Table 30A-2-001. KNO_3. Solubility A in H_2O [62Kaf].

A [wt%]	T [°C]	A [wt%]	T [°C]
12.2	0	45.5	50
17.5	10	51.5	60
24.0	20	57.5	70
27.5	25	62.5	80
31.2	30	67.0	90
38.0	40	71.0	100

Table 30A-2-002. KNO_3. Unit cell parameters in various phases.

Phase	T [°C]	Unit cell parameters [Å]	Ref.
II	25	a = 5.4119, b = 9.1567, c = 6.4213	73Nim
III	91 *)	a = 5.487(1), c = 9.156(3) **)	76Nim
I	151	a = 5.425(1), c = 9.836(4) **)	76Nim

*) A quenched state. The temperature region where phase III is observed depends on previous treatment. In this study it was lower than those reported by other authors (see subsection 1b).
**) For the hexagonal cell.

Table 30A-2-003. KNO_3. Structure of phase II [73Nim]. Fractional coordinates and anisotropic temperature parameters obtained by neutron diffraction. b_{ij} is defined by Eq. (b) in Introduction. R factor: 0.058 at 25 °C, 0.141 at 100 °C.

T[°C]		x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
25 (1)	K	0.2500	0.4166 (1)	0.7568 (2)	0.0184 (5)	0.0061 (1)	0.0180 (4)	0	0	0.0005 (2)
	N	0.2500	0.7548 (1)	−0.0848 (1)	0.0184 (2)	0.0071 (1)	0.0111 (2)	0	0	0.0001 (1)
	O (1)	0.2500	0.8902 (1)	−0.0893 (2)	0.0273 (4)	0.0066 (1)	0.0249 (3)	0	0	−0.0024 (1)
	O (2)	0.4492 (1)	0.6866 (1)	−0.0849 (1)	0.0173 (3)	0.0097 (1)	0.0236 (2)	0.0019 (1)	−0.0027 (1)	0.0016 (1)
100 (1)	K	0.2500	0.4155 (3)	0.7646 (8)	0.0158 (5)	0.0101 (3)	0.0238 (16)	0	0	−0.0089 (6)
	N	0.2500	0.7539 (1)	−0.0829 (2)	0.0256 (4)	0.0083 (1)	0.0181 (4)	0	0	0.0018 (2)
	O (1)	0.2500	0.8890 (2)	−0.0900 (6)	0.0425 (9)	0.0090 (3)	0.0258 (10)	0	0	0.0011 (5)
	O (2)	0.4442 (2)	0.6849 (1)	−0.0835 (5)	0.0247 (4)	0.0116 (2)	0.0332 (7)	0.0017 (3)	−0.0048 (5)	−0.0007 (3)

Table 30A-2-004. KNO_3. Structure of phase II [73Nim]. Interatomic distances and bond angles obtained by neutron diffraction. Numbering of atoms: see Fig. 30A-2-003, Fig. 30A-2-004.

			25 °C	100 °C
Uncorrected interatomic distances [Å]				
	Metal-oxygen	K_4–O_3 (1)	2.845 (4)	2.926 (13)
		K_4–O_1 (2)	2.885 (3)	2.864 (8)
		K_4–O_4 (1)	2.925 (1)	2.951 (5)
		K_4–O'_2 (2)	2.828 (2)	2.815 (6)
		K_4–O_4 (2′)	2.884 (3)	2.938 (7)
	Within the NO_3 group	N–O (1)	1.241 (2)	1.241 (5)
		N–O (2) } N–O (2′) }	1.246 (1)	1.229 (3)
		O (1)–O (2)	2.155 (2)	2.150 (4)
		O (2)–O (2′)	2.157 (1)	2.106 (2)
Corrections to be added [Å]				
	(i) Assuming rigid-body motion of the NO_3 group	N–O (1)	0.017 (6)	0.014 (6)
		N–O (2) } N–O (2′) }	0.012 (4)	0.016 (4)
		O (1)–O (2)	0.031 (11)	0.035 (10)
		O (2)–O (2′)	0.027 (10)	0.040 (10)
	(ii) Assuming "riding" motion of the O on N	N–O (1)	0.016 (1)	0.018 (1)
		N–O (2) } N–O (2′) }	0.014 (1)	0.018 (1)
Uncorrected bond angles [°]				
	O (2)–N–O (1)		120.06 (8)	121.02 (17)
	O (2)–N–O (2′)		119.85 (15)	117.90 (34)

Table 30A-2-005. KNO_3. Structures of phases I and III [76Nim]. Fractional coordinates and anisotropic temperature parameters. b_{ij} is defined by Eq. (b) in Introduction. R factor: 0.18 for phase III, 0.13 for phase I.

Phase		x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
III (91 °C)*)	K	0	0	0	0.038 (6)	b_{11}	0.030 (5)	$b_{11}/2$	0	0
	N	0	0	0.405 (6)	0.09 (3)	b_{11}	0.00 (1)	$b_{11}/2$	0	0
	O	0.131 (2)	$\bar{x}$	0.434 (3)	0.05 (2)	b_{11}	0.007 (4)	0.03 (2)	−0.001 (3)	$-b_{13}$
I (151 °C)	K	0	0	0	0.109 (7)	b_{11}	0.029 (3)	$b_{11}/2$	0	0
	N	0	0	$\frac{1}{2}$	0.03 (2)	b_{11}	0.06 (1)	$b_{11}/2$	0	0
	O	0.130 (2)	$\bar{x}$	0.475 (5)	0.05 (2)	b_{11}	0.10 (1)	0.04 (2)	0.008 (8)	$-b_{13}$

*) A quenched state. See footnote of Table 30A-2-002.

Table 30A-2-006. KNO_3. Structures of phases I and III [76Nim]. Interatomic distances and bond angles.

Phase	III (91 °C)*)	I (151 °C)
Interatomic distances [Å]		
K⋯O	2.87 (2)	2.68 (4)
	2.91 (1)	3.07 (2)
N–O	1.28 (2)	1.25 (2)
Interatomic angles [°]		
O–N–O	116 (2)	116 (1)

*) A quenched state. See footnote of Table 30A-2-002.

Table 30A-2-007. KNO_3. Structures of high pressure phase IV [86Wor]. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction. p = 0.36 GPa, T = RT.

Atom	x	y	z	B [Å^2]
K	0.4863(5)	0.25	0.6897(5)	1.32(7)
N	0.3465(2)	0.25	0.1321(2)	1.09(3)
O(1)	0.4411(3)	0.25	0.2806(4)	1.46(5)
O(2)	0.2985(3)	0.4432(3)	0.0556(3)	1.64(3)

Table 30A-2-008. KNO_3. Linear thermal expansion coefficients. $\alpha_{[111]}$: thermal expansion coefficient along the [111] direction.

Phase	T [°C]	α_{ii} [$\cdot 10^{-4}$ K^{-1}]			Ref.
II	–180…20	α_{11} = 1.36	α_{22} = 0.20	α_{33} = 0.16	63Gut
III	120	$\alpha_{[111]}$ = 3.33			65Kaw
I	125	$\alpha_{[111]}$ = 3.15			65Kaw

Table 30A-2-009. KNO_3. Variation of unit cell parameters and unit cell volume at different pressures [88Ada]. T = RT. Space group of high pressure phase IV is taken as Pnma– D_{2h}^{16}.

p [GPa]	a [Å]	b [Å]	c [Å]	V [Å^3]
0.35	7.487(3)	5.565(2)	6.763(3)	281.75(30)
1.60	7.395(18)	5.507(15)	6.696(18)	272.70(120)
2.00	7.331(18)	5.462(14)	6.656(17)	266.50(120)
2.58	7.295(15)	5.449(12)	6.662(24)	264.80(130)
3.00	7.282(16)	5.441(13)	6.650(16)	263.50(100)
4.58	7.219(38)	5.400(27)	6.639(54)	258.85(280)
5.10	7.175(26)	5.346(18)	6.613(38)	253.69(190)
7.36	7.097(49)	5.288(35)	6.571(71)	246.60(350)
9.30	6.944(18)	5.236(11)	6.461(13)	234.94(90)

Table 30A-2-010. KNO_3. Transition heats and transition entropies [93Wes].

Transition	ΔQ_m [$\cdot 10^3$ J mol^{-1}]	ΔS_m [J K^{-1} mol^{-1}]
II–I	5.065	12.53
I–III	2.603	6.61
III–II	2.084	5.30

Table 30A-2-011. KNO_3, $CsNO_3$. Elastic stiffnesses [90Hau].

	T	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
	[K]	[$\cdot 10^{10}$ Pa]								
KNO_3	293	3.716	2.989	2.037	0.680	0.543	0.835	1.680	1.096	1.114
	398	3.313	2.643	1.834	0.599	0.495	0.739	1.491	1.018	1.002
$CsNO_3$	293	3.098	$= c_{11}$	2.968	0.967	$= c_{44}$	0.898	1.303	1.375	$= c_{13}$
	425	2.590	$= c_{11}$	2.464	0.768	$= c_{44}$	0.726	1.14	1.32	$= c_{13}$
	430	2.53	$= c_{11}$	2.43	0.75	$= c_{44}$	0.71	1.11	1.32	$= c_{13}$

Table 30A-2-012. KNO_3. Refractive indices [62Kor].

λ nm	n_α	n_β	n_γ
253.0	1.367	*)	1.698
260.0	1.349	*)	1.671
270.0	1.361	*)	1.644
280.0	1.358	*)	1.624
290.0	1.356	*)	1.608
300.0	1.3543	*)	1.5450
310.0	1.3526	*)	1.5861
320.0	1.3514	*)	1.5782
330.0	1.3499	*)	1.5703
350.0	1.3479	*)	1.5582
366.3	1.3460	*)	1.5502
396.9	1.3435	*)	1.5384
435.8	1.3410	*)	1.5279
589.3	1.3346	*)	1.5056
686.8	1.3328	*)	1.4988
405	1.3384	1.5299	1.5304
436	1.3368	1.5224	1.5229
486	1.3347	1.5139	1.5144
546	1.3330	1.5072	1.5077
656	1.3310	1.4998	1.5002
706	*)	1.4975	1.4979
768	*)	1.4951	1.4955
527	1.3365	1.5124	1.5135
589	1.3346	1.5056	1.5064
687	1.3328	1.4988	1.4994

*) No value given.