

**Table 41A-3-001.** RbLiSO<sub>4</sub>. Structure of phase I [87Kun].  $T = 220$  °C. Fractional coordinates [ $\cdot 10^4$ ] and isotropic temperature parameters.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B [\text{\AA}^2]$
Li	2500	4148(25)	3301(19)	3.90(46)
Rb	7500	2129(1)	5020(1)	3.45(2)
S	2500	848(2)	2064(2)	2.10(4)
O(1)	2500	915(15)	444(9)	7.55(36)
O(2)	1671(22)	2244(11)	2659(17)	6.66(43)
O(3)	4909(22)	473(11)	2642(13)	4.57(29)
O(4)	696(22)	−248(13)	2527(14)	5.45(35)

**Table 41A-3-002.** RbLiSO<sub>4</sub>. Structure of phase IV [87Kun].  $T = 190$  °C. Fractional coordinates [ $\cdot 10^4$ ] and isotropic temperature parameters.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B [\text{\AA}^2]$
Li(i)	2419(50)	4196(24)	1629(12)	2.87(42)
Li(ii)	2434(61)	866(33)	4106(14)	4.39(59)
Rb(i)	7524(4)	2161(1)	2515(1)	3.09(2)
Rb(ii)	7408(3)	2850(1)	5007(1)	3.21(2)
S(i)	2474(8)	833(3)	1031(2)	1.81(5)
S(ii)	2450(8)	4162(3)	3528(2)	1.88(5)
O(1i)	2499(28)	871(18)	211(5)	6.08(38)
O(1ii)	2478(38)	4066(18)	2719(7)	6.61(41)
O(2i)	1610(24)	2208(12)	1308(8)	4.93(32)
O(2ii)	1625(26)	2813(13)	3874(9)	5.68(34)
O(3i)	4880(20)	457(13)	1335(7)	3.93(26)
O(3ii)	4998(20)	4471(12)	3806(6)	3.64(25)
O(4i)	718(21)	−277(13)	1267(7)	3.98(27)
O(4ii)	743(26)	5302(14)	3754(9)	6.10(34)

**Table 41A-3-003.**  $\text{RbLiSO}_4$ . Structure of phase V [87Kun].  $T = 170^\circ\text{C}$ . Fractional coordinates [ $\cdot 10^4$ ] and isotropic temperature parameters.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B [\text{\AA}^2]$		$x$	$y$	$z$	$B [\text{\AA}^2]$
Li(i)	2368(156)	4360(85)	657(22)	4.77(207)	O(1vi)	2402(55)	4181(43)	5086(6)	4.91(96)
Li(ii)	2264(97)	865(66)	1647(15)	2.54(149)	O(1vii)	2556(54)	944(44)	6083(7)	5.09(108)
Li(iii)	2463(151)	4056(82)	2668(21)	4.48(182)	O(1viii)	2485(55)	4055(46)	7091(7)	5.50(101)
Li(iv)	2294(89)	816(62)	3648(14)	2.22(146)	O(1ix)	2515(51)	833(41)	8076(7)	4.75(100)
Li(v)	2287(129)	4041(77)	4640(18)	3.72(199)	O(1x)	2615(55)	3992(42)	9085(7)	4.68(88)
Li(vi)	2640(87)	877(52)	5664(14)	1.82(117)	O(2i)	1558(47)	2212(26)	525(7)	3.32(67)
Li(vii)	2559(122)	4136(80)	6669(17)	3.59(172)	O(2ii)	1639(60)	2781(35)	1520(11)	6.39(122)
Li(viii)	2563(101)	786(56)	7649(15)	2.44(147)	O(2iii)	3416(47)	2172(24)	2548(8)	3.61(69)
Li(ix)	2663(137)	4142(88)	8668(20)	4.49(206)	O(2iv)	1716(66)	2788(37)	3516(12)	6.59(126)
Li(x)	2607(103)	814(62)	9653(13)	2.32(131)	O(2v)	1465(45)	2162(26)	4543(7)	3.15(68)
Rb(i)	7513(6)	2150(4)	1004(1)	2.98(7)	O(2vi)	3349(61)	2810(35)	5526(11)	6.00(123)
Rb(ii)	7402(6)	2824(4)	2006(1)	2.76(6)	O(2vii)	3400(48)	2183(27)	6542(8)	3.70(70)
Rb(iii)	7576(6)	2166(4)	3004(1)	2.94(7)	O(2viii)	1516(62)	2831(34)	7562(10)	5.71(102)
Rb(iv)	7527(6)	2840(4)	4005(1)	2.77(6)	O(2ix)	3431(46)	2203(27)	8526(8)	3.71(70)
Rb(v)	7400(6)	2176(4)	5006(1)	2.98(6)	O(2x)	3252(58)	2763(33)	9551(11)	5.68(120)
Rb(vi)	7476(6)	2833(4)	6004(1)	2.80(6)	O(3i)	4835(35)	508(23)	549(5)	1.80(46)
Rb(vii)	7595(6)	2175(4)	7005(1)	2.87(6)	O(3ii)	4994(42)	4438(27)	1521(17)	2.77(67)
Rb(viii)	7410(6)	2836(4)	8006(1)	2.75(6)	O(3iii)	4351(37)	−283(24)	2532(6)	2.39(47)
Rb(ix)	7463(7)	2165(4)	9004(1)	3.00(7)	O(3iv)	4944(41)	4491(27)	3543(6)	2.58(68)
Rb(x)	7583(6)	2832(3)	5(1)	2.72(7)	O(3v)	4933(37)	470(24)	4539(5)	2.04(46)
S(i)	2479(12)	827(7)	413(2)	1.22(12)	O(3vi)	4384(40)	5235(25)	5529(7)	2.71(53)
S(ii)	2442(12)	4144(8)	1413(2)	1.26(12)	O(3vii)	4282(35)	−293(24)	6528(6)	2.16(50)
S(iii)	2519(12)	811(7)	2414(2)	1.26(11)	O(3viii)	5024(39)	4519(26)	7526(7)	3.19(69)
S(iv)	2476(12)	4179(8)	3413(2)	1.36(12)	O(3ix)	4281(35)	−256(25)	8529(6)	2.32(67)
S(v)	2440(12)	835(7)	4414(2)	1.30(12)	O(3x)	4382(39)	5264(25)	9521(7)	2.74(68)
S(vi)	2557(12)	4189(7)	5411(2)	1.27(12)	O(4i)	948(47)	−434(28)	480(7)	3.37(74)
S(vii)	2571(12)	829(7)	6410(2)	1.25(12)	O(4ii)	841(58)	5334(38)	1476(9)	5.22(94)
S(viii)	2473(12)	4187(7)	7414(2)	1.30(12)	O(4iii)	121(48)	458(29)	2521(7)	3.89(76)
S(ix)	2535(11)	828(7)	8410(2)	1.22(12)	O(4iv)	805(58)	5366(36)	3470(9)	5.13(94)
S(x)	2541(12)	4159(8)	9412(2)	1.34(12)	O(4v)	1033(53)	−364(33)	4479(7)	3.90(81)
O(1i)	2539(56)	870(43)	82(7)	5.04(107)	O(4vi)	−96(51)	4540(34)	5519(7)	3.92(83)
O(1ii)	2377(59)	4044(48)	1086(7)	5.52(105)	O(4vii)	163(51)	416(31)	6533(7)	3.57(78)
O(1iii)	2399(55)	924(45)	2084(7)	5.44(115)	O(4viii)	935(49)	5433(29)	7448(7)	3.72(77)
O(1iv)	2533(58)	4129(44)	3085(7)	5.34(98)	O(4ix)	34(54)	474(32)	8527(7)	3.98(79)
O(1v)	2405(56)	946(49)	4084(7)	5.89(120)	O(4x)	52(57)	4438(36)	9501(8)	4.36(86)

**Table 41A-3-004.**  $\text{RbLiSO}_4$ . Structure of phase VI [87Kun].  $T = 160^\circ\text{C}$ . Fractional coordinates [ $\cdot 10^4$ ] and isotropic temperature parameters.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B [\text{\AA}^2]$
Li	2449(29)	4131(16)	3268(17)	3.22(34)
Rb	7405(1)	2177(1)	5030(1)	2.39(2)
S	2473(3)	808(2)	2064(2)	1.17(3)
O(1)	2523(13)	928(10)	425(7)	5.15(21)
O(2)	1587(11)	2176(6)	2718(8)	3.96(15)
O(3)	4975(10)	481(6)	2644(7)	2.86(15)
O(4)	776(10)	−355(6)	2493(8)	3.57(15)

**Table 41A-3-005.** RbLiSO<sub>4</sub>. Structure [87Kun].  $T = 220, 190, 170, 160$  °C. Bond lengths [Å] and angles [°] of SO<sub>4</sub> tetrahedra.

	220 °C	190 °C		170 °C	160 °C
		i	ii		
S–O(1)	1.411(14)	1.428(11)	1.411(11)	1.437(13)	1.434(1)
S–O(2)	1.452(15)	1.423(11)	1.441(11)	1.440(24)	1.451(5)
S–O(3)	1.420(12)	1.424(11)	1.463(11)	1.464(20)	1.450(5)
S–O(4)	1.448(12)	1.438(12)	1.436(13)	1.427(43)	1.443(6)
Average	1.433(20)	1.428(20)	1.438(20)	1.442(16)	1.445(8)
O(1)–S–O(2)	108.6(8)	108.7(7)	111.6(7)	109.3(26)	109.4(4)
O(1)–S–O(3)	111.4(8)	111.7(7)	109.4(9)	112.6(17)	110.3(3)
O(1)–S–O(4)	108.0(8)	108.0(7)	109.0(8)	105.9(41)	109.0(3)
O(2)–S–O(3)	111.2(8)	112.1(6)	107.9(6)	107.4(32)	109.6(3)
O(2)–S–O(4)	108.2(8)	108.6(7)	108.4(7)	113.0(41)	109.3(3)
O(3)–S–O(4)	109.3(7)	107.7(6)	110.6(6)	108.4(37)	109.2(3)
Average	109.5(15)	109.5(19)	109.5(14)	109.4(28)	109.5(5)