

TABLE 5—Continued

MOL.	STATES	N	DO (EV)	EQUILIBRIUM CONSTANT					MAX. ER.	PARTITION FUNCTION					MAX. ER.
				B0	B1	B2	B3	B4		A0	A1	A2	A3	A4	
CS	CL	1	4.5800	9.9334	-1.1912	2.8233	-3.8854	-0.5854	2.7110	6.0479	-2.3133	0.2312	0.1311		0.0048
BA	CL	10	4.5500	9.9594	-1.9957	0.9232	2.2392	-2.6168		6.0299	-2.5102	1.0500	-0.5580		0.0031
YB	CL	3		9.6866	-1.0826	3.0713	-6.6055	4.3000		5.9687	-2.1767	0.2766			0.0029
AU	CL	1	3.5000	10.4491	-0.9692	0.4074	-0.2975			5.5640	-2.0523	0.2002			0.0008
HG	CL	1	1.0400	9.6012	-0.4731	-0.0125	-0.2218			6.0249	-2.1049	-0.0366	0.2703		0.0031
TL	CL	2	3.8200	10.2434	-0.7136	-0.0901	0.0752			5.7692	-2.2258	0.4817	-0.2245		0.0013
PB	CL	3	3.1000	9.8253	-1.2422	0.4309	0.9152	-1.2224		5.9996	-2.2534	0.4921	-0.1698		0.0010
AL	SE	2	3.4600	10.7857	-0.7858	-0.1407				5.4873	-2.0722	0.2604			0.0024
SI	SE	1	5.6400	11.3895	-0.9755	-0.0901				5.1075	-2.0100	0.2322			0.0011
CU	SE	3	2.5800	10.0783	-0.9668	-0.9568	-0.6674			6.1556	-2.3030	0.1452			0.0023
GE	SE	1	4.9800	11.2384	-1.1163	0.3775				5.5644	-2.0873	0.2463			0.0023
K	BR	1	3.9100	9.7968	-0.7823	1.8098	-3.8842	2.5552		6.0128	-2.3146	0.1345	0.2360		0.0053
SI	TE	1	4.6400	11.1445	-1.0274	0.2402	-0.1432			5.3406	-1.9922	0.1831			0.0013
GE	TE	1	4.2400	11.0317	-1.1431	-0.1381	-0.0535			5.8258	-2.0901	0.2184			0.0027
K	I	1	3.3100	9.6625	-0.7210	1.8703	-3.9239	2.5006		6.1888	-2.3327	0.2099	0.1594		0.0052
H	H	1	4.4781	11.1759	-0.8735	-0.7470	0.2748			1.6498	-1.6265	0.7472	-0.2751		0.0007
H	H	1	2.6508	9.9835	-0.0664	-1.4979	-0.0195	0.7486		2.5410	-2.4336	1.4979	0.0192	-0.7483	0.0054
HE	HE	1	2.3650	10.2190	-0.4011	-0.6310				3.2041	-2.0989	0.6310			0.0029
LI	LI	4	1.0460	9.4736	-0.3274	1.1962	-3.5541	2.4491		4.6515	-2.5580	0.5835			0.0041
B	B	2	3.0200	11.0585	-0.4932	0.3893				4.2793	-2.0492	0.4345			0.0029
C	C	8	6.2100	11.4576	-0.4458	-0.1818				4.3091	-2.2406	0.4865	-0.2049		0.0012
C	C	1	5.3200	11.4535	-0.7842	-0.0300	-0.3124			4.1166	-1.8188	0.2984			0.0041
N	N	1	9.7594	11.8838	-0.8915	0.2929	-1.4220	0.9007		3.2643	-1.7303	0.4192			0.0025
N	N	4	8.7128	11.8072	-0.4420	-0.5843	-0.9278	0.8821		3.6830	-2.1583	0.9929	-0.2181		0.0031
O	O	6	5.1156	11.8558	-0.5309	-0.6214				4.0636	-2.0779	0.7660	-0.2111		0.0016
O	O	2	6.6630	11.5549	-0.7335	-0.3005	-0.1753			4.0194	-1.8480	0.4661			0.0027
F	F	1	1.6020	11.6249	-0.3917	-0.5115	-0.1205			4.0355	-2.1726	0.4608			0.0036
NE	NE	1	1.3000	10.2518	-0.6359	-0.2103				4.6665	-1.9305	0.1411			0.0026
NA	NA	4	0.7200	9.2096	-0.1176	1.1635	-5.6561	8.6389	-4.7450	5.6752	-2.6810	0.6626	-0.1283		0.0020
MG	MG	2	0.0501	8.6463	-1.6726	1.6431	-3.3322	2.4266		5.6533	-1.0891	-0.0121	-0.1854		0.0008
AL	AL	2	1.5500	10.3474	-0.2333	-0.2761	-0.7144	0.6243		5.5538	-2.3365	0.5754	-0.2119		0.0011
SI	SI	3	3.2100	11.0799	-0.7830	-0.3694	0.8076	-0.8107		5.2617	-2.1485	0.5647	-0.2985		0.0037
P	P	4	5.0330	11.2490	-0.9821	0.2367	0.8887	-1.3142		4.4984	-2.1415	1.1375	-1.8111	1.2663	0.0017
P	P	6	4.9900	10.7616	-0.8035	0.3322	0.0919	-0.7295		5.2762	-2.2351	0.4167	-0.1852		0.0039
S	S	2	4.3693	11.2917	-0.6065	-0.1125	-0.3562			5.0796	-2.1967	0.4101			0.0030
S	S	1	5.3700	10.9811	-0.9318	0.4797	-0.6452			5.0598	-1.8928	0.2034			0.0034
CL	CL	1	2.4794	11.2793	-0.5356	-0.4665				4.7438	-2.1109	0.3280			0.0033
K	K	4	0.5140	8.9949	-1.1018	3.7043	-6.1302	3.2656		6.2963	-2.3873	0.2118			0.0041
CU	CU	3	2.0300	10.1749	-0.9712	1.1405	-0.8963			5.4806	-2.4706	0.8867	-0.4736		0.0018
AS	AS	5	3.9600	11.0864	-0.7253	-0.2214	1.2187	-1.1896		5.2506	-2.4520	1.5981	-1.9349	0.9330	0.0023
SE	SE	2		11.0950	-0.9844	0.0343	0.2123			5.7320	-2.1070				0.0029
SB	SB	1	3.0900	11.0023	-1.2817	1.0114	0.0151	-0.7954		5.7012	-2.0571	0.1630			0.0012
TE	TE	2	2.6770	10.7951	-0.7579	0.4198	0.9161	-1.1418		6.1915	-2.4514	0.0164	0.1181		0.0035
I	I	1	1.5424	10.6380	-0.4931	-0.0491				5.9902	-2.2284	0.0271			0.0028