Table 43A-8-001. $K_2Mn_2(SO_4)_3$. Fractional coordinates of atoms and the isotropic temperature parameters *B* determined by neutron diffraction at RT [88Oel]. *B* is defined by Eq. (e) in Introduction.

Atom	*x*	*y*	*z*	*B*
K(1)	0.8065(15)	0.8065	0.8065	2.9(8)
K(2)	0.0515(19)	0.0515	0.0515	4.6(10)
Mn(1)	0.3299(96)	0.3299	0.3299	–2.3(2)
Mn(2)	0.5983(19)	0.5983	0.5983	3.5(9)
S	0.2198(20)	0.3799(29)	0.0136(26)	2.5(4)
O(1)	0.3010(11)	0.2694(15)	0.9575(12)	3.6(4)
O(2)	0.0838(12)	0.3350(12)	0.0061(10)	3.4(3)
O(3)	0.2308(10)	0.4909(12)	0.9280(11)	3.1(3)
O(4)	0.2609(12)	0.4147(12)	0.1473(13)	2.4(3)

Table 43A-8-002. $K_2Mn_2(SO_4)_3$. Fractional coordinates of atoms based on a disordered model at 20 °C [81Yam]. L and R stand for two ordered sites with equal occupancies.

Atom	*x*	*y*	*z*
K(1)	0.1846(119)	0.3154(120)	0.6846(108)
K(2)	0.0510(155)	0.0510(126)	0.0510(135)
Mn(1)	0.3335(64)	0.3335(55)	0.3335(64)
Mn(2)	0.4062(65)	0.0938(55)	0.9062(57)
S(1)	0.2213(7)	0.3754(7)	0.0149(6)
$O(1)^L$	0.3082(62)	0.2683(60)	0.9735(60)
$O(1)^R$	0.3144(51)	0.2854(56)	0.9449(63)
$O(2)^L$	0.0861(51)	0.3155(56)	0.0207(74)
$O(2)^R$	0.0844(46)	0.3386(49)	0.9940(50)
$O(3)^L$	0.2304(73)	0.4818(55)	0.9209(57)
$O(3)^R$	0.2464(69)	0.5080(57)	0.9539(65)
$O(4)^L$	0.2703(73)	0.4184(65)	0.1409(51)
$O(4)^R$	0.2459(56)	0.3986(76)	0.1587(45)

Table 43A-8-003. $K_2Mn_2(SO_4)_3$. Anisotropic temperature parameters [$\cdot 10^{-5}$] for disordered cubic phase at 20 °C [81Yam]. b_{ij} is defined by Eq. (b) in Introduction. L and R stand for two ordered sites with equal occupancies.

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
K(1)	544(423)	557(393)	377(96)	153(111)	28(335)	4(402)
K(2)	598(734)	417(101)	588(786)	−54(509)	−34(634)	108(148)
Mn(1)	364(222)	157(58)	325(261)	−6(173)	−149(48)	−3(167)
Mn(2)	336(81)	208(126)	237(178)	88(174)	−44(234)	−98(71)
S(1)	194(4)	203(4)	202(4)	51(4)	6(4)	14(4)
$O(1)^L$	598(51)	508(48)	537(50)	350(43)	22(42)	−151(40)
$O(1)^R$	299(35)	446(42)	676(52)	135(34)	84(36)	−186(41)
$O(2)^L$	240(33)	425(41)	1013(69)	−161(33)	250(43)	−138(45)
$O(2)^R$	249(30)	357(34)	433(37)	−103(28)	−47(30)	80(32)
$O(3)^L$	998(72)	329(39)	402(43)	−108(46)	−68(48)	207(36)
$O(3)^R$	648(51)	316(37)	659(54)	−171(36)	−150(47)	156(39)
$O(4)^L$	977(72)	532(49)	253(35)	−141(53)	−191(42)	−60(35)
$O(4)^R$	462(42)	1026(71)	116(27)	−80(48)	−48(30)	75(39)

Table 43A-8-004. $K_2Mn_2(SO_4)_3$. Structure of phase I [95Uke]. Fractional coordinates and temperature parameters [$\cdot 10^{-2}$ Å^2] at 296 K. SO_4 takes two arrangements discriminated by primed and double primed symbols with equal probabilities. U_{ij} is defined by Eq. (d) in Introduction.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	0.33363(8)	0.33363(8)	0.33363(8)	1.57(2)	1.57(2)	1.57(2)	–0.25(2)	–0.25(2)	–0.25(2)
Mn(2)	0.59387(8)	0.59387(8)	0.59387(8)	1.44(2)	1.44(2)	1.44(2)	–0.03(2)	–0.03(2)	–0.03(2)
K(1)	0.81553(16)	0.81553(16)	0.81553(16)	2.71(5)	2.71(5)	2.71(5)	–0.22(5)	–0.22(5)	–0.22(5)
K(2)	0.05076(18)	0.05076(18)	0.05076(18)	2.93(5)	2.93(5)	2.93(5)	0.04(6)	0.04(6)	0.04(6)
S	0.22123(4)	0.37538(4)	0.01494(4)	1.17(1)	1.17(1)	1.15(1)	0.27(1)	0.03(1)	0.10(1)
O(1′)	0.31273(65)	0.28892(50)	0.94903(89)	1.74(13)	1.27(18)	4.61(34)	0.88(13)	0.55(16)	–0.82(17)
O(1″)	0.30787(93)	0.26312(56)	0.97092(107)	4.23(30)	1.66(23)	4.61(35)	1.98(22)	–0.09(24)	–0.40(21)
O(2′)	0.08800(98)	0.31593(95)	0.02416(74)	1.99(22)	3.39(33)	6.04(50)	–0.90(22)	1.21(33)	–1.43(34)
O(2″)	0.08489(78)	0.33420(82)	–0.00518(54)	1.13(11)	2.38(18)	1.95(13)	–0.45(11)	–0.21(11)	–0.22(12)
O(3′)	0.23194(101)	0.48057(57)	0.92101(66)	8.13(49)	1.93(21)	2.90(26)	–0.50(25)	0.08(28)	1.51(18)
O(3″)	0.24504(66)	0.50689(52)	0.95084(66)	3.08(17)	1.71(18)	3.96(31)	–0.34(15)	–0.36(19)	1.27(17)
O(4′)	0.26617(98)	0.41867(81)	0.14212(67)	5.08(44)	2.92(22)	1.65(23)	–0.54(23)	–1.03(22)	–0.52(19)
O(4″)	0.24619(85)	0.39730(94)	0.15811(71)	2.57(18)	5.39(44)	1.21(13)	–0.73(22)	–0.38(12)	0.73(19)

Table 43A-8-005. $K_2Mn_2(SO_4)_3$. Structure of phase I [95Uke]. Interatomic distances [Å] and bond angles [°] in the SO_4 tetrahedron for average structure.

	296 K	263 K	233 K	213 K	203 K	193 K	190 K	186 K
S–O(1^i)	1.497(3)	1.494(3)	1.494(3)	1.485(3)	1.497(3)	1.488(3)	1.504(4)	1.506(6)
–O(2)	1.489(2)	1.484(2)	1.486(2)	1.483(2)	1.483(3)	1.486(3)	1.481(3)	1.475(5)
–O(3^i)	1.486(3)	1.481(4)	1.485(4)	1.498(4)	1.481(4)	1.501(4)	1.477(5)	1.509(8)
–O(4)	1.502(3)	1.500(3)	1.505(3)	1.494(3)	1.503(3)	1.498(3)	1.509(4)	1.520(6)
O(1^i)–O(2)	2.433(3)	2.428(4)	2.431(4)	2.427(4)	2.430(4)	2.430(4)	2.436(5)	2.430(7)
–O(3^i)	2.378(4)	2.372(5)	2.372(5)	2.371(5)	2.367(5)	2.375(5)	2.353(7)	2.344(9)
–O(4)	2.492(4)	2.486(4)	2.494(5)	2.465(5)	2.494(5)	2.469(5)	2.498(7)	2.506(10)
O(2)–O(3^i)	2.460(4)	2.454(5)	2.458(5)	2.466(5)	2.447(5)	2.470(5)	2.451(6)	2.540(10)
–O(4)	2.472(4)	2.470(4)	2.478(4)	2.461(4)	2.482(5)	2.470(5)	2.489(6)	2.493(9)
O(3^i)–O(4)	2.392(4)	2.381(5)	2.382(5)	2.401(5)	2.382(5)	2.407(6)	2.383(7)	2.385(11)
O(1^i)–S–O(2)	109.1(1)	109.2(2)	109.4(2)	109.7(2)	109.2(2)	109.6(2)	109.4(2)	109.2(3)
O(1^i)–S–O(3^i)	105.7(2)	105.7(2)	105.6(2)	105.3(2)	105.3(2)	105.3(2)	104.3(3)	102.1(4)
O(1^i)–S–O(4)	112.4(2)	112.3(2)	112.5(2)	111.7(2)	112.5(2)	111.6(2)	112.1(3)	111.8(4)
O(2)–S–O(3^i)	111.6(2)	111.7(2)	111.7(2)	111.6(2)	111.3(2)	111.6(2)	112.0(3)	116.7(4)
O(2)–S–O(4)	111.5(2)	111.7(2)	111.9(2)	111.5(2)	112.4(2)	111.8(2)	112.7(3)	112.6(4)
O(3^i)–S–O(4)	106.4(2)	106.0(2)	105.6(2)	106.8(2)	105.9(2)	106.7(2)	105.9(3)	103.9(4)

Symmetry code: (i) x, y, z–1.

Table 43A-8-006. $K_2Mn_2(SO_4)_3$. Structure of phase I [95Uke]. Metal-oxygen distances [Å] for disordered structure. Prime and double prime discriminate two arrangements of disordered SO_4.

	296 K	263 K	233 K	213 K	203 K	193 K	190 K	186 K
Mn(1)–O($3^{i, ii, iii}$)′	2.182(7)	2.189(6)	2.187(6)	2.184(5)	2.186(5)	2.182(5)	2.202(8)	2.239(12)
Mn(1)–O($3^{i, ii, iii}$)″	2.156(6)	2.143(5)	2.145(5)	2.146(5)	2.141(4)	2.144(4)	2.156(7)	2.151(11)
Mn(1)–O($4^{iv, v, vi}$)′	2.228(7)	2.228(9)	2.231(6)	2.225(7)	2.221(7)	2.221(7)	2.225(9)	2.215(14)
Mn(1)–O($4^{iv, v, vi}$)″	2.087(8)	2.079(10)	2.064(7)	2.061(7)	2.070(7)	2.056(8)	2.039(11)	2.015(17)
Mn(2)–O($1^{vii, viii, ix}$)′	2.232(6)	2.217(7)	2.205(6)	2.207(6)	2.208(5)	2.208(5)	2.212(6)	2.203(8)
Mn(2)–O($1^{vii, viii, ix}$)″	2.087(7)	2.094(9)	2.103(7)	2.093(7)	2.099(6)	2.092(6)	2.071(8)	2.083(12)
Mn(2)–O($2^{x, xi, xii}$)′	2.173(10)	2.172(9)	2.162(7)	2.156(8)	2.165(7)	2.162(7)	2.164(11)	2.150(15)
Mn(2)–O($2^{x, xi, xii}$)″	2.193(8)	2.192(7)	2.193(5)	2.190(6)	2.185(6)	2.185(6)	2.180(9)	2.194(13)
K(1)–O($1^{vii, viii, ix}$)′	2.988(9)	2.975(9)	2.972(8)	2.968(8)	2.961(6)	2.965(6)	2.965(8)	2.958(11)
K(1)–O($1^{vii, viii, ix}$)″	3.201(11)	3.214(11)	3.216(9)	3.196(10)	3.207(8)	3.201(8)	3.201(12)	3.226(16)
K(1)–O($3^{vii, viii, ix}$)′	2.959(7)	2.942(6)	2.930(6)	2.906(6)	2.909(6)	2.902(5)	2.881(8)	2.899(12)
K(1)–O($3^{vii, viii, ix}$)″	3.376(7)	3.379(6)	3.378(5)	3.375(5)	3.376(5)	3.385(5)	3.380(8)	3.412(12)
K(1)–O($4^{xiii, xiv, xv}$)′	2.770(8)	2.748(9)	2.760(7)	2.756(7)	2.751(7)	2.758(7)	2.755(10)	2.753(16)
K(1)–O($4^{xiii, xiv, xv}$)″	3.002(10)	3.007(10)	2.999(8)	3.010(8)	3.008(8)	3.006(9)	3.013(13)	3.028(22)
K(2)–O($1^{xvi, xvii, xviii}$)′	2.905(7)	2.897(8)	2.882(7)	2.876(7)	2.868(6)	2.864(6)	2.873(7)	2.880(10)
K(2)–O($1^{xvi, xvii, xviii}$)″	3.105(9)	3.094(10)	3.109(8)	3.117(8)	3.124(7)	3.137(7)	3.126(10)	3.135(13)
K(2)–O($2^{iv, v, vi}$)′	2.724(10)	2.704(9)	2.706(8)	2.703(8)	2.701(7)	2.695(7)	2.705(10)	2.703(15)
K(2)–O($2^{iv, v, vi}$)″	2.945(9)	2.944(7)	2.935(6)	2.933(6)	2.934(4)	2.935(6)	2.947(8)	2.947(13)
K(2)–O($3^{xvi, xvii, xviii}$)′	3.255(10)	3.245(10)	3.244(9)	3.253(9)	3.263(9)	3.265(9)	3.242(13)	3.149(20)
K(2)–O($3^{xvi, xvii, xviii}$)″	3.149(7)	3.143(6)	3.141(5)	3.133(5)	3.137(5)	3.137(5)	3.117(7)	3.121(11)

For the symmetry code, see Table 43A-9-007.

Table 43A-8-007. $K_2Mn_2(SO_4)_3$. Structure of phase I [95Uke]. Metal-oxygen distances [Å] for average structure.

	296 K	263 K	233 K	213 K	203 K	193 K	190 K	186 K
Mn(1)–O($3^{i, ii, iii}$)	2.135(4)	2.133(4)	2.129(4)	2.112(4)	2.128(4)	2.111(4)	2.141(5)	2.178(8)
Mn(1)–O($4^{iv, v, vi}$)	2.120(3)	2.115(3)	2.109(3)	2.103(3)	2.104(3)	2.097(3)	2.092(4)	2.081(7)
Mn(2)–O($1^{vii, viii, ix}$)	2.123(3)	2.117(3)	2.117(3)	2.121(3)	2.109(3)	2.117(3)	2.102(4)	2.095(6)
Mn(2)–O($2^{x, xi, xii}$)	2.163(3)	2.161(3)	2.156(3)	2.150(3)	2.156(3)	2.148(3)	2.153(4)	2.153(5)
K(1)–O($1^{vii, viii, ix}$)	3.080(4)	3.075(4)	3.067(4)	3.067(4)	3.057(5)	3.066(5)	3.051(6)	3.057(8)
K(1)–O($3^{vii, viii, ix}$)	3.188(4)	3.185(4)	3.190(4)	3.174(5)	3.179(5)	3.173(5)	3.177(6)	3.173(9)
K(1)–O($4^{xiii, xiv, xv}$)	2.854(4)	2.843(4)	2.835(4)	2.853(4)	2.834(4)	2.852(4)	2.835(6)	2.830(9)
K(2)–O($1^{xvi, xvii, xviii}$)	2.986(4)	2.974(4)	2.969(3)	2.961(4)	2.966(4)	2.965(4)	2.962(5)	2.972(6)
K(2)–O($2^{iv, v, vi}$)	2.841(4)	2.834(4)	2.834(4)	2.831(4)	2.836(4)	2.830(4)	2.840(4)	2.839(6)
K(2)–O($3^{xvi, xvii, xviii}$)	3.180(5)	3.167(5)	3.162(5)	3.158(5)	3.158(5)	3.158(5)	3.132(6)	3.017(9)

Symmetry code:

(i) $z - 0.5, 0.5 - x, 1 - y$
(ii) $1 - y, z - 0.5, 0.5 - x$
(iii) $0.5 - x, 1 - y, z - 0.5$
(iv) x, y, z
(v) z, x, y
(vi) y, z, x
(vii) $0.5 + y, 1.5 - z, 1 - x$
(viii) $1 - x, 0.5 + y, 1.5 - z$
(ix) $1.5 - z, 1 - x, 0.5 + y$
(x) $0.5 + z, 0.5 - x, 1 - y$
(xi) $1 - y, 0.5 + z, 0.5 - x$
(xii) $0.5 - x, 1 - y, 0.5 + z$
(xiii) $0.5 + x, 1.5 - y, 1 - z$
(xiv) $1 - z, 0.5 + x, 1.5 - y$
(xv) $1.5 - y, 1 - z, 0.5 + x$
(xvi) $x - 0.5, 0.5 - y, 1 - z$
(xvii) $1 - z; x - 0.5, 0.5 - y$
(xviii) $0.5 - y, 1 - z, x - 0.5$

Table 43A-8-008. $K_2Mn_2(SO_4)_3$. Fractional coordinates of atoms in orthorhombic phase at –90 °C [81Yam]. Non-primed, primed and double-primed atoms constitute three SO_4 molecules which are related by the triad symmetry axis in phase I to each other.

Atom	x	y	z
K(1)	0.1711(14)	0.3128(14)	0.6909(14)
K(2)	0.0372(15)	0.0558(15)	0.0577(14)
Mn(1)	0.3128(9)	0.3450(9)	0.3361(9)
Mn(2)	0.3924(10)	0.0947(9)	0.9194(9)
S(1)	0.2114(15)	0.3725(15)	0.0258(15)
S(1′)	0.3833(15)	0.0117(15)	0.2386(15)
S(1″)	0.0025(15)	0.2131(15)	0.3687(15)
O(1)	0.3008(47)	0.2583(49)	0.0155(47)
O(2)	0.0732(43)	0.3316(46)	0.9947(46)
O(3)	0.2558(47)	0.4727(42)	0.9275(47)
O(4)	0.2169(46)	0.4268(45)	0.1621(45)
O(1′)	0.3018(45)	0.9348(45)	0.3330(45)
O(2′)	0.3300(47)	0.9923(49)	0.1031(46)
O(3′)	0.5194(46)	0.9577(47)	0.2477(50)
O(4′)	0.3879(50)	0.1516(46)	0.2776(46)
O(1″)	0.9368(47)	0.2809(48)	0.2569(49)
O(2″)	0.0497(50)	0.0824(47)	0.3223(49)
O(3″)	0.9048(50)	0.1958(50)	0.4752(46)
O(4″)	0.1163(47)	0.2919(45)	0.4183(49)

Table 43A-8-009. $K_2Mn_2(SO_4)_3$. Anisotropic temperature parameters [$\cdot 10^5$] for orthorhombic phase at –90 °C [81Yam]. b_{ij} is defined by Eq. (b) in Introduction. See also the caption of Table 43A-8-008 about the non-primed, primed and double-primed atoms.

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
K(1)	149(11)	136(11)	166(12)	22(10)	−6(11)	0(10)
K(2)	193(12)	236(12)	113(12)	−28(11)	7(11)	−17(11)
Mn(1)	58(8)	69(8)	63(8)	1(7)	−12(7)	−13(7)
Mn(2)	66(8)	68(7)	63(8)	10(7)	−11(7)	2(7)
S(1)	54(12)	62(12)	57(11)	−4(11)	−2(10)	0(10)
S(1′)	72(12)	68(12)	48(12)	15(11)	18(10)	−4(11)
S(1″)	71(12)	73(12)	47(12)	−26(11)	5(11)	19(11)
O(1)	222(42)	118(39)	134(41)	46(37)	12(38)	10(35)
O(2)	58(39)	132(41)	132(41)	−35(33)	−4(33)	−29(36)
O(3)	108(38)	82(42)	143(40)	16(36)	18(36)	55(36)
O(4)	186(42)	120(40)	64(38)	4(34)	−31(35)	−27(34)
O(1′)	87(37)	142(39)	90(38)	−6(34)	47(35)	25(35)
O(2′)	152(42)	182(41)	71(39)	−32(38)	−31(36)	21(36)
O(3′)	91(43)	192(42)	160(40)	−9(35)	0(37)	8(37)
O(4′)	274(44)	48(38)	174(42)	−3(39)	−49(39)	−52(36)
O(1″)	147(42)	181(43)	151(42)	42(36)	−30(36)	46(37)
O(2″)	272(43)	103(40)	166(43)	36(38)	32(39)	−29(37)
O(3″)	194(43)	299(46)	52(39)	−9(41)	41(38)	15(37)
O(4″)	109(40)	102(39)	220(43)	−34(36)	−33(39)	3(36)

Table 43A-8-010. $K_2Mn_2(SO_4)_3$. Structure of phase I [95Uke]. Fractional coordinates and temperature parameters [$\cdot 10^{-2}$ Å^2] at 296 K. See also the caption of Table 43A-8-006 about the primed and double-primed atoms.

Atom	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	0.33361(8)	0.33361(8)	0.33361(8)	1.55(2)	1.55(2)	1.55(2)	–0.36(2)	–0.36(2)	–0.36(2)
Mn(2)	0.59387(8)	0.59387(8)	0.59387(8)	1.24(2)	1.24(2)	1.24(2)	–0.02(2)	–0.02(2)	–0.02(2)
K(1)	0.81540(13)	0.81540(13)	0.81540(13)	2.10(4)	2.10(4)	2.10(4)	–0.21(4)	–0.21(4)	–0.21(4)
K(2)	0.05088(15)	0.05088(15)	0.05088(15)	2.31(4)	2.31(4)	2.31(4)	–0.05(4)	–0.05(4)	–0.05(4)
S	0.22123(4)	0.37538(4)	0.01490(4)	0.98(1)	1.01(1)	0.94(1)	0.27(1)	0.06(1)	0.11(1)
O(1)′	0.31568(59)	0.28935(39)	0.94687(60)	1.61(11)	1.18(13)	3.50(23)	0.55(11)	0.61(14)	–0.74(13)
O(1)″	0.30378(71)	0.26125(49)	0.97409(79)	2.96(26)	2.05(21)	4.85(35)	1.86(20)	0.20(22)	–0.38(19)
O(2)′	0.08855(73)	0.31468(68)	0.02731(68)	1.75(18)	3.01(27)	6.51(45)	–0.74(19)	1.23(30)	–1.80(29)
O(2)″	0.08455(58)	0.33452(55)	–0.00664(40)	1.04(9)	1.77(13)	1.59(10)	–0.32(9)	–0.23(9)	–0.20(9)
O(3)′	0.22946(85)	0.47742(45)	0.91858(52)	9.86(51)	1.74(16)	2.52(20)	–1.14(23)	0.40(27)	1.24(14)
O(3)″	0.24529(43)	0.50865(37)	0.95264(50)	2.31(12)	1.45(13)	4.03(24)	–0.46(11)	–0.55(15)	1.52(14)
O(4)′	0.26522(97)	0.41880(62)	0.14207(59)	5.80(48)	2.25(16)	1.65(22)	–0.06(21)	–1.73(24)	–0.74(16)
O(4)″	0.24806(89)	0.39506(87)	0.15877(68)	2.78(18)	6.90(63)	1.11(13)	–1.10(29)	–0.41(12)	0.56(22)

Table 43A-8-011. $K_2Mn_2(SO_4)_3$. Atomic coordinates determined by neutron diffraction at 4.2 K [88Oel]. Space group: $P2_12_12_1$.

Atom	*x*	*y*	*z*
K(1)	0.1771(39)	0.3237(55)	0.6799(43)
K(2)	0.0218(35)	0.0519(33)	0.0483(45)
Mn(1)	0.2746(35)	0.3558(29)	0.3461(37)
Mn(2)	0.3856(41)	0.0809(44)	0.9307(47)
S(1)	0.2709(2)	0.3349(48)	0.0414(72)
S(2)	0.3914(46)	0.0233(37)	0.2114(64)
S(3)	0.9702(48)	0.2171(41)	0.3677(78)
O(1)	0.3130(42)	0.2578(58)	0.0125(32)
O(2)	0.0782(62)	0.3312(69)	0.9885(50)
O(3)	0.2697(94)	0.4712(47)	0.9387(52)
O(4)	0.2196(47)	0.4275(59)	0.1610(60)
O(5)	0.2995(49)	0.9243(46)	0.3252(50)
O(6)	0.8195(34)	0.9899(60)	0.1072(52)
O(7)	0.5158(55)	0.9573(45)	0.2445(49)
O(8)	0.3778(48)	0.1527(52)	0.2928(35)
O(9)	0.9577(54)	0.2748(51)	0.2598(34)
O(10)	0.0582(72)	0.0768(48)	0.3398(66)
O(11)	0.9152(36)	0.1799(78)	0.4823(57)
O(12)	0.1250(73)	0.2827(41)	0.4345(62)

Table 43A-8-012. $K_2Mn_2(SO_4)_3$, $Rb_2Cd_2(SO_4)_3$, $Tl_2Cd_2(SO_4)_3$. $(d\Theta/dp)_{p=0}$ [80Hik].

Crystal	Transition	$(d\Theta/dp)_{p=0}$ [K GPa^{-1}]
$Tl_2Cd_2(SO_4)_3$	I–II	+ 4
	II–III	+ 12
	III–IV	+ 3
$Rb_2Cd_2(SO_4)_3$	I–II	+ 37
	II–III	– 24
$K_2Mn_2(SO_4)_3$	I–II	+ 69

Table 43A-8-013. $K_2Mn_2(SO_4)_3$. Positions of peaks [cm^{-1}] of absorption spectra [89Bre].

Term	ν_{SA}^{exp}	Term	ν_{SA}^{exp}
	17000	$^2E(t_2^3\,^2Ee^2\,^3A_2)$	
		$^2T_2(t_2^3\,^2T_1e^2\,^1E)$	
$^4T_1(t_2^4\,^3T_1e)$	19600	$^2T_1(t_2^4\,^1T_2e)$	
		$^4A_2(t_2^3\,^4A_2e^2\,^1A_1)$	
$^4T_2(t_2^4\,^3T_1e)$	23200		40000
		$^4T_1(t_2^3\,^2T_2e^2\,^3A_2)$	
		$^2T_2(t_2^4\,^3T_1e)$	
		$^2T_1(t_2^3\,^2T_2e^2\,^1E)$	
$^4E(t_2^3\,^2Ee^2\,^3A_2)$	25000	$^2E(t_2^3\,^2Ee^2\,^1E)$	
	26000		42500
		$^2A_1(t_2^4\,^1Ee)$	
$^2T_2(t_2^5)$		$^2A_2(t_2^3\,^2Ee^2\,^1E)$	
		$^4T_2(t_2^2\,^3T_1e^3)$	44000
$^4T_2(t_2^3\,^2T_1e^2\,^3A_2)$	28100	$^2T_2(t_2^3\,^2T_1e^2\,^3A_2)$	
		$^2T_1(t_2^3\,^2T_1e^2\,^1E)$	
$^4E(t_2^3\,^4A_2e^2\,^1E)$	29600	$^2E(t_2^4\,^1A_1e)$	
		$^2T_2(t_2^2\,^1T_2e^3)$	
		$^2T_1(t_2^2\,^3T_1e^3)$	48500
$^2A_2(t_2^4\,^1Ee)$		$^2T_1(t_2^3\,^2T_2e^2\,^3A_2)$	
$^4T_1(t_2^2\,^3T_1e^3)$	31800	$^2A_2(t_2^2\,^1Ee^3)$	
$^2T_1(t_2^4\,^3T_1e)$		$^2A_1(t_2^3\,^2Ee^2\,^1E)$	
			49800
$^2T_2(t_2^4\,^1T_2e)$	33800		
$^2E(t_2^4\,^1Ee)$			
$^2A_1(t_2^3\,^4A_2e^2\,^3A_2)$			

Table 43A-8-014. $K_2Mn_2(SO_4)_3$. Raman and infrared frequencies [cm^{-1}] and their symmetry assignments [82Kre].

	Description of vibration	Cubic				Orthorhombic
		Raman			Infrared	Raman
		Z(*YY*)*X* A, E	*Z*(*YZ*)*X* T	45° rotated *Z*(*YZ*)*X* E	T	unpolarized
SO_4^-	ν_3	1230 vw		1228 vvw		
Internal			1224 vw			1223 sh
		1218 sh				1215 m
						1207 sh
						1179 ?
					1167 sh	
		1162 vvw		1160 vvw		
			1153 vvw			1156 s
		1149 sh				
			1138 vvw		1136 s	1139 m
					1121 sh	1130 vvw
		1121 sh				1119 s
		1112 sh	1113 vvw			
		1105 s	1107 vw	1107 vw		1107 sh
						1102 vs
	ν_1					1058 vvw
		1030 vvs	1031 m	1032 w		1030 vvs
						1024 s
			1022 sh		1021 sh	1021 sh
						1006 vvw
	ν_4					665 vvw
			651 vvw			
		648 sh	645 vw		645 m	646 s
		641 m		641 vw		642 s
		629 sh	628 w		626 m	628 m
		620 s	620 w	620 w		619 s
					611 m	
		603 w	604 w	604 vw		602 m
			597 sh			
			590 vvw			
						578 ?
						529 ?
	ν_2		473 sh			473 m
		467 sh		469 vw	468 w	468 m
		461 m	461 w			460 vvw
		449 sh		449 vw		451 m
			447 w			444 w
			436 vvw		438 vw	436 w
		431 vvw				
			426 vvw			
						381 vw

(continued)

Table 43A-8-014 (continued)

Description of vibration	Cubic				Orthorhombic
	Raman			Infrared	Raman
	Z(*YY*)*X* A, E	*Z*(*YZ*)*X* T	45° rotated *Z*(*YZ*)*X* E	T	unpolarized
External		unpolarized			
				286 ?	
				265 m	
		244 vvw			248 vvw
		230 sh		237 m	227 sh
		221 vw		227 sh	221 w
		212 vw			215 vvw
		205 vw		204 sh	207 vw
		190 vvw		193 m	195 vw
					180 vvw
		170 vvw		167 vw	168 vw
				154 sh	
		149 w		148 m	149 vvw
		132 vvw		139 ?	132 vvw
		119 vvw		129 sh	119 vvw
		112 vv		111 sh	
		103 vvw		104 sh	102 vw
		90 vvw		97 w	92 w
		83 vvw		84 ?	86 vvw
		74 sh		75 m	75 vw
		68 w		67 sh	69 vw
		61 sh			
		52 vw		57 ?	53 vvw
		42 vvw			43 vvw
		35 vvw		35 ?	36 vvw
					31 vvw
		29 vvw		28 ?	27 vvw

vvs: very very strong
vs: very strong
s: strong
vvw: very very weak

vw: very weak
w: weak
m: medium
sh: shoulder