

TABLE 5—Continued

MOL.	N STATES	D0 (EV)	EQUILIBRIUM CONSTANT					MAX. ER.	*	PARTITION FUNCTION					MAX. ER.
			B0	B1	B2	B3	B4			A0	A1	A2	A3	A4	
B H +	2	1.9500	10.3048	-0.7004	-0.5024			0.0005	*	3.0915	-1.8213	0.5252			0.0020
C H +	4	4.0850	10.7018	0.0994	-1.4610	-0.8279	1.3625	0.0035	*	2.8849	-2.6920	1.6342	0.6912	-1.3638	0.0038
N H +	4	3.3900	9.6574	-0.6294	-0.6294	0.1927		0.0014	*	3.5792	-1.9573	0.9387	-0.4781		0.0040
O H +	3	5.0900	10.4950	-0.6799	-0.9224	0.3310		0.0029	*	3.0879	-1.8739	0.9959	-0.4405		0.0034
H F +	2	3.4230	10.6684	-0.6549	-0.9526	0.2645		0.0009	*	3.2093	-1.9027	0.9429	-0.3415		0.0012
NE H +	1	2.0800	10.1080	-0.8691	-0.4086			0.0022	*	2.5352	-1.6309	0.4086			0.0022
MG H +	2	2.0800	9.4108	-0.5435	0.0987	-1.7288	1.3461	0.0035	*	3.2458	-2.0802	0.6259			0.0039
AL H +	2		9.7925	-0.7214	0.4948	-0.8627		0.0012	*	3.6272	-1.8270	-0.3655	0.6606		0.0031
SI H +	2	3.1700	10.5758	-0.7532	-0.6480	0.1410		0.0036	*	3.0519	-1.9409	0.7783	-0.2512		0.0027
P H +	1	3.3600	9.7604	-1.1045	0.3654	-0.5871		0.0022	*	3.5374	-1.7004	0.3861			0.0033
S H +	1	3.4800	10.2741	-0.9924	-0.2456	-0.2060		0.0009	*	3.3283	-1.6545	0.4028			0.0026
H CL +	2	4.6530	10.4094	-0.8021	-0.6304			0.0025	*	3.4719	-1.8460	0.7283	-0.2012		0.0018
ZN H +	2	2.5000	9.5271	-0.4794	-0.5934			0.0043	*	3.1362	-2.0520	0.7530	-0.1462		0.0014
H BR +	2	3.8940	10.2047	-0.9225	-0.5992	0.2723		0.0020	*	3.5928	-1.8837	0.7143	-0.1815		0.0016
CD H +	2	2.1000	9.4122	-0.4222	-0.6361			0.0037	*	3.2572	-2.0778	0.6361			0.0037
HG H +	1	2.9930	9.5121	-0.5024	-0.6184			0.0036	*	3.1604	-2.0039	0.6274			0.0041
C N	3	7.7600	11.4479	-0.4840	-0.4160	-0.9435	0.8380	0.0015	*	4.0078	-2.1514	0.9226	-0.1671		0.0033
C O	2	11.0920	12.2263	-0.8829	-0.1230	-0.3226		0.0011	*	3.6076	-1.7608	0.4172			0.0024
C F	3	5.6700	11.1538	-0.6431	-0.4255			0.0035	*	4.5449	-1.9879	0.4598			0.0037
SI C	1	4.6400	10.8445	-0.9184	0.1532	-0.3771		0.0012	*	5.1477	-1.8671	0.2404			0.0038
C P	4	5.2800	11.0579	-0.4737	0.1729	-1.2021	0.5631	0.0025	*	4.6258	-2.3994	0.7464	0.0605		0.0044
C S	4	7.3550	11.8298	-0.8130	-0.5170	1.1553	-1.2249	0.0036	*	4.1646	-1.9348	0.8034	-1.3669	1.1561	0.0030
C CL	2		10.7975	-0.5818	-0.3397			0.0015	*	5.0103	-2.0870	0.3565			0.0034
C SE	2	5.9800	11.6323	-0.8887	-0.4754	0.8627	-0.7308	0.0020	*	4.4060	-2.0380	0.6731	-0.3284		0.0053
C BR	1	4.1100	10.5031	-0.8128	0.0167			0.0033	*	5.3299	-1.9319	0.1386			0.0025
RH C	4	6.0100	11.8689	-1.0481	-0.5630	0.3225		0.0012	*	4.7382	-2.2834	0.9149	-0.3151		0.0014
IR C	4	6.4500	11.6317	-1.0444	0.0162			0.0042	*	4.9037	-2.3935	0.6410			0.0028
PT C	4	6.2800	12.0345	-0.6227	-0.8549	0.2473		0.0034	*	4.4772	-2.3097	1.1982	-0.6348		0.0039
C N +	3	4.8500	12.0523	-0.3741	-0.6714	-0.7355	0.6846	0.0010	*	3.7429	-2.2415	0.9459	-0.1119		0.0043
C O +	2	8.3380	11.5907	-0.7647	-0.4319			0.0019	*	3.9001	-1.8498	0.6943	-0.2230		0.0029
B N	2		10.6476	-0.6812	-0.0958	-0.3121		0.0018	*	4.5916	-1.9257	0.4475			0.0025
N O	2	6.4968	11.2253	-0.8143	0.0446	-0.4529		0.0033	*	4.3073	-1.8255	0.3765			0.0019
N F	3	3.5000	10.8509	-0.5611	-0.4198			0.0038	*	4.5511	-2.0680	0.5972	-0.1613		0.0019
AL N	2		10.1571	-0.5225	-0.1325	-0.2400		0.0021	*	5.3348	-2.1160	0.5845	-0.2548		0.0035
SI N	6		11.0504	-0.4223	-0.4462	-0.2266		0.0042	*	4.6570	-2.3587	0.8819	-0.1642		0.0023
P N	2	6.3600	11.2316	-1.0111	0.6714	-0.8076		0.0029	*	4.1665	-1.8848	0.3521			0.0026
N S	5	4.8000	10.9036	-0.7786	0.0941	-0.3808		0.0010	*	4.8052	-1.9619	0.3140			0.0019
N CL	2		10.6045	-0.6697	-0.0703	-0.2794		0.0021	*	4.9171	-1.9905	0.3045			0.0010
TI N	1	4.9000	11.7421	-1.7267	1.5855	-1.3639		0.0022	*	4.5568	-1.8253	0.2914			0.0041
AS N	1		11.1252	-0.9863	0.6970	-0.7720		0.0022	*	4.4116	-1.9312	0.3194			0.0023
N SE	6	4.0000	10.7173	-0.6078	-0.4482	0.3251		0.0033	*	5.0500	-2.2744	0.7939	-0.5283		0.0064
ZR N	1	5.8100	11.6496	-1.8280	0.8730	-0.7237		0.0020	*	4.7625	-1.8648	0.2434			0.0038
NB N	1		11.4059	-1.6909	0.9973	-1.1792		0.0022	*	5.2229	-1.8645	0.2439			0.0038
N O +	1	10.9506	11.6210	-0.8373	0.0676	-1.0507	0.6864	0.0007	*	3.5649	-1.7328	0.4241			0.0024
N S +	1	6.3000	11.2307	-0.8277	0.5112	-1.3707	0.7033	0.0005	*	4.1450	-1.8975	0.3832			0.0020
LI O	2	3.4900	10.0377	-0.4691	0.7661	-2.2854	1.3395	0.0016	*	4.9296	-2.2751	0.2384	0.2587		0.0016
BE O	6	4.6000	10.6366	0.5176	-0.4647	-3.7714	3.3677	0.0045	*	4.1294	-3.1941	1.1968	2.3269	-2.4715	0.0035
B O	4	8.2800	11.6221	-0.7011	-0.4788			0.0022	*	3.9953	-1.8665	0.5965	-0.1617		0.0033
F O	1	2.2300	11.0588	-0.6355	-0.2688	-0.1683		0.0007	*	4.7283	-1.9565	0.3311			0.0018
NA O	1	2.6000	10.0152	-0.8008	1.1032	-2.6609	1.7389	0.0033	*	5.3711	-1.9284	0.1449			0.0026

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