

**Table 30A-3-001.** RbNO<sub>3</sub>. Solubility  $A$  in H<sub>2</sub>O [62Kaf].

$A$ [wt%]	$T$ [°C]	$A$ [wt%]	$T$ [°C]
16.3	0	66.7	60
24.8	10	71.5	70
34.6	20	75.6	80
44.8	30	78.9	90
53.9	40	81.9	100
60.9	50		

**Table 30A-3-002.** RbNO<sub>3</sub>. Crystal structure of phase IV. Fractional coordinates [ $\cdot 10^4$ ] and isotropic temperature parameters [92Poh].  $T = 296$  K (upper line) and  $372$  K (lower line).  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B [\text{\AA}^2]$
Rb(1)	4474(2)	5575(2)	6483(4)	2.5(1)
	4373(2)	5491(2)	6900(5)	2.9(1)
Rb(2)	1231(1)	2201(1)	0	2.5(1)
	1147(2)	2241(1)	0	3.3(1)
Rb(3)	-2161(1)	2299(1)	6242(1)	2.4(1)
	-2107(1)	2348(1)	6485(6)	3.0(1)
N(1)	4612(7)	5915(7)	1628(15)	2.4(3)
	4400(9)	5665(12)	2169(23)	2.3(4)
N(2)	1009(8)	2047(8)	-4784(15)	2.2(3)
	1253(11)	2035(10)	-5191(17)	2.5(4)
N(3)	-2337(9)	2260(6)	959(14)	1.7(3)
	-2279(10)	2331(10)	1317(29)	2.4(4)
O(1)	4495(7)	6778(7)	2713(8)	3.7(2)
	4432(9)	6649(9)	3105(16)	4.2(3)
O(2)	3927(8)	4597(7)	1935(10)	5.0(3)
	3538(11)	4373(9)	2618(21)	6.1(4)
O(3)	5465(7)	6419(8)	389(9)	4.0(2)
	5172(12)	6030(15)	901(15)	5.6(5)
O(4)	22(6)	1101(6)	-3799(9)	3.4(2)
	1121(11)	1076(10)	-6178(17)	5.5(4)
O(5)	2310(6)	2476(7)	-4432(10)	4.3(2)
	2124(11)	2314(10)	-3889(16)	5.2(4)
O(6)	637(7)	2519(7)	-6081(8)	3.9(3)
	602(14)	2673(13)	-5341(19)	6.9(5)
O(7)	-2729(9)	1458(8)	2269(9)	4.6(9)
	-2674(13)	1479(11)	2541(14)	5.2(4)
O(8)	-1034(6)	3091(7)	553(11)	4.4(2)
	-1010(9)	3200(10)	942(18)	5.6(4)
O(9)	-3315(6)	2246(7)	-15(8)	3.4(2)
	-3306(10)	2242(9)	330(18)	4.8(4)

**Table 30A-3-003.** RbNO<sub>3</sub>. Interatomic distances [Å] and bond angles [°] [92Poh]. *T* = 296 K, 372 K. Symmetry code: (i) *x*, *y*, 1 + *z*; (ii)  $-y$ ,  $x - y$ ,  $1/3 + z$ ; (iii)  $-y$ , 1 +  $x - y$ ,  $1/3 + z$ ; (iv)  $-y$ ,  $x - y$ ,  $4/3 + z$ ; (v) 1 - *y*, 1 +  $x - y$ ,  $1/3 + z$ ; (vi) 1 - *y*, 1 +  $x - y$ ,  $4/3 + z$ ; (vii)  $-1 + y - x$ ,  $-x$ ,  $2/3 + z$ ; (viii)  $y - x$ ,  $-x$ ,  $-1/3 + z$ ; (ix)  $y - x$ ,  $-x$ ,  $2/3 + z$ ; (x)  $y - x$ , 1 - *x*,  $-1/3 + z$ ; (xi)  $y - x$ , 1 - *x*,  $2/3 + z$ .

	296 K	372 K	296 K	372 K	296 K	372 K		
Rb(1)–O(1)	3.072(6)	3.073(11)	Rb(2)–O(1) <sup>x</sup>	3.097(6)	3.095(8)	Rb(3)–O(2) <sup>ii</sup>	2.961(6)	3.008(10)
Rb(1)–O(1) <sup>v</sup>	3.131(6)	3.107(8)	Rb(2)–O(2)	3.043(6)	3.086(12)	Rb(3)–O(3) <sup>xi</sup>	2.993(5)	3.005(10)
Rb(1)–O(1) <sup>xi</sup>	3.124(7)	3.149(10)	Rb(2)–O(3) <sup>x</sup>	3.391(7)	3.407(13)	Rb(3)–O(4) <sup>†</sup>	3.110(6)	3.146(10)
Rb(1)–O(2)	3.501(8)	3.369(14)	Rb(2)–O(4) <sup>*</sup>	3.078(7)	3.100(12)	Rb(3)–O(5) <sup>iv</sup>	3.137(6)	3.385(12)
Rb(1)–O(2) <sup>v</sup>	3.662(8)	3.471(12)	Rb(2)–O(4) <sup>ii</sup>	3.082(5)	3.147(11)	Rb(3)–O(6) <sup>i</sup>	3.311(7)	3.017(11)
Rb(1)–O(3) <sup>i</sup>	3.068(7)	3.078(11)	Rb(2)–O(4) <sup>ix</sup>	3.104(7)	3.123(10)	Rb(3)–O(7) <sup>iii</sup>	3.059(7)	3.053(11)
Rb(1)–O(3) <sup>xi</sup>	3.286(6)	3.434(12)	Rb(2)–O(5)	3.452(7)	3.069(12)	Rb(3)–O(7) <sup>iii</sup>	3.407(8)	3.425(10)
Rb(1)–O(5) <sup>i</sup>	2.963(6)	3.030(9)	Rb(2)–O(5) <sup>ii</sup>	3.502(7)	3.260(10)	Rb(3)–O(8) <sup>i</sup>	3.376(8)	3.490(13)
Rb(1)–O(6) <sup>vi</sup>	2.992(6)	2.985(11)	Rb(2)–O(6) <sup>i</sup>	3.026(6)	3.592(14)	Rb(3)–O(8) <sup>vii</sup>	3.502(7)	3.495(12)
Rb(1)–O(7) <sup>ix</sup>	3.378(8)	3.331(12)	Rb(2)–O(6) <sup>ix</sup>	3.394(6)	3.707(13)	Rb(3)–O(9) <sup>i</sup>	3.026(6)	3.115(13)
Rb(1)–O(8) <sup>v</sup>	3.089(7)	3.105(10)	Rb(2)–O(7) <sup>viii</sup>	2.968(6)	3.016(9)	Rb(3)–O(9) <sup>iii</sup>	3.158(6)	3.108(12)
Rb(1)–O(9) <sup>ix</sup>	3.100(6)	3.104(9)	Rb(2)–O(8)	2.979(6)	2.988(10)	Rb(3)–O(9) <sup>vii</sup>	3.075(5)	3.115(9)
N(1)–O(1)	1.26(1)	1.24(1)	N(2)–O(4)	1.25(1)	1.20(1)	N(3)–O(7)	1.22(2)	1.20(2)
N(1)–O(2)	1.22(1)	1.24(2)	N(2)–O(5)	1.24(1)	1.27(2)	N(3)–O(8)	1.23(1)	1.21(1)
N(1)–O(3)	1.21(1)	1.18(2)	N(2)–O(6)	1.23(1)	1.18(2)	N(3)–O(9)	1.25(1)	1.27(2)
O(1)–N(1)–O(2)	119(1)	117(2)	O(4)–N(2)–O(5)	119(1)	116(1)	O(7)–N(3)–O(8)	124(1)	125(2)
O(1)–N(1)–O(3)	118(1)	117(1)	O(4)–N(2)–O(6)	118(1)	124(2)	O(7)–N(3)–O(9)	118(1)	115(1)
O(2)–N(1)–O(3)	123(1)	125(1)	O(5)–N(2)–O(6)	122(1)	126(1)	O(8)–N(3)–O(9)	119(1)	120(2)

\* At 296 K there is no superscript, at 372 K superscript (i).

† At 296 K superscript (i), at 372 K superscript (iv).

**Table 30A-3-004.** RbNO<sub>3</sub>. Structure of phase III. Fractional coordinates and isotropic temperature parameters [80Ath].  $T = 463$  K.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$	$B$ [Å <sup>2</sup> ]
Rb	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	7.7 (2)
N	0.065 (5)	0	0	8.6 (8)
O (1)	0.350	0	0	8.4 (14)
O (2)	0	0.244 (6)	−0.100 (7)	

**Table 30A-3-005.** RbNO<sub>3</sub>. Structure of phase II. Fractional coordinates and overall isotropic temperature parameters [80Ath].  $T = 503$  K.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$
Rb	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
N	−0.0318 (7)	−0.0318	−0.0318
O	−0.0726 (7)	−0.0726	0.2463 (7)

 $B(\text{overall}) = 8.0 (1) \text{ Å}^2$ **Table 30A-3-006.** RbNO<sub>3</sub>. Structure of phase I. Fractional coordinates and overall isotropic temperature parameters [80Ath].  $T = 568$  K.  $B$  is defined by Eq. (e) in Introduction.

	$x$	$y$	$z$
Rb	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
N	−0.0373 (16)	−0.0373	−0.0373
O	0.0659 (21)	0.0659	0.1562 (20)

 $B(\text{overall}) = 10.8 (6) \text{ Å}^2$ **Table 30A-3-007.** RbNO<sub>3</sub>. Interatomic distances [Å] and bond angles [°] in phases III, II, I [80Ath]. Numbers in brackets represent the bonds involved.

Phase	III		II		I	
N—O (1)	1.25 Å	[1]	1.24 (2) Å	[3]	1.77 (5) Å	[1]
N—O (2)	1.10 (8) Å	[2]			1.17 (4) Å	[2]
O (1)—N—O (2)	104 (2)°	[2]	102 (2)°	[3]	101 (4)°	[2]
O (2)—N—O (2)	120°	[1]			158 (4)°	[1]
O (1)—O (2)	1.92 (4) Å	[2]	2.15 (4) Å	[3]	2.30 (4) Å	[3]
O (2)—O (2)	2.13 (6) Å	[1]				
Rb—O (1)	3.16 (1) Å	[4]	3.06 (2) Å	[6]	2.61 (2) Å	[6]
Rb—O (2)	3.01 (3) Å	[2]				

**Table 30A-3-008.** RbNO<sub>3</sub>. Unit cell parameters at various  $T$  [92Poh].

$T$ [K]	$a$ [Å]	$c$ [Å]
296(0.1)	10.474(1)	7.443(1)
372(3)	10.506(3)	7.469(2)
413(5)	10.537(4)	7.493(3)
437(9)	10.560(6)	7.503(5)
299(0.1) *)	10.455(1)	7.421(1)

\*) Values for the previously heated crystal.