

Table 28A-2-001. AgNa(NO₂)₂. Unit cell parameters and X-ray densities at different temperatures [87Ish].

Phase	<i>T</i> [K]	<i>a</i>	<i>b</i>	<i>c</i>	ρ_{x} [·10 ³ kg m ⁻³]
		[Å]			
II	118(1)	7.607(1)	10.665(1)	10.945(1)	3.33
	218(1)	7.728(1)	10.680(1)	10.918(1)	3.29
	268(1)	7.830(3)	10.698(1)	10.877(1)	3.25
	297(1)	7.928(4)	10.717(1)	10.820(2)	3.22
	308(1)	8.038(2)	10.742(3)	10.763(2)	3.19
I	323(1)	8.062(1)	10.748(3)	10.754(2)	3.18
	334(1)	8.077(2)	10.749(3)	10.751(2)	3.17
	343(1)	8.089(1)	10.753(2)	10.744(1)	3.17

Table 28A-2-002. AgNa(NO₂)₂. Structure of phases I and II [87Ish]. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-1} \text{ \AA}^2$]. B is defined by Eq. (e) in Introduction. In the analysis, it is assumed that the two configurations of disordered NO₂[−] ion are related to each other by pseudo-mirror perpendicular to the b axis. Asterisk denotes disordered N atoms.

Phase I

	x	y	z	B
323 K				
Ag	0	0	0	41(1)
Na	0	5000	0	31(1)
N11*	0	1973(9)	0	29(1)
N12*	0	2687(4)	0	29(1)
O11	−474(4)	2604(7)	905(3)	40(1)
O12	−474(4)	2056(4)	905(3)	40(1)

Phase II

	x	y	z	B
118 K				
Ag	0	0	0	11(1)
Na	0	4881(6)	0	9(1)
N11*	0	2099(4)	0	8(1)
N12*	0	2956(112)	0	8(1)
N21	0	7327(5)	0	10(1)
O11	−326(3)	2728(4)	945(2)	11(1)
O12	−326(3)	2327(110)	945(2)	11(1)
O21	397(3)	7969(3)	918(2)	13(1)
308 K				
Ag	0	0	0	38(1)
Na	0	5016(12)	0	30(1)
N11*	0	1983(10)	0	24(2)
N12*	0	2609(21)	0	24(2)
N21*	0	7263(12)	0	28(2)
N22*	0	7875(141)	0	28(2)
O11	−502(10)	2599(14)	943(8)	39(2)
O12	−502(10)	1994(18)	943(8)	39(2)
O21	454(9)	7902(10)	872(6)	36(2)
O22	454(9)	7237(142)	872(6)	36(2)

Table 28A-2-003. AgNa(NO₂)₂. Structure of phases I and II [87Ish]. Interatomic distances [Å] and angles [°]. Values for NO₂⁻ (12) and NO₂⁻ (22) are equal to those in NO₂⁻ (11) and NO₂⁻ (21), respectively, because of the mirror constraint; see caption of Table 28A-2-002.

	118 K	218 K	268 K	297 K	308 K	323 K	334 K	343 K
N(11)–O(11)	1.258(4)	1.254(6)	1.249(6)	1.251(7)	1.277(12)	1.246(4)	1.248(5)	1.244(5)
O(11)–N(11)–O(11 ⁱ)	115.5(4)	115.9(7)	116.3(6)	116.0(7)	117.6(11)	114.1(4)	114.0(5)	114.1(5)
Ag...N(11)	2.239(5)	2.230(8)	2.223(8)	2.220(8)	2.130(11)	2.121(10)	2.123(12)	2.117(12)
Ag...O(12)	2.70(11)	2.56(12)	2.45(4)	2.47(2)	2.404(18)	2.445(4)	2.445(4)	2.445(4)
Na...N(12)	2.05(12)	2.23(14)	2.36(5)	2.36(3)	2.59(3)	2.486(4)	2.485(5)	2.489(5)
Na...O(11)	2.530(7)	2.552(12)	2.574(11)	2.621(16)	2.817(18)	2.779(7)	2.777(8)	2.786(9)
N(21)–O(21)	1.253(4)	1.249(8)	1.252(7)	1.238(9)	1.218(10)	–	–	–
O(21)–N(21)–O(21 ⁱ)	113.7(4)	114.0(10)	113.1(8)	113.1(11)	111.5(11)	–	–	–
Ag...O(21)	2.406(3)	2.409(5)	2.415(5)	2.417(6)	2.469(10)	–	–	–
Na...N(21)	2.609(8)	2.615(17)	2.604(15)	2.589(21)	2.414(18)	–	–	–
Ag...N(22)	–	–	–	–	2.28(15)	–	–	–
Na...O(22)	–	–	–	–	2.59(14)	–	–	–
Symmetry code: (i) – x, y, – z.								

Table 28A-2-004. AgNa(NO₂)₂. Population parameters of N atoms at different temperatures [87Ish]. Positions of N(ij) (i, j = 1, 2) are shown in Fig. 28A-2-004.

Phase II

<i>T</i> [K]	118	218	268	297	308
N(11)	0.974(12)	0.957(17)	0.898(11)	0.733(12)	0.496(21)
N(12)	0.026(12)	0.043(17)	0.102(11)	0.267(12)	0.504(21)
N(21)	1	1	1	1	0.952(26)
N(22)	0	0	0	0	0.048(26)

Phase I

<i>T</i> [K]	323	334	343
N(11)	0.277(6)	0.277(7)	0.274(7)
N(12)	0.723(6)	0.723(7)	0.726(7)