Table 28A-1-001. $NaNO_2$. Solubility A in H_2O [62Kaf].

A [wt%]	41.63	43.7	45.07	52.00	54.07	56.95	61.5
T [°C]	0	15	22	56.8	64.7	79.5	99.9

Table 28A-1-002. $NaNO_2$. Fractional coordinates, temperature parameters, occupancy factors. b_{ij} is defined by Eq. (b) in Introduction. f_1: fraction in the observed position in phase III, f_2: fraction in the reverse position.

T [°C]		RT	145	150	162	185	225
Ref.		75Kay				72Kay	
N	y	0.1188(4)	0.0727(11)	0.0723(6)	0.0764(6)	0.0719(4)	0.0704(5)
O	y	0	–0.0435	–0.0457	–0.0408(15)	–0.0435(10)	–0.0468(8)
	z	0.1953(4)	0.1949(9)	0.1937(6)	0.1931(6)	0.1920(4)	0.1912(4)
Na	y	0.5830(11)	0.5346(23)	0.5353(13)	0.5439(12)	0.5390(20)	0.5337(43)
N	b_{11}	0.0501(20)	0.0784(44)	0.0912(33)	0.0935(38)	0.117(2)	0.130(4)
	b_{22}	0.0081(9)	0.0140(14)	0.0165(11)	0.0216(11)	0.032(1)	0.032(1)
	b_{33}	0.0109(11)	0.0191(23)	0.0217(16)	0.0237(13)	0.030(1)	0.033(1)
O	b_{11}	0.0562(19)	0.0900(44)	0.0939(33)	0.1009(36)	0.116(3)	0.131(3)
	b_{22}	0.0135(11)	0.0292(29)	0.0288(18)	0.0337(17)	0.045(3)	0.044(3)
	b_{33}	0.0113(7)	0.0163(16)	0.0210(12)	0.0231(12)	0.031(1)	0.0352(8)
	b_{23}	0.0011(10)	0.0044(22)	0.0006(13)	0.0040(13)	0.004(1)	0.007(1)
Na	b_{11}	0.0300(38)	0.0594(91)	0.0599(61)	0.0689(58)	0.069(4)	0.082(4)
	b_{22}	0.0130(17)	0.0231(48)	0.0220(22)	0.0170(28)	0.031(6)	0.036(9)
	b_{33}	0.0139(19)	0.0174(36)	0.0247(24)	0.0253(23)	0.028(1)	0.032(2)
f_1				0.883	0.768(5)		
f_2				0.117	0.232(5)		

Table 28A-1-003. $NaNO_2$. Interatomic distances, bond angles, principal values of root-mean-square amplitudes of thermal vibrations. μ_{xx}, μ_{yy}, μ_{zz}: root-mean-square amplitudes along the principal axes of the thermal vibration ellipsoids in the x, y, z directions. μ_y, μ_z: refer to the amplitudes along the principal axes close to y and z. Angle denotes the angle between the major principal axis of oxygen in the (100) plane and the y axis.

T [°C]		RT	145	150	162	185	225
Ref.		75Kay				72Kay	
N–O	[Å]	1.244(4)	1.237(5)	1.236(4)	1.229(4)	1.217(5)	1.214(6)
O–N–O	[°]	115.6(3)	115.8(6)	114.7(4)	114.8(4)	114.9(6)	113.2(6)
Na–O	[Å]	2.554(8)	2.605(15)	2.587(29)	2.566(9)	2.579(13)	2.597(19)
Na–N	[Å]	2.590(10)	2.611(17)	2.617(32)	2.642(10)	2.648(13)	2.642(24)
Root mean square amplitudes of motion							
N	μ_{xx} [Å]	0.180(4)	0.230(7)	0.203(9)	0.251(5)	0.282(3)	0.300(4)
	μ_{yy} [Å]	0.126(6)	0.167(10)	0.193(10)	0.187(5)	0.227(3)	0.232(4)
	μ_{zz} [Å]	0.113(6)	0.150(8)	0.193(10)	0.186(5)	0.210(3)	0.218(4)
O	μ_{xx} [Å]	0.190(3)	0.247(6)	0.253(5)	0.261(5)	0.282(3)	0.300(4)
	μ_y [Å]	0.148(6)	0.218(11)	0.219(7)	0.237(6)	0.273(9)	0.276(10)
	μ_z [Å]	0.127(5)	0.154(8)	0.180(5)	0.179(5)	0.208(3)	0.214(5)
	Angle [°]	17.2(14)	5.1(80)	0.6(70)	15.1(46)	10(3)	21(5)
Na	μ_{xx} [Å]	0.143(9)	0.200(15)	0.203(9)	0.216(9)	0.217(4)	0.238(7)
	μ_{yy} [Å]	0.143(10)	0.194(20)	0.193(10)	0.192(9)	0.229(2)	0.243(28)
	μ_{zz} [Å]	0.139(9)	0.160(16)	0.193(10)	0.1666(14)	0.203(4)	0.212(6)

Table 28A-1-004. $NaNO_2$. Structure of phase II [85Kuc]. $T = \Theta_{III–II} + 0.2$ K. Modulations of occupation probability and displacement are expressed as: $p(x) = 1/2 + p_c\cos(2\pi qx) + p_s\sin(2\pi qx)$, $u_y = u_y^c \cos(2\pi qx) + u_y^s \sin(2\pi qx)$, where q is the modulation wave number.

(a) Fractional coordinates of the average structure

Atom	x	y	z
Na	0	0.53771(6)	0
N	0	0.07787(9)	0
O	0	–0.04058(9)	0.19297(5)

(b) Anisotropic temperature parameters of the average structure

Atom	B_{11}	B_{22}	B_{33}	B_{23}
Na	0.0721(3)	0.0239(1)	0.0248(1)	0
N	0.1039(5)	0.0223(1)	0.0169(1)	0
O	0.1147(3)	0.0325(2)	0.0295(1)	0.0053(1)

(c) Modulational parameters

Atom	p_c	p_s	u_y^c	u_y^s
Na	0.219(3)	0	0.0134(3)	–0.0022(8)
N, O	0.231(3)	–0.102(5)	0.0069(1)	–0.0028(4)

Table 28A-1-005. $NaNO_2$. $c_{\lambda\mu}$, $s_{\lambda\mu}$ [70Hau]. $T = 21$ °C.

$c_{\lambda\mu}[10^9$ N m$^{-2}]$								
c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
30.1 (2)	55.8 (2)	63.4 (3)	12.0 (2)	10.0 (2)	4.8 (2)	12.3 (30)	16.4 (30)	17.0 (30)
$s_{\lambda\mu}[10^{-11}$ m^2 N$^{-1}]$								
s_{11}	s_{22}	s_{33}	s_{44}	s_{55}	s_{66}	s_{12}	s_{13}	s_{23}
4.06	2.05	1.91	8.33	10	20.8	−0.63	−0.80	−0.39

Table 28A-1-006. $NaNO_2$. n_c, n_b vs. λ [74Che].

λ μm	n_c	n_b
1.014	1.631_3	1.405
1.3673	1.621_4	1.401_8
1.5295	1.616_0	1.401_0
1.7109	1.613_6	1.401_0
2.25	1.610_2	1.399_7
3.4	1.593_3	1.398_0
4.4	1.540_0	1.395_0
5.4	1.495_0	1.390_7
6.	1.462_6	1.388_0

Table 28A-1-007. $NaNO_2$. Piezooptic constants measured by Brillouin scattering [75Shi].

$\lvert p_{11}\rvert = 0.44$	$\lvert p_{12}\rvert = 0.37$	$\lvert p_{13}\rvert = 0.36$
$\lvert p_{21}\rvert = 0.39$	$\lvert p_{22}\rvert = 0.33$	$\lvert p_{23}\rvert = 0.27$
$\lvert p_{31}\rvert = 0.18$	$\lvert p_{32}\rvert = 0.19$	$\lvert p_{33}\rvert = 0.15$

Table 28A-1-008. $NaNO_2$. ν_0/c, γ_{TO}/c at RT. ν_0: frequency of phonon mode, γ_{TO}: damping constant.

	ν_0/c [cm^{-1}] (IR)				ν_0/c [cm^{-1}] (Raman)						γ_{TO}/c [cm^{-1}]	Dielectric transition strengths [a]	Assignment
	[68Axe]		[68Bar]		[67Chi]		[68Tsu]		[72Har]				
	TO	LO	TO	LO	TO	LO	TO	LO	TO	LO		S	
A_1	194	269	186.8									2.085 [b]	
	826	829	825.3		825		830		827.5	829	1.5	0.0715 [b]	sym. stretch
	1323	1336	1320.5		1327		1323		1326	1328	7.5	0.0041 [b]	sym. bend
A_2					119		117		119.5		10	0.000	libration
B_1	157	163	150.9		153		158		154	165	8	1.519	libration
	188	250	180.7		177		191		184.5	236	15	1.420	translation
	1235	1368	1227.3		1280		1230		1225	1356	14	0.608	asym. stretch
B_2	149	193	145.7						149.5	201	16	2.085	translation
	223	261	231.7		220		223		227.5	254	25	0.178	libration

[a]) Calculation was made by Eq. (5) of [71Har] using the values of [72Har].
[b]) Calculation used the three LO and TO frequencies of the A_1 external mode of [68Axe].

Table 28A-1-009. $NaNO_2$. Vibration frequencies [cm^{-1}] at $\boldsymbol{k} = 0$.

Species	Assign.	Mode	T = 295 K [80Cas]	T = 4 K [94Sig]
B_1	ν_3	LO	1358	1363
		TO	1225	1229
A_1	ν_1	LO	1328	1332
		TO	1326	1329
A_1	ν_2	LO	829	832
		TO	827	831
A_1	T_b	LO	270	>280
		TO	190	208
A_2	R_b		119	133
B_1	T_c	LO	236	251
	T_c; R_a	TO	184	195
B_1	R_a	LO	165	178
	R_a;T_c	TO	154	165
B_2	R_c; T_a	LO	254	280
	R_c	TO	227	240
B_2	T_a; R_c	LO	201	210
	T_a	TO	149	160

Table 28A-1-010. $NaNO_2$. Activation energy of resistivity, $\rho = \rho_0 \exp(\Delta U/kT)$.

Temperature range	ΔU [eV] in			
	a direction	*b* direction		*c* direction
T < 155 °C	1.2_5	1.5_5	1.05	1.8_5
165 °C < T < 178 °C			1.39	
T < 178 °C	1.2_5	1.3	1.23	1.1_5
Ref.	62Asa	62Asa	67Tak	62Asa