TABLE 5

COEFFICIENTS FOR MOLECULAR PARTITION FUNCTIONS AND EQUILIBRIUM CONSTANTS

MOL.	N STATES	DO (EV)	EQUILIBRIUM CONSTANT B0	B1	B2	B3	B4	B5	MAX. ER.	*	PARTITION FUNCTION A0	A1	A2	A3	A4	MAX. ER.
LI H	1	2.4287	9.9506	-0.5163	0.1833	-1.7211	1.2805		0.0031	*	3.2564	-2.1799	0.7236	-0.1052		0.0026
BE H	3	2.0340	9.6644	-0.6592	-0.2541	-0.2677			0.0033	*	3.2507	-2.0115	0.8852	-0.3258		0.0030
B H	5	3.4200	10.5064	0.1929	-0.3299	-1.4246	0.6362		0.0034	*	3.1862	-2.6821	0.5142	0.6959		0.0056
C H	5	3.4650	10.5263	-0.5284	-0.7239				0.0027	*	3.3586	-2.0656	0.9624	-0.2239		0.0008
N H	4	3.4700	10.4609	-0.7387	-0.5713				0.0034	*	3.0735	-1.8501	0.9607	-0.3935		0.0019
O H	2	4.3920	10.7881	-0.8762	-0.5436				0.0022	*	3.0929	-1.6778	0.6743	-0.1874		0.0007
H F	1	5.8690	11.2835	-0.9228	-0.5642				0.0040	*	2.4164	-1.6132	0.6357	-0.1767		0.0008
NA H	3	1.8800	9.7127	-0.3175	0.2445	-2.4962	2.0335		0.0053	*	3.5453	-2.3457	0.8557	-0.1685		0.0032
MG H	4	1.3400	9.2846	-0.3587	-0.1220	-1.5627	1.3047		0.0034	*	3.6704	-2.2682	0.9354	-0.2597		0.0011
AL H	4	3.0600	10.3999	0.0733	-1.6121	0.0063	0.7650		0.0058	*	3.3209	-2.5909	1.7415	-0.7636		0.0057
SI H	2	3.0600	10.2379	-0.7143	-0.6404	0.1156			0.0031	*	3.6908	-1.9801	0.7704	-0.2247		0.0021
P H	4	3.0200	10.1061	-0.7236	-0.2853	-0.2032			0.0014	*	3.4957	-2.0871	0.9617	-0.2598		0.0007
S H	3	3.5500	10.4145	-0.8190	-0.5524				0.0014	*	3.4935	-1.8385	0.5852			0.0036
H CL	1	4.4336	10.9013	-0.8274	-0.5974				0.0025	*	2.8005	-1.7476	0.5310			0.0024
K H	1	1.8600	9.5373	-0.6621	1.4043	-3.7901	2.5004		0.0034	*	3.7667	-2.2837	0.5043	0.1196		0.0051
CA H	9	1.7000	9.1952	-0.8802	1.1610	-2.5221	1.3514		0.0015	*	3.8411	-2.3891	1.3578	-0.6893		0.0042
CR H	2		9.8937	-1.2266	1.1519	-1.9385	0.9790		0.0025	*	4.0929	-2.2491	0.8923	-0.1787		0.0031
MN H	2	2.5000	9.5870	-0.7116	0.8607	-2.8120	1.8726		0.0028	*	4.1860	-2.1839	0.8747	-0.2513		0.0016
CO H	2		10.3877	-0.8745	-0.0412	-1.7427	1.4621		0.0022	*	4.1047	-2.2620	0.4803	0.2721		0.0060
NI H	4	3.0700	10.7821	-0.4987	-1.0040	0.3197			0.0037	*	3.6736	-2.3271	1.0818	-0.5338		0.0037
CU H	3	2.7300	10.2359	-0.8631	-0.2045	0.5079	-0.7366		0.0027	*	3.1001	-2.1456	1.1944	-0.5914		0.0054
ZN H	4	0.8510	9.3436	-0.3528	-0.0866	-1.2327	0.8192		0.0005	*	3.6197	-2.1349	0.3017	0.3458		0.0035
GA H	3	2.8400	10.3713	-0.3071	-1.3737	0.0238	0.5134		0.0055	*	3.3100	-2.3703	1.4724	-0.7575		0.0046
GE H	2	3.3000	10.0536	-0.8571	-0.8573				0.0013	*	3.7954	-2.0472	0.6234			0.0036
AS H	1	3.6000	10.1156	-1.1074	0.3885	-0.5746			0.0019	*	3.5022	-1.7207	0.3759			0.0036
SE H	1	3.2000	10.2854	-1.1036	-0.3013				0.0017	*	3.5571	-1.6887	0.3912			0.0031
H BR	1	3.7580	10.7059	-0.8545	-0.5918	0.1995			0.0012	*	2.9356	-1.8051	0.5439			0.0023
RB H	2		9.4673	-0.6489	1.3539	-3.5418	2.2686		0.0026	*	3.8516	-2.2990	0.4213	0.2106		0.0058
SR H	6	1.6600	9.1300	-1.0867	1.9505	-3.5983	1.8586		0.0025	*	3.9406	-2.3979	1.2564	-0.5865		0.0029
PD H	1		10.0979	-2.2770	-0.0175	2.7905	-2.2384		0.0054	*	3.3378	-1.7316	0.3697			0.0037
AG H	6	2.2800	10.0411	-0.4123	-0.7461	0.1382			0.0015	*	3.2301	-2.0994	0.8105	-0.2140		0.0011
CD H	4	0.6780	9.2759	-0.4191	-0.6388	0.1624			0.0029	*	3.6946	-2.0809	0.6389	-0.1625		0.0030
IN H	4	2.4800	10.1447	-0.3957	-1.7087	0.5557	0.5123		0.0044	*	3.4418	-2.4303	1.4516	-0.6835		0.0047
SN H	1	2.7300	9.8503	-1.4863	-0.6936	0.2966			0.0036	*	3.8321	-1.7739	0.3402			0.0041
SB H	1		9.9235	-1.0973	0.4311	-0.4708			0.0032	*	3.7208	-1.7994	0.3179			0.0041
TE H	1		10.0058	-1.0836	-0.0154	-0.1301			0.0017	*	3.7592	-1.7365	0.3667			0.0037
H I	1	3.0541	10.4946	-0.7350	-0.4527				0.0025	*	3.1038	-1.8753	0.5591			0.0028
CS H	1	1.8100	9.4674	-1.1765	2.7899	-4.0266	-0.5222	2.6745	0.0048	*	3.9070	-2.2534	0.3373	0.2409		0.0052
BA H	9	1.9500	9.2562	-0.9600	-1.9128	2.8211	3.7826	-6.1227	0.0101	*	4.1275	-3.4445	3.4729	-1.6164	-0.6508	0.0128
LA H	1		10.5707	-2.0868	0.6501	-0.3842			0.0029	*	3.8330	-1.8516	0.2606			0.0040
YB H	5	1.9300	9.1165	-0.8337	2.3885	-6.1903	4.1950		0.0063	*	3.8992	-2.3567	1.0469	-0.3525		0.0029
LU H	1		10.5132	-1.1430	0.3964	-1.8500	1.4373		0.0026	*	3.4069	-2.0439	0.5556			0.0035
PT H	6	3.4400	10.5855	-0.8305	-0.9753	0.7861	-0.6278		0.0012	*	3.6862	-2.0426	1.1143	-0.5023		0.0045
AU H	2	3.2200	10.3037	-1.0665	-0.0737	0.4760	-0.7257		0.0023	*	3.0587	-1.9182	0.7472	-0.2103		0.0020
HG H	3	0.3744	9.2184	-0.5946	0.1954	-0.5625			0.0021	*	3.7548	-1.9107	-0.1771	0.5461		0.0020
TL H	1	1.9700	9.8718	-0.4509	-0.8717	0.5256	-0.0995		0.0042	*	3.4880	-2.4274	1.2776	-0.4865		0.0054
PB H	3	1.5900	9.1386	-0.9871	-0.4793	1.3671	-1.1166		0.0040	*	4.0319	-2.4374	1.4150	-0.5829		0.0058
BI H	3	2.9000	9.6707	-0.2999	-0.2473	-1.0153	0.6873		0.0004	*	3.9292	-2.3670	0.8067			0.0038
HE H +	1	1.8450	10.1667	-0.4814	-0.6444	-0.7916	0.8534		0.0015	*	2.3613	-1.9733	0.6761	0.0794		0.0060
BE H +	2	3.1400	9.7188	-0.7267	0.0041	-1.0889	0.7404		0.0010	*	2.8969	-1.9119	0.5829			0.0036