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Empirical parameters for calculating cation–oxygen bond valences

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NO	INDCA	1965	314	0.000 (1)	K2 #B CO (N=02) B
CA(2)-O					
60	AMMIA	1966	50	1.000 (2)	CA AL B.04
61	AMMIA	14	675	1.000 (2)	CA MG (C.03)2
62	ACORA	10	567	1.030 (2)	*CALCITE* CA C.03
63	CHBAA	75	27	2.000 (1)	*ARAGONITE* CA C.03
64	JCPSA	26	503	1.000 (1)	CA (O.H)2
65	ACORA	17	585	2.020 (3)	CA O
66	FRJUA	6	725	2.020 (3)	BA CA FE4.08
67	CHDCA	270	572	1.000 (2)	CA V2.06
68	ACBCA	27	648	1.000 (2)	GAMMA CA2 51.04
69	ACBCA	27	648	1.000 (2)	GAMMA CA2 51.04
70	ZEKGA	125	255	1.070 (1)	CA2 NA H 513.09
71	ZEKGA	125	255	1.070 (1)	CA2 NA H 513.09
72	TIPMA	10	11	1.000 (2)	M6 CA 51.04
73	ACORA	20	295	1.110 (2)	CA12 BE17 O29
74	ACORA	20	295	1.110 (2)	CA12 BE17 O29
75	ACORA	21	337	1.060 (2)	CA3 V10.02B (H2.O)17
76	ACORA	21	337	1.070 (2)	CA3 V10.02B (H2.O)17
77	ACBCA	27	2611	1.050 (1)	CA2 FE AF O5
78	AMMIA	52	707	2.010 (2)	CA MN (SI.03)2
79	AMMIA	52	707	2.030 (3)	CA MN (SI.03)2
80	ACBCA	27	648	1.000 (2)	CA2 MN (P.04)2 (H2.O)2
81	ACBCA	27	648	1.000 (1)	CA B2.04-III
82	ACBCA	25	555	1.000 (1)	CA B2.04-III
83	ACBCA	25	555	1.000 (1)	CA B2.04-III
84	ACBCA	26	1140	1.000 (1)	CA2 FE2 O5
85	INDCA	7	1140	1.000 (1)	ALPHA CA2 P2.07
86	INDCA	7	1140	1.000 (2)	ALPHA CA2 P2.07
87	ACORA	16	690	1.000 (1)	CA B2.04-I
88	ZEKGA	132	241	1.000 (1)	CA B3.05 (O.H)
89	ZEKGA	132	241	1.000 (1)	CA3 B2.06
90	AMMIA	1969	142	1.000 (1)	CA N.04
91	ACORA	16	665	1.000 (1)	CA NA2 (S.04)2
92	ZEKGA	122	170	1.000 (2)	CA3 AL2 (SI.04)3
93	ZEKGA	122	170	1.000 (1)	CA B SI.04 O.H
94	ACORA	21	442	2.010 (2)	BETA-CA2 P2.07
95	ACORA	21	442	1.000 (2)	BETA-CA2 P2.07
96	ACORA	21	442	1.000 (2)	BETA-CA2 P2.07
97	ACORA	21	442	2.000 (2)	BETA-CA2 P2.07
SC(3)-O					
67	ZEKGA	122	136	3.000 (1)	SC2.05
68	ZEKGA	122	136	2.000 (1)	SC2.03
69	ICXN	45	451	2.000 (3)	SC2 SC2.07
70	ZAACCA	45	130	3.000 (3B)	LI SC.02
71	JCPSA	45	245	3.000 (2B)	SC2 (H.04)3
72	ZAACCA	45	245	2.000 (2B)	CA SC2.04
73	ZAACCA	45	245	2.000 (2B)	CA SC2.04
74	ACORA	5	677	3.000 (1B)	SC P.04
75	JCPSA	56	154	3.310 (1B)	CA V.04
TI(4)-O					
74	ZAACCA	408	50	4.130 (14)	CA2 TI.03
75	ACBCA	29	2006	3.950 (5)	CA2 TI.04
76	ACBCA	24	1327	4.110 (17)	CA TI.05
77	CHDCA	270	572	3.000 (5)	CA2 TI.05
78	ZEKGA	125	255	4.000 (2.0)	CA2 TI.05 SI2.07
79	JCPSA	26	503	4.000 (2)	*MUTILE* TI.02
80	ACORA	17	585	4.000 (1)	*MUTILE* TI.02
81	ACORA	17	585	4.000 (1)	*MUTILE* TI.02
82	ACORA	17	585	4.000 (2)	CA TI.03
83	ACORA	17	585	4.000 (2)	CA TI.07
84	ACORA	17	585	4.000 (2)	CA TI.07
85	ACORA	17	585	4.000 (2)	CA TI.07
86	ACORA	17	585	4.000 (2)	CA TI.07
87	ACORA	17	585	4.000 (2)	CA TI.07
88	ACORA	17	585	4.000 (2)	CA TI.07
89	ACORA	17	585	4.000 (2)	CA TI.07
90	ACORA	17	585	4.000 (2)	CA TI.07

66	ACORA	21	974	4.11(12)	TH T12 06
60	JOPSA	32	1515	3.95(12)	BA T14 09
60	JOPSA	32	1515	4.03(10)	BA T14 09
69	ACBCA	25	1444	4.20(13)	BA5 T15 011
69	ACBCA	25	1444	3.92(9)	BA5 T15 011
69	ACBCA	25	1444	4.03(9)	BA5 T15 011
69	ACBCA	25	1444	4.05(10)	BA5 T15 011
69	ACBCA	25	1444	3.82(6)	BA5 T15 011
72	CSGMC	1	1	3.95(3)	BA T16 013
72	CSGMC	1	1	3.96(3)	BA T16 013
72	CSGMC	1	1	4.01(3)	BA T16 013
72	CSGMC	1	1	4.02(2)	BA T16 013
72	CSGMC	1	1	3.85(3)	BA T16 013
72	CSGMC	1	1	3.97(3)	BA T16 013
69	ZEKGA	129	222	4.11(2)	BA T1 S13.09
70	ACBCA	26	1645	3.72(6)	BA6 T117 040
70	ACBCA	26	1645	3.59(9)	BA6 T117 040
70	ACBCA	26	1645	4.33(9)	BA6 T117 040
70	ACBCA	26	1645	3.69(9)	BA6 T117 040
70	ACBCA	26	1645	3.90(7)	BA6 T117 040
70	ACBCA	26	1645	4.32(9)	BA6 T117 040
70	ACBCA	26	1645	4.15(6)	BA6 T117 040
70	ACBCA	26	1645	3.59(9)	BA6 T117 040
70	ACBCA	26	1645	3.82(7)	BA6 T117 040
70	ACBCA	26	1645	4.20(6)	BA6 T117 040
70	ACBCA	26	1645	3.66(6)	BA6 T117 040

TI(3)-0

66	ACORA	9	121	2.93(15)	T12 CA.04
63	PHRVA	130	2230	3.02(9)	T12.03

V(5)-0

73	CJCHA	51	1004	3.05(7)	ZN2 V2 07
68	ACBCA	24	252	3.13(12)	Y V.04
71	CJCHA	49	1825	4.34(4)	MG3 (V.04) 2
73	ACBCA	29	2304	4.94(5)	CO3 (V.04) 2
73	ACBCA	29	2304	4.74(2)	N13 (V.04) 2
71	CJCHA	49	3056	4.93(9)	ZN3 (V.04) 2
67	CJCHA	49	2297	4.98(16)	CO2 V2.07
72	JSSCB	4	29	3.03(5)	FE V.04
72	JSSCB	4	29	4.69(5)	FE V.04
72	JSSCB	4	29	4.93(5)	FE V.04
73	JSSCB	5	536	4.96(1)	LI3 V.04
73	JSSCB	6	536	5.00(2)	LI3 V.04
74	ACBCA	30	2907	4.92(7)	CO2 V2.07
74	ACBCA	30	2907	4.65(6)	CO2 V2.07
70	INOCA	9	2259	3.11(5)	GA2 V.04 CL
71	ACBCA	27	2124	3.36(6)	NA3 V.04 (H2.0) 12
73	ZEKGA	137	67	3.20(6)	CA3 (V.04) 2
73	ZEKGA	137	67	3.31(11)	CA3 (V.04) 2
73	ZEKGA	137	67	3.37(15)	CA3 (V.04) 2
60	ZEKGA	114	257	4.93(26)	N-H4 V.03
60	ZEKGA	114	257	4.90(7)	K V.03
66	INOCA	5	1604	4.90(13)	CS V3.06
68	INOCA	5	1606	5.30(11)	CS V3.06
72	CJCHA	50	3619	5.14(2)	MG V2.06
74	ACBCA	33	736	4.96(15)	CU V2.06
70	CHUCA	270	952	5.10(7)	CA V2.06
60	CANLA	6	446	4.55(22)	CA V2.06 (H2.0) 2
60	CANLA	6	446	5.45(24)	CA V2.06 (H2.0) 2
74	ACBCA	30	2491	3.14(2)	MG2 V2.07
74	ACBCA	30	2491	4.62(1)	MG2 V2.07
60	ZEKGA	114	257	4.00(15)	K V.03 H2.0
66	ACORA	21	397	3.05(3)	CA3 V10.026 (H2.0) 17
66	ACORA	21	397	3.09(3)	CA3 V10.026 (H2.0) 17
66	ACORA	21	397	3.01(3)	CA3 V10.026 (H2.0) 17
66	ACORA	21	397	3.06(3)	CA3 V10.026 (H2.0) 17
66	INOCA	5	967	4.97(5)	Z2 ZN2 V10.026 (H2.0) 16
66	INOCA	5	967	5.46(5)	Z2 ZN2 V10.026 (H2.0) 16
66	INOCA	5	967	4.95(5)	Z2 ZN2 V10.026 (H2.0) 16
66	INOCA	5	967	4.97(5)	Z2 ZN2 V10.026 (H2.0) 16
66	INOCA	5	967	4.95(5)	Z2 ZN2 V10.026 (H2.0) 16
72	JSSCB	4	432	3.20(5)	P.05
72	JSSCB	4	432	3.10(5)	P.05
75	ACBCA	26	1794	3.24(6)	FE V.04 V2.07

V(4)-O

70	ACSAA	24	420	4.00(1)	V.02
70	JSSCB	1	394	3.69(26)	V.0 S.04
72	JSSCB	5	314	3.95(14)	ALPHA TE V.04
74	ACBCA	30	2834	4.25(6)	V SE2.06
74	ACBCA	30	2834	4.18(8)	V SE2.06
74	ACBCA	30	2834	4.11(7)	V SE2.06
66	ACSAA	20	722	3.61(10)	V.0 MO.04
65	ACSAA	19	1905	4.01(11)	V.0 S.04
72	JSSCB	5	446	4.12(2)	CU V.03
73	ACBCA	29	269	4.13(22)	CA V3 07
73	ACHCA	29	269	4.10(20)	CA V3 07
65	AMMIA	46	661	4.52(36)	V.02
73	ACBCA	29	2732	4.11(2)	V.0 S.04 (H2.0)3
66	JAGSA	90	5305	4.03(3)	V.0 S.04 (H2.0)5
73	ACBCA	31	1598	4.05(4)	CA V.0 SI4.010 H2.0
73	ACBCA	31	1598	3.62(23)	CA V.0 SI4.010 H2.0
75	ACBCA	31	1614	4.04(3)	V.0 IN2.05
75	ACBCA	31	1794	4.24(4)	K2 V.0 V2.07

V(3)-O

69	PRVBA	2	3771	3.07(1)	V2.03
75	ACBCA	31	1153	3.05(1)	V2.03
69	ZAACA	369	306	2.93(6)	ZH V2.04
69	ZAACA	369	306	2.91(7)	CD V2.04

CR(6)-O

70	ACBCA	26	437	6.05(3)	(N,H4)2 CR.04
65	ACACB	25	5115	5.82(7)	AG2 CR2.07
65	ACACB	25	5116	5.82(7)	AG2 CR2.07
69	BUFDA	92	264	5.53(12)	CO CR.04
69	BUFDA	92	264	5.63(26)	NI CR.04
70	ACSAA	24	211	6.49(13)	(PH3 SI)2 CR.04
70	AMMIA	55	1103	5.79(26)	ZN PB10 F2 (CR.04)6 (SI.04)2
70	AMMIA	55	1103	5.78(26)	ZN PB10 F2 (CR.04)6 (SI.04)2
70	AMMIA	55	1103	5.64(20)	ZN PB10 F2 (CR.04)6 (SI.04)2
68	CJCHA	46	933	6.02(3)	K2 CR2.07
68	CJCHA	46	933	6.00(3)	K2 CR2.07
68	CJCHA	46	933	5.96(3)	K2 CR2.07
68	CJCHA	46	933	5.99(3)	K2 CR2.07
70	ACECA	26	222	5.96(4)	CR.03
71	ACSAA	25	35	5.97(12)	RB2 CR2.07-X
71	ACSAA	25	44	6.24(15)	RB2 CR2.07-VII
71	ACSAA	25	44	6.24(15)	RB2 CR2.07-VII
70	CJCHA	46	537	6.20(5)	RB2 CR2.07-VIII
70	CJCHA	46	537	6.09(4)	RB2 CR2.07-VIII
70	CJCHA	46	537	6.05(5)	RB2 CR2.07-VIII
70	CJCHA	46	537	6.29(5)	RB2 CR2.07-VIII
71	JSSCB	3	364	5.69(11)	AG2 CR.04
74	AMMIA	55	1166	5.47(90)	*YEDLINITE* PB6 CL2 CR.06 (H2.0)2

CR(5)-O

60	ACSAA	14	441	5.31(26)	K3 CR (02)4
69	ACBCA	29	2170	4.93(3)	CA2 CR.04 CL
65	ACSAA	19	177	5.47(22)	CA O.H. (CR.04)3

CR(4)-O

62	JAPIA	33	1193	4.59(11)	CR.02
67	SICOA	5	663	3.65(18)	SF CR.03
67	SICOA	5	663	3.40(16)	SF CR.03
67	IRKEA	26	157	4.05(1)	SF2 CR.04

CR(3)-O

62	ZERGA	117	235	2.69(6)	CR2.03
67	ACGRA	10	423	3.05(32)	H CR.02
65	ACSAA	12	1965	3.09(13)	K CR.02
65	INDIA	4	2326	3.04(13)	CR MO6 (24 H) (H2.0)8
67	ACSAA	24	3627	2.95(4)	CR.012
67	ACBAA	24	3627	2.92(3)	NB2 CR3.08 O.H
67	ACBAA	24	3627	2.92(3)	K2 CR3.08 O.H

MN(7)-0

66	ACCRA	21	681	6.90(59)	SR (MN.04)2 (H2.0)3
66	ACCRA	21	681	7.03(77)	SR (MN.04)2 (H2.0)3
66	ACBGA	24	1053	6.91(9)	AG MN.04
67	INOCA	6	503	6.96(7)	K MN.04
74	ACIEA	13	603	6.48(37)	(H3.0)2 MN (MN.04)6 (H2.0)11

MN(4)-0

67	JCP5A	46	3776	4.02(3)	DY MN2.05
54	ACCRA	7	246	3.89(25)	MG6 MN.06
55	ACCRA	8	165	3.67(21)	ZN MN3.07 (H2.0)3

MN(3)-0

67	JCP5A	46	3776	3.04(3)	DY MN3.05
63	ACCRA	16	957	2.89(20)	Y MN.03
63	ZEKGA	118	303	3.06(8)	GAMMA MN 0 0.H
68	ACBGA	24	1233	3.01(2)	ALPHA MN 0 0.H
67	ACSAA	21	2671	3.07(3)	ALPHA MN2.03
67	ACSAA	21	2671	3.02(3)	ALPHA MN2.03
67	ACSAA	21	2671	2.95(2)	ALPHA MN2.03
67	ACSAA	21	2671	2.96(2)	ALPHA MN2.03
67	ACSAA	21	2671	2.95(2)	ALPHA MN2.03

MN(2)-0

69	ZAACA	369	306	1.97(5)	MN V2 04
62	CINCA	24	23	2.02(5)	MN CX2 04
62	ZEKGA	117	331	2.05(2)	CA MN S12 06
70	PEPIA	3	161	2.07(4)	BETA MN2 GE.04
70	PEPIA	3	161	1.99(3)	BETA MNC GE.0-
70	PEPIA	3	161	1.99(3)	BETA MN2 GL.0-
68	ZAACA	355	125	2.13(6)	MN SE.04
69	ZEKGA	130	139	2.09(3)	MN GE.03
69	ZEKGA	130	139	1.79(3)	MN GE.03
65	AMMIA	50	1884	2.45(6)	*LAUEITE* MN FE2 (P.04)2 (O.H)2 (H2.0)
65	AMMIA	50	1884	2.01(3)	*LAUEITE* MN FE2 (P.04)2 (O.H)2 (H2.0)
63	ZEKGA	119	117	1.84(1)	ZN2 MN (O.H)2 S1.04
58	NJNMA	19	556	1.97(6)	MN S.04
60	ACCRA	13	323	1.97(2)	LI MN P.04
68	AMMIA	53	733	1.86(7)	MN7 (O.H)6 (AS.04)2
68	AMMIA	53	733	1.96(7)	MN7 (O.H)6 (AS.04)2
68	AMMIA	53	733	2.05(7)	MN7 (O.H)6 (AS.04)2
68	AMMIA	53	733	2.00(7)	MN7 (O.H)6 (AS.04)2
70	AMMIA	55	2023	1.75(4)	MN9 (O.H)9 (H2.0)2 AS3.011
70	AMMIA	55	2023	1.96(4)	MN9 (O.H)9 (H2.0)2 AS3.011
70	AMMIA	55	2023	2.05(4)	MN9 (O.H)9 (H2.0)2 AS3.011
70	AMMIA	55	2023	2.05(4)	MN9 (O.H)9 (H2.0)2 AS3.011
70	AMMIA	55	2023	1.96(4)	MN9 (O.H)9 (H2.0)2 AS3.011
67	ACSAA	21	590	1.98(6)	MN2 V2.07
70	JCP5A	14	1352	2.09(8)	MN T1.03
65	ACBGA	26	640	1.97(2)	CA2 MN (P.04)2 (H2.0)2
65	JCP5A	43	2533	2.15(1)	ALPHA MN M0.04
65	JCP5A	43	2533	2.15(1)	ALPHA MN M0.04
70	ZEKGA	132	1	1.86(2)	MN5 (O.H)2 (S1.04)2
70	ZEKGA	132	1	1.96(2)	MN5 (O.H)2 (S1.04)2
70	NJMIA	113	1	2.05(3)	MN7 NA12 (S.04)13 (H2.0)15
70	NJMIA	113	1	2.10(2)	MN7 NA12 (S.04)13 (H2.0)15
69	ZEKGA	129	427	1.76(2)	FE3 MN2 (GE.04)3
69	ACSAA	23	1219	2.09(16)	MN SN (O.H)6

FE(3)-0

61	ACCRA	14	1051	3.00(10)	G03 FE3 012
61	ACCRA	14	1051	3.00(10)	G03 FE3 012
70	SSCOA	8	1743	3.11(6)	H03 FE3 012
70	SSCOA	8	1743	2.93(7)	H03 FE3 012
70	SSCOA	8	1743	3.09(10)	I03 FE3 012
60	ACCRA	13	971	2.97(4)	S03 FE3 012
60	ACCRA	13	971	2.97(4)	S03 FE3 012
60	ACCRA	13	971	2.83(5)	T03 FE3 012
60	ACCRA	13	971	2.83(5)	T03 FE3 012
65	ACCRA	19	971	3.05(5)	Y3 FE3 012
65	ACCRA	19	971	2.95(5)	Y3 FE3 012
65	ACCRA	19	971	3.10(4)	Y3 FE3 012
65	ACCRA	19	971	3.10(4)	Y3 FE3 012

65	ACCRA	19	471	3.04 (7)	LU3 FE5 012
71	MRBUA	6	6725	2.96 (7)	UA CA FE4 06
67	ACCRA	22	766	3.14 (4)	NA3 FE5 09
67	ACCRA	22	766	2.98 (4)	NA3 FE5 09
67	ACCRA	22	766	2.84 (4)	NA3 FE5 09
70	ACBCA	26	1469	2.97 (2)	CA2 FE2 05
70	ACBCA	26	1469	3.02 (2)	CA2 FE2 05
71	JSSCB	4	1	3.03 (4)	FE V.04
71	JSSCB	4	1	3.10 (3)	FE V.04
71	JSSCB	4	1	3.05 (3)	FE V.04
71	AMMIA	56	1917	3.06 (2)	K FE (S.04) 2 (H2.0) 4
71	AMMIA	56	1917	3.20 (3)	K FE (S.04) 2
65	AMMIA	50	1923	3.14 (3)	K FE (S.04) 2 H2.0
69	MSAPA	2	31	2.95 (1)	MA FE S12 06
69	MSAPA	2	31	2.93 (1)	LI FE S12 06
70	ACBCA	26	2008	2.90 (1)	PR FE 03
70	ACBCA	26	2008	3.06 (1)	NO FE 03
70	ACBCA	26	2008	2.98 (1)	SM FE 03
70	ACBCA	26	2008	2.98 (1)	SU FE 03
70	ACBCA	26	2008	2.17 (2)	GO FE 03
70	ACBCA	26	2008	2.99 (1)	TB FE 03
70	ACBCA	26	2008	2.89 (1)	DY FE 03
70	ACBCA	26	2008	3.00 (1)	HO FE 03
70	ACBCA	26	2008	2.99 (1)	ER FE 03
70	ACBCA	26	2008	2.99 (1)	TM FE 03
70	ACBCA	26	2008	3.00 (2)	YS FE 03
70	ACBCA	26	2008	3.01 (2)	LU FE 03
69	ACBCA	25	1524	3.07 (1)	FA FE3 B3 AL6 S16 030 F
68	JCPSA	46	1094	3.04 (5)	FE2 FE2 GA3 J12
66	AMMIA	51	123	2.93 (3)	FE2 03
68	ZEKGA	127	261	3.07 (4)	FE2 (S.04) 2 (H2.0) 7
68	ZEKGA	127	261	2.96 (4)	FE2 (S.04) 2 (H2.0) 7
72	SSCGA	10	9	2.93 (6)	CA3 FE2 GE3 012
69	ZEKGA	129	427	3.13 (6)	FE2 MN3 GE3 012
65	JCPSA	42	3957	2.94 (4)	GA FE 03

CO (4)-0

71	ZAACA	386	1	3.66 (7)	BA2 CO.04
73	ZAACA	398	54	3.77 (26)	LI6 CO 06
74	ZAACA	408	79	3.60 (12)	CS2 CO 03
74	ZAACA	409	152	3.94 (6)	K6 CO2.07

CO (2)-0

69	ZAACA	369	306	1.98 (6)	CO V2.04
68	CJCHA	46	3472	2.05 (20)	CO3.04
71	ACBCA	27	2437	2.26 (7)	CO (O3 H6 03)
71	NATUA	169	442	1.85 (2)	CO.0
70	CJCHA	48	881	2.00 (2)	CO3 (AS.04) 2
70	CJCHA	48	881	1.97 (2)	CO3 (AS.04) 2
70	CJCHA	48	881	1.92 (1)	CO3 (AS.04) 2
70	CJCHA	48	3124	1.77 (2)	CO6 AS3 016
70	CJCHA	48	3124	1.65 (3)	CO6 AS3 016
68	ZEKGA	126	299	1.92 (3)	CO GE.03
68	ZEKGA	126	299	1.98 (3)	CO GE.03
64	ACCRA	17	240	1.92 (4)	CO TI.03
73	ACBCA	29	2304	2.18 (2)	CO3 (V.04) 2
73	ACBCA	29	2304	2.17 (2)	CO3 (V.04) 2
70	PEPIA	3	161	1.95 (4)	CO2 S1.04
70	PEPIA	3	161	2.81 (4)	CO2 S1.04
70	PEPIA	3	161	1.92 (2)	CO2 S1.04
70	PEPIA	3	161	1.63 (1)	CO2 S1.04
71	HOAGA	54	1621	1.98 (5)	CO3 (O.H) 2 (S.04) 2 (H2.0) 2
71	HOAGA	54	1621	2.15 (4)	CO3 (O.H) 2 (S.04) 2 (H2.0) 2
62	ACCRA	149	1219	2.85 (5)	CO S.04 (H2.0) 6
67	ACCRA	149	775	1.93 (5)	CO S.04 (H2.0) 6
65	ACCRA	149	269	2.84 (3)	CO (H.H4) 2 (S.04) 2 (H2.0) 6
65	ACCRA	149	269	2.13 (2)	CO MO.04
68	ZANCA	885	129	2.47 (3)	CO MO.04
74	ACBCA	30	2907	1.96 (3)	CO SE.04
74	ACBCA	30	2907	2.19 (1)	CO2 V2.07
74	ACBCA	30	2907	2.08 (1)	CO2 V2.07
73	ACBCA	29	2741	2.11 (1)	CO (H2.0) 6 S1.F6

NI(2)-O

73	ZAACA	400	311	2.00(13)	K2 NI O2
69	BUFCA	92	264	2.20(14)	NI CR O2
69	IHOCA	8	1304	2.11(2)	NI6 (C.F3 C.O C.H2 C.O C.H3)10 (O.H)2 (H2.O)2
69	IHOCA	8	1304	2.06(2)	NI6 (C.F3 C.O C.H2 C.O C.H3)10 (O.H)2 (H2.O)2
69	IHOCA	8	1304	2.10(2)	NI6 (C.F3 C.O C.H2 C.O C.H3)10 (O.H)2 (H2.O)2
73	ACBCA	29	2304	2.01(9)	NI3 (V.O4)2
73	ACBCA	29	2304	2.12(11)	NI3 (V.O4)2
70	BUFCA	93	426	2.19(10)	NI (U.O2)2 (V.O4)2 (H2.O)4
70	ZAACA	378	129	2.10(4)	SR2 NI TE O6
70	JUPSA	14	1352	1.83(10)	NI TI O3
70	ZAACA	379	207	2.02(7)	NI (H2.O)6 SE.O4
70	BAPUA	15	47	1.94(7)	NI2 P2.O7
70	BAPUA	15	47	1.94(6)	NI2 P2.O7
70	ZAACA	392	193	2.10(11)	LI NI O2
70	ACORA	21	705	1.99(3)	NI (H2.O)6 S.O4
70	ACORA	10	209	1.90(14)	NI H.O4
70	ACORA	6	609	1.82(5)	NI (C.H3 C.O2)2 (H2.O)4
70	ZAACA	358	129	2.02(6)	NI SE.O4
70	IHOCA	5	1074	2.10(33)	AG3 NI (O5 H7 O2)3 (N.O3)2 H2.O
70	ACBCA	30	2907	2.11(1)	NI2 V2.O7
70	ACBCA	30	2907	2.05(1)	NI2 V2.O7
70	ACBCA	29	2741	2.08(1)	NI (H2.O)6 SI.F6
70	ACBCA	30	37	1.91(3)	NI3 (B.O3)2
70	ACBCA	30	37	1.87(2)	NI3 (B.O3)2

CU(2)-O

71	ZAACA	379	157	1.73(5)	LI2 CU O2
69	NEACA	130	231	1.83(5)	CU ZN2 AS2 O8
69	JUPSA	48	2619	2.13(3)	CU MO.O4
69	JUPSA	48	2619	2.17(2)	CU MO.O4
69	JUPSA	48	2619	2.17(3)	CU MO.O4
69	ACSA	23	15	1.91(3)	CU3 W.O6
73	ACBCA	29	1338	2.07(3)	CU5 V2.O10
73	ACBCA	29	1338	1.91(3)	CU5 V2.O10
73	ACBCA	29	1338	2.02(3)	CU5 V2.O10
73	ACBCA	29	1338	1.96(3)	CU5 V2.O10
73	ACBCA	29	1338	1.95(3)	CU5 V2.O10
73	ACBCA	29	1338	1.95(3)	CU5 V2.O10
69	ACORA	16	1009	2.06(6)	CU2 O S.O4
69	ACORA	16	1009	2.06(9)	CU2 U S.O4
71	ACBCA	27	2066	2.13(6)	CU3 MO2 O9
71	AMMIA	55	193	2.03(1)	CU2 CA2 S13 O10 (H2.O)2
71	AMMIA	56	193	2.08(1)	CU2 CA2 S13 O10 (H2.O)2
69	CJCHA	46	917	2.04(6)	CU3 AS2 O8
69	CJCHA	46	917	1.99(7)	CU3 AS2 O8
69	CJCHA	46	917	2.02(6)	CU3 AS2 O8
69	ACORA	18	777	2.03(4)	CU3 AS.O4 (O.H)3
69	ACORA	18	777	2.05(4)	CU3 AS.O4 (O.H)3
69	ACORA	18	777	2.03(4)	CU3 AS.O4 (O.H)3
69	ACORA	11	169	1.77(7)	*CALLAGHANITE* CU8 HG8 (C.O3)4 (O.H)24 (H2.O)
70	ACORA	26	8	1.95(1)	CU.O
69	PREAA	266	95	1.97(4)	CU S.O4 (H2.O)5
69	PREAA	266	95	2.05(4)	CU S.O4 (H2.O)5
69	ACBCA	29	676	1.91(1)	CU (H2.O)2 (S.O4)2 (H2.O)6
69	ACORA	21	437	1.96(3)	CU2 AS.O4 O.H (H2.O)3
69	ACORA	21	437	1.93(3)	CU2 AS.O4 O.H (H2.O)3
69	JSSCB	5	446	1.77(1)	CU 7.O3
69	ACORA	22	665	2.08(2)	ALPHA CU2 P2.O7
69	CJCHA	46	605	1.95(6)	BETA CU2 P2.O7
69	ACBCA	24	506	2.07(2)	CU S.O4 (H2.O)3
69	NATUA	197	70	2.02(11)	CU3 S.O4 (O.H)4
69	NATUA	197	70	2.06(7)	CU3 S.O4 (O.H)4
69	ACBCA	27	2066	1.97(7)	CU3 MO2 O9
69	ACBCA	27	2066	2.01(11)	CU 7.O4
69	CJCHA	50	619	2.06(11)	CU3 V2 O8
69	CJCHA	50	619	2.08(2)	CU3 V2 O8
69	ACORA	14	136	2.03(12)	NA2 U (S.O4)2 (H2.O)2
69	ACBCA	27	1203	2.03(1)	(CU (N.O3)2)2 (H2.O)2
69	ACBCA	27	677	1.80(3)	CU 7.O4
69	ACBCA	31	136	1.92(1)	CU 7.O4
69	ACBCA	31	136	2.07(1)	*KROENKITE* NA2 CU (S.O4)2 (H2.O)2

SR(2)-0

71	AMMIA	56	758	2.15(2)	SR C.03
69	ACBCA	25	714	2.40(3)	SR (CG H11 06)2
66	ACCRA	20	274	1.99(4)	SR B4.07
69	ACBCA	25	1047	1.84(1)	SR BE3.04
70	ZEKGA	131	499	2.12(2)	SR C.03
69	ACBCA	25	787	1.99(3)	SR2 U.05
69	ACBCA	25	787	1.83(3)	SR2 U.05
69	ACBCA	25	787	2.33(13)	SR3 U.06
69	ACECA	25	787	1.90(10)	SR3 U.06
69	ACBCA	25	787	1.88(8)	SR3 U.06
69	ACBCA	25	787	1.91(1)	SR U.04
71	JCPSA	55	1093	2.03(2)	SR NO.04
71	JCPSA	55	1093	2.10(1)	SR W.04
66	ACCRA	21	681	2.15(12)	SR (NO.04)2
66	ARKEA	26	157	2.01(6)	SR2 CR.04
66	ARKEA	26	157	2.25(7)	SR2 CR.04
66	NJNHA	1966	253	2.02(7)	SR2 CR.05
66	NJNHA	1966	253	2.00(7)	SR2 B2.05
71	AMMIA	56	1934	2.20(4)	SR2 (B3.08 (O.H))2 B (O.H)3 H2.0
71	AMMIA	56	1934	2.06(4)	SR2 (B3.08 (O.H))2 B (O.H)3 H2.0
71	ACBCA	27	2429	2.01(1)	SR (H C.02)2 (H2.0)2
71	NJNHA	1971	241	2.05(3)	SR AL3 (P.04)2 (O.H)2 H2.0
72	ZEKGA	135	399	2.22(9)	SR S2.06 (H2.0)4
72	JSSCB	4	87	1.75(3)	BETA SR2 V2.07
72	JSSCB	4	87	1.88(4)	BETA SR2 V2.07
72	JSSCB	4	87	2.12(4)	BETA SR2 V2.07
72	JSSCB	4	87	1.92(4)	BETA SR2 V2.07
72	ACBCA	28	679	1.94(2)	SR (1.03)2 H2.0
72	ACBCA	28	3000	2.02(1)	SR5 (P.04)3 U.H
72	ACBCA	28	3000	1.97(1)	SR5 (P.04)3 U.H
72	ZEKGA	135	137	1.80(7)	SR (1.03)2 (H2.0)4

Y(3)-0

69	ACBCA	25	791	3.03(12)	Y2 SI BE2.07
65	ACCRA	19	971	3.15(3)	AL5 Y3 012
65	ACCRA	19	971	3.62(2)	GA5 Y3 012
65	ACCRA	19	971	2.90(3)	FE5 Y3 012
69	ACBCA	25	2140	3.05(2)	Y2.03
69	ACBCA	25	2140	3.01(3)	Y2.03
68	ACBCA	24	1327	3.10(14)	Y2 TI 05
68	ACBCA	24	1327	2.88(12)	Y2 TI 05
67	ACCRA	22	354	3.03(1)	Y2 BE.04
67	ACCRA	22	354	3.01(1)	Y2 BE.04
70	ZEKGA	131	270	3.05(1)	Y2 TI2.07
71	KRISA	16	909	2.87(12)	Y2 SI2.07
71	KRISA	16	909	2.51(13)	Y2 SI2.07
67	AMMIA	52	1603	2.08(14)	MN2 Y (O.H)4 AS.04
73	ACBCA	29	141	3.20(1)	Y V.04

ZR(4)-0

71	ACBCA	27	602	4.06(26)	ZR TE3.08
71	ACBCA	27	494	3.93(8)	NA2 ZR (S.04)3 (H2.0)3
71	AMMIA	56	782	3.96(1)	ZR SI.04
69	ZEKGA	130	133	4.11(5)	K ZR2 (P.04)2
69	ACBCA	25	2658	4.10(5)	ZR (AS.04)2 H2.0
71	ACBCA	27	1373	4.17(8)	K2 ZR (S.04)3 (H2.0)2
61	ACCRA	14	129	3.81(15)	ZR (1.03)4
70	ACBCA	26	1129	4.80(9)	GAMMA ZR (S.04)2 H2.0
70	ACBCA	26	1131	4.13(9)	ALPHA ZR (S.04)2 H2.0
70	ACBCA	26	1140	4.36(12)	ALPHA ZR (S.04)2
69	ACBCA	25	1596	3.83(7)	ZR2 (S.04)4 (H2.0)14
69	ACBCA	25	1560	4.12(11)	ALPHA ZR2 (S.04)4 (H2.0)10
69	ACBCA	25	1572	3.88(5)	BETA ZR2 (S.04)4 (H2.0)10
70	JSSCB	2	410	3.59(12)	K2 ZR.03
70	JSSCB	2	378	3.74(14)	BETA K2 ZR2 05
73	ACSAF	27	177	4.05(3)	ZR4 (O.H)6 (CR.04)5 H2.0
73	ACSAF	27	177	4.04(3)	ZR4 (O.H)6 (CR.04)5 H2.0
70	ACSAF	27	1390	4.00(4)	ZR (CG)5 H2.0

NB(S)-O

69	ACBCA	25	851	5.021 (8)	NA NB.03
70	AMHIA	55	90	4.93 (5)	CA NB2 06
72	CSCMC	1	83	5.01 (4)	LI NB3 08
72	CSCMC	1	83	4.96 (4)	LI NB3 08
72	CSCMC	1	83	4.93 (4)	LI NB3 08
72	CJCHA	50	3648	5.30 (30)	GD2 NB2 07
65	ACCRA	18	874	4.90 (8)	GA NB.04
70	JSSCB	1	454	5.16 (12)	NA2 NB4 011
70	JSSCB	1	454	4.91 (16)	NA2 NB4 011
70	JSSCB	1	454	5.02 (22)	NA2 NB4 011
71	ACSAA	25	3337	5.02 (4)	LI NB3 08
71	ACSAA	25	3337	5.04 (4)	LI NB3 08
71	ACSAA	25	3337	5.00 (4)	LI NB3 08
67	ACCRA	22	634	4.88 (5)	K NB.03
73	ACBCA	29	2171	5.14 (2)	N-NA NB 03
70	ACBCA	26	105	4.92 (3)	BA3 S14 NB6 026
69	JCP5A	50	4352	5.25 (15)	BA4 NA2 NB10 030
69	JCP5A	50	4352	5.07 (14)	BA4 NA2 NB10 030

MO(S)-O

65	ACCRA	19	269	5.65 (12)	CO MO.04
65	ACCRA	19	269	5.74 (13)	CO MO.04
71	ACBCA	27	2900	5.93 (30)	CU3 MO2 09
71	ACBCA	27	2900	6.16 (33)	CU3 MO2 09
70	KRISA	15	577	5.75 (20)	LI AL (MO.04) 2
70	KRISA	15	577	5.45 (18)	LI AL (MO.04) 2
71	JCP5A	50	1093	5.66 (16)	CA MO.04
69	ZETKA	10	504	6.13 (32)	NA2 MO.04 (H2.0) 2
69	ACSAA	25	415	5.32 (27)	MO4 O10 (O.H) 2
71	KRISA	16	2922	5.78 (33)	K IN (MO.04) 2
71	KRISA	16	2922	5.35 (39)	K IN (MO.04) 2
71	KRISA	16	742	5.70 (39)	K2 MO2 07
71	KRISA	16	742	6.15 (42)	K2 MO2 07
72	ACBCA	28	2222	6.07 (3)	MO.03 (H2.0) 2
72	ACBCA	28	2222	5.61 (3)	MO.03 (H2.0) 2
72	ACBCA	28	2222	6.20 (3)	MO.03 (H2.0) 2
72	ACBCA	28	2222	5.94 (3)	MO.03 (H2.0) 2
72	ACBCA	28	3097	5.70 (21)	CU3 MO2 09
72	ACBCA	28	3097	6.24 (26)	CU3 MO2 09
72	ACBCA	28	60	6.05 (10)	GD2 (MO.04) 3 LOW TEMP
72	ACBCA	28	60	6.05 (10)	GL2 (MO.04) 3 LOW TEMP
72	ACBCA	28	60	6.15 (10)	GD2 (MO.04) 3 LOW TEMP
72	ACBCA	28	60	6.23 (13)	GD2 (MO.04) 3 HIGH TEMP
72	ACBCA	28	60	5.56 (23)	GD2 (MO.04) 3 HIGH TEMP
65	ZEKGA	121	158	5.71 (39)	PB MO.04
64	ACCRA	17	190	5.91 (10)	NA CO2.3 (MO.04) 3
64	ACCRA	17	190	5.72 (13)	NA CO2.3 (MO.04) 3
73	ACBCA	29	2074	5.61 (13)	LA2 (MO.04) 3
73	ACBCA	29	2074	5.60 (18)	LA2 (MO.04) 3
73	ACBCA	29	2074	5.79 (13)	LA2 (MO.04) 3
73	ACBCA	29	2074	5.61 (13)	LA2 (MO.04) 3
73	ACBCA	29	2074	5.74 (13)	LA2 (MO.04) 3
72	KRISA	17	264	5.02 (18)	CS PR (MO.04) 2
74	ACIEA	13	525	5.84 (10)	(N.H4) 2 MO2.07
74	ACIEA	13	525	5.87 (20)	(N.H4) 2 MO2.07
73	ACBCA	29	2433	5.99 (10)	Bi2 (MO.04) 3
73	ACBCA	29	2433	5.90 (10)	Bi2 (MO.04) 3
73	ACBCA	29	2433	5.75 (10)	Bi2 (MO.04) 3
70	JSSCB	1	484	5.53 (27)	Ag6 MO10 033
70	JSSCB	1	484	5.95 (31)	Ag6 MO10 033
70	JSSCB	1	484	5.74 (28)	Ag6 MO10 033
70	JSSCB	1	484	5.71 (27)	Ag6 MO10 033
70	JSSCB	1	484	5.82 (25)	Ag6 MO10 033
70	ACSAA	25	271	5.88 (13)	LI MO.03 AS.04
73	ACBCA	29	2433	5.68 (23)	Bi2 MO.06
74	ACBCA	30	46	5.90 (7)	(N.H4) 5 MO6 027 (H2.0) 4
74	ACBCA	30	46	5.64 (7)	(N.H4) 5 MO6 027 (H2.0) 4
74	ACBCA	30	46	5.87 (7)	(N.H4) 5 MO6 027 (H2.0) 4
74	ACBCA	30	46	5.54 (7)	(N.H4) 5 MO6 027 (H2.0) 4
74	ACBCA	30	46	5.12 (7)	(N.H4) 5 MO6 027 (H2.0) 4

Ag(1)-O

72	ACBCA	28	1774	1.27(4)	AG FE 02
72	ACBCA	28	2951	1.05(1)	AG (O2 P (O C2.H5) 2)
69	ACSAA	23	2261	0.97(4)	AG2 S.03
72	ACBCA	28	1485	1.07(2)	N.H2 C.H2 C O O.H AG N.03
70	JSSCB	1	484	1.10(5)	AG6 MO10 033
70	JSSCB	1	484	0.88(4)	AG6 MO10 033
70	JSSCB	1	484	0.79(3)	AG6 MO10 033
61	ACCRA	14	779	0.88(3)	AG P.03
61	ACCRA	14	779	0.88(4)	AG P.03
68	ACBCA	24	1853	1.04(2)	AG MN.04
65	ACCRA	18	777	1.88(3)	AG2 89.04
65	ACCRA	18	777	0.93(2)	AG2 89.04
65	ADAOB	25	3116	1.08(1)	AG2 CK2.07
65	ADAOB	25	3116	1.17(1)	AG2 CK2.07
71	JCSIA	1971	2058	0.93(1)	AG N.03

Co(2)-O

72	ZAACA	392	289	1.73(8)	K2 CO 02
71	ZAACA	382	270	2.87(11)	K2 CO2 03
72	ACBCA	28	2567	2.33(6)	K2 CO (S.04)2 (H2.0)1.5
67	CJCHA	45	2257	2.03(7)	CO2 V2 07
69	CJCHA	47	3409	2.73(3)	CO2 P2 07
65	CJCHA	47	3409	2.09(4)	CO2 P2 07
71	ACSAA	25	1477	2.38(5)	C3 H5 07 P CO (H2.0)3
72	JCUTB	1972	956	1.95(1)	CO (H3.0 C O2) (H2.0)2
74	USCNC	3	757	1.91(2)	CO (H.03)2 (H2.0)2
72	CJCHA	50	3646	2.12(5)	CO2 NE2 07
69	ACBCA	25	1603	2.24(7)	CO (N.03)2 (H2.0)4
70	ACBCA	20	1003	2.03(15)	CO (H3 1.06) (H2.0)3
66	ACCRA	21	715	2.13(7)	CO (N.03)2 (H2.0)3
73	COXMC	2	163	2.17(2)	K2 CO (SE 04)2 (H2.0)2
72	INOCA	11	1459	2.15(2)	(2-AMIAZOLISINONE)6 CO CL 04
69	USCFA	1969	736	2.14(17)	BETA CO V2 06
72	ACBCA	28	2667	2.32(8)	K2 CO (S.04)2 (H2.0)1.5

IN(3)-O

74	ZAACA	409	97	2.54(27)	R82 IN4 07
74	ZAACA	409	97	3.17(26)	R92 IN4 07
70	JSSCB	2	276	2.53(27)	NA IN (W.04)2
71	KRISA	16	292	3.15(16)	K IN (H0.04)2
68	ACBCA	24	388	3.13(13)	CU2 IN2 05
66	ACBCA	24	388	3.83(12)	CU2 IN2 05
68	ACBCA	24	388	3.22(13)	CU2 IN2 05
68	ACBCA	24	388	2.63(11)	CU2 IN2 05
66	ACCRA	28	723	2.64(16)	IN2.03
66	ACCRA	28	723	2.64(11)	IN2.03
61	ACCRA	14	1140	3.06(17)	IN P.04 (H2.0)2
70	ACSAA	24	1662	2.92(2)	IN O O.H

Sn(4)-O

68	CJCHA	46	859	4.02(35)	SN2 SN2 07
5	ACBCA	31	511	4.00(2)	K4 SN 04
68	CJCHA	46	859	4.12(13)	Y2 SN2 07
71	ACBCA	27	502	4.42(35)	SN TE3 08
69	ACSAA	23	1214	3.35(39)	NA SN (OH)6
70	ACSAA	24	1267	4.43(10)	NA4 SN2 GE2 012 (OH)5
70	ACSAA	24	1267	4.43(10)	NA4 SN2 GE2 012 (OH)4
68	CJCHA	46	859	3.78(6)	LA2 SN2 07
70	JACSA	92	3636	3.89(3)	SN OH (C7 H5 O2)3

Sr(5)-O

64	PCSLA	1	400	5.34(9)	BETA SB2.04
70	AMBLA	55	1400	4.70(3)	HR7 SB AS 012
74	ACBCA	30	945	4.95(16)	K2 SB4 011
74	ACBCA	30	945	5.14(15)	K2 SB4 011
74	ACBCA	30	945	4.83(10)	K2 SB4 C11
74	ACSBA	30	945	5.85(22)	K3 SB5 014
74	ACBCA	30	945	5.15(16)	K3 SB5 014
74	ACBCA	30	945	4.83(10)	K3 SB5 014
74	ACBCA	30	945	5.23(12)	K3 SB5 014
70	UOTLA	17	376	5.13(6)	U SB3 010
70	UOTLA	18	356	5.27(4)	U SB3 010

TE(6)-O

69	ACSAA	23	3062	4.98(11)	NA2 K4 (TE2 O8 (O.H)2) (H2.O)14
66	ACSAA	20	2138	5.17(8)	K4 (TE2 O6 (O.H)4) (H2.O)7
73	ACBCA	29	956	5.89(6)	H2 TE2 O6
73	ACBCA	29	643	5.88(4)	TE2 O5
71	ACBCA	27	815	5.93(6)	MG3 TE.O6
71	ACBCA	27	815	5.93(6)	MG3 TE.O6
70	ZAAGA	378	124	6.10(21)	SR2 NI TE O6
73	ACSAA	27	85	6.06(1)	TE (O.H)6
73	ACSAA	27	85	6.02(1)	TE (O.H)6
72	ZAAGA	492	124	5.64(31)	BA2 NI TE O6
72	ZAAGA	392	124	5.68(27)	BA2 NI TE O6

I(7)-O

70	ACBCA	26	1782	6.67(16)	NA I.O4
70	ACBCA	26	1075	6.66(36)	MG (O.H2)6 (I O6 H3)
65	ACCRA	19	623	7.12(13)	K4 (I2 O10 H2) (H2.O)3
66	ACCRA	20	765	7.52(19)	H5 I.O6
70	ACBCA	26	1069	6.76(34)	CU (H3 I.O6) (H2.O)3

CS(1)-O

72	ACBCA	26	806	1.00(2)	CS TL (S.O4)2 (H2.O)12
72	ZAACA	393	13	0.97(6)	CS2 PB.O3
72	ZAACA	393	97	0.98(1)	CS2 MH2 (C2.O4)3 (H2.O)3
66	INOCA	9	1500	1.13(2)	CS V3 O8
66	ACCRA	21	383	0.93(1)	CS AL (S.O4)2 (H2.O)12
67	ACCRA	23	427	1.04(2)	CS BY O14
67	CJCHA	45	1305	1.02(2)	CS C.H3 S.O3
72	CSCHC	1	109	1.02(1)	CS2 CU (H2.O)6 (S.O4)2
74	ACBCA	30	1178	1.03(1)	CS2 B6 O10
74	ACBCA	30	602	1.02(1)	CS TI (S.O4)2 (H2.O)12
71	JSSCB	3	31	1.06(3)	CS V2 O8
72	KRISA	17	284	1.10(7)	CS PR (MO.O4)2
71	JCSIA	1971	1997	0.94(2)	CS H (C4 H4 O4) H2.O
70	INOCA	9	1404	0.93(4)	CS2 (B3 C2 H11)2 FE2 (C.O)4 C.H3 S.O H2
74	ZAACA	408	75	0.93(2)	CS2 CU O3
74	ZAACA	408	75	1.16(2)	CS2 CU O3
74	FEROA	8	623	1.30(1)	CS 43 (SE.O3)2

BA(2)-O

69	ACBCA	25	787	2.19(2)	BA J.O4
69	ACBCA	25	1444	2.29(4)	BA TI5 O11
72	CSCHC	1	1	2.19(1)	BA TI6 O13
73	ACBCA	29	2009	1.63(1)	BA2 TI.O4
73	ACBCA	29	2009	2.02(1)	BA2 TI.O4
69	AGBCA	25	1811	2.12(1)	BA (B (O.H)4)2 H2.O
69	ZEKGA	129	222	1.61(1)	BA TI (S13 O9)
71	JCPSA	55	1093	2.23(1)	BA H.O4
72	CSCHC	1	193	2.06(2)	BA C.H3 C.H2 C C.O2 H2.O
70	ACBCA	26	1688	1.79(2)	ALPHA BA (AL (O.H)2)2
70	ACBCA	26	1587	1.69(6)	BA H2 (C2 O4)2 (H2.O)2
74	ACBCA	26	867	2.30(4)	BA2 AL2 (O.H)10
72	ACBCA	28	1219	2.36(1)	BA4 CR13 O25
72	ACBCA	28	784	1.63(3)	GAMMA BA (AL O (O.H)2)2
72	ACBCA	28	956	1.66(2)	BA TR.O3
72	ACBCA	28	956	1.62(16)	BA SE.O3
72	ACBCA	28	956	1.56(12)	BA PR.O3
70	ACBCA	26	1645	2.26(2)	BA6 TI17 O40
70	ACBCA	26	1645	2.17(2)	BA6 TI17 O40
70	ACBCA	26	1645	2.16(2)	BA6 TI17 O40
71	ACSAA	25	3837	2.05(1)	BA TE O3 H2.O
71	AMHIA	56	758	2.28(2)	BA C.O3
66	ADCPA	20	619	2.09(16)	BA B2 O4
66	ADCPA	20	619	1.96(4)	BA B2 O4
65	ADCPA	19	297	2.35(4)	BA B4 O7
65	ADCPA	19	297	1.66(3)	BA B4 O7
73	ACBCA	26	1924	2.04(1)	BA2 (CU (O.H)6)
72	ZAAGA	492	124	2.22(3)	BA2 NI TE O6
72	ZAAGA	392	124	2.18(3)	BA2 NI TE O6
74	ACBCA	30	2694	2.53(2)	BA TI2 O5
74	ACBCA	30	2694	2.53(2)	BA TI2 O5
71	ACBCA	27	1603	1.82(8)	BA FE2 O4
71	ACBCA	27	1263	2.05(7)	BA FE2 O4

71	ZAACA	306	1	2.25(3)	BA2 CO.04
71	ZAACA	366	1	1.66(2)	BA2 CO.04
75	ACBCA	31	1148	2.07(1)	BA2 CU (P.03)6
75	ACBCA	31	1148	1.96(1)	BA2 CU (P.03)6
74	CSGMC	3	599	1.75(1)	BA2 SI.04
74	CSGMC	3	599	2.25(2)	BA2 SI.04
75	ACBCA	31	580	1.80(1)	BA GA2 SI2 08
74	ACBCA	30	178	2.21(1)	BA (CO H6 O9 S) (H2.O)2
70	ZEKGA	131	161	2.22(6)	BA3 (V.04)2
70	ZEKGA	131	161	2.10(4)	BA3 (V.04)2
70	ACBCA	26	105	2.08(2)	BA3 SI4 NB0 026
72	ACBCA	28	2348	2.08(4)	BA NA P3.09

LA(3)-0

73	ACBCA	29	2074	3.01(4)	LA2 (MO.04)3
73	ACBCA	29	2074	3.01(4)	LA2 (MO.04)3
73	ACBCA	29	2074	3.03(4)	LA2 (MO.04)3
65	CJCHA	46	859	2.95(2)	LA2 SN2 07
65	ACBCA	24	1468	2.92(3)	LA4 RE6 019

PR(3)-0

70	ACBCA	26	1843	3.10(6)	PR (C.H3 ACAC)3
70	ACBCA	26	1843	3.05(6)	PR (C.H3 ACAC)3
71	ZEKGA	133	364	2.66(5)	PR2 SI2 07
71	ZEKGA	133	364	3.15(5)	PR2 SI2 07
71	ZEKGA	133	364	3.03(6)	PR2 SI2 07
71	ZEKGA	133	364	3.02(7)	PR2 SI2 07
71	ZEKGA	133	364	2.60(+2)	PR2 SI2 07 HIGH TEMP
71	ZEKGA	133	364	3.10(+3)	PR2 SI2 07 HIGH TEMP
72	KRISA	17	281	3.42(28)	CS PR (MO.04)2
70	ACBCA	26	2008	3.04(1)	PR FE.03

ND(3)-0

70	ACBCA	26	484	2.75(3)	ND2 SI2.07
70	ACBCA	26	484	3.14(4)	ND2 SI2.07
70	ACSAA	24	3406	3.48(3)	ND4 RE2 011
70	ACSAA	24	3406	3.13(4)	ND4 RE2 011
74	ACBCA	30	488	3.42(3)	ND P5 014
75	JCPSA	62	759	3.37(4)	ND (1.05)3 H2.0
70	ACSAA	24	3527	3.03(4)	NA5 ND (CL H4 O5)3 (CL.04)2
70	ACBCA	26	2008	3.07(1)	ND FE.03

SN(3)-0

65	ACCRA	19	971	3.10(3)	SM3 FE5 012
70	KRISA	15	250	2.90(4)	SM2 SI2 07
70	KRISA	15	250	2.85(4)	SM2 SI2 07
70	KRISA	15	250	3.04(4)	SM2 SI2 07
70	KRISA	15	250	2.87(4)	SM2 SI2 07
69	ACBCA	25	621	3.06(6)	SM (BR.03)3 (H2.O)9
68	CJCHA	46	859	2.93(16)	SM2 SN2 07
70	ACBCA	26	2008	3.06(1)	SN FE.03

EU(3)-0

65	INOCA	8	1760	3.45(5)	CS (F6ACAC)4 EU
70	ACBCA	26	2008	3.07(1)	EU FE.03
63	ACCRA	16	762	3.06(6)	EU2 (H.04)3

GD(3)-0

72	ACBCA	28	60	3.14(3)	GD2 (MO.04)3
72	ACBCA	28	60	3.14(3)	GD2 (MO.04)3
72	ACBCA	28	60	3.14(3)	GD2 (MO.04)3 HIGH TEMP
65	ACCRA	19	971	3.21(4)	GD3 AL5 012
70	ACBCA	26	484	2.70(3)	GD2 SI2 07
70	ACBCA	26	484	3.08(4)	GD2 SI2 07
64	ACSAA	23	1792	3.03(5)	GD (H2O C.H2 C.02)3
70	ACBCA	26	2008	2.96(2)	GD FE.03
61	ACCRA	17	1051	2.45(6)	GD3 FE5 012

TS(3)-0

70	ACBCA	26	2008	2.97(1)	TS FE.03
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OY(3)-0

75	ACGRA	19	971	2.92(3)	OY3 FE5 012
76	ACBCA	26	2008	2.93(1)	OY FE.03

HO(3)-0

74	ACBCA	30	2613	3.11(8)	HO (C2.H5 S.03)3 (H2.0)4
70	ACBCA	26	2008	2.96(1)	HO FE.03
69	ACSAA	23	1253	3.21(4)	ER (H.O C.H2 C.02) (D C.H2 C.02) H2.O) H2.O

ER(3)-0

78	ACBCA	26	2008	2.94(1)	ER FE.03
79	ACBCA	26	184	2.97(2)	ER2 SI2 07
72	ACBCA	28	2339	3.34(3)	ER (C.H3 ACAC)3

TM(3)-0

71	ACBCA	28	2008	2.92(1)	TM FE 03
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YJ(3)-0

78	ACBCA	26	484	3.03(2)	Y32 SI2 07
70	KRISA	14	985	3.09(3)	Y82 SI 05
75	KRISA	14	985	3.09(3)	Y82 SI 05
69	ACGRA	19	971	3.04(4)	Y83 AL5 012
69	ACGRA	19	971	2.92(4)	Y83 GA5 012
69	ACGRA	19	971	2.93(4)	Y83 FE5 012
70	ACSAA	24	3527	2.73(2)	Y85 (Y8 (C+ H+ 05)3 (CL.04)2
70	ACBCA	26	2008	2.97(2)	Y8 FE.03

LU(3)-0

73	ACBCA	29	141	3.25(2)	LU P.04
73	ACBCA	29	141	3.19(1)	LU AS.04
69	ACGRA	19	971	3.09(4)	LU3 AL5 012
69	ACGRA	19	971	2.88(5)	LU3 GA5 012
69	ACGRA	19	971	2.81(5)	LU3 FE5 012
70	ACBCA	26	2008	2.97(2)	LU FE.03

HF(4)-0

71	ACBCA	27	602	4.32(25)	HF TE3 08
69	ACSAA	23	3541	4.27(6)	HF (O.H)2 S.04 H2.O

TA(5)-0

70	JSSCB	-1	454	5.11(10)	CA TA4 011
70	JSSCB	-1	454	4.97(25)	CA TA4 011
70	ACBCA	31	408	5.09(17)	CA TA4 011
70	ACBCA	31	408	5.10(20)	CA TA4 011

K(6)-0

70	KRISA	17	1135	5.42(43)	K IN (H.O)2
61	JOPSA	40	584	5.63(8)	CA H.04
71	JOPSA	55	1093	2.97(5)	BA H.04
71	JOPSA	55	1093	6.01(6)	SR H.04
72	ACBCA	28	3174	6.63(27)	BETA SN W.04
72	ZENBA	27	203	5.92(23)	ALPHA SN W.04
63	ACCPRA	16	762	6.95(34)	EUB (H.04)3
63	ACCPRA	16	762	6.25(25)	EUB (H.04)3
75	ACBCA	31	1200	6.94(13)	NAS H2 07
75	ACBCA	31	1200	6.24(12)	NAS H2 07
70	JSSCB	-2	278	6.11(45)	NAL IN (H.04)2
69	ACSAA	23	221	6.07(24)	CU3 H.06

RE(7)-0

61	INOCA	8	436	7.53(27)	RE2.07
61	INOCA	8	436	6.65(23)	RE2.07
61	INOCA	6	436	7.81(26)	RE2.07
61	INOCA	6	436	7.67(25)	RE2.07
70	ZAACA	376	87	6.63(31)	RE2.07 (H2.0)2
70	ZAACA	376	87	6.53(31)	RE2.07 (H2.0)2
75	ACBCA	31	1764	7.24(24)	K RE.04

HG(2)-0

73	ACBCA	29	367	2.11(12)	ALPHA HG2 V2.07
73	ACBCA	29	367	2.13(9)	ALPHA HG2 V2.07
69	ACSAA	23	1607	1.93(8)+	HG2 SE.04
74	ACBCA	30	144	1.98(8)+	HG2 (C.F3 C.02)2
73	ACBCA	29	1666	1.98(8)+	HG2 AS.04
73	ACBCA	29	1666	1.97(8)+	HG2 AS.04
73	ACBCA	29	1666	1.98(8)+	HG2 AS.04

* ASSUMING THE HG - HG BOND HAS A VALENCE OF 1.0

TL(1)-0

73	CHOCA	277	863	0.97(5)	TL4 O3
73	CHOCA	277	863	1.08(6)	TL4 O3
73	CHUCA	277	863	1.08(5)	TL4 O3
73	CHUCA	276	1735	1.07(4)	TL3 P.04
73	CHUCA	276	1735	1.05(6)	TL3 S.03
72	CSCMC	1	371	0.89(1)	TL2 CU (H2.0)6 (S.04)2
74	CJCHA	52	3539	1.89(2)	TL V.03
75	ACBCA	31	369	0.95(1)	TL N.03 - I11
73	ACSAA	27	349	0.99(1)	TL2 CU (S.03)2

PB(2)-0

73	ACBCA	29	2242	1.67(4)	PB6 B10 O21
73	ACBCA	29	2242	1.91(3)	PB6 B10 O21
73	ACBCA	29	2242	2.07(4)	PB6 B10 O21
74	ACBCA	30	1634	1.96(3)	PB T13 O7
70	ZEKGA	132	99	2.07(6)	PB2 O S.04
70	ZEKGA	132	99	2.13(8)	PB2 O S.04
73	CJCHA	51	78	2.01(2)	PB2 V2.07
73	CJCHA	51	78	1.95(2)	PB2 V2.07
65	ZEKGA	121	156	2.04(6)	PB M0.04
72	TMPMA	17	196	1.80(1)	PB SE.03
73	ACBCA	29	1986	1.89(6)	CU2 PB5 (S.04)3 C.03 (O.H)6
73	ACBCA	29	1986	2.11(5)	CU2 PB5 (S.04)3 C.03 (O.H)6
73	ACBCA	29	1986	2.15(6)	CU2 PB5 (S.04)3 C.03 (O.H)6
75	CJCHA	53	42	1.84(7)	PB3 (P.04)2
75	CJCHA	53	42	2.03(7)	PB3 (P.04)2
70	ZEKGA	132	226	2.12(6)	LOW PB3 (P.04)2
70	ZEKGA	132	226	1.96(5)	LOW PB3 (P.04)2
69	JCSIA	1969	366	2.15(2)	K2 PB CU (N.02)6

B(13)-0

73	ACBCA	29	2436	2.72(19)	B12 M0.06
73	ACBCA	29	2436	2.75(14)	B12 M0.06
73	ACBCA	29	2433	3.23(3)	B12 (M0.04)3
73	ACBCA	29	2433	3.14(4)	B12 (M0.04)3
69	ACSAA	23	1925	2.67(7)	B1 (O2 C.H)3
69	ACSAA	23	1925	2.75(7)	B1 (O2 C.H)3
69	ACSAA	23	1925	2.99(7)	B1 (O2 C.H)3

U(b)-0

71	ZSTKA	12	94	6.93(29)	Rb2 U.02 (N.03)+
65	ACGRA	19	205	6.74(18)	Rb U.02 (N.03)3
73	ACBCA	29	1251	6.10(18)	U-TE 05
69	ACBCA	25	787	5.94(3)	SR U.04
69	ACBCA	25	787	5.97(7)	SR2 U.05
69	ACBCA	25	787	5.78(7)	SR2 U.05
69	ACBCA	25	787	5.81(20)	SR3 U.06
69	ACBCA	25	787	5.65(14)	CA3 U.06
69	ACBCA	25	787	5.68(9)	CA2 U.05
69	ACBCA	25	787	5.73(6)	CA2 U.05
69	ACBCA	25	787	5.92(3)	UA U.04
69	ACBCA	25	787	6.28(1)	CA U.04
71	ACBCA	27	1088	6.34(32)	ALPHA U.02 (O.H)2
70	ACBCA	26	1775	5.95(18)	BETA U.02 (O.H)2
72	ACBCA	28	3489	5.95(18)	GAMMA U.02 (O.H)2
70	ACBCA	26	855	6.12(6)	BETA U3.05
72	ACBCA	28	117	6.27(18)	H2 U3 010
72	ACBCA	28	117	6.75(21)	H2 U3 010
74	ACBCA	30	151	5.50(22)	U2 U3 010
74	ACBCA	30	151	6.34(33)	U2 U3 010
72	INOCA	11	1848	6.43(13)	U.02 H2.0 (CO (N.H2)2)4 (N.03)2
74	ACBCA	30	407	6.14(9)	C.02 C.H2 0 C.H2 C.02 U.02
75	ACBCA	31	1140	6.45(6)	(U.02)2 GE.04 (H2.0)2
75	ACBCA	31	1133	6.90(29)	CU (H2.0)4 (U.02 4 GE.04)2 (H2.0)2

LIST OF JOURNAL CODENS USED

ACACB	ACTA CRYST A
ACBCA	ACTA CRYST B
ACGRA	ACTA CRYST
ACIEA	ANGEN CHEM (INTERNAT EON)
ACSAA	ACTA CHEM SCAND
AMMIA	AMER MIN
ARKEA	ARK KEMI
BAPCA	BULL ACAD POLON SCI SER SCI CHEM
BSCFA	BULL SOC CHIN FR
BUFCA	BULL SOC FR MINER CRYST
CAMIA	CANAD MINER
CHBCA	C R ACAD SCI PARIS SEC C
CUCHA	CANAD J CHEM
CUPHA	CANAD J PHYS
CJGMC	CRYST STRUCT COMM
CSRPA	CHEM SRIPTA
FEROA	FERRICELECTRICS
INOCA	INORG CHEM
INOCA	INORG NUCL CHEM LETTERS
JAGSA	J AMER CHEM SOC
JAPIA	J APP PHYS
JCOIB	J CHEM SOC DALTON TRANS.
JUPSA	J CHEM PHYS
JUSIA	J CHEM SOC A
JUTLA	J CATALYSIS
JINDA	J INORG NUCL CHEM
JNBAA	J RES NAT BUREAU STAND A
JSSCB	J SOLID STATE CHEM
JUPSA	J PHYS SOC JAPAN
KRISA	KRISTALLOGRAFIYA
MOCHA	MONATSH CHEM
NRBUA	MATER RES BULL
MSAPA	MINER SOC AMER SPEC PAPERS
NATLA	NATURF O
NJHIA	NEUES JAHRBK MINER ABHANDLUNGEN
NJHIA	NEUES JAHRBK MINER MONATSH
PCSLA	PROC CHEM SOC LOND
PEPIA	PHYS EARTH PLANETARY INTERIORS
PHISA	PHYS SOC JAPAN SER A
PSCOA	SOLID STATE COMM
TIPHA	TSCHEKHAUS MITTEIL PETROL MITT
ZARCA	Z ANORG ALLGEME CHEM
ZEKVA	Z KRIST
ZENBA	Z NATURF O