.400	†
C3H3 Allenyl Radical CH <sub>2</sub> =C=CH*	39.05592	348.427	352.384	±8	55.262	253.192	11.905	#
C3H3 CycloPropenyl Radical	39.05592	488.064	492.719	±8	50.459	232.865	11.207	#
C3H3+ [CH <sub>2</sub> =C=CH] <sup>+</sup> cation	39.05537	1201.645	1198.416	±8	59.173	239.329	12.894	#
CLC3H3 1-Chloro-1-propyne	74.50862	184.711	189.553	±8	71.364	283.822	15.611	#
C3H3Cl CH <sub>2</sub> Cl-CCH	74.50952	162.729	167.78		73.747	296.899		
3-C3H3Cl CY	74.50952	218.333	225.43		66.257	281.203		
C3H3Cl CHCl=C=CH <sub>2</sub>	74.50952	160.851	163.18		70.089	290.465		
C3H3F2 *CF <sub>2</sub> -CH=CH <sub>2</sub>	77.05273	-224.438	-216.93	±8	89.452	316.769		#
C3H3F3 CF <sub>3</sub> -CH=CH <sub>2</sub>	96.05113	-631.131	-619.51	±6.	90.704	319.468		#
C3H3I CH <sub>2</sub> ICCH Propargyl Iod.	165.96039	269.072	276.353	±12.5	74.028	310.672	15.180	#
C3H3I CH <sub>2</sub> =C=CHI Allenyl Iod.	165.96039	264.117	272.127	±12.5	70.463	305.857	14.451	#
C3H3N CH <sub>2</sub> =CHCN	53.06266	184.037	190.874	±8	59.387	263.290	13.361	#
C3H3O CH <sub>2</sub> =CHC*=O	55.05532	88.530	94.601	±8	61.410	300.654		#
C3H3O *CH <sub>2</sub> -CH=C=O	55.05532	93.560	98.877	±8	68.927	293.760		#
H4C3 PROPYNE	40.06386	184.9	191.966		60.731	248.429	13.031	†
C3H4 ALLENE	40.06386	190.92	198.412		58.88	243.630	12.605	†
C3H4 CYCLOPROPENE	40.06386	277.1	285.823		52.883	243.605	11.374	†
C3H4Cl *CH=CH-CH <sub>2</sub> Cl	75.51656	250.253	259.680	±8.	73.850	303.749	15.261	#
CLC3H4 *CH <sub>2</sub> -CH=CHCl	75.51656	137.444	147.12	±8.	71.705	303.390	15.012	#
C3H4N CH <sub>3</sub> -CH*-CN	54.07060	222.706	232.213	±8.	72.044	298.672	14.925	#
C3H4N2 1,3-DIAZOLE	68.07824	140.959		±28	65.701	273.426		
1,3,3 TRI-NITRO-AZETIDINE	192.08812	128.449	171.220	±8.	134.987	357.315	20.706	
C3H4O ACROLEIN	56.06416	-68.065	-57.913	± 8	64.332	297.025		#
C3H4O2 CH <sub>2</sub> =CH-C(O)-OH	72.06266	-326.051	-312.52	± 8	79.301	313.570	15.243	#
C3H5 Symmetric Allyl Radical	41.0727	163.594			63.387	258.886		†
T-C3H5 CH <sub>3</sub> C*=CH <sub>2</sub> “ “	41.0727	237.651			61.663	266.064		
S-C3H5 CH <sub>3</sub> CH=CH* “ “	41.07180	265.533	276.287	±8.	63.362	271.305	13.577	#
C3H5 Cyclo	41.07180	279.91	292.716	±10.5	55.701	251.486		#
C3H5Cl 1-Chloro-1-propene	76.5245	-8.100	+4.937	± 8.	76.450	299.193	15.884	#
C3H5Cl 3-Chloro-1-propene	76.5245	0.369	14.052	±8.	74.210	307.919	15.239	#
C3H5N PROPIONITRILE	55.07944	53.191	66.974	±8.	72.039	285.205	14.883	#
CH3CH=CHNO <sub>2</sub> Nitropropylene	87.07824	9.987	29.046	±8.9	93.59	330.004	18.288	
C3H5NO <sub>2</sub> NitroCycloPropane	87.07824	21.033	41.466	±8.	90.786	311.278	16.913	#
C3H5N3O <sub>9</sub> NITROGLYCERINE	227.08752	-279.073	-246.14	±2.7	234.24	545.865	43.458	
C2H5CO Propanal	57.0712	-32.83	-19.862	± 8.	67.859	314.290		#
CH2COCH3 Acetone Radical	57.0712	-33.34	-20.617	± 8.	72.843	307.518		#
C3H5O Propylene Oxide Radical	57.0712	104.069	118.072	± 8.	71.197	293.196		#
C3H5O2 Propanoic acid Radical	73.07060	-213.175	-197.658	± 8.	79.370	337.845	17.494	#
C3H5O2 CH <sub>3</sub> -C(O)-OCH <sub>2</sub> *	73.07060	-221.639	-205.562	± 8.	85.269	316.985	16.934	#
C3H6 PROPYLENE	42.07974	20.000	35.014		64.433	266.668	13.551	†
C3H6 CYCLOPROPANE	42.07974	53.30	70.455		55.572	237.488	11.410	†
C3H6N2O <sub>2</sub> N-NITRO-AZETIDIN	102.09292	114.123	141.198		100.656	328.954	18.840	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C3H6N6O6 RDX Solid	222.11748	79.078	--		248.95	259.8	--	
C3H6N6O6 RDX 135 Triazine	222.11748	192.000	233.285		230.174	482.441	39.331	
C2H5CHO Propionaldehyde	58.08004	-192.046			80.73	304.51		
CH3COCH3 ACETONE	58.08004	-214.814	-198.10	$\pm 0.26$	74.207	295.660	16.193	†#
C3H6O PROPYLENE OXIDE	58.07914	-92.760	-74.271	$\pm 8.$	72.671	281.487	14.415	#
C3H6O CY OXETANE	58.07914	-81.086	-61.49	$\pm 8.$	61.826	274.672	13.499	#
C3H6O Vinylmethylether	58.07914	-100.378	-83.824	$\pm 8.$	76.313	308.229	16.351	#
C3H6O Cyclopropanol	58.08004	-101.504	-81.907	$\pm 8.$	70.158	277.454	13.308	#
C3H6O2 Propionic acid	74.07854	-450.868	-431.289	$\pm 8.$	82.546	333.431	17.666	#
C3H6O2(liq) Methylacetate liq.	74.07854	-445.89						X
C3H6O2 Methylacetate ester.	74.07854	-415.170	-396.272	$\pm 8.$	85.346	321.527	18.347	#
C3H6O2(liq.) Ethylformate ester	74.07854	-394.2		$\pm 0.8$				X
C3H6O2 Ethylformate ester	74.07854	-377.188	-357.631	$\pm 8.$	84.642	329.799	17.688	#
C3H6O3 Lactic Acid	90.07794	-610.278	-587.408	$\pm 8.$	101.214	354.204	18.715	#
C3H6S THIETHANE	74.14574	65.220	84.226	$\pm 8.$	70.419	282.055	13.971	#
N-C3H7 PROPYL RADICAL	43.0883	101.32	119.149	$\pm 1$	71.309	290.460	14.970	†#
I-C3H7 ISOPROPYL RADICAL	43.0883	90.19	108.237	$\pm 2$	65.545	290.109	14.725	†#
1-C3H7I Iodopropane	169.99305	-31.999		$\pm 2$	85.883	332.737		
2-C3H7I 2-Iodopropane	169.99305	-40.865		$\pm 2$	91.193	334.082		
C3H5NH2 CY-PROPYLAMINE	57.09499	77.389			89.045	285.464	16.956	*
C3H7N AZETIDINE	57.09532	98.198			67.14	267.274		
C3H7NO2 Nitropropane	89.09412	-124.265	-97.795	$\pm 0.4$	104.085	350.046	19.344	
C3H7NO3 NPN Propylnitrate	105.09262	-174.054	-146.91	$\pm 1.3$	123.239	362.601	23.008	
C3H7NO3 L-Serine (gas)	105.09262	-579.107	-551.829	$\pm 8.$	118.076	404.228	22.876	#
C3H7NO3 L-Serine (solid)	105.09262	-732.73		$\pm 0.28$		149.16		X
C3H7O N-PROPOXY RAD.	59.08798	-37.656			81.634	309.616		
C3H7S C <sub>3</sub> H <sub>7</sub> S* Thiopropyl Rad.	75.15368	75.513	95.137	$\pm 8.$	87.069	324.010	17.687	#
C3H7S CH <sub>3</sub> CHS*CH <sub>3</sub>	75.15368	70.131	89.714	$\pm 8.$	87.941	313.855	17.688	#
C3H8 PROPANE	44.09562	-104.68	-82.388	$\pm 0.6$	73.589	270.315	14.741	†
C3H7OH PROPANOL	60.09592	-255.2	-231.35		84.978	323.367	17.519	†
(CH3)2CHOH 2-Propanol	60.09592	-272.7	-248.59		89.594	309.226	17.265	†
C3H8O2 CH <sub>3</sub> -O-CH <sub>2</sub> -O-CH <sub>3</sub>	76.0953	-346.967	-321.13	$\pm 8.$	100.842	347.098		#
C3H8O3 (L) Glycerol (liq)	92.09382	-669.6		$\pm 0.6$	218.9	37.87(s)		X
C3H8O3 Glycerol	92.09382	-577.9	-552.153	$\pm 1.1$	131.648	400.000	24.306	
C3H7SH	76.16162	-64.890	-42.311	$\pm 8.$	89.535	343.373	18.866	#
C3H9Bi TriMethylBismutine	254.08394	194.		$\pm 14.$	125.791	360.814	23.738	#
C3H9Sb Sb(CH <sub>3</sub> ) <sub>3</sub>	166.86356	38.5	62.9	$\pm 4.2$	113.001	361.073	23.510	#
C3N2O NC-CO-CN	80.0449	247.5	246.523	$\pm 6.4$	80.854	310.032	17.148	#
C3O2	68.0318	-93.64			67.37	276.816		†
C4 singlet <sup>1</sup> A <sub>g</sub>	48.04280	1055.713	1046.544	$\pm 8$	58.639	245.962	13.383	#
C4 triplet <sup>3</sup> Σ <sub>g</sub> <sup>-</sup>	48.04280	1059.720	1050.435	$\pm 8$	59.078	255.801	13.499	#†
C4Cl2 Cl-CC-CCl	118.94820	453.592	447.208	$\pm 8.$	93.858	319.209	19.779	#
C4CL6 Perchloro-1,3-Butadiene	260.7590	-7.209	-7.411	$\pm 8.$	158.984	460.208	31.959	#
C4F2 FCC-CCF	86.03961	215.309	210.191	$\pm 8.$	88.863	294.682	18.157	#
C4F6 Perfluoro 1,3-Butadiene	162.0343	-1004.122			137.272	388.442	24.949	*
F6C4 Perfluorocyclobutene	162.03439	-1210.843			131.589	379.256	25.135	*
C4F8 Perfluorocyclobutane	200.03123	-1513.6			145.483	405.3		
C4F10 FC-3110 Perfluorobutane	238.02803	-2137.417			189.038	480.624		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C4H	49.05074	780.	775.015	$\pm 50.$	64.851	256.088	13.433	#
C4H2 Butadiyne	50.05988	458.299	456.653	$\pm 8$	73.738	249.613	14.328	#†
C4H2N2 Fumaronitrile	78.07216	330.996	334.8	$\pm 8.$	85.445	308.998	17.549	#
C4H3 E,1-butene-3-yne-1-yl	51.06662	543.104	545.65	$\pm 8$	71.773	281.767	14.371	#
C4H3 i,1-butene-3-yne-2-yl	51.06662	501.829	502.00	$\pm 8.$	77.383	305.368	16.739	#
C4H3 1,2,3-butatriene-4-yl	51.06662	501.829	Resonant	with	former	species		X
C4H4 1-Butene 3-yne	52.07456	287.859	294.717	$\pm 8.$	71.612	277.319	14.292	#
C4H4 Cyclobutadiene	52.07456	431.722	440.911	$\pm 8.$	58.200	251.074	11.961	#†
C4H4N2 PYRAZINE	80.08804	195.811	212.069	$\pm 1.3$	73.945	280.378	13.562	#
C4H4N2 PYRIMIDINE	80.08804	196.648	212.864	$\pm 1.$	73.69	280.677	13.645	#
C4H4N2 SUCCINONITRILE	80.08804	209.7	221.172	$\pm 0.9$	92.458	325.114	18.349	#
C4H4O FURAN	68.07516	-34.685			65.407	267.251		
C4H4O VINYL-KETENE	68.07516	22.719	31.98	$\pm 8.$	81.797	309.171	16.229	#
C4H4O2 1,4-DIOXIN	84.07456	-86.0	-71.5	$\pm 7.$	81.291	284.693		#
C4H4O4 Fumaric acid <i>trans</i>	116.07216	-696.469	-679.388	$\pm 8.$	117.504	376.826	21.430	#
C4H4S Thiophene	84.14056	115.96	128.240	$\pm 8.$	72.818	278.908	13.282	#
E-C4H5 1,3-butadiene 1-yl	53.08250	363.339	373.360	$\pm 8.$	74.144	303.589	15.362	#
I-C4H5 1,3-butadiene-2-yl	53.08250	315.223	325.419	$\pm 8.$	77.138	290.119	15.188	#
T-C4H5 1,2,3-butadiene-4-yl	53.08250	315.223	Resonant with the former species					X
C4H5 1-butyne-3-yl	53.08250	318.432	327.890	$\pm 8.$	81.537	293.840	15.926	#
C4H5 2-butyne-1-yl	53.08250	306.085	314.862	$\pm 8.$	77.774	300.775	16.607	#
C4H5N PYRROLE	67.09044	108.18		$\pm 0.81$	71.6	270.722		
C4H5N Cyclopropanecarbonitrile	67.09044	184.096		$\pm 0.84$	78.734	321.389		
C4H5O *CH <sub>2</sub> CH <sub>2</sub> CH=C=O	69.08190	119.072	129.592	$\pm 8.$	94.588	343.805	19.205	#
C4H5O CH <sub>3</sub> CH*CH=C=O	69.08190	67.500	77.848	$\pm 8.$	90.390	342.574	19.377	#
C4H5O2 *CH=CHC(O)-OCH <sub>3</sub>	85.08130	-56.053	-42.208	$\pm 8.$	100.313	351.572	20.219	#
C4H5O2 CH <sub>2</sub> =C*C(O)-OCH <sub>3</sub>	85.08130	-57.300	-44.908	$\pm 8.$	105.344	372.811	21.672	#
C4H6 1-Butayn Ethyl-acetylen	67.09044	165.2	178.798	$\pm 0.88$	81.820	291210	16.020	†
C4H6 2-ButaynDimethylacetylen	54.09044	146.314	159.388	$\pm 8.$	77.886	291.909	16.544	†#
1,3-C4H6 Butadiene	54.09044	110.834	125.118	$\pm 8.$	74.219	293.330	15.335	†#
1,2-C4H6 Butadiene	54.09044	161.314	175.436	$\pm 2.$	78.663	290.993	15.496	#
C4H6 Cyclobutene	54.09164	156.7	173.761		64.414	262.076	12.558	†
C4H6CL2 1,4-Dichlorobutene	124.99584	-51.882	-34.587	$\pm 8.$	108.341	386.083	21.505	#
CL2C4H6 3,4-Dichlorobutene	124.99584	-53.572	-36.121	$\pm 8.$	109.803	379.398	21.349	#
C4H6O CH <sub>3</sub> CH <sub>2</sub> CH=C=O	70.08984	-88.303	-72.169	$\pm 8.$	91.448	343.487	17.824	#
C4H6O 2,5 Di-Hydro FURAN	70.08984	-108.78	-89.313		75.600	284.250	14.401	
C4H6O2 CH <sub>2</sub> =CHC(O)-OCH <sub>3</sub>	86.08924	-309.386	-291.690	$\pm 8.$	101.460	360.043	20.603	#
C4H6O2 liq Diacetyl liquid	86.08924	-364.908		$\pm 0.637$				X
C4H6O2 CH <sub>3</sub> -C(O)-C(O)-CH <sub>3</sub>	86.08924	-325.482	-308.273	$\pm 0.987$	102.375	351.425	21.089	#
C4H6O4 liq. Succinic acid	118.08804	-940.237		$\pm 0.132$				X
C4H6O4 HOOC-CH <sub>2</sub> CH <sub>2</sub> -COOH	118.08804	-817.729	-794.955	$\pm 0.59$	124.337	424.442	24.204	#
C4H6O4 CH <sub>3</sub> -CO-OO-CO-CH <sub>3</sub>	118.08804	-500.	-477.02	$\pm 10$	122.291	390.682	23.944	#
2,5 C4H6S Dihydrothiophene	86.15644	85.872	104.666	$\pm 8.$	80.794	295.466	15.237	#
C4H7 tt-1-Butene-1-yl	55.09838	245.871	262.755	$\pm 8.$	83.705	311.281	16.968	#
C4H7 cc-1-Butene-1-yl	55.09838		264.85	$\pm 8.$	-	-		X
C4H7 trans 1-Butene-2-yl	55.09838	231.162	248.45	$\pm 8.$	83.973	300.371	16.425	#
C4H7 cis 1-Butene-2-yl	55.09838		248.11	$\pm 8.$	-	-		X
C4H7 trans-2-Butene-2-yl	55.09838	223.853	239.743	$\pm 8.$	83.237	313.256	17.962	#
C4H7 cis-2-Butene-2-yl	55.09838		243.09	$\pm 8.$	-	-		X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C4H7 <i>trans</i> 3-Butene 1-yl Rad.	55.09838	204.595	220.915	$\pm 8.$	84.719	317.348*	17.533	#
C4H7 <i>cis</i> 3-Butene-1-yl Radical	55.09838		223.01	$\pm 8.$	-	-		X
C4H7 <i>trans</i> (CH <sub>2</sub> =CH*CHCH <sub>3</sub> )	55.09838	136.111	153.553	$\pm 8.$	80.787	306.087*	16.411	#
C4H7 <i>cis</i> -1-Methylallyl Radical	55.09838		156.48	$\pm 8.$	-	-		X
C4H7 2-Methyl-Allyl Radical	55.09838	137.603	155.226	$\pm 5.$	82.196	300.803	16.229	#
C4H7 Cyclobutyl Radical	55.09838	230.306	249.366	$\pm 8.$	73.070	286.490	14.792	#
C4H7N C3H7CN Propylcyanide	69.10512	31.200	51.765	$\pm 8.$	91.422	310.996	17.622	#
C4H7O *CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH=O	71.09778	2.494	21.652	$\pm 8.$	96.363	368.530	19.034	#
C4H7O CH <sub>3</sub> *CHCH <sub>2</sub> CH=O	71.09778	-12.510	5.510	$\pm 8.$	101.188	356.878	20.172	#
C4H7O CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> *C=O	71.09778	-51.313	-32.787	$\pm 8.$	97.923	352.974	19.666	#
C4H7O 2-Butanone Radical	71.09778	-75.994	-57.670	$\pm 8.$	97.420	344.655	19.868	#
C4H7O CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> O*	71.09778	55.748	75.378	$\pm 8.$	96.143	334.259	18.562	#
C4H7O2 CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(O)O*	87.09718	-234.007	-212.646	$\pm 8.$	103.763	378.873	21.172	#
C4H7O2 *CH <sub>2</sub> CH <sub>2</sub> C(O)OCH <sub>3</sub>	87.09718	-229.166	-208.651	$\pm 8.$	111.373	376.723	22.018	#
C4H7O2 CH <sub>3</sub> C(O)OCH <sub>2</sub> CH <sub>2</sub> *	87.09718	-236.773	-216.138	$\pm 8.$	108.389	381.911	21.898	#
C4H8 CH <sub>2</sub> =CH-CH <sub>2</sub> -CH <sub>3</sub>	56.10632	-0.031	20.819	$\pm 0.47$	85.601	305.372	17.236	#†
H8C4 CH <sub>2</sub> =C(CH <sub>3</sub> ) <sub>2</sub> isobutene	56.10632	-17.574	4.293	$\pm 0.52$	86.018	287.454	16.220	#†
C4H8 2-Butene <i>trans</i>	56.10632	-11.185	9.391	$\pm 0.5$	87.670	296.330	17.510	†
C4H8 2-Butene <i>cis</i>	56.10632	-7.340	13.946	$\pm 0.52$	80.150	301.310	16.800	†
C4H8 CYCLOBUTANE	56.10632	28.4	52.952		70.565	264.509	13.534	†
C4H8CL2S Mustard	159.07772	-124.77	-100.66		136.283	420.586	27.569	#
Beta HMX solid	296.15664	74.894	--		307.302	320.0	--	
C4H8N8O8 HMX	296.15664	187.862	245.304	$\pm 25.1$	275.455	568.833	50.045	
C4H8O 2-Methyl-Allyl Alcohol	72.10572	-161.143	-137.34	$\pm 2$	100.007	316.183	18.622	#
C4H8O n-Butanal	72.10572	-206.137	-182.183	$\pm 8.$	95.543	327.343	18.473	#
C4H8O 2-BUTANONE	72.10572	-238.362			102.432	339.991		
H8C4O 2,3-Dimethyloxirane	72.10572	-137.658	-113.00	$\pm 8.$	95.471	303.780	17.777	#
OC4H8 ETHYL-OXYRANE	72.10572	-115.960	-91.115	$\pm 8.$	91.134	316.499	17.582	#
C4H8O Tetrahydrofuran, Oxolan	72.10572	-184.18	-156.421		76.25	302.41	14.667	
C4H8O2 (liq) Butyric acid	88.10512	-533.92		$\pm 0.59$				
C4H8O2 Butyric acid	88.10512	-455.780	-429.750	$\pm 8.$	102.582	367.660	20.736	#
C4H8O2 Methyl Propionate	88.10512	-437.291	-412.905	$\pm 8.$	107.873	375.707	22.381	#
C4H8O2 Ethyl Acetate	88.10512	-448.550	-424.136	$\pm 8.$	107.786	377.409	22.352	
C4H8O2 1,4 DIOXANE	88.10632	-314.428		$\pm 7.$	92.568	294.582		
(CH <sub>3</sub> COOH) <sub>2</sub> Acetic Acid dimer	120.1048	-929.015	-901.62		137.254	414.396	28.053	†
C4H8O4 Tetraoxocan	120.10512	-620.2			116.255	340.343		
C4H8S Tetrahydrothiophen	88.17232	-30.702	-4.196	$\pm 8.$	87.38	300.156	15.993	#
1,4-C4H8S2 Dithiane	120.23832	20.635	48.493	$\pm 8.$	109.655	326.500	19.053	#
1,3-C4H8S2 Dithiane	120.23832	4.945	32.593	$\pm 8.$	110.433	333.844	19.263	#
C4H9,n-Butyl Radical	57.11426	81.80	105.91	$\pm 8.$	94.555	307.628		#†
<i>i</i> -C4H9 iso-Butyl Radical	57.11426	73.785	97.92	$\pm 8.$	98.111	304.662	18.063	#
<i>s</i> -C4H9 sec-Butyl Radical	57.11426	70.224	94.945	$\pm 8.$	86.395	327.417	17.538	#
C4H9,t-Butyl Radical	57.11426	55.041	79.719	$\pm 8.$	82.410	323.393	17.010	#
C4H9N PYROLIDINE	71.12100	-3.59	26.889	$\pm 0.8$	82.112	309.206	16.177	#
C4H9NO2 Nitrobutane	103.121	-143.93	-109.63		115.119	369.874	21.040	
C4H9O n-BUTOXY RAD	73.11366	-56.350	-29.003	$\pm 8.$	101.794	349.126	19.314	#
C4H9O <i>i</i> -BUTOXY RAD	73.11366	-65.070	-36.703	$\pm 8.$	101.777	319.038	18.294	#
C4H9O <i>s</i> -BUTOXY RAD	73.11366	-69.84	-41.88	$\pm 8.$	102.025	327.058	18.700	#
C4H9O <i>t</i> -BUTOXY RAD	73.11366	-86.923	-58.899	$\pm 8.$	106.062	309.188	18.637	#



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C4H9O C <sub>2</sub> H <sub>5</sub> -O-CH <sub>2</sub> CH <sub>2</sub> *	73.11366	-44.095	-18.932	±8.	109.732	366.749	21.498	#
C4H9O C <sub>2</sub> H <sub>5</sub> -O-CH*CH <sub>3</sub>	73.11366	-74.697	-49.959	±8.	109.080	370.674	21.922	#
C4H9O2 Peroxy n-Butane RAD	89.11306	-63.530	-34.746	±8.	111.895	381.549	22.217	#
C4H9O2 Peroxy s-Butane RAD	89.11306	-84.557	-55.898	±8.	116.539	380.506	22.482	#
C4H9O2 Peroxy T-Butane RAD	89.11306	-106.412	-78.159	±8.	122.218	367.903	22.748	#
C4H10 n-Butane	58.123	-125.790	-98.46	±0.67	98.651	309.884	19.227	†
I-C4H10 ISOBUTANE	58.123	-134.990	-106.37	±0.63	96.643	295.493	17.936	†
C4H10FO2P SARIN	140.09437	-963.157	-927.62	±40	161.667	412.013	29.468	#
C4H10N2 1,4-Piperazine	86.13568	32.058	70.65	±8.	96.860	301.189	16.633	#
C4H10O-N 1-BUTANOL	74.1228	-274.68			108.168	361.616		
C4H10O-S 2-BUTANOL	74.1228	-292.629			111.134	363.877		
C4H10O-T 2-Methylpropanol	74.1228	-312.628			113.481	329.72		
C4H10O DiEthylEther	74.1216	-254.948	-224.468	±8.	105.009	345.73	20.415	#
C4H10O2 nButyl Hydroperoxide	90.1210	-202.602	-171.262	±8.	122.721	373.151	23.895	#
C4H12Sn Sn(CH <sub>3</sub> ) <sub>4</sub>	178.84808	-20.502	+11.004	±4.2	145.919	410.093	29.840	#
C4H12Sn H <sub>2</sub> Sn(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	178.84808	56.484	90.910	±4.2	143.567	410.046	26.920	#
C4N2 Carbon Subnitrid	76.0574	529.2	524.285	±0.8	86.326	290.524	17.799	†
C5 <sup>1</sup> Σ <sub>g</sub> <sup>+</sup> singlet	60.05350	1072.112	1061.180	±8.	75.507	271.677	16.192	†#
C5Cl6 PerChloroCycloPentadiene	272.76970	-11.7	-11.066	±4.4	165.769	449.904	32.177	#
C5F6 PerFluoroCycloPentadiene	174.04392	-932.986	-928.15	±8.	144.089	393.515	26.906	#
C5F12 FC 4-1-12	288.03584	-2543.311			229.036	555.108		
C5H	61.06144	860.	853.43	±75.	80.114	281.338	16.071	#
C5H2	62.0709	691.412			82.981	266.639	14.674	*
C5H2CL2O CY	148.97418	-12.17	-5.59		111.295	349.650		#
C5H2CL3 CY	168.42748	152.68	158.05		118.207	369.726		#
C5H2Cl3 ClHC=C=CCl-CCl=CH*	168.42748	460.064	462.152	±8.	131.611	413.831	25.420	#
C5H3 1,3-Pentadiyne-5-yl Rad.	63.07882	602.58			87.499	295.196		
C5H3 HC≡C-CH*CH≡CH	63.07882	564.61		±43	93.241	306.147		
C5H3 Cyclopentatriene-yl	63.07882	697.77		±75	70.898	281.721		
C5H3Cl3 1,2,4-triCl-2,4-CYdiene	169.43542	61.513	71.033	±8.	118.468	372.260	22.221	#
C5H3Cl3O CY	185.43482	-104.72	-93.65	±8.	139.671	397.902		#
C5H3N HC≡C-CH=CH-CN	77.08406	422.613	426.538	±8.	93.766	318.598	18.380	#
C5H4 1,3-Pentadiyne	64.08526	411.835	416.818	±8.	86.669	291.342	17.221	#
C5H4 1,4-Pentadiyne	64.08526	451.964	434.773	±8.	89.940	305.243	17.191	#
C5H4 Pentane-Tetraene	64.08526	444.466	449.702	±8.	86.132	287.480	16.968	#
H4C5 1,2-Pentadiene-4-yne	64.08526	433.354	438.929	±8.	86.751	301.509	16.628	#
C5H4 1,2,4-Cyclo-Pentatriene.	64.08526	551.485		±9.	73.235	279.6		
C5H4N *CH=CH-CH=CH-CN	78.09200	502.942	510.320	±8.	97.601	341.652	19.160	#
C5H4N meta-Pyridyl Radical	78.09200	405.241	418.146	±8.	74.123	292.227	13.634	#
C5H4O Cyclopentadiene-1-one	80.08616	55.229			80.941	289.977		
C5H4O2 3 ketene	96.08556	-105.834	-95.030	±8	101.982	361.789	20.080	#
C5H5 1-Pentyne-3-ene-5-yl	65.09320	384.93	394.23	±8.	92.828	310.776	17.130	#
C5H5 CY Cyclopentadienyl Rad.	65.09320	266.102			76.605	279.485		
C5H5N CH <sub>2</sub> =CH-CH=CH-CN	79.09994	238.944	250.471	±8.	99.632	336.825	19.246	#
C5H5N PYRIDINE	79.10144	140.37		±0.54	77.746	282.759		
C5H4OH CYCLO RAD	81.0941	66.526			95.625	310.007		
1,3C5H5O CY RADICAL	81.0941	59.8			90.023	307.695		
1,4C5H5O CY RADICAL	81.0941	103.3			90.479	307.805		
2,4-c-C5H5O CY RADICAL	81.0941	221.758			83.1	302.922		*

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C5H5O2 2-pentenedialdehyde R	97.0935	-83.638			110.293	391.33		
C5H5O2 2-pentenedialdehyde R	97.0935	-72.76			113.89	387.94		
C5H6 1,2,4-Pentatriene	66.10264	252.295	264.571		93.878	318.687		
C5H6 1-ene-2-yne	66.10264	249.366			89.238	320.076		
C5H6 3-enE-1-yne	66.10264	256.479			94.424	314.637		
C5H6 CYCLOPENTADIENE	66.10264	134.3	151.43	$\pm 1.5$	75.368	274.152	13.535	†
C5H6N2 2-AMINOPYRIDINE	94.11612	118.616		$\pm 0.84$	103.84	309.401		
2,4-C5H5OH	82.10204	7.9			91.437	304.61		
1,3-C5H5OH	82.10204	-24.3			94.957	304.343		
1,4 C5H5OH	82.10204	-27.2			95.023	304.565		
C5H7 1,3-Pentadien-5-yl	67.10908	205.455	222.877	$\pm 8.$	92.672	325.606	17.484	#
C5H7 1,4-Pentadien-3-yl	67.10908	205.455	223.086	$\pm 8.$	93.92	323.195	17.275	#
C5H7 Cy 1-penten-1-yl	67.10908	172.623	192.745	$\pm 8.$	79.939	296.325	14.785	#
C5H7 Cy 1-penten-4-yl	67.10908	223.94	243.815	$\pm 8.$	80.499	290.579	15.031	#
C5H7CL	102.56178	58.091	76.235	$\pm 8$	110.072	374.067	21.352	#
C5H7CL2	138.01448	110.926	128.756	$\pm 8$	132.403	444.862	26.257	#
C5H7NO	97.11672	-108.7			120.7	387.6		
C5H7O 1-Cypenten-4-oxy Rad.	83.10848	95.04	117.53	$\pm 8.$	92.705	317.69		#
C5H8 1,3-Pentadiene	68.11702	84.157	105.770	$\pm 8.$	94.718	318.284	17.527	#
C5H8 ISOPRENE	68.11852	75.73			104.6	315.641		
C5H8 Cyclopentene	68.11852	33.9	58.183		81.275	291.379	14.857	†
C5H8CL CH2CICH=CHCH2CH2	103.56972	158.197	179.288	$\pm 8.$	119.551	399.520	22.640	#
PETN Solid	316.13828	-538.481		$\pm 0.84$	353.757	?		
C5H8N4O12 PETN	316.13828	-387.02	-332.00		294.758	614.706	53.542	
C5H8O Cyclopentanone	84.11642	-197.401	-171.29	$\pm 5.4$	97.436	309.296	17.366	#
C5H8O 1,5-Cyclopenten-2-ol	84.11642	-126.579	-99.582	$\pm 8.$	96.604	315.064	16.583	#
C5H9 CY	69.12496	111.131	138.404	$\pm 8.$	88.092	298.784	16.101	#
C5H9 2-PENTEN-5-YL	69.12496	174.615	196.937	$\pm 8.$	110.968	357.785	21.052	#
H9C5 2-PENTEN-1-YL	69.12496	116.700	140.617	$\pm 8.$	106.281	347.013	19.457	#
C5H9 3M-1-BUTEN3YL	69.12496	102.479	126.521	$\pm 8.$	106.535	329.883	19.332	#
C5H9 3M-1-BUTEN1YL	69.12496	219.091	243.190	$\pm 8.$	105.817	335.407	19.275	#
C5H9 3M-1-BUTEN4YL	69.12496	180.356	204.114	$\pm 8.$	108.450	348.534	19.616	#
C5H9N	83.1332	75.312		$\pm 8.4$	99.27	274.978		
C5H9O2 C4H9C(O)O* Valeryl	101.12376	-255.550	-226.845	$\pm 8.$	125.431	377.951	23.349	#
C5H9O2 C3H7C(O)OCH2* C0	101.12376	-258.818	-232.358	$\pm 8.$	131.482	414.869	25.594	#
C5H9O2 C2H5CH*C(O)OCH3 C2	101.12376	-281.328	-255.386	$\pm 8.$	129.041	424.815	26.112	#
C5H9O2 CH3CH*CH2C(O)OCH3	101.12376	-260.388	-235.465	$\pm 8.$	132.918	426.760	26.931	#
C5H9O2 CH2*C2H4C(O)OCH3	101.12376	-251.668	-225.677	$\pm 8.$	131.262	419.488	26.064	#
C5H10 1-PENTENE	70.13290	-21.28	+4.648		108.200	347.110	21.680	†
C5H10 2-PENTENE	70.1344	-31.757			108.449	340.41		
C5H10 2MB-1ene	70.1344	-36.317			109.956	339.532		
C5H10 2MB-2ene	70.1344	-42.551			105.018	338.569		
C5H10 2MB-3ene	70.1344	-28.953			118.616	333.465		
C5H10 Cyclopentane	70.1344	-77.1	-44.515		82.760	293.007	15.023	†
C5H10O TetraHydroPYRAN	86.1338	-224.283	-189.04	$\pm 0.84$	96.359	301.959	16.710	#
C5H10O2 Pentanoic (Valeric) acid	102.13170	-477.018	-444.615	$\pm 8.$	122.513	393.642	23.886	#
C5H10O2(liq) MethylButyrate	102.13170	-497.1						X
C5H10O2 MethylButyrate	102.13170	-457.884	-426.201	$\pm 8.$	125.394	373.612	24.605	#
C5H10O2(liq) Ethyl Propionate	102.13170	-505.59		$\pm 0.5$				X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C5H10O2 Ethyl Propionate	102.13170	-470.696	-439.503	$\pm 8.$	124.994	402.675	25.096	#
N-C5H11 n-pentyl	71.14234	45.81	73.23		119.150	368.649	24.422	†
S-C5H11 1-methyl-butyl	71.14234	45.564			119.653	369.949		
T-C5H11	71.14084	32.6	64.8	$\pm 8.$	98.855	366.474	19.644	†
C5H11 neopentyl	71.14234	34.392			118.84	333.423		†
C5H11NO2 Nitropentane	117.14788	-164.431	-123.37	$\pm 2.1$	137.100	390.905	23.792	
C5H12 PENTANE	72.14878	-146.76	-114.87		120.040	349.560	24.184	†
I-C5H12 Isopentane	72.14878	-153.70	-119.63		118.870	343.740	22.008	†
CH3C(CH3)2CH3 Neopentane	72.14878	-167.92	-135.02		120.830	306.000	23.179	†
C5H12O liquid MTBE	88.14968	-313.6	-293.85		187.510	265.650		
C5H12O Me-Tertiary Butyl Ether	88.14968	-283.7	-247.14	$\pm 0.8$	138.010	355.489		#
C5O5Fe Fe(CO) <sub>5</sub>	See Fe(CO) <sub>5</sub>							
C6 linear singlet 1A <sub>1</sub>	72.0642	1227.3	1216.08	$\pm 8.$	83.768	288.457	17.550	#
C6 linear triplet <sup>3</sup> $\Sigma_g^-$	72.0642	1283.971	1272.522	$\pm 8.$	84.585	300.600	17.770	#
C6CL6 Hexachlorobenzene	284.78040	-42.526	-41.486	$\pm 8.$	174.696	438.879	32.824	#
C6D5 Deuterated phenyl radical	82.13651	315.700	327.525		94.997	300.504	15.919	†
C6D6 Deuterated Benzene	84.14881	58.157	73.86		100.398	282.629	16.325	†
C6F6 Hexafluorobenzene	186.05642	-956.63			157.938	384.457		
C6F14 FC 51-14Perfluorohexane	338.04364	-2949.201			269.551	629.592		
C6H	73.07394	1000.	991.8	$\pm 75.$	95.617	305.418	18.757	#
C6HCL5 Pentachlorobenzen	250.33564	-31.589	-27.707	$\pm 8.$	159.291	427.213	29.625	#
C6H2	74.08188	700.82			104.103	299.19		†
C6H2CL4 1,2,3,4-Chlorobenzen	215.89088	-13.071	-6.239	$\pm 8.$	143.507	398.859	26.320	#
C6H2CL4 1,2,3,5-Chlorobenzen	215.89088	-18.464	-11.75	$\pm 8.$	143.922	400.437	26.439	#
C6H2CL3O Trichlorophenoxy ra	196.43758	-27.48	-20.29		140.508	398.583		#
C6H2CL3O Trichlorophenol Rad	196.43758	101.51	107.37		144.581	410.077		#
C6H2CL3O3 Peroxybicyclo Rad.	228.43638	131.42	142.99		174.462	429.942		#
C6H2CL3O3 Peroxybicyclo Rad	228.43638	28.95	40.414		171.330	433.035		#
C6H3	75.08802	682.016			100.896	319.344		
C6H3 Cy o-Benzyne-o-yl Rad.	75.08802	728.911	733.879	$\pm 8.$	75.851	293.013	14.055	#
C6H3Cl3 1,2,3-trichlorobenzen	181.44612	6.711	14.425	$\pm 8.$	127.690	370.460	23.081	#
C6H3Cl3 1,3,5-trichlorobenzen	181.44612	-4.314	5.25	$\pm 8.$	128.171	364.132	23.231	#
C6H3CL3O Trichlorophenol	197.44552	-189.07	-176.92		142.427	397.903		#
C6H3CL3O linear	197.44552	-19.83	+17.3		39.200	109.923		
C6H3CL3O2 CY	213.44492	-277.25	-263.99		162.216	420.242		#
C6H3I o-Iodo-Benzyne	201.99249	534.715	542.244	$\pm 12.$	96.910	340.309	18.093	#
C6H3(NO2)3 Trinitrobenzene	213.10464	62.342	82.617		205.633	485.335	37.794	
1,2-C6H4 o-BENZYNE	76.09596	461.135	470.128	$\pm 8.$	78.406	283.240	14.265	#
1,3-C6H4 m-BENZYNE	76.09596	523.690	532.497	$\pm 8.$	80.202	283.810	14.451	#
1,4-C6H4 p-BENZYNE	76.09596	574.254	582.364	$\pm 8.$	85.476	282.239	15.147	#
C6H4 TRANS	76.09596	523.105	527.104	$\pm 8.$	102.894	317.187	19.328	#
C6H4 CIS	76.09596	524.218	528.632	$\pm 8.$	101.969	317.563	18.843	#
C6H4 HEXAPENTAENE	76.09596	568.263	572.160	$\pm 8.$	99.977	309.859	19.359	#
C6H4 TRIENE-5YNE	76.09596	559.706	563.792	$\pm 8.$	101.909	325.109	19.172	#
C6H4CL -ortho Radical	111.55046	303.173		$\pm 28.9$	100.842	329.678		#
C6H4CL -metha Radical	111.55046	297.02		$\pm 28.0$	101.165	329.135		#
C6H4CL -para Radical	111.55046	298.86		$\pm 28.0$	101.264	329.476		#
C6H4CLO o-Chlorophenoxy Rad	127.54806	32.895	45.773	$\pm 8.$	109.172	338.965	19.310	#
C6H4CLO CyHexadiene Rad	127.54806	225.91	237.50		112.226	359.349		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C6H4CL2 o-Dichlorobenzen	147.00136	28.464	40.970	$\pm 8.$	111.879	347.871	19.933	#
C6H4CL2 m-Dichlorobenzen	147.00136	22.656	35.089	$\pm 8.$	112.361	343.476	20.005	
C6H4CL2 p-Dichlorobenzen	147.00136	23.104	35.493	$\pm 8.$	112.303	337.735	20.049	#
C6H4CL2O Z 2,4- Dichlorophenol	163.00076	-158.009	-143.023	$\pm 8.$	128.644	364.031	21.793	#
C6H4CL2O E 2,4- Dichlorophenol	163.00076	-145.398	-131.202	$\pm 8.$	130.914	368.913	22.582	#
C6H4N4O2 4-Nitro-Phenyl-Azide	164.12172	389.7	410.723	$\pm 5.2$	157.694	420.170	28.254	#
o-C6H4I Radical	203.00043	427.186	439.032		97.752	346.415	18.010	#
o-C6H4I2	329.90490	248.95	263.625	$\pm 5.9$	113.052	386.892	21.778	#
m-C6H4I2	329.90490	243.509	257.766		118.125	384.828	22.196	#
p-C6H4I2	329.90490	242.700	257.177		114.640	365.746	21.976	#
C6H4O2 O=C6H4=O	108.09656	-122.9			108.485	333.212		
C6H5 CHAIN	77.1057	531.368			109.472	339.195		
C6H5 PHENYL RAD	77.10390	339.740	353.657	$\pm 2.5$	76.656	286.072		#
C6H5 FULVENYL RAD	77.10390	467.315	479.324	$\pm 8.$	87.147	297.813	15.482	#
C6H5 FULVENYL Rad. Melius	77.1057	490.365		$\pm 52.$	93.077	307.123		
C6H5Br Bromobenzen	157.0079	101.253	123.571	$\pm 8.$	97.507	324.774	17.433	#
C6H5BrO 2-Bromophenol (Z) cis	173.00730	-63.72	-39.09	$\pm 8.$	113.188	350.929	19.051	#
C6H5BrO 2-Bromophenol-Etrans	173.00730	-70.208	-46.085	$\pm 8.$	115.810	356.656	19.968	#
C6H5CL Chlorobenzen	112.55660	52.287	67.461	$\pm 8.$	96.152	313.366	16.908	#
C6H5CLO o-Chlorophenol (Z)	128.55600	-130.942	-113.250	$\pm 8.$	112.581	341.454	18.729	#
C6H5CLO o-Chlorophenol (E)	128.55600	-117.834	-100.912	$\pm 8.$	114.787	346.205	19.500	#
C6H5CLO 2,4-Cy-hexadiene...	128.55600	-35.75	-19.81		113.199	352.445		#
C6H5CLO 2,5 Cy-hexadiene...	128.55600	-55.87	-39.79		113.969	346.868		#
C6H5F Fluorobenzen	96.10230	-113.914	-97.973	$\pm 8.$	92.385	301.688	15.963	#
C6H5I Iodobenzen	204.00837	165.	181.038	$\pm 6.$	99.918	334.751	18.051	#
C6H5NO NITROSOBENZENE	107.11004	198.075	215.586	$\pm 8.$	106.354	332.852	18.655	#
C6H5NO2 NITRO-BENZENE	123.11124	68.534	88.137		120.38	348.800	20.903	
C6H5O PHENOXY RAD	93.10330	54.		$\pm 10.$	97.682	311.871		
C6H5O Cy-hexadiene-1one-2yl	93.10330	246.58	260.42		98.386	332.759		#
C6H5OO PEROXYPHENYL rad	109.10270	141.612	158.975	$\pm 8.$	108.706	339.197	18.808	#
C6H6(L)	78.11184	49.08	50.695		135.95	173.44	30.110	†
C6H6 BENZENE	78.11184	82.88	100.41		81.934	269.158	14.195	†
C6H6 FULVENE	78.11364	236.814		$\pm 10$	90.362	294.123		
C6H6 BENZVALENE	78.11364	384.9	403 ?	$\pm 8.3$	80.825	284.701		#
C6H6 1,5-Hexadiyne	78.11364	417.166	428.062	$\pm 8.$	111.036	336.936	20.829	#
C6H6 2,4-Hexadiyne	78.11364	369.100	379.830	$\pm 8.$	103.026	335.627	20.995	#
C6H6 1,3-Hexadiyne	78.11364	392.363	404.299	$\pm 8.$	107.021	328.174	19.790	#
C6H6 1,2,4,5 Hexatetraene	78.11364	396.229	407.942	$\pm 8.$	102.421	343.852	20.012	#
C6H6 1,2-Hexadiene-5-yne	78.11364	412.542			107.68	336.912		
C6H5OH PHENOL	94.11124	-83.847	-58.807	$\pm 8.$	103.338	315.238	17.497	†
C6H6O 2,4-Cyclohexadiene1one	94.11124	-21.63	-3.31		99.188	322.935		#
C6H5OOH Hydroperoxyphenyl	110.11064	-2.678	18.039	$\pm 8.$	114.440	350.539	19.688	#
C6H7 1,4 CYCLO Radical	79.11798	200.589		$\pm 35$	97.618	305.835		
C6H7 1,3,5-Hexatriene-6-yl	79.11798	431.387	446.410	$\pm 8.$	110.758	363.629	20.937	#
C6H7-1 CY C5H5-1-CH2*	79.11798	334.092	351.954	$\pm 6.3$	100.095	326.062	18.098	#
C6H7-3 CY C5H5-3-CH2*	79.11798	247.316	265.583	$\pm 19.2$	101.756	321.686	17.693	#
C6H7-1 CY C5H4-1-*.CH3	79.11798	226.773	244.638	$\pm 12.5$	103.103	314.389	18.094	#
C6H5NH2(L) aniline	93.12832	31.50	37.774		191.92	191.060	34.020	†
C6H7N ANILINE	93.12832	87.04	--		108.385	319.27	--	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C6H8 DIHYDROBENZVALENE	80.12772	230.12	255.3	$\pm 8.3$	89.425	293.780		#
C6H8 CY 1,3-C5H5-5-CH3	80.12772	112.257	135.267	$\pm 8.$	95.574	310.854	17.183	#
C6H8 CY 1,3-C5H5-3-CH3	80.12772	99.303	121.918	$\pm 8.$	97.546	312.884	17.579	#
C6H8 1,3,5-HEXATRIENE	80.12772	152.214			107.911	330.388		
H8C6 (1,3-CYCLO)	80.12772	106.3			94.168	303.419		
C6H8 (1,4-CYCLO)	80.12772	109			94.053	296.34		
C6H9 1,3 hexadiene 5-yl Rad.	81.13566	173.49	195.692	$\pm 8.$	119.775	370.613	22.225	#
1,3-C6H9 hexadiene 6-yl Rad.	81.13566	265.533	286.651	$\pm 8.$	120.582	389.084	22.990	#
C6H9 Cyclohexenyl-3	81.13566	131.47	159.011	$\pm 8.$	97.860	313.685	16.886	#
C6H9 CY 1- C5H6-4-CH3-4-yl	81.13566	188.468	214.322	$\pm 8.$	103.489	321.009	18.574	#
C6H9 CY 1- C5H7-4-CH2*	81.13566	215.731	241.534	$\pm 8.$	106.551	323.588	18.625	#
C6H9 CY 1-C5H7-3-CH2*	81.13566	212.464	237.965	$\pm 8.$	104.037	333.573	18.926	#
C6H9 CY 1-C5H7-1-CH2*	81.13566	124.89			94.663	323.377		
C6H9I CY 1-C6H9-3-I	208.04013	69.0	99.331	$\pm 21.$	116.001	360.644	20.731	#
C6H10 1,3-HEXADIENE	82.14360	58.513	84.568	$\pm 8.$	120.575	372.675	22.606	#
C6H10 Cyclohexene	82.14360	-4.6	+26.79		101.464	310.632	17.271	†
C6H10 C5H7-CH3 Cypentene-4	82.14360	8.46	38.49	$\pm 8.$	101.249	309.518	17.208	#
C6H11 CH2=CHC3H6CH2*	86.15334	162.502	190.886	$\pm 8.$	127.963	417.768	24.512	#
C6H11 CH3CH=CHC2H4CH2*	86.15334	153.862	181.880	$\pm 8.$	129.760	404.206	24.878	#
C6H11 trans 3-hexene-6-yl Rad	83.15334	154.540	183.164	$\pm 8$	128.546	401.219	24.272	#
C6H11 CH2=C(CH2*)C3H7	83.15334	95.340	125.298	$\pm 8$	125.511	391.885	22.942	#
C6H11 CH2=C(CH3)C3H6*	83.15334	149.787			130.797	390.786		
C6H11 CH3C(CH2*)=CHC2H5	83.15154	90.847	121.134	$\pm 8.$	122.131	383.848	22.609	#
C6H11 CH3C(CH3)=CHC2H4*	83.15334	141.838			124.52	387.438		
C6H11 (CH3)2C=CHCH*CH3	83.15154	72.91	101.569	$\pm 8.$	128.105	375.530	24.237	#
C6H11 (CH3)CHCH*CH=CH2	83.15154	91.232	119.916	$\pm 8.$	135.913	384.042	24.212	#
C6H11 2-Methyl-1-pentene-4-yl	83.15154	136.913	165.834	$\pm 8.$	127.708	386.671	23.975	#
C6H11 Cyclohexyl Radical	83.15154	75.839	110.421	$\pm 8.$	106.108	317.527	18.513	#
C6H11I Iodo-CycloHexane	210.05601	-50.0	-11.926	$\pm 4.7$	121.960	363.668	21.420	#
C6H11O2 Caproyl Radical	115.15034	-278.4	-243.938	$\pm 12.5$	145.374	434.509	27.114	#
C6H12 TRANS-3-HEXENE	84.16128	-50.417	-17.218	$\pm 8.$	128.815	365.867	23.931	#
C6H12 1-HEXENE	84.16128	-41.95	-11.06		130.800	386.850	26.240	†
C6H12 2MP-1ene	84.16128	-59.371			135.603	382.167		
C6H12 2MP-2ene	84.16128	-66.86			126.608	378.443		
C6H12 4MP-2ene CIS	84.16128	-57.446			133.553	373.338		
C6H12 4MP-2ene TRANS	84.16128	-61.463			141.419	368.276		
C6H12 CYCLOHEXANE	84.15948	-123.3	-83.715		105.343	297.389	17.545	†
C6H12O2 liq. Caproic acid (liq.)	116.15828	-581.8		$\pm 1.1$	225.1??			X
C6H12O2 C5H11COOH Caproic	116.15828	-498.206	-459.568	$\pm 8.$	142.527	421.649	27.172	#
C6H12O2 liq. Methyl Valerate	116.15828	-514.2		$\pm 7.1$				X
C6H12O2 C4H9COOCH3 Valerate	116.15828	-448.847	-411.914	$\pm 8.$	148.507	441.134	28.876	#
C6H12O2 liq. Ethyl Butyrate (liq)	116.15828	-528.4		$\pm 0.79$				X
C6H12O2 C3H7COOC2H5 Butyrate	116.15828	-462.863	-425.524	$\pm 8.$	144.783	443.565	28.471	#
N-C6H13 n - HEXYL RAD.	85.16742	25.10	57.480		141.790	408.339	28.983	†
2-C6H13 2-HEXYL RAD.	85.16922	28.158	61.309	$\pm 8.$	147.533	428.452	28.213	#
C6H13 2MP-1YL	85.16922	35.635	70.799	$\pm 8$	140.892	399.411	26.200	#
C6H13 2MP-5YL	85.16922	32.367	67.427	$\pm 8.$	139.391	414.154	26.304	#
C6H13-S 2ME - 4PENTYL	85.16922	20.079	55.023	$\pm 8.$	141.737	402.960	26.420	#
C6H13-T 2ME 2PENTYL	85.16922	17.209	52.180	$\pm 8.$	139.289	404.566	26.392	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C6H14(L) n-Hexan	86.17716	-198.660	-179.98		195.480	296.090	46.920	†
C6H14 n-Hexane	86.17716	-166.92	-130.02		142.59	388.85	28.702	†
H14C6 2-METHYLPENTANE	86.17716	-174.55			142.21	380.98		
C6H14 3MP	86.17716	-171.97			140.21	383.03		
C6H14 2,2-DMBUTANE	86.17716	-184.68			141.46	358.34		
C6H14 2,3-DMBUTANE	86.17716	-176.8			139.41	365.92		
C6H14O (L) 1-Hexanol (liq)	102.17476	-377.5		$\pm 0.44$	243.2	287.4		X
C6H14O 1-Hexanol	102.17476	-314.7	-269.230	$\pm 1.4$	139.043	376.040	24.468	#
C6H15Bi Bi(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>		216.		$\pm 17.$				X
C6H15Sb Sb(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>		-0.837	+41.	$\pm 11.$				X
C6N6O6 BENZOTRIFUROXAN	252.10284	N/A	N/A		200.972	416.395		
C7 linear singlette $^1\Sigma_g^+$	84.0749	1322.34	1309.34	$\pm 8.$	98.927	314.106	20.372	#
C7F16 Perfluoroheptane	124.9	-3383.969			300.804	704.075		
C7H	85.08284	1090.	1080.1	$\pm 100.$	110.882	330.513	21.504	#
C7H4	69.036	676.13	682.585		100.798	312.080		#
C7H5N C6H5-CN Benzonitrile	103.12134	213.066	227.443	$\pm 8.$	105.310	328.810	18.503	#
TNT Solid	227.13122	-63.178		$\pm 5.0$	244.68	284.9		
C7H5N3O6 TNT	227.13122	24.1	53.992	$\pm 8.4$	215.417	481.936	37.698	#
C7H5N5O8 Tetryl Solid	287.1456	41.003			302.08	330.1		
C7H5O C <sub>6</sub> H <sub>5</sub> -C* <sub>2</sub> =O	105.11400	124.604	138.295	$\pm 8.$	108.240	342.800	19.194	#
C7H6O BENZALDEHYDE	106.12404	-39.179	-21.320	$\pm 8.$	111.428	336.148	19.260	#
C7H7 2,4,6-Cycloheptatriene-1-yl	91.13048	280.696	298.308	$\pm 8.$	109.167	332.619	19.401	#
C7H7 BENZYL RADICAL	91.13048	208.0	226.8	$\pm 1.9$	109.700	318.229	18.178	#
C7H7 Quadricyclene Appex Rad.	91.13048	534.519	556.275	$\pm 2.2$	95.877	297.781		#
C7H7 Quadricyclene Basis Rad.	91.13048	581.346	603.316	$\pm 2.2$	90.683	299.778		#
C7H7 Quadricyclene Shoulder R	91.13048	588.94	611.424	$\pm 2.2$	90.774	299.687		#
C7H7O C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> O*	107.12988	125.909	146.9	$\pm 8.$	117.167	351.816	20.362	#
TOLUENE(L)	92.13842	12.18	19.957		157.29	221.030	33.470	†
C7H8 TOLUENE	92.13842	50.17	73.476		103.279	320.187	17.940	†
C7H8 (liq) Norbornadiene	92.13842	179.172		$\pm 1.$	----	----		X
C7H8 Norbornadiene	92.13842	212.5	238.345	$\pm 1.17$	98.054	295.528	15.402	#
C7H8 (liq) Quadricyclene	92.13842	302.1		$\pm 2.2$	----	----		X
C7H8 Quadricyclene	92.13842	337.23	363.987	$\pm 2.2$	91.551	228.420		#
C7H8 1,3,5-Cycloheptatriene	92.14052	182.8			106.251	316.365		
C7H8 1,6-Heptadiyne	92.14052	395.8			134.202	379.7		
C7H8O CRESOL	108.13782	-132.298	-108.55		128.026	360.116	21.838	†
C7H8O BENZYL-ALCOHOL	108.13782	-94.6	-70.081	$\pm 3.0$	119.290	360.634	21.068	#
C7H9 2-CH <sub>3</sub> -4=CH <sub>2</sub> -1-CyPenten	93.14636	190.862	216.044	$\pm 8.$	118.751	344.962	20.298	#
C7H10 Cyclopentyl-Acetylene	94.15430	166.096	194.511	$\pm 8.$	118.125	349.171	21.300	#
C7H10 5,5 dimethyl-1,3-CPD	94.15430	81.211	109.705	$\pm 8.$	122.658	333.143	21.221	#
C7H10 2,5 dimethyl-1,3-CPD	94.15430	74.659	103.023	$\pm 8.$	120.843	341.862	21.352	#
C7H10 2,4 dimethyl-1,3-CPD	94.15430	63.513	91.186	$\pm 8.$	121.800	347.404	22.042	#
C7H10 2,3 dimethyl-1,3-CPD	94.15430	61.894	89.955	$\pm 8.$	117.103	344.813	21.654	#
C7H10 NORBORNENE	94.15640	90.	123.4	$\pm 30.$	103.136	306.087	16.310	
C7H10N2O2 Cyclo(Pro-Gly)	154.16658	-341.012	-301.25	$\pm 12.5$	158.210	401.299	27.301	#
C7H12 NORBORNANE	96.17228	-53.723		$\pm 8.4$	103.291	307.66		#
C7H12 CY-HEPTENE	96.17018	-7.866	30.578	$\pm 8.$	120.515	324.394	19.739	#
C7H13 Cycloheptanyl Radical	97.17812	77.739	118.315	$\pm 8.$	126.683	353.102	21.841	#
C7H13 1-Heptyl-4/5 ene	97.17812	132.2	194.632		148.532	435.136	--	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C7H13 1-Heptene-4-yl	97.17812	129.7	192.117		149.900	505.000	--	
C7H14 n-HEPTENE	98.18816	-62.76	-26.9		153.500	425.600	30.790	†
C7H14 CY-HEPTANE	98.18816	-118.2			131.171	336.512		
C7H14O2 (liq) Enanthic acid	130.18486	-608.5		±0.9				X
C7H14O2 n-Heptanoic acid	130.18486	-534.3	-489.48	±12.5	162.604	448.539	30.514	#
C7H14O2 Me-Hexanoate	130.18486	-505.43	-461.8	±12.5	169.320	451.890	31.739	#
C7H14O2 Ethyl Pentanoate	130.18486	-512.65						X
C7H15 n-HEPTYL RAD.	99.1940	4.39	41.732		164.430	448.029	33.543	†
C7H15 NEOHEPTYL-1	99.1961	3.347	44.329		164.117	426.788	29.704	#
C7H15 NEOHEPTYL-2	99.19400	-2.926	37.433	±8.	168.595	430.562	30.526	#
C7H15O 3,3dimethyl1-pentanoxy	115.1955	-142.256			171.86	328.026		
C7H16(L) n-Heptan	100.20194	-224.35	-201.87		224.980	328.560	52.640	†
C7H16 n-HEPTAN	100.20194	-187.78	-145.88		165.180	429.099	33.221	†
C7H16 iso-Heptan	100.20194	-194.600	-150.40		164.500	420.500	30.920	†
C7H16 NEOHEPTAN	100.20194	-209.87			166.955	395.221		
C7H15OH n-Heptanol	116.20344	-339.741		±1.6	178.605	480.449		
C7H15OH Neoheptanol	116.20344	-359.657			179.907	448.901		
C8 (1A <sub>g</sub> ) linear singlette	96.08560	1458.866	1445.44		107.988	330.429	21.848	#
C8 ( <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ) linear triplete	96.08560	1513.8	1500.3	±8.	100.651	301.647	21.932	#
C8H CH≡C-C≡C-C≡C-C*	97.09354	1230.	1218.5	±100.	125.662	354.191	24.131	#
C8H2 CH≡C-C≡C-C≡C-CH	98.10388	900.	891.8	±60.	134.364	348.303	25.093	#
C8H5 CH≡C-CH=CH-CH=C*-C≡CH	101.12530	808.453	812.494	±8.	141.494	402.387	26.558	#
C8H5 C <sub>6</sub> H <sub>5</sub> C≡C*	101.12530	654.934	665.190	±8.	108.279	334.534	19.342	#
C8H6 C <sub>6</sub> H <sub>5</sub> C≡CH	102.13324	320.886	330.632	±8.	125.784	334.300	20.883	#
C8H6 Benzocyclobutene	102.13324	410.015	426.377	±8.	105.597	312.114	17.471	#
C8H6O BENZOFURANE	118.13264	17.0	37.048	±1.5	111.964	326.193		#
C8H6O2 Benzodioxin	134.13204	-71.2	-49.95	±6.	128.967	347.408		#
C8H6S BENZOTHIOPHENE	134.20164	166.272			131.558	337.481		
C8H7 n-STYRYL RADICAL	103.14358	393.5	411.737	±8.	117.820	349.841	19.830	#
C8H7 i-STYRYL RADICAL	103.14118	367.686	385.134	±8.	120.881	355.861	20.618	#
C8H7 o-C <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>	103.14118	401.827	420.034	±8.	116.318	350.846	19.860	#
C8H7 1,3,5,7Cy-octateraene-1-yl	103.14118	503.921	522.020	±8.	118.407	340.591	19.948	#
C8H7 2,3,5,7Cy-octateraene-1-yl	103.14118	503.795	521.914	±8.	118.425	340.577	19.948	#
C8H7N INDOLE	117.15032	156.5		±1.25	121.264	332.373		
C8H8 CUBANE	104.14912	651.7		±30	98.47	271.426		
C8H8 STYRENE	104.14912	148.3	169.66	±2.	120.190	344.770	20.940	†
C8H8 1,3,5,7 Cyclooctateraene	104.14912	297.6	319.294	±1.3	122.616	327.102	20.607	#
C8H8 2,3,5,7 Cyclooctateraene	104.14912	389.434	411.499	±8.	118.990	338.828	20.235	#
C8H8 Benzocyclobutane	104.14912	200.476	224.662	±8.	109.342	317.617	18.115	#
C8H9 C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> *	105.15706	237.714	262.114	±8.	130.543	364.717		#
C8H9 1,3-BiMeBenzen-5-yl	105.15706	266.3	--		124.9	376.7	--	
C8H10 C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> H <sub>5</sub>	106.16500	29.790	58.81	±8.	129.799	337.688	22.280	†#
C8H10 Di METHYLBENZENE	106.16500	19.652	50.476	±8.	118.286	352.115	19.944	#
C8H12 3,6-di-CH <sub>3</sub> -1,4-hexadiene	108.18088	52.622	88.364	±8.	139.021	352.015	23.495	#
C8H14 CH(-CH <sub>2</sub> -CH <sub>2</sub> -) <sub>3</sub> CH	110.19676	-99.035	-51.705	±1.	125.174	327.572	20.374	#
C8H15 1-Octen-4-yl	111.20710	109.1	181.039		172.717	481.400	---	
1-C8H16 1-OCTENE	112.2144	-83.59	-42.768		176.100	464.840	35.350	†
C8H16 CycloOctane	112.21264	-124.4	-72.762	±1.	146.194	366.725		#
C8H16O2 (liq) Caprylic acid	144.21144	-634.8		±0.8				X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C8H16O2 n-Octanoic acid	144.21144	-553.96	-502.584	$\pm 12.5$	185.105	476.251	33.476	#
N-C8H17 N-OCTYL RAD	113.2223	-16.32	+25.983		187.070	488.879	38.103	†
C8H18(L) n-Octane	114.22852	-250.260	-227.11		254.150	361.071	61.490	†
C8H18 OCTANE	114.22852	-208.75	-161.89		187.780	468.480	37.780	†
C8H18(L) isooctane	114.22852	-259.160	-224.71		239.000	328.110	50.190	†
C8H18 ISO-OCTANE	114.22852	-224.01	-171.54		188.410	423.090	32.170	†
(CH <sub>3</sub> ) <sub>3</sub> C-OO-C(CH <sub>3</sub> ) <sub>3</sub> Liquid	146.22732	-380.8	---	$\pm 2.0$				X
C8H18O2 (CH <sub>3</sub> ) <sub>3</sub> C-OO-C(CH <sub>3</sub> ) <sub>3</sub>	146.22732	-343.	---		219.150	482.400	---	
C8H20Pb (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> Pb Liquid	323.4444	53.0		$\pm 5.$				X
C8H20Pb (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> Pb Gas	323.4444	109.6	169.315	$\pm 5.1$	233.217	477.890		#
C9 ( $^1\Sigma_g^+$ )	108.0963	1563.57	1553.48	$\pm 8.$	122.991	356.062	24.670	#
C9H	109.10424	1310.	1296.8	$\pm 125.$	140.858	379.086	26.889	#
C9H4 C(CCH) <sub>4</sub>	112.12806	913.78	918.435		126.858	330.747		#
C9H7 INDENYL	115.15188	285.6	304.521	$\pm 22$	128.21	342.843	20.199	#
C9H7N QUINOLINE	129.15862	200.52	223.454		129.153	344.075	20.521	#
C9H7N ISOQUINOLINE	129.15862	204.61	227.487		128.983	344.568	20.578	#
C9H8 INDENE	116.15982	164.138	187.693	$\pm 1$	124.226	335.846	19.799	#
C9H10 METHYLSTYRENE	118.1784	112.968			146.858	383.673		
C9H11 C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> * Rad	119.18364	214.639			148.114	410.869	--	
C9H12 C(CH=CH <sub>2</sub> ) <sub>4</sub>	120.19158	250.6	279.18		174.032	417.887	31.734	#
C9H12 1,3,5-Trimethylbenzene	120.19158	-16.067	44.22 ?		147.800	385.300	---	
C9H12 1,2,4-Trimethylbenzene	120.19158	-13.933	46.36 ?		154.508	395.765	---	
C9H12 Propylbenzene	120.19158	7.95	68.240		151.461	399.990	---	
C9H17 1-Nonenyl Radical	125.23398	88.400	169.860		195.709	520.900	---	
C9H18 1-Nonene	126.24192	-432.207			200.269	505.000		
C9H18O2 (liq) Pelargic acid	158.23802	-658.0		$\pm 0.9$				X
C9H18O2 n-Nonanoic acid	158.23802	-573.6	-516.938	$\pm 12.5$	206.200	515.713	37.686	#
C9H18O6 cyTriAcetoneTriPeroxy	222.23562	-395.472	-331.52	$\pm 22$	302.788	499.584	47.780	#
N-C9H19 n-NONYL RAD	127.2491	-37.03	+10.234		209.710	527.419	42.664	†
N-C9H20 liq. NONANE	128.2578	-275.475			284.386	393.673		
N-C9H20 NONANE	128.2578	-228.907	-177.09		210.413	506.431	42.342	
C10 ( $^1A_1'$ ) cyclic?	120.10700	1459.363	1443.5		132.726	373.758	26.376	#
C10 ( $^3\Sigma_g^-$ )	120.10700	1741.11	1725.189		133.694	382.818	26.460	#
C10D8 NAPHTHALENE-D8	136.21982	118.050	139.214		156.120	350.531	23.647	#
C10H	121.11494	1450.	1435.2	$\pm 125.$	155.644	402.686	29.534	#
C10H2	122.12288	1120.	1108.5	$\pm 80.$	164.350	396.743	30.501	#
C10H4Cl4 2,3,6,7-Cl-Naphthalen	265.94956	50.21	62.584		192.982	449.224	32.457	#
C10H6 Naphtyne	126.15764	500.825	515.5		132.178	347.542	21.264	
C10H7 Naphtyl Radical	127.16558	396.225	415.418		132.216	352.133	20.980	
C10H7 C <sub>6</sub> H <sub>5</sub> CH=CH-C $\equiv$ C*	127.16558	687.515	701.677	$\pm 20$	144.738	406.909	26.011	#
C10H7 C <sub>6</sub> H <sub>4</sub> *CH=CH-C $\equiv$ CH	127.16558	630.612	645.066	$\pm 20$	148.770	402.203	25.719	#
C10H7 C <sub>6</sub> H <sub>4</sub> (C <sub>2</sub> H)CH=CH*	127.16558	617.140	634.110		144.841	367.587	23.203	
C10H7I (L) 1-Iodobenzene Liq.	254.06705	162.		$\pm 6.3$				X
C10H7I 1-Iodobenzene	254.06705	234.	----	$\pm 8.8$	158.574	394.133	-----	
C10H7O* Naphthol Radical	143.15498	115.478	136.47		146.882	373.015	23.522	
H8C10 AZULENE	128.17352	279.932			128.868	338.065	20.368	*
C10H8 NAPHTHALENE	128.17352	150.582	174.276	$\pm 1.5$	131.920	333.267	20.713	†
C10H8O Naphtol	144.17292	-30.794	-6.37		154.318	368.709	24.318	#



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C10H9 2-HydroNaphthalen Rad	129.17846	229.534	255.533		143.289	363.659	22.643	
C10H9 C <sub>6</sub> H <sub>5</sub> CH=CHCH=CH*	129.17846	444.508	466.692	±20	152.314	419.069	26.458	#
C10H9 1-Methyl-1-Indenyl Rad	129.17846	262.337	287.549	±20	144.004	369.098	23.429	#
C10H9 1-Methylene-Indene Rad	129.17846	337.649	363.520	±20	144.045	364.065	22.771	#
C10H9 2-Methylene Indene Rad	129.17846	266.5		±20	-	-		X
C10H10 1,2-DihydroNaphthalene	130.1864	117.152	147.213		143.955	359.383	22.797	
C10H10 1,1'-BiCyclo-Pentadiene	130.1864	291.625	320.336		143.016	385.011	24.164	#
C10H10 2,2''-BiCycloPentadiene	130.1864	291.056	318.773		150.301	386.504	25.159	#
C10H10 1-Methyl Indene	130.1864	184.933	214.695	±20	144.346	360.391	23.113	#
C10H10 2-Methyl Indene	130.1864	173.636	202.811	±20	146.240	364.509	23.701	#
C10H10 3-Methyl Indene	130.1864	173.218	202.400	±20	146.056	364.755	23.694	#
C10H13 C5H7-C5H6*	133.21322	197.15	----	±20	149.452	395.356	---	
C10H14 3,3-C5H7-C5H7 bicyclo	134.21816	108.784	152.131	±20	155.753	401.109	26.465	#
11-C10H15 JP-10 apex Radical	135.22910	105.650	157.726		142.526	359.233	21.970	#
6-C10H15 JP-10 Tert side Rad.	135.22910	96.32	149.14		138.190	355.345	21.225	#
C10H15 C5H8*-C5H7	135.22910	171.54	218.396	±125.5	155.918	417.467		
C10H16 JP-10	136.23404	-87.139	-31.556		153.679	355.323	22.696	†
C10H18 (liq) 1,1'-Bicyclopentyl	138.24992	-179.3		±1.0	238.9			
C10H18 1,1'-Bicyclopentyl	138.24992	-127.8	-70.05 ??		167.750	427.551	29.001	#
C10H19 1-Decenyl 4/5 Radical	139.26086	67.900	158.882		218.653	560.300	-----	
C10H19 1-Decenyl 3 Radical	139.26086	2.600	93.582		221.077	567.300	-----	
C10H20 1-Decene	140.26880	-123.900			223.362	544.500		
C10H20 2-Decene-trans	140.26880	-136.200			222.222	541.000		
C10H20 3-Decene-trans	140.26880	-135.500			220.659	542.600		
C10H20O2 (liq) Capric acid	172.26460	-713.7		±0.9				X
C10H20O2 n-Decanoic acid	172.26460	-593.7	-529.69	±12.5	225.282	524.779	39.879	#
N-C10H21 n-DECYL 1-Radical	141.27374	-57.74	-5.514		232.350	567.109	47.224	†
C10H21 n-Decyl – 2-Radical	141.27674	-58.100			230.534	567.300		
C10H21 n-Decyl-3/4 Radical	141.27674	-58.200			230.534	567.300		
N-C10H22 liq DECANE	142.28468	-301.039			314.511	425.889		
N-C10H22 gas-DECANE	142.28468	-249.534	-192.75		233.049	545.677	46.903	#
C11 singlet	132.11770	1792.06	1775.137	±8.	144.086	394.396	28.517	#
C11H radical	133.12564	1530.	1513.5	±150.	170.848	427.700	32.321	#
HC11N HC10CN	147.13238	1270.	1253.8	±100.	190.022	458.112	36.314	#
1-C10H7C*O Naphtaldehyde Rd.	155.17598	174.891	193.741		161.693	399.949	26.717	
1-C10H7CHO Naphtaldehyde	156.18392	30.543	54.59		162.397	383.881	25.754	
1-C10H7-CH2* Methyl-Naphthyl	141.19246	272.797	297.846		158.090	378.770	24.645	
1-C10H7-CH3 MethylNaphthalen	142.20040	116.106	145.0		157.922	381.348	25.026	
C11H22O2 n-Undecanoic acid	186.29118	-612.96	-543.14	±12.5	245.847	577.079	43.603	#
C11H24 N-UNDECANE	156.31156	-270.286	-208.54		255.684	584.923	51.463	#
C11N *C10-CN Radical	146.12444	1500.	1479.45	±150.	185.004	462.108	36.477	#
C12 Σ <sub>g</sub> <sup>+</sup> linear singlet	144.12840	1913.7	1895.3	±12.5	158.347	416.774	31.035	#
C12 linear triplet	144.12840	1964.1	1945.56	±12.5	159.729	427.047	31.198	#
O-C12D9 O-BIPHENYL Radical	162.25532	386.5	407.176		194.573	428.719	30.527	#
C12D10 BIPHENYL – D	164.26942	138.410	163.029		199.244	413.432	30.868	#
C12H	145.13634	1670.	1651.89	±150.	185.671	451.233	34.985	#
C12H2	146.14428	1340.	1325.2	±100.	194.154	445.249	35.889	#
C12H4CL4O 2,3,6,7	305.97036	-50.	-35.924	±10	225.108	496.028	38.205	
C12H4CL4O 2,4,6,8	305.97036	-58.	-44.108	±10	225.552	493.238	38.388	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C12H4CL4O2 2,3,7,8	321.96976	-136.1	-120.71	$\pm 10$	241.524	513.049	41.226	#
C12H4CL4O2 1,3,6,8	321.96976	-174.10	-158.934	$\pm 10$	241.685	520.954	41.454	#
C12H4CL4O2 1,3,7,9	321.96976	-174.130	-158.961	$\pm 10$	241.657	520.551	41.452	
C12H4CL4O3 1,3,6,8	337.97276	-295.37	-278.36		256.811	533.525	43.948	
C12H4CL5O2 spiro radical	357.42246	-95.550	-80.345	$\pm 10$	264.387	571.035	46.006	#
C12H4CL5O2 6-2' ether radical	357.42246	-125.900	-112.30	$\pm 10$	266.495	600.066	47.612	#
C12H4CL6O2 2-6' ether	392.87516	-201.95	-187.778	$\pm 10$	287.872	625.238	51.630	#
C12H4CL6O2 Biphenyl-diol	392.87876	-321.92	-305.6	$\pm 33.5$	286.707	573.925	49.483	
C12H5CL3O3 2,4,7 trichloro	303.52800	-348.99	-329.03		241.279	505.020	40.642	
C12H5CL4O2 6-6' ether radical	322.98130	-85.52	-69.659	$\pm 25.1$	250.467	582.730	44.993	
C12H5CL4O3 radical	338.97710	-432.42	-412.55	$\pm 62.8$	265.578	551.043	45.331	
C12H5CL4O3 radical	338.97710	-321.79	-301.82	$\pm 62.8$	263.787	550.127	45.226	
C12H5CL5O2 6-6' ether	358.43040	-265.590	-247.196	$\pm 10.$	272.572	577.900	47.051	#
C12H6CL2O DCDF	237.08084	5.2	25.245	$\pm 24.7$	192.255	439.242		#
C12H6CL2O2 DCDD	253.08024	-89.3	-67.92	$\pm 26.6$	209.088	461.386		#
C12H6CL4O2 6-2' ether	323.98564	-207.57	-187.21		256.821	561.466	44.729	
1-C10H7-C $\equiv$ C* EthynylNaphthyl	151.18758	694.962	710.644		162.077	397.847	26.598	
C12H7 5-Acenaphtylenyl Rad.	151.18398	525.300	544.948	$\pm 8.$	146.923	338.218	22.633	#
C12H8 Acenaphthylene	152.19552	259.7	283.489	$\pm 5.9$	148.772	338.676	22.726	#
C10H7-C $\equiv$ CH EthynylNaphthalen	152.19552	379.070	398.592		169.895	391.974	26.992	
C12H8Cl2O2	255.09612	-231.794	-167.418?		238.488	528.021		
C12H8O Di-Benzo-Furan	168.19492	55.2	80.812	$\pm 4.8$	163.566	375.274	25.229	
C12H8O2 Di-Benzo-p-Dioxin	184.19432	-50.1	-23.24	$\pm 2.2$	180.004	396.647	28.336	#
1-C10H7-CH=CH* Vinyl-Naphthy	153.20346	469.863	492.963		172.891	404.234	27.649	
1-C10H7-C*=CH2	153.20346	412.208	434.879		175.034	407.260	28.077	
O-C12H9 O-BIPHENYL RAD	153.2031	427.73	451.889		163.048	405.110	26.589	†
C12H9CL	188.65616	148.55			178.868	433.51		
C12H9N CARBAZOLE	167.2102	200.7			176.877	388.305		
1-C10H7-CH=CH2	154.21140	215.058	242.302		173.671	400.851	27.738	
C12H10 BIPHENYL	154.21140	182.13	210.329	$\pm 0.7$	166.179	388.941	26.783	†
C12H10 1-C10H7-CH2CH2*	155.21934	292.88	322.861		185.266	418.370	29.235	
C12H10 1-C10H7-CH*-CH3	155.21934	220.497	250.340		184.272	426.717	29.373	
1-C10H7-C2H5 EthylNaphthalen	156.22728	96.901	131.723		181.943	406.323	28.829	
C12H12O 1-C10H7CH2CH2OH	172.22668	-52.718	-16.807		195.002	447.806	31.880	
C12H23 liquid JET-A(L)	167.31102	-303.469	--		350.336	448.112	--	†
C12H23 JET-A (Kerosine)	167.31102	-211.46	--		293.494	612.539	--	†
C12H23O2 O=CH(CH2) <sub>10</sub> CH2O*	199.30982	-303.2			294.1	691.2	---	
C12H23O2 C <sub>6</sub> H <sub>13</sub> C(O)CH2CHO*C <sub>3</sub> H <sub>7</sub>	199.30982	-351.0			295.8	676.97	---	
C12H24O2 n-Dodecanoic acid	200.31776	-775.1						X
C12H24O2 n-Dodecanoic acid	200.31776	-633.0	-510.1??	$\pm 15.$	294.554	629.27	---	
C12H26 N-DODECANE	170.33844	-290.872	-224.17		278.32	624.253	56.024	
C12H26O (liq.) 1-Dodecanol	186.33424	-528.5	--	$\pm 0.8$	438.42			X
C12H26O 1-Dodecanol	186.33424	-775.714	-648.646		294.554	674.879	--	
C13H9 1-Phenalenyl Radical	165.21056	264.3	291.327	$\pm 8.$	164.097	376.488	24.775	#
C13H9N ACRIDINE	179.2212	273.9			177.643	394.998		
C13H9N PHENANTHRIDINE	179.2212	240.5			184.131	391.6		
C13H10 Fluorene	166.21850	175.	205.189		166.651	381.181	25.847	#
C13H10 Phenalene	166.21850	189.4	219.636	$\pm 8.$	167.435	385.909	25.800	#
C13H26O2 liq n-Tridecanoic acid	214.34434	-807.2						X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C13H26O2 Methyl-Dodecanoate	214.34434	-623.4	-490.9???	$\pm 15.$	313.382	666.511	---	
C13H28 n-TriDecane (liquid)	184.36142	-377.7		$\pm 1.6$				X
C13H28 n-TriDecane	184.36142	-311.5	-179.251?	$\pm 1.6$	303.340	661.449	--	
C14H6(NO2)6 solid HNS	450.23068	58.07		$\pm 10.$				X
C14H6(NO2)6 HexaNitroStilbene	450.23068	238.4	285.396		411.150	773.618	71.248	#
C14H9 1-Antryl	177.22126	480.2	504.75	$\pm 8.$	184.7	408.7	28.300	
C14H9 2-Antryl	177.22126	478.5	503.06	$\pm 8.$	184.9	408.5	28.300	
C14H9 9-Antryl	177.22126	488.0	512.66	$\pm 8.$	184.2	409.1	28.300	
C14H9 1-Phenantryl	177.22126	458.0	482.65	$\pm 8.$	184.1	409.5	28.200	
C14H9 2-Phenantryl	177.22126	457.0	481.56	$\pm 8.$	184.4	409.5	28.300	
C14H9 3-Phenantryl	177.22126	456.4	480.96	$\pm 8.$	184.4	409.3	28.300	
C14H9 4-Phenantryl	177.22126	450.8	475.45	$\pm 8.$	183.8	408.3	28.200	
C14H9 9-Phenantryl	177.22126	456.2	480.75	$\pm 8.$	184.3	409.8	28.300	
C14H10 ANTHRACENE	178.2334	230.1		$\pm 4.6$	184.993	392.693		
C14H10 PHENANTHRENE	178.2334	207.1			186.787	394.614		
C14H10O Phenanthrenol (any loc)	194.22860	33.			217.3	429.78		
C14H12 solid t-Stilbene	180.24508	136.73		$\pm 10.$				X
C14H12 trans-Stilbene	180.24508	223.3	255.957	$\pm 4.$	203.066	447.878	32.901	#
C14H14 BIBENZYL	182.26096	135.6	175.94	$\pm 1.3$	202.411	477.207	33.684	#
C14H28O2(liq) Myristic acid	228.37092	-834.1						X
C14H28O2 Myristic acid	228.37092	-672.369		$\pm 15.$	338.486	688.268	---	
C14H28O2 (liq) Ethyl Dodecanoate	228.37092	-732.6						X
C14H28O2 Ethyl Dodecanoate	228.37092	-657.7	-515.7	$\pm 15.$	333.465	702.915	---	
C15H30O2(liq) MethylMyristate	242.3975	-759.4						X
C15H30O2 MethylMyristate	242.3975	-662.746		$\pm 15.$	360.242	731.782	--	
C16H9 1-Pyrenyl Radical	201.24266	476.9	501.96	$\pm 8.$	201.5	418.9	29.9	
C16H9 2-Pyrenyl Radical	201.24266	473.8	498.76	$\pm 8.$	202.0	419.0	30.00	
C16H9 4-Pyrenyl Radical	201.24266	479.2	504.26	$\pm 8.$	201.7	419.2	29.9	
C16H10 PYRENE	202.2554	225.7	---		202.501	407.513	--	
C16H29O2 Palmitoleate Rad. O*	253.40026	-348.5	-260.537?	$\pm 25.$	336.544	708.254	60.334	#
C16H30O2 Palmitoleic acid	254.40820	-585.342		$\pm 25.$	368.192	794.960	--	
C16H31O2 Palmitate Radical O*	255.41614	-475.3	-380.46	$\pm 12.5$	343.345	714.875	61.951	#
C16H32O2 (liq) Palmitic acid	256.42408	-848.8		$\pm 2.2$				X
C16H32O2 Palmitic acid	256.42408	-711.698		$\pm 25.$	385.346	764.835	--	
C16H32O2(liq) EthylMyristate	256.42408	-802.9						X
C16H32O2 EthylMyristate	256.42408	-697.054		$\pm 15.$	379.070	769.019	--	
C16H33 2-HEXADECYL Rad.	225.43802	-181.67	-25.09?		366.100	818.976	--	#
C16H34 n-HEXADECANE	226.44596	-374.51	-213.7?		370.284	780.943	--	#
C17H31O2 Margaroleate Rad O*		-368.2		$\pm 25.$				
C17H31O2 MePalmitoleate-C0-yl	267.42684	-378.6	-285.249	$\pm 15.$	366.327	740.672	64.495	#
C17H32O2 MargarOleic acid	268.43478	-605.425		$\pm 25.$	389.112	842.658	--	
C17H32O2(liq) MethylPalmitoleate	268.43478	-674.29						X
C17H32O2 cis-MethylPalmitoleate	268.43478	-576.14		$\pm 15.$	386.183	835.545	---	
C17H33O2 Margareate Rad O*	269.44272	-494.967	-394.08	$\pm 15.$	363.591	741.763	65.427	#
C17H33O2 MePalmitate-C16-yl	269.44272	-492.04		$\pm 8.$	409.39	897.8	---	
C17H34O2 Margaric acid	270.45066	-731.363		$\pm 25.$	405.430	786.592	---	
C17H34O2(liq) MethylPalmitate	270.45066	-1441.8		$\pm 3.8$				X
C17H34O2 MethylPalmitate	270.45066	-702.075		$\pm 25.$	404.174	796.634	---	
C18H12 Naphthacene	228.28788	302.	337.48	$\pm 15.$	227.829	440.252	34.291	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C18H12 (s) Triphenylene solid	228.28788	146.5		$\pm 1.5$				X
C18H12 Triphenylene	228.28788	278.0	312.98	$\pm 10.$	227.580	446.288	34.792	#
C18H15N (s) TriPhenylAmine		235.		$\pm 3.$				X
C18H15N (C6H5)3N	245.31844	327.	371.585	$\pm 4.2$	260.410	523.427	42.224	#
C18H29O2 Linolenate Rad. O*	277.42166	-132.63		$\pm 25.$	363.702	754.722	64.877	#
C18H30O2 (liq) $\alpha$ Linolenic acid	278.42960	-508.8						X
C18H30O2 $\alpha$ Linolenic acid	278.42960	-369.45			389.112	841.4	----	
C18H31O2 Linoleate Radical O*	279.43754	-258.153	-165.4??	$\pm 25.$	367.963	769.453	66.170	#
C18H32O2 (liq) Linoleic acid	280.44548	-634.7						X
C18H32O2 Linoleic acid	280.44548	-494.97			397.9	875.29	----	
C18H33O2 Oleate Radical O*	281.45342	-388.275	-288.418	$\pm 12.5$	374.717	776.117	67.510	#
C18H34 1-Octadecyne	250.46256	-123.579	-35.485		402.668	836.131	74.726	#
C18H34O2 (liq) Oleic acid	282.46136	-764.8						X
C18H34O2 Oleic acid	282.46136	-624.67			397.9	878.64	-----	
C18H34O2 EthylPalmitOleate	282.46136	-610.03			409.614	863.996		
C18H35O2 Stearate Radical O*	283.46930	-514.63	-413.734	$\pm 25.$	402.870	833.512	74.937	#
C18H36 1-Octadecene	252.47844	-289.03	-193.548		406.768	852.030	75.906	#
C18H36O2 Stearic acid	284.47724	-751.028	-570.96 ?	$\pm 31.$	423.421	834.29		
C18H36O2 (liq) Ethyl Palmitate	284.47724	-860.2						X
C18H36O2 Ethyl Palmitate	284.47724	-736.384	-556.31?	$\pm 25.$	423.421	834.29		
C18H38 (l) n-Octadecane liquid	254.49432	-505.4		$\pm 2.7$		696.6		X
C18H38 n-Octadecane	254.49432	-414.55	-318.039	$\pm 2.7$	414.132	859.812	83.345	#
C19H32O2(liq) MethylLinolenate	292.45618	-472.75						X
C19H32O2 MethylLinolenate	292.45618	-358.15	-193.96 ?	$\pm 20.$	406.266	868.6		
C19H34O2(liq) MethylLinoleate	294.47206	-604.88						X
C19H34O2 MethylLinoleate	294.47206	-485.762	-313.11 ?	$\pm 15.$	418.400	887.01		
C19H36O2(liq) Methyl Oleate	296.48794	-727.64						X
C19H36O2 Methyl Oleate	296.48794	-615.885	-434.76 ?	$\pm 15.$	430.115	932.195		
C19H38O2(S) Methyl Stearate	298.50382	-945.6						X
C19H38O2 Methyl Stearate	298.50382	-741.82	-552.23 ?	$\pm 35.$	450.617	861.9	---	
C20H10 Corannulene	250.29340	463.712	495.843	$\pm 7.3$	216.018	412.967	31.264	#
C20H12 Perylene	252.30928	306.0	340.0	$\pm 0.8$	254.201	475.499	37.878	#
C20H12 Benzo[a]Pyrene	252.30928	289.5			254.800	468.700		
C20H14 Alpha BiNaphtyl	254.32516	315.055	395.402		278.654	513.795	----	
C20H34O2 Ethyl Linolenate	306.48276	-392.04	-218.33?		428.44	889.1	----	
C20H36O2 Ethyl Linoleate	308.49864	-522.58	-340.4 ?		445.18	918.39	----	
C20H38O2(liq) Ethyl Oleate	310.51452	-773.25						X
C20H38O2 Ethyl Oleate	310.51452	-649.775	-459.13?		452.29	981.86	----	
C20H39O2 Archidate Rad. O*	311.52246	-554.	-440.4?	$\pm 25.$	442.784	890.297	82.276	#
C20H40O2(liq) Arachidic acid	312.53040	-1012.6						X
C20H40O2 Arachidic acid	312.53040	-790.36	-591.25?	$\pm 22.6$	474.05	893.7	----	
C20H40O2 MeNanodecanoate	312.53040	-763.5	-----		477.8	1000.7	----	
C20H40O2 (S) Ethyl Stearate	312.53040	-984.6						X
C20H40O2 Ethyl Stearate	312.53040	-775.7	-576.6 ?	$\pm 50.$	467.35	905.	----	
C20H42 (l) n-Eicosane liquid	282.54748	-556.5		$\pm 3.1$				X
C20H42 n-Eicosane	282.54748	-455.8	-349.366	$\pm 3.1$	459.403	938.053	92.466	#
C21H42O2 Methyl Eicosanate	326.55698	-781.153	-572.5 ?	$\pm 35.$	495.804	924.246	---	
C22H14 Pentacene	278.34656	389.000	428.03	$\pm 15.$	277.388	494.673	41.423	#
C22H14 Pentafene	278.35315	345.000			282.920	501.187		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C22H18 (C <sub>10</sub> H <sub>7</sub> -CH <sub>2</sub> ) <sub>2</sub>	282.37832	279.073	378.46 ??		320.9	597.89	----	
C22H44O2 EthylEicosanate	340.58356	-815.043		±35.	512.958	962.32	----	
C24CL12 Perchloro-coronene	713.68920	146.6	146.7	±35.	458.824	803.678	80.264	#
C24H12 Coronene	300.35208	307.5	345.262	±10.	262.602	458.935	38.331	#
C24H17 Triphenylbenzene Rad.	305.39898	623.2			323.134	652.000		
C24H18 Triphenylbenzene	306.39972	373.38	432.36	±15.	320.200	604.870	51.514	#
C24H20Pb(S) TetraPhenylLead	515.6156	515.		±15.				X
C24H20Pb Pb(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	515.6156	674.	727.7	±15.	371.099	722.859	63.103	#
C25H20 C(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	320.42630	393.	449.2	±6.3	334.652	654.026	54.783	#
C30H10 Half-BuckminsterFullerene	370.40040	1139.303	1168.575	±12.	323.869	494.466	44.674	#
C32H13 Ovalenyl Radical	397.44562	663.541	701.746	±20.	359.727	558.246	50.510	#
C32H14 Ovalene	398.45356	418.4	460.8	±12.	361.353	546.813	50.580	#
C60 Buckminster Fullerene	720.66	2585.7		±105.	560.816	591.403		
C70 Footballene	840.77	2652.	2660.33	±34.	558.171	589.537		#
JET-A(L)	167.31102	-303.469	-		350.336	448.112	-	†
JET-A(G) (C12H23)	167.31102	-211.46	-		293.494	612.539	-	†
Ca (S) REFERENCE ELEMENT	40.07800	0.	0.		25.75	42.536		±
Ca (gas)	40.07800	177.8	177.386	±0.8	20.786	154.887		†
Ca+	40.07740	773.2		±0.2	20.786	160.650		
CL	35.4527	121.302	119.620	±0.008	21.838	165.192	6.272	†
CL+	35.45215	1378.80	1370.807	±0.002	22.959	167.558	6.388	†
CL -	35.45325	-233.543	-228.952	±0.003	20.786	253.358	6.197	†
CuCl (see under Cu)								
DCL	37.4668	-93.547	-93.333	±0.21	29.170	192.773	8.661	†
DOCL	53.4662	-79.539	-76.648	±2.1	38.585	240.321	10.325	†
CLF	54.4511	-55.701	-55.706	±0.42	32.085	217.943	8.908	†
CLF3	92.44791	-164.6	-160.5	±5.	64.061	282.152	13.728	†
CIF5	130.44472	-238.	-229.277	±7.	97.167	310.257	17.930	†
HCL	36.46094	-92.31	-92.125	±0.10	29.136	186.901	8.640	†
HCL+	36.46009	1143.81	1137.794	±0.005	29.146	193.202	8.643	#
HOCL	52.46004	-76.149	-73.205	±0.6	37.264	236.971	10.221	#
ICL	162.35717	17.39	19.029	±0.041	35.532	247.451	9.549	#
CIONO2 Chloronitrate	97.45764	22.389	29.466	±8.	68.705	302.565	14.869	#
CLO	51.4521	-101.669	-101.984	±0.04	33.804	233.421	9.246	#†
CLO2 (O=ClO*)	67.4515	99.035	101.518	±6.3	41.921	257.555	10.788	#†
CLOO*	67.4518	101.671	102.712	±4.0	47.463	276.894	12.230	#
HCLO2	68.45944	20.92	25.94	±1.67	50.512	281.726	12.531	#
CLO3	83.45090	185.351	190.574	±1.67	56.096	282.289	12.388	#
CLO3F	102.4493	-23.799	-15.076		64.927	278.989	13.299	†
HCLO3 HO-ClO <sub>2</sub>	84.45884	-10.878	-3.200	±1.25	63.375	299.446	14.166	#
HCLO4 HO-ClO <sub>3</sub>	100.45824	-0.418	+11.234	±1.	69.774	300.191	14.532	#
CL2 REFERENCE ELEMENT	70.9054	0	0		33.949	223.082	9.181	*±
Cl2Cu (see under Cu)								
CL2O	86.90480	78.743	80.569	±0.67	47.811	267.951	11.695	#†
CL2O2	102.9042	138.976			65.034	295.883		
CL2O7 ClO <sub>3</sub> -O-ClO <sub>3</sub>	182.90120	275.726	293.029	±8.4	118.323	400.922	22.258	#
CL3Cu3 (See under Cu)								
Cr(cr) REFERENCE ELEMENT	51.9961	0	0		23.434	23.618	4.057	±†
Cr	51.9961	397.48		±4.2	20.786	174.313		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CrCl	87.4488	129.9	129.159	$\pm 2.7$	34.684	249.790	9.389	#
CrClO		-117.9		$\pm 9.6$		301.01	13.574	X
CrClO2		-310.3		$\pm 21.6$		309.81	14.449	X
CrCl2	122.9015	-117.6	-120.00	$\pm 1.7$	59.00	319.36	15.638	X
CrCl2O		-336.5		$\pm 22.5$		333.03	16.784	X
CrCl2O2	154.90030	-519.2	-515.35	$\pm 4.2$	84.052	329.53	18.066	#
CrCl3		-283.		$\pm 6.1$		347.03	19.101	X
CrCl3O		-507.8		$\pm 3.0$		357.32	20.049	X
CrCl4		-396.5		$\pm 13.8$		371.92	22.480	X
CrCl5		-389.6				407.16	26.602	X
CrCl6	264.71230	-345.3	-344.58	+50. ?	143.573	414.95	30.878	#
CrN(s)	66.00284	-117.152	-116.465	$\pm 8.4$	52.677	37.711	7.705	†
CrN	66.00284	505.009	504.523	$\pm 20.9$	30.754	230.556	8.778	†
CrO	67.9955	188.285		$\pm 41.8$	31.33	239.27		*
CrO2	83.9949	-108.043	-106	$\pm 15.$	41.971	265.575	10.694	†
CrO3	99.9943	-322.037	-318.00	$\pm 15.$	58.658	269.408	13.040	†
CrO3-	99.9949	-738.9	-729.049	$\pm 34.$	60.322	277.590	13.423	#
Cr2N(s)	117.99894	-125.520		$\pm 12.6$	66.065	64.921	---	†
Cr2O3(s)	151.9904	-1140.6	-1134.766	$\pm 8.4$	120.08	81.100	15.300	†
Cr2FeO4	223.8348	-1458.124			133.69	141.963		
Cr3C2(S)	180.0103	-85.354			99.326	85.437		
Cr7C3(S)	400.0057	-160.666			209.764	200.999		
C6Cr23	1267.9763	-328.444			628.117	612.119		
CuCl	98.99870	91.090	91.213	$\pm 1.67$	35.262	237.210	9.471	†
CuCl2(S)	134.4520	-205.85			71.84	108.0		X
CuF	82.54440	-12.550	-12.217	$\pm 16.7$	33.380	226.498	9.083	†
CuF2	101.54281	-266.940	-265.167	$\pm 12.55$	47.988	267.090	12.056	†
CuO	79.54540	306.270	305.863	$\pm 41.8$	35.693	234.621	9.751	†
Cu2	127.0920	485.340	485.418	$\pm 12.6$	36.585	241.724	9.934	†
Cu3Cl3	296.9961	-258.270	-258.510	$\pm 2.09$	124.572	429.553	28.724	†
D	2.0141	221.717	219.804	$\pm 0.001$	20.786	123.352	6.197	†
D+	2.01355	1540.320	1532.210	$\pm 0.001$	20.786	117.585	6.197	†
D-	2.01465	142.753	147.037		20.786	117.592	6.197	†
DF	21.01251	-276.228	-276.169	$\pm 0.8$	29.137	179.705	8.638	†
HD	3.02204	0.322	0.332		29.200	143.801	8.509	†
HD+	3.02149	1496.793	1490.50		29.334	155.552	8.614	†
HDO	19.02144	-245.280	-242.35		33.798	199.517	9.926	†
HDO2	35.02084	-140.242	-134.38		43.779	243.581	11.335	†
OD	18.01350	37.226	36.852		29.939	189.666	8.999	†
OD-	18.01405	-145.378	-139.2		29.143	178.409	8.642	†
DO2	34.0129	6.487	9.387		35.845	232.883	10.065	†
DO2-	34.01345	-104.796	-95.713		36.041	227.860	10.080	†
SD	34.080102	140.14	140.17	$\pm 0.52$	29.239	198.212	8.666	#
D2 REFERENCE ELEMENT	4.0282	0	0		29.195	144.96	8.569	±
D2+	4.02766	1498.586	1492.29		29.510	156.735	8.651	†
D2-	4.02875	235.161	241.213		30.315	158.261	8.714	†
D2O	20.0276	-249.209	246.261	$\pm 0.067$	34.265	198.342	9.960	†
D2O2	36.027	-144.3	-138.61		45.252	242.085	11.563	†
D2S	36.0942	-24.047	-21.114	$\pm 0.8$	35.795	215.316	10.089	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
ELECTRON GAS e-	0.00055	0	0		20.786	20.979	6.197	* $\pm$
F	18.9984	79.39	77.274	$\pm 0.3$	22.747	158.752	6.518	†
F+	18.99785	1766.661	1758.165	$\pm 0.159$	23.497	182.644	6.197	†
F-	18.99895	-255.459	-251.046	$\pm 0.159$	20.786	145.578	6.197	†
HF	20.00634	-273.3	-273.25	$\pm 0.7$	29.137	173.778		
HF+ <sup>a</sup>		1281.847		$\pm 0.16$				X
HOF	36.00574	-96.898	-94.		35.94	226.757		
FO	34.9978	111.267	110.632	$\pm 0.69$	31.995	216.396	9.388	†
FO+ <sup>a</sup>		1348.997		$\pm 1.11$				X
FO2 O-F-O	50.9972	378.6	381.154	$\pm 20$	41.126	251.289	10.538	†
FO2 F-O-O	50.9972	25.4		$\pm 2$	44.453	259.511	11.256	†
FO2+ F-O-O+	50.99665	1201.51	1197.864	$\pm 6.44$	40.240	247.719	10.541	#
F2 REFERENCE ELEMENT	37.99681	0	0		31.304	202.792	8.825	†
F2 <sup>-a</sup>		-299.174		$\pm 1.72$				X
HF2+ <sup>a</sup>		779.197		$\pm 10.$				X
HF2- <sup>a</sup> FHF-		-719.47		$\pm 5.63$				X
H2F2	40.01269	-569.924	-566.5		58.132	260.905		
F2O F-O-F	53.99621	24.5	26.754	$\pm 2$	43.495	247.508	10.912	†
F2O2 F-O-O-F	69.99561	32.87	36.597	$\pm 1.3$	62.073	277.214	13.778	†
F2O2+ F-O-O-F+	69.95506	1292.427	1290.26	$\pm 9.08$	57.747	279.484	13.475	#
F3 <sup>a</sup>		87.88		$\pm 6.11$				X
F3+ <sup>a</sup>		1533.41		$\pm 6.67$				X
F3- <sup>a</sup>		-357.45		$\pm 7.28$				X
H3F3	60.01903	-883.677	-873.		73.884	280.947		
H4F4	80.02537	-1186.932	-1174.		104.022	350.016		
H5F5	100.03172	-1490.188	-1475.		134.161	417.286		
H6F6	120.03806	-1805.545	-1788.		163.735	486.619		
H7F7	140.0444	-2099.699	-2080.		194.438	548.654		
Fe(a) REFERENCE ELEMENT	55.847	0	0		25.094	27.321	4.507	†
Fe	55.847	415.5	413.128	$\pm 1.3$	25.675	180.49	6.850	†
Fe+	55.84645	1181.144	1175.59		26.068	181.859	6.936	†
Fe-	55.84755	393.338	397.4		25.023	180.2	6.642	†
FeC5O5 (liq) Fe(CO) <sub>5</sub> liquid	195.8955	-766.09	-787.55	$\pm 7.1$	233.785	337.078	52.934	†
FeC5O5 Fe(CO) <sub>5</sub>	195.8955	-727.850	-729.521	$\pm 7.1$	170.705	439.291	33.145	†
FeCL	91.2997	251.036	249.76	$\pm 84.$	38.223	257.577	10.377	†
FeClO(s) Iron Oxychloride	107.2971	-410.994	-410.497	$\pm 0.92$	70.5	82.55	12.940	†
FeCL2(s)	126.7524	-341.833	-344.418	$\pm 0.42$	76.664	117.947	16.273	†
FeCL2	126.7504	-141	-141.59	$\pm 2.1$	57.571	299.287	14.277	†
FeCL3(s)	162.2051	-399.237	-400.399	$\pm 0.84$	96.943	147.821	19.441	†
FeCL3	162.2031	-253.13	-253.07	$\pm 5$	77.703	344.210	18.214	†
Fe0.947O(s) Wustite	71.8444	-272.037			47.990	57.488		†
FeO	71.8464	251.040	251.050	$\pm 20.9$	31.406	241.926	8.837	†
Fe(OH)2(s)	89.85968	-574.045		$\pm 2.9$	97.069	87.864		†
Fe(OH)2	89.85968	-330.536	-323.09	$\pm 2.1$	71.505	283.092	14.209	†
Fe(OH)3(s)	106.86702	-832.627		$\pm 12.6$	101.671	104.600		†
FeS(a)	87.911	-101.818	-100.116	$\pm 0.8$	50.543	60.312	9.414	†
FeS(G)	87.911	370.767			34.002	252.344		†
FeSO4(s)	151.9086	-928.848	-919.338	$\pm 8.4$	100.583	120.955	16.769	†
FeS2(s) Pyrite	119.9770	-171.544	-167.854	$\pm 2.1$	62.124	52.915	9.641	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Fe2CL4	253.5008	-431.370	-433.843	$\pm 4.2$	125.876	464.506	29.849	†
Fe2CL6	324.4062	-654.378	-658.268	$\pm 8.4$	173.665	536.945	40.448	†
Fe2O3(S) Solid-A Hematite	159.6882	-817.088			103.763	87.404		†
Fe2(SO4)3 Solid	399.8808	-2582.992		$\pm 1.7$	264.722	307.524		†
Fe3C (S) Solid-A	179.546	25.104			105.868	104.6		
Fe3O4(S) Solid-A Magnetite	231.5326	-1118.383	-1112.264		150.791	146.147	24.762	†
Ge(S) Reference Element	72.61	0.	0.		23.222	31.090	4.636	†
Ge	72.61	372.		$\pm 2.$				X†
Ge <sup>-</sup>		248.9		$\pm 1.$				X
GeBr	152.5140	137.438	144.470	$>\pm 4.2$	37.250	257.225	9.864	†
GeBr2	232.4180	-60.963	-46.00	$\pm 5.$	55.757	319.172	14.193	†
GeBr3	312.3220	-119.031	-96.164	$>\pm 50.$	78.139	363.175	18.549	†
GeBr4	392.2260	-291.	-261.29	$\pm 6.$	101.687	396.195	23.963	†
GeCl	108.0627	69.030	68.66	$\pm 18.$	36.990	245.904	9.599	†
GeCl2 singlet	143.5154	-166.9	-166.39	$\pm 5.$	53.806	296.332	13.307	†#
GeCl2 triplet	143.5154	102.3	102.525	$\pm 5.$	54.217	307.835	13.593	#
GeCl3	178.9681	-234.4	-233.69	$\pm 5.$	76.149	338.232	17.700	†#
GeCl4	214.4208	-500.9	-498.55	$\pm 5.$	95.975	348.572	21.150	†#
GeH3Cl	111.08652	57.70	67.63	$\pm 5.$	54.795	273.113	11.995	#
GeH4	76.64176	90.3	101.125	$\pm 5.$	45.011	217.303	10.748	†#
H	1.00794	217.998	216.034	$\pm 0.001$	20.786	114.718	6.197	†
H+	1.00739	1536.244	1528.084	$\pm 0.001$	20.786	108.948	6.197	†
H-	1.00849	139.031	143.246	$\pm 0.001$	20.786	108.961	6.197	†
HI	127.91241	26.5	28.676	$\pm 0.1$	29.153	206.589		*
HNO	31.01408	106.842	109.809	$\pm 0.125$	33.880	220.920	9.942	†
HNO2	47.01348	-78.452	-72.8	$\pm 0.6$	46.320	254.071	11.597	†
HNO3	63.01288	-134.3	-124.58	$\pm 0.5$	54.092	266.816	11.876	#
HNO3 <sup>+</sup> <sup>a</sup>		1026.247		$\pm 0.692$				X
OH	17.00734	37.3	37.1	$\pm 0.3$	29.886	183.737	8.813	#
OH A <sup>2</sup> $\Sigma^+$ (excited)	17.007340	430.5	425.189		29.153	179.131	13.887	#
OH+	17.00679	1299.213	1292.987	$\pm 0.042$	29.196	182.746	8.603	†
OH-	17.00789	-145.256	-139.091	$\pm 0.036$	29.141	172.542	8.606	†
HO2	33.00674	12.296	15.208	$\pm 0.25$	34.893	229.106	10.002	†#
HO2+	33.00619	1113.774	1110.565	$\pm 0.586$	33.515	225.293	9.926	#
HO2-	33.00728	-97.677	-88.811	$\pm 0.438$	37.720	226.610	10.245	†#
HPO	47.9811	-56.869			35.81	235.685		
SH	33.07394	141.87	141.212	$\pm 0.52$	32.446	195.751	9.274	#
SH-	33.074489	-86.574	-80.377	$\pm 0.12$	29.146	186.638	8.646	†
S-OH	49.07334	-6.694	-3.857	$\pm 15.$	36.704	239.812	10.149	#
HS=O	49.07334	-21.757	-18.825	$\pm 15.$	35.699	241.683	10.055	#
HO2S	65.07274	-255.88		$\pm 6$	50.708	276.742		
HSO3 HO-SO2	81.07214	-385			67.209	294.061		
HS2 Hydrothiosulpheno Radical	65.13994	104.60	107.145	$\pm 10.46$	39.703	253.304	10.484	#
H2 REFERENCE ELEMENT	2.01588	0	0		28.836	130.679	8.468	*†
H2+	2.015331	1494.677	1488.365	$\pm 7 \times 10^{-5}$	29.289	142.370	8.583	†
H2-	2.016429	235.168	241.213	$\pm 42.$	29.556	143.747	8.621	†
H2O(L)	18.01528	-285.83	-286.922		75.351	69.939	13.278	†
H2O	18.01528	-241.826	-238.922	$\pm 0.04$	33.588	188.829	9.934	†



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
H <sub>2</sub> O+	18.01473	981.815	978.491	±0.033	33.683	195.378	9.934	†
H <sub>2</sub> O <sub>2</sub> (L)	34.01468	-187.778	-193.58		89.328	109.604	22.949	†
H <sub>2</sub> O <sub>2</sub>	34.01468	-135.88	-129.89	±0.2	42.416	234.542	11.162	#
H <sub>2</sub> O <sub>2</sub> +	34.01413	895.122	894.847	±0.621	38.931	243.420	11.226	#
H <sub>2</sub> S	34.08188	-20.6	-17.67	±0.5	34.255	205.817	9.958	†
H <sub>2</sub> SO <sub>4</sub> (L)	98.07948	-814.01			138.594	156.907		*†
H <sub>2</sub> SO <sub>4</sub>	98.07948	-732.7	-720.85	±2.0	90.235	311.333	18.391	#
H <sub>2</sub> S <sub>2</sub>	66.14788	15.500	21.243		48.745	251.070	11.549	
H <sub>3</sub> O+	19.02267	603.417	604.215	±1.05	35.485	193.139	10.046	†
H <sub>3</sub> PO <sub>3</sub> gas (P(OH) <sub>3</sub> )	81.99578	-771.02	-755.56	±8.	84.344	312.678	15.622	#
H <sub>3</sub> PO <sub>3</sub> O=PH(OH) <sub>2</sub>	81.99578	-820.754	-804.3	±8.	75.978	307.665	14.635	#
H <sub>3</sub> PO <sub>4</sub> (S) Orthophosphoric acid	97.995181	-1284.5	-1266.0		106.0	110.5	16.980	X†
H <sub>3</sub> PO <sub>4</sub> (L) Orthophosphoric acid	97.995181	-1271.66	--		145.049	150.777	--	†
H <sub>3</sub> PO <sub>4</sub> (g) Orthophosphoric acid	97.995181	-1118.71	-1100.5	±8.	95.715	327.316	17.211	#
He REFERENCE ELEMENT	4.0026	0	0		20.786	126.154	6.197	*‡
He+	4.00205	2378.519	2372.322	±0.001	20.786	131.915	6.197	†
Hg(cr,L) REFERENCE ELEMENT	200.5900	0	0		27.978	76.028	9.343	†
Hg (gas)	200.5900	61.38	64.53	±0.04	20.786	174.972	6.197	†
HgBr <sub>2</sub> (solid)	360.3980	-175.31	--		75.312	170.314	---	†
HgBr <sub>2</sub> (gas)	360.3980	-91.312	-73.107		60.277	320.227	15.658	†
HgCl (gas) Calomel	236.0427	78.45			36.34	260.0		
HgCl <sub>2</sub> (solid)	236.0427	-230.12						X
HgCl <sub>2</sub> (liquid)	236.0427	-213.22						X
HgCl <sub>2</sub> (gas) from 1500 K and up	271.4954	-146.29			----	-----		
HgO (solid)	216.5894	-90.789	-86.210	±0.1	44.062	70.270	9.104	†
I	126.90447	106.76	107.161	±0.04	20.786	180.789	6.197	†
I+	126.90392	1121.345	1115.548	±0.039	20.786	182.644	6.197	†
I-	126.90502	-194.594	-187.996	±0.039	20.786	169.262	6.197	†
INO <sub>2</sub> NITRO-IODINE	172.91001	60.25		±4.2	59.366	294.432		
IO	142.90387	126		±18	33.117	239.835		
IO <sub>2</sub> O-O-I	158.90327	116.5		±40	48.727	296.374		
IO <sub>2</sub> O-I-O	158.90327	159.3		±25	46.697	281.231		
IO <sub>3</sub>	174.90267	241.9		±50	61.56	292.975		
I <sub>2</sub>	253.8089	62.444	65.500	±0.08	36.889	260.584	10.116	*
I <sub>2</sub> O I-I-O	269.80834	106.7		±40	52.359	330.647		
I <sub>2</sub> O I-O-I	269.80834	119.5		±25	51.874	308.111		
K(S) REFERENCE ELEMENT	39.09830	0	0		29.6	64.680	7.088	‡
K (gas)	39.09830	89.0	89.82	±0.4	20.786	160.470	6.197	†
K+	39.09775	514.0	508.7	±0.4	20.786	154.578	6.197	†
K <sup>-</sup>	39.09885	34.418	41.5		20.786	154.579	6.197	X†
KNO <sub>3</sub> (S)	101.10320	494.0	-488.31	±0.5	95.060	132.900		†
KNO <sub>3</sub>	101.10320	-315.833	-307.31		68.358	311.473	15.917	†
KO	55.09770	64.733	66.68	±20.	35.352	241.198	9.481	†
K <sub>2</sub> +	78.19605	524.66	521.778		38.133	259.959	10.861	X†
K <sub>2</sub> CO <sub>3</sub>	138.2055	-871.65	-862.9	±20.	89.939	345.508	19.516	†
K <sub>2</sub> O	94.19600	-74.09	-69.429		54.180	286.548	13.858	†
K <sub>2</sub> O <sub>2</sub>	110.19540	-191.566	-185.0		70.589	306.461	16.290	†
Kr REF ELEMENT	83.8	0	0		20.786	164.086	6.197	*‡
Kr+	83.79945	1356.954	1350.76	±0.001	20.786	175.613	6.197	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Mg (S) REFERENCE ELEMENT	24.30500	0	0		24.775	32.535	4.979	$\pm$
Mg(L)	24.30500	4.79			---	---	---	†
Mg (G)	24.30500	-147.10	145.90	$\pm 0.8$	20.786	148.649	6.197	†
Mg+	24.30445	891.047	883.65	$\pm 1.3$	20.786	154.412	6.197	†
MgAl2O4 (S)	142.26568	-2299.11	-2332.17	$\pm 1.3$	116.198	88.692	64.480	†
MgAl2O4 (L)	142.26568	-2106.53			---	---		†
MgBr	104.2090	6.163	13.814	$\pm 20.$	35.664	244.976	9.588	†
MgBr2(S)	184.1130	-526.0	-512.0	$\pm 2.5$	73.219	117.0	15.500	†
MgBr2(L)	184.1130	-490.41			---	---	---	†
MgBr2	184.1130	-306.743	-292.0	$\pm 10.$	58.550	296.432	14.757	†
MgCO3(S) Magnesium Carbonat	84.31390	-1096.	-1088.58	$\pm 3.$	76.108	65.090	11.630	†
MgCl	59.75770	-54.705	-54.498	$\pm 6.$	34.837	233.423	9.363	†
MgCl+	59.75715	640.196	640.196	$\pm 84.$	35.447	228.559	9.516	†
MgClF	78.75610	-569.02		$\pm 21.$	49.912	265.994		
MgCl2 (S)	95.21040	-644.3	-643.910	$\pm 0.7$	71.384	89.620	13.770	†
MgCl2(L)	95.21040	-601.58			---	---	---	†
MgCl2	95.21040	-399.170	-398.91	$\pm 5.$	56.548	272.242	13.901	†
MgF	43.30340	-232.267	-231.844	$\pm 10.$	32.580	221.097	8.969	†
MgF+	43.30285	516.868	511.093	$\pm 38.$	32.606	215.334	8.969	†
MgF2(S)	62.30181	-1124.2	-1120.3	$\pm 1.3$	61.587	57.200	9.920	†
MgF2(L)	62.30181	-1072.35			---	---	---	†
MgF2	62.30181	-735.498	-734.316	$\pm 16.7$	52.293	247.556	12.622	†
MgF2+	62.30126	582.692	577.884	$\pm 20.9$	52.450	258.148	12.415	†
MgH	25.31294	229.786	230.317	$\pm 6.$	29.587	193.197	8.682	†
MgOH	41.31234	-132.429	-130.	$\pm 12.$	46.497	232.622	11.124	†
MgOH+	41.31179	615.769	612.937	$\pm$	43.216	220.827	10.188	†
MgH2 (S)	26.32088	-75.7	-67.563	$\pm 2.$	35.35	31.1	5.31	†
Mg(OH)2(S)	58.31968	-924.35	-935.76	$\pm 2.1$	77.111	63.180	11.410	†
Mg(OH)2 gas	58.31968	-551.996	-547.	$\pm 20$	80.668	271.597	17.132	†
MgI	151.20947	61.206	63.042	$\pm 20.$	36.078	252.815	9.741	†
MgI2(S)	278.11394	-370.	-368.825	$\pm 2.0$	74.475	134.0	17.000	†
MgI2(L)	278.11394	-342.25 ?			---	---		†
MgI2	278.11394	-171.706	-168.825	$\pm 15.$	59.364	313.820	15.294	†
MgN	38.31174	288.7	289.02	$\pm 25.1$	32.733	224.838	8.989	†
MgO(S)	40.30440	-601.6	-597.441	$\pm 0.3$	37.237	26.950	5.160	†
MgO(L)	40.30440	-532.61	---		---	---	---	†
MgO	40.30440	32.261	32.671	$\pm 25.1$	32.111	213.318	8.909	†
MgS(S)	56.37100	-348.	-346.939	$\pm 4.2$	45.560	50.330	8.330	†
MgS	56.37100	120.649	120.806	$\pm 30.$	34.237	225.448	9.234	†
MgSO4(S) II	120.36860	-1288.8	-1277.45	$\pm 20.9$	96.399	91.600	15.400	†
MgSO4(L)	120.36860	-1246.59			---	---		†
MgSiO3 (S)	100.38870	-1548.92	-1539.813	$\pm 4.2$	81.927	67.768	12.113	†
MgSiO3 (L)	100.38870	-1494.86		$\pm 20.9$	---	---		†
MgTiO3(S)	120.18320	-1562.24	-1552.74	$\pm 6.3$	91.881	74.59	3.240	†
MgTiO3(L)	120.18320	-1497.63		$\pm 6.3$	---	---		†
MgTi2O5(S)	200.06200	-2491.14	-2477.25	$\pm 10.5$	146.858	135.603	5.363	†
MgTi2O5 (L)	200.06200	-2382.31		$\pm 8.4$	---	---		†
Mg2	48.61000	276.555	276.971	$\pm 0.06$	24.199	240.843	9.542	†
Mg2F4	124.60361	-1718.37	-1711.9	$\pm 37.7$	107.502	337.018	21.143	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Mg <sub>2</sub> SiO <sub>4</sub> (S)	140.69310	-2163.93	-2150.67	±4.2	118.688	95.140	4.130	†
Mg <sub>2</sub> SiO <sub>4</sub> (L)	140.69310	-2113.88		±20.9	---	---		†
Mg <sub>2</sub> TiO <sub>4</sub> (S)	160.48760	-2164.35	-2151.048	±6.3	128.574	115.102	18.836	†
Mg <sub>2</sub> TiO <sub>4</sub> (L)	160.48760	-2046.33			---	---		†
Mg <sub>3</sub> N <sub>2</sub> (S) cubic	100.92848	-461.300	-448.183?	±2.	92.049	85.00	10.500	†
MnO (S)	70.93745	-385.221			44.102	59.71		
MnO <sub>2</sub> (S)	86.93685	-520.029			54.415	53.049		
Mn <sub>2</sub> O <sub>3</sub> (S)	157.8743	-959.002			99.034	110.499		
Mn <sub>3</sub> O <sub>4</sub> Solid-A	228.81175	-1387.799			140.515	155.599		
Mn <sub>5</sub> N <sub>2</sub> (S)	302.70373	-204.2			175.724	187.443		
MnS Solid	87.00405	-214.2			49.943	78.199		
MnS <sub>2</sub> (S)	119.07005	-223.844			70.075	99.914		
Mo(cr) REFERENCE ELEMENT	95.94	0	0		23.933	28.605		*‡
MoC Solid-C	107.951	-28.451			30.878	36.652		
MoO <sub>2</sub> Solid	127.9388	-588.94			55.982	46.275		
MoO <sub>2</sub>	127.9388	-8.314			34.002	252.344		
Mo <sub>2</sub> C(S)	203.891	-53.137			60.207	65.814		
N	14.00674	472.68	470.818	±0.4	20.786	153.302	6.197	†
N+	14.00619	1881.903	1872.924	±0.044	21.285	159.799	7.117	†
N-	14.00729	485.27	489.304	±4.10	21.009	159.930	6.498	†
ND	16.0208	355.739	355.710	±8.	29.159	187.234	8.648	†
NHD Radical	17.02878	178.165	181.106	±8.	33.703	205.600	9.912	#
ND <sub>2</sub>	18.0349	181.937	184.878	±8.	34.415	204.335	9.962	†
ND <sub>2</sub> H	19.04288	-52.748	-45.684		35.976	209.279	10.074	#
ND <sub>3</sub>	20.04901	-54.501	-47.546	±0.4	38.225	203.931	10.234	†#
NF	33.00514	232.99	233.	±3.	30.228	212.908	8.738	†
NF <sub>2</sub>	52.00355	34.421	37.000	±5.	41.058	249.638	10.582	†
NF <sub>3</sub>	71.00195	-131.7	-125.98	±1.	53.497	260.812	11.855	†
NH	15.01468	358.792	358.76	±0.37	29.193	181.227	8.601	†
NH+	15.01413	1665.795	1656.29		32.775	187.651	9.495	†
NHF	34.01308	112.0	114.952	±15	35.234	230.806	10.030	†
NHF <sub>2</sub>	53.01149	-103	-96.413	±15	43.384	252.814	10.807	†
NH <sub>2</sub> AMIDOGEN RADICAL	16.02258	186.2	189.1	±1.0	33.663	194.868	9.911	#
NH <sub>2</sub> +	16.02207	1269.973	1266.648	±0.169	33.609	189.481	9.931	#
NH <sub>2</sub> -	16.02316	105.910	114.987	±0.479	33.460	189.662	9.924	#
NH <sub>2</sub> D	18.03672	-48.697	-41.627		35.157	205.591	10.018	#
NH <sub>2</sub> F	35.02102	-75	-67.889	±15.	36.474	229.534	10.105	†
NH <sub>2</sub> O	32.02202	66.270	72.925	±8.	39.380	228.059	10.488	#
NH <sub>3</sub> AMONIA RRHO calc	17.03056	-45.567	-38.513	±0.03	34.597	192.475	9.984	#
NH <sub>3</sub> AMONIA Anharmonic calc	17.03056	-45.567	-38.946	±0.03	35.630	192.770	10.043	†
NH <sub>3</sub> + cation	17.03001	943.294	944.04	±0.03	36.034	198.847	10.094	#
NH <sub>2</sub> OH Hydroxyl Amine	33.02996	-43.95	-33.809	±0.55	46.472	236.181	11.236	†#
NH <sub>4</sub> + AMONIUM ION	18.03795	644.905	637.358	±0.37	34.764	186.095	9.987	†
NH <sub>4</sub> Cl crystal	53.4912	-314.553	-311.389		86.441	94.860	22.698	†
NH <sub>4</sub> CLO <sub>4</sub> (l)	117.4888	-295.767	-277.78		128.072	184.18	25.238	†
NO	30.00614	91.271	90.767		29.862	210.748	9.179	†
NO+	30.00559	990.807	982.137	±60.	29.123	198.234	8.670	†
NO- <sup>a</sup>		81.988		±0.356				X
NOCL	65.45884	52.524	54.425	±0.5	44.623	261.590	11.364	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
NOF	49.00454	-65	-62.633	$\pm 2.0$	41.530	248.224	10.720	†
NOF3	87.00135	-187	-178.78	$\pm 7.$	68.067	277.731	13.698	†
NO2	46.00554	34.193	37.0	$\pm 0.5$	37.177	240.171	10.208	†
NO2+ <sup>a</sup> ONO+		964.409		$\pm 0.2$				X
NO2-	46.00609	-191.518	-182.482	$\pm 0.47$	37.215	236.241	10.177	†
NO2CL	81.45824	12.5	17.901	$\pm 1.$	53.246	272.128	12.205	†
NO2F	65.00394	-109	-102.92	$\pm 20$	48.999	259.287	11.347	†
NO3	62.00494	74.628	81.024	$\pm 0.69$	46.935	252.623	10.959	†
NO3+	62.00439	1292.57	1291.2	$\pm 1.09$	52.621	255.193	12.519	#
NO3-	62.00549	-312.185	-299.405	$\pm 0.65$	44.724	245.638	10.733	†#
NO3F	81.00334	15			66.958	293.171		†
N2 REFERENCE ELEMENT	28.01348	0	0		29.124	191.607	8.670	±†
N2+	28.01293	1509.509	1503.310	$5.5 \cdot 10^{-4}$	29.137	197.663	8.671	†
N2-	28.01403	148.183	154.377	$\pm 96.4$	29.194	204.539	8.674	†
N2D2 Cis	32.0416	202.857	209.788		39.025	224.095	10.308	†#
N2F2	66.01029	62.374	67.	$\pm 10$	56.569	268.216	12.869	†
N2F4	104.00709	-22	-13.491	$\pm 10$	88.384	317.531	17.812	†
N2H	29.02142	251.776	254.707	$\pm 8.$	34.662	224.507	9.973	#
N2H2	30.02936	211.859	219.	$\pm 10$	35.045	218.333	9.997	†
NH2NO2 NITRAMIDE	62.02816	-26.000	-12.346	$\pm 10$	56.672	268.548	12.164	†
H3N2 HYDRAZINE RAD	31.0373	220.659	209.946	$\pm 8.$	34.358	236.791	10.634	#
N2H4(L) Hydrazin	32.04524	50.38	--		98.839	121.545	--	†
N2H4 HYDRAZIN	32.04524	95.18	109.337	$\pm 0.5$	48.43	238.466	11.449	†
NH4NO3 (solid)	80.04344	-365.6	--	$\pm 1$	139.080	150.810	--	†
N2O (NNO)	44.01288	81.6(82.6)	85.029	$\pm 0.1$	38.628	220.01	9.581	†
N2O+	44.01233	1333.399	1329.146	$\pm 0.63$	42.263	233.859	10.623	†
N2O3	76.01168	86.631	91.2		72.733	314.736	17.121	†
N2O3+	76.01113	1036.847	1033.763	$\pm 8.99$	76.843	320.915	18.577	#
N2O3- <sup>a</sup> ONONO-		-112.297		$\pm 10.9$				X
N2O4	92.01108	11.111	20.4	$\pm 0.14$	79.168	304.451	16.741	†#
N2O5	108.01048	15.437	25.010	$\pm 0.74$	95.332	355.717	20.797	†#
N3 AZIDE RADICAL	42.02022	453.54	456.97	$\pm 3.5$	36.175	223.072	9.571	†#
N3+	42.01967	1526.92	1523.347	$\pm 3.64$	41.979	224.004	10.388	#
N3-	42.02077	187.61	197.458	$\pm 3.63$	37.031	218.207	9.354	#
N3H (s) Azidic Acid	43.02816	261.59		$\pm 0.77$				X
N3H AZIDIC ACID	43.02816	291.713	298.005	$\pm 0.65$	44.219	239.330	10.947	†#
N3H+	43.02761	1334.177	1333.176	$\pm 0.957$	47.155	248.163	11.158	#
N4H4 NH4N3 (cr)		114.14		$\pm 0.94$				X
N4H4 NH4N3 (g) ??		179.7 ?	doubtful	Existence				X
Na(cr) REFERENCE ELEMENT	22.98977	0.	0.		28.230	51.300	6.460	†
Na(g)	22.98977	107.5	107.763	$\pm 0.7$	20.786	153.719	6.197	†
Na+	22.98922	609.34	--		20.785	147.953	6.197	†
NaO2(cr)	54.98857	-261.	-264.16	$\pm 3.$	72.130	115.900	18.300	†
Na2O(cr)	61.97894	-417.98	(-413.15)	$\pm 4.2$	69.103	75.042	12.399	*†
Na2O(liq)	61.97894	-372.843	--		104.600	91.607	--	†
Na2O (g)	61.97894	-16.56	-13.710	$\pm 10.$	56.773	271.324	14.410	†
Na2O2(cr)	77.97834	-513.21	(-507.34)	$\pm 5.$	89.266	94.801	15.707	*†
Na2O2(g)	77.97834	-123.93	-117.895	$\pm 30.$	68.503	289.595	15.565	†
Ne REFERENCE ELEMENT	20.1797	0	0		20.786	146.33	6.197	*†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Ne+	20.17915	2086.966	2080.66	$\pm 0.001$	22.120	158.310	6.304	†
Ni(cr) REFERENCE ELEMENT	58.6934	0	0		25.987	29.87	4.786	*‡
NiO Solid-A	74.689	-8.314			44.309	37.991		
NiS(b) Crystal	90.7594	-87.869		$\pm 6.3$	47.121	52.986		*
NiS2(s)	122.8254	-131.381		$\pm 16.7$	70.627	71.966		*
Ni3S2(l)	240.2122	-216.325		$\pm 5$	117.75	133.871		*
Ni3S4(s)	304.3442	-301.121		$\pm 25.1$	164.813	186.484		*
O	15.99940	249.175	246.79	$\pm 0.1$	21.912	161.06	6.725	†
O singlet (excited)	15.99940	438.523	436.666	$\pm 0.002$	20.786	156.816	6.197	#
O+	15.99885	1568.787	1560.752	$\pm 0.00$ 2	20.786	154.961	6.197	†
O-	15.99995	101.846	105.813	$\pm 0.00$ 2	21.685	157.797	6.571	†
O2 REFERENCE ELEMENT	31.99880	0	0		29.378	205.149	8.680	*‡
O2 singlet (excited)	31.99880	94.418	94.409		29.485	201.915	8.689	#
O2+	31.99825	1171.828	1165.	$\pm 0.009$	30.67	205.393	9.311	†
O2-	31.99935	-48.028	-42.5		31.422	209.336	9.350	†
O3 OZONE	47.9982	141.8	144.454		39.378	239.011	10.366	†
O3+	47.99765	1356.140	1352.45	$\pm 0.33$	40.631	239.385	10.511	†
O3- Ozone Anion	47.99875	-67.049	-58.463	$\pm 0.203$	41.790	247.593	10.631	#
P(cr,white) REF. ELEMENT	30.97376	0.	0.		23.824	41.090	5.360	†
P(cr,red)	30.97376	-17.460	-15.707		21.187	22.853	3.607	
P	30.97376	316.39		$\pm 1$	20.786	163.2		†
PCL	66.42646	134.615	135.275	$\pm$	33.991	236.883	9.291	†
PCL2	101.87916	-54.292	-52.	$\pm 6.$	50.935	285.127	12.249	†
PCL2-	101.87971	-356.285	-348.	$\pm 40.$	50.861	281.466	12.453	†
PCL3	137.33186	-289.5	-286.3	$\pm 2.0$	71.592	311.708	15.932	†
PCL5	208.23726	-376.	-370.993	$\pm 2.0$	113.318	367.208	23.305	†
PF	49.97217	-52.377		$\pm 20.9$	31.616	224.968		*†
PF2	68.97057	-488.269		$\pm 20.9$	44.716	262.958		*†
PF3	87.96897	-958.457		$\pm 3.8$	58.801	273.073		*†
PF5	125.96578	-1593.300	-1582.415	$\pm 1.3$	84.703	301.026	16.538	†
PH	31.9817	230.752	231.698	$\pm 33.5$	29.175	196.381	8.648	†
PH2 Phosphonium Radical	32.989641	135.474	139.333	$\pm 8.$	34.272	212.710	9.969	#†
PH2- Phosphonium anion	32.990190	-9.265	+0.800	$\pm 10.$	34.124	205.247	9.960	†
PH3 PHOSPHINE RRHO	33.997581	11.786	19.712	$\pm 8.$	37.102	210.245	10.137	#†
P(OH)3 Metaphosphoric acid	See H3PO3							
O=P(OH)3 Orthophosphoric acid	See H3PO4							
PN	44.9805	104.776			29.667	211.126		*
PO	46.97316	-29.597		$\pm 4.2$	31.725	222.768		*
PO2	62.97256	-314.533			41.397	253.682		*
P2	61.94752	143.651		$\pm 2.1$	32.057	218.135		*
P4	123.89505	58.917		$\pm 2.1$	67.326	280.022		*
P4O6	219.89145	-2144.519		$\pm 33.5$	143.998	345.664		*
P4O10(s)	283.88904	-3010.100	-2979.479	$\pm 3.2$	215.569	231.000	34.220	†
P4O10	283.88905	-2904.154		$\pm 8.9$	188.827	403.974		*
Pb (cr) REFERENCE RLEMENT	207.2	0.	0.		24.430	36.899	6.870	†
Pb (gas)	207.2	195.2	195.88	$\pm 0.8$	20.786	175.377	6.197	†
PbBr	287.1040	64.821	73.805	$\pm 20$	36.916	272.744	10.146	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
PbBr <sub>2</sub>	367.0080	-103.908	-87.54	$\pm 7.$	56.966	339.673	15.022	†
PbBr <sub>3</sub>	446.9120	-104.011	-80.330	$\pm 80.$	80.540	385.255	19.969	†
PbBr <sub>4</sub>	526.8260	-182.436	-152.4	$\pm 80.$	104.468	427.724	25.871	†
PbCl	242.65270	8.819	10.493	$\pm 12.$	36.215	261.306	9.787	†
PbCl <sub>2</sub>	278.10540	-175.046	-173.5	$\pm 5.$	55.299	315.621	14.003	†
PbCl <sub>3</sub>	313.55810	-177.654	-175.27	$\pm 80.$	77.918	351.604	18.256	†
PbCl <sub>4</sub>	349.0108	-327.43	-325.65	$\pm 80.$	100.537	381.682	23.449	†
PbF	226.19840	-98.072	-96.853	$\pm 10.$	34.401	249.962	9.268	†
PbF <sub>2</sub>	245.19681	-443.427	-440.30	$\pm 11.$	50.981	291.532	12.573	†
PbF <sub>3</sub>	264.19521	-489.573	-485.0	$\pm 60.$	70.582	316.287	15.535	†
PbF <sub>4</sub>	283.1936	-799.925	-795.03	$\pm 60.$	90.232	331.825	19.626	†
PbI	344.10447	108.904	112.033	$\pm 4.$	37.152	280.413	10.339	†
PbI <sub>2</sub>	461.00894	-10.253	-5434	$\pm 5.$	57.182	352.613	15.247	†
PbI <sub>3</sub>	587.91341	21.755	27.35	$\pm 80.$	81.624	411.532	21.065	†
PbI <sub>4</sub>	714.81788	-41.281	-35.485	$\pm 80.$	106.276	463.806	27.521	†
PbO(S)	223.19940	-218.6	-216.61	$\pm 0.5$	46.414	67.840	9.225	†
PbO	223.19940	68.187	70.385	$\pm 4.5$	32.513	240.045	8.962	†
PbO <sub>2</sub> (S)	239.19880	-276.0	-271.41	$\pm 1.5$	60.997	71.920	10.962	†
PbO <sub>2</sub>	239.19880	136.153	139.452	$\pm 100.$	51.721	261.093	12.251	†
PbS(S)	239.2660	-99.475	-99.703	$\pm$	49.499	91.200	11.510	†
PbS	239.2660	127.945	129.797	$\pm 1.5$	35.085	251.414	9.430	†
PbS <sub>2</sub>	271.3320	244.049	245.722	$\pm 10.$	57.511	286.141	14.021	†
PbN <sub>6</sub> (S) Lead Azide	291.3	469.						X
Pd(S) REFERENCE ELEMENT	106.42	0.	0.		25.982	37.823		X
Pd	106.42	376.56			20.786	167.059		X
Pt(S) REFERENCE ELEMENT	195.084	0.	0.		25.852	41.631		X
Pt	195.084	564.840			25.542	192.406		X
Rn REFERENCE ELEMENT	222.01760	0.	0.		20.786	176.238	6.197	†
S(S) REFERENCE ELEMENT	32.066	0.	0.		22.690	33.070	4.412	††
S	32.066	277.17	274.925	$\pm 0.25$	23.674	167.832	6.657	†
SCL	67.5187	156.47	155.648	$\pm 16.7$	37.542	237.328	9.819	†
SCL <sub>2</sub>	102.9714	-17.573	-16.425	$\pm 3.3$	50.896	281.633	12.445	†
SCL <sub>2</sub> +	102.97085	901.383	896.326	$\pm 2.$	50.861	287.327	12.453	†
SF	51.0644	15.446	14.8	$\pm 6.3$	35.180	225.282	9.470	†
SF+	51.06385	994.570	988.333	$\pm 10.$	31.679	225.410	8.864	†
SF-	51.06495	-231.347	-225.2	$\pm 50.$	31.787	216.351	8.875	†
SF <sub>2</sub>	70.06281	-293.189	-291.	$\pm 10.$	44.415	256.582	11.048	†
SF <sub>2</sub> +	70.06226	706.016	701.821		44.937	263.528	11.234	†
SF <sub>2</sub> -	70.06336	-394.795	-387.485	$\pm 42.$	50.165	267.450	12.125	†
SF <sub>3</sub>	89.06121	-504.101	-500.	$\pm 20.$	63.148	285.616	13.548	†
SF <sub>3</sub> +	89.06066	393.583	392.627	$\pm 33.5$	56.224	268.977	12.409	†
SF-	89.06176	-790.124	-780.	$\pm 7.$	64.068	281.593	13.773	†
SF <sub>4</sub>	108.05961	-760.	-753.321	$\pm 20.$	76.673	296.714	15.383	†
SF <sub>4</sub> +	108.05906	416.112	415.471	$\pm 50.$	80.396	311.676	16.506	†
SF <sub>4</sub> -	108.06016	-887.464	-877.685	$\pm 33.5$	89.189	312.967	18.480	†
SF <sub>5</sub>	127.05802	-902.663	-895.	$\pm 10.$	100.085	322.275	18.811	†
SF <sub>5</sub> +	127.05746	172.644	176.574	$\pm 20.9$	89.844	298.157	16.347	†
SF <sub>5</sub> -	127.05856	-1204.622	-1191.	$\pm 10.$	101.065	317.070	19.050	†
SF <sub>5</sub> Br	206.96202	-972.8		$\pm 59$	107.075	333.654		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
SF5CL	162.51072	-1038.9		$\pm 10.5$	104.344	319.936		
SF6	146.05642	-1219.4	-1205.453	$\pm 1.5$	97.069	291.678	16.940	†
SF6-	146.05697	-1341.876	-1322.282	$\pm 29.3$	99.986	302.865	17.491	†
SN	46.07274	267.388	266.742	$\pm 50$	31.795	222.096	9.393	†
SO	48.06540	4.760	4.714	$\pm 0.18$	30.176	221.942	8.798	†
SO-	48.06595	-105.968	-100.486	$\pm 5.0$	34.425	223.679	9.467	†
SOF2	86.06221	-584.952	-580.	$\pm 50.$	57.095	279.138	12.625	†
SO2	64.0648	-296.81	-294.266	$\pm 0.21$	39.842	248.222	10.548	†
SO2-	64.06535	-408.606	-400.066	$\pm 3.5$	41.795	256.027	10.749	†
SO2CLF	118.5159	-556.472	-549.070	$\pm 21$	71.593	302.854	14.701	†
SO2CL2	134.9702	-354.802	-348.559	$\pm 2.1$	77.096	311.101	16.029	†
SO2F2	102.06161	-760.	-751.573	$\pm 8.4$	65.776	283.543	13.490	†
SO3	80.06420	-395.9	-390.156	$\pm 0.71$	50.619	256.547	11.688	†
S2	64.13200	128.60	128.292	$\pm 0.3$	32.505	228.167	9.132	†
S2-	64.13255	-37.132	-31.708	$\pm 4.0$	37.193	228.430	9.597	†
S2CL	99.58470	78.6	79.540	$\pm$	50.968	292.162	12.474	†
S2CL2	135.0374	-16.736	-16.734	$\pm 4.2$	72.776	327.237	16.521	†
S2F2 (S=SF <sub>2</sub> ) Thiothionyl fluoride	102.12881	-401.413	-397.482	$\pm 41.8$	63.128	292.833	13.718	†
FS2F (FSSF) Fluorodisulfane	102.11681	-336.435	-333.381	$\pm 41.8$	66.042	294.088	14.595	†
S2F10	254.11603	-2064.386		$\pm 29.3$	176.702	397.041		
S2O	80.1314	-56.035	-54.	$\pm 1.4$	44.114	266.968	11.129	†
S3	96.1980	144.738	146.	$\pm 4.$	48.964	276.296	11.974	†
S4	128.2640	135.632	139.	$\pm 3.$	65.944	293.565	14.280	†
S5	160.3300	132.993	136.	$\pm 4.$	87.870	354.088	19.053	†
S6	192.3960	101.315	105.	$\pm 3.$	113.165	357.812	22.787	†
S7	224.4620	111.890	116.5	$\pm 3.$	133.866	404.855	26.274	†
S8	256.528	101.277	105.	$\pm 2.$	156.503	432.546	31.573	†
Sb(s) REFERENCE ELEMENT	121.760	0	0		25.2	45.522	5.90	#
Sb(g)	121.760	264.588.			20.786	180.264	6.20	#
SbCl singlet	157.21270	177.820		$\pm 11.4$	37.948	248.179	9.750	#
SbCl2 DichloroAntimon Radical	192.66540	-98.742	-97.32	$\pm 4.27$	43.229	280.788	11.032	#
SbCl3 TrichloroAntimon.	228.11810	-313.382	-312.0	$\pm 4.48$	77.389	341.080	18.207	#
SbCl5 PentachloroAntimon	299.0235	-433.044		$\pm 9.12$	122.115	422.234	27.003	#
SbF	140.7584	-74.128			35.992	236.617	9.301	#
SbF3 TriFluoroAntimon	178.75521	-812.533			68.256	303.031		#
SbOH singlet	138.76734	68.199		$\pm 19.8$	39.595	273.714	10.471	#
SbOH triplet	138.76734	21.34		$\pm 6.4$	40.422	263.403	10.573	#
Sb(OH)2	155.77468	-279.073		$\pm 6.3$	66.186	308.869	14.798	#
SbH3 Antimonium Hydride	124.78382	144.766	153.218	$\pm 4.2$	41.217	232.745	10.493	#
Sb(OH)3	172.78202	-638.478		$\pm 4.5$	97.581	333.671	19.140	#
Sb2(g)	243.520	236.			36.412	255.882	9.894	#
Sb4(g)	487.04000	205.			79.318	354.711	18.880	#
Si(cr) REFERENCE ELEMENT	28.0855	0.	0.		19.789	18.81	3.217	†
Si	28.0855		448.32	$\pm 0.84$				X
SiC(b) Silicon carbide	40.09620	734.946	730.	$\pm 20.$	31.032	226.213	9.217	†
SiC2	52.10690	631.361	625.0	$\pm 12.$	44.227	252.239	11.685	†
SiCl	63.53820	142.363	140.327	$\pm 40.$	35.783	237.840	9.884	†
SiCl2	98.99090	-163.069	-163.2	$\pm 4.2$	51.274	281.618	12.529	†
SiCl3	134.44360	-336.272	-335.	$\pm 10.$	70.563	316.646	15.717	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/ mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
SiHCl <sub>3</sub>	135.45154	-496.222	-491.150	±4.2	75.457	313.722	16.152	†
SiCl <sub>4</sub>	169.89630	-662.2	-660.076	±0.8	90.406	331.452	19.455	†
SiF <sub>2</sub> DifluoroSilylene	66.08231	-627.014	-626.2	±16.8	44.707	256.710	11.228	#
SiF <sub>3</sub> TrifluoroSilyl Radical	85.08071	-993.365	-990.4	± 8.	59.613	282.433	13.398	#
SiHF <sub>3</sub> TriFluoroSilane	86.08865	-1207.67	-1200.5	± 5.4	63.486	277.351	13.545	#
SiF <sub>4</sub> TetrafluoroSilane	104.07911	-1614.98	-1609.4	± 4.2	73.534	282.615	15.325	#
SiO <sub>2</sub> (Lqz) Quarz	60.08430	-910.7	-905.718	±1.0	44.602	41.460	9.916	†
Si <sub>2</sub> N <sub>2</sub> O(s) Silicon Oxynitride	100.18388	-947.711			67.46	46.06		
Si <sub>3</sub> N <sub>4</sub> (a) Silicon Nitride	140.28346	-744.77			99.579	112.968		*
SiS <sub>2</sub> Solid	92.2175	-213.384			77.482	80.333		#
SnCl <sub>4</sub> TetraChloroStanum	260.52080	-478.650	-476.30	±4.2	98.459	364.549	22.340	†#
SnH <sub>3</sub> TriHydroStanum Radical	121.73382	258.153	266.252	±4.2	44.818	240.204	10.926	#
SnH <sub>4</sub> TetraHydroStanum	122.74176	162.758	174.594	±4.2	51.108	228.991	11.423	#
W(cr) Reference Element	196.8507	0	0		35.378	32.374	---	†
WO <sub>3</sub> (cr)	231.83820	-841.300	-836.587		79.705	81.640	13.280	X†
WO <sub>3</sub> gas	231.83820	-319.725	-315.000		59.164	283.127	13.268	X†
Xe REFERENCE ELEMENT	131.29	0	0		20.786	169.686	6.197	*‡
Xe+	131.28945	1176.552	1170.35		20.786	181.212	6.197	†
Zn(cr) REFERENCE ELEMENT	65.39	0	0		25.390	41.630	5.657	‡
ZnCL <sub>2</sub>	136.29540	-265.684	-		56.902	276.672	-	
ZnSO <sub>4</sub> (cr)	161.4536	-980.144	-969.95	± 4.2	99.035	110.541	17.238	†
Zr(cr) REFERENCE ELEMENT	91.2240	0.	0.		25.202	38.869	5.497	†
Zr	91.2240	599.319	598.0	± 20.9	26.642	181.346	6.816	†
ZrCl <sub>2</sub>	162.12940	-185.750	-185.316	± 20.9	57.677	292.562	14.244	#
ZrCl <sub>4</sub>	233.0348	-869.980	-868.682	± 2.1	98.234	367.710	22.561	#
ZrF	110.22240	82.84	83.666	± 20.9	33.420	243.7	9.084	#
ZrF <sub>2</sub>	129.22080	-558.150	-555.657	± 20.9	48.652	283.430	11.829	#
ZrF <sub>4</sub>	167.21762	-1673.6	-1669.395	± 3.3	86.810	319.300	18.942	#
ZrN(cr)	105.23074	-371.238	-367.996		40.443	38.861	6.590	†
ZrN	105.23074	713.372	714.341		31.661	233.491	8.863	†
ZrO	107.22340	83.923	84.790		34.374	228.400	8.970	†
ZrO <sub>2</sub> (cr)	123.22280	-1100.3	-1094.874	±0.7	55.920	50.390	8.751	†
ZrO <sub>2</sub>	123.22280	-317.043	-314.874	±>15.	46.062	273.750	12.008	†

<sup>a</sup> Values from Active Thermochemical Tables ATcT A

\* The polynomials are pinned at 1000 K, therefore the property values are not exact at 298 K. All other polynomials are pinned at 298 K, therefore the property values are exact.

# 9 term NASA polynomials are available in the NEWNASA.TXT file for this species.

† 9-term NASA polynomials are available in <http://cea.grc.nasa.gov>

‡ 9-term NASA polynomials for all Reference Elements are available in the ELEMENTS.DAT file.

X Polynomials not available



Table 6 (continued)