Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Sodium 2,4-dinitrophenolate monohydrate

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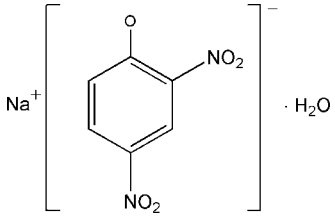
Received 30 April 2007; accepted 12 May 2007

Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.040; data-to-parameter ratio = 6.7.

The title compound, $Na^+\cdot C_6H_3N_2O_5^-\cdot H_2O$, was obtained by the reaction of sodium hydroxide with 2,4-dinitrophenol in water. The crystal packing shows a laminated structure with intercalated coordinated 2,4-dinitrophenolate spacers, where Na^+ cations and water molecules lie on twofold rotation axes. The laminated structure consists of NaO_6 chains linked by 2,4-dinitrophenolate ligands. Each Na^+ cation exhibits a distorted octahedral geometry. One cation is surrounded by four water molecules and two O atoms from two 4-nitro groups. The other is surrounded by two O atoms from two 2-nitro groups and four phenolate O atoms.

Related literature

For general background, see: Prondzinski *et al.* (2007); Zaderenko *et al.* (1997). For a related structure, see: In *et al.* (1997).



Experimental

Crystal data

$Na^+\cdot C_6H_3NO_5^-\cdot H_2O$
M_r = 224.11
Monoclinic, $C2$
a = 19.962 (3) Å
b = 11.4615 (17) Å
c = 3.5291 (5) Å
β = 95.136 (12)°
V = 804.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 203 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.959, T_{max} = 0.979
5696 measured reflections
971 independent reflections
716 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.040
S = 0.90
971 reflections
145 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O8—H2···O3^{i}	0.80 (3)	2.25 (3)	3.035 (3)	171 (3)
O7—H1···O5^{ii}	0.92 (3)	2.07 (3)	2.925 (3)	154 (3)

Symmetry codes: (i) $x-\frac{1}{2}, y+\frac{1}{2}, z-1$; (ii) $-x-\frac{1}{2}, y-\frac{1}{2}, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL* and local programs.

We are grateful to the Deutsche Forschungsgemeinschaft (SFB 558 Metall-Substratwechselwirkungen in der heterogenen Katalyse) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2061).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m1687 [**doi:10.1107/S1600536807023409**]

Sodium 2,4-dinitrophenolate monohydrate

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Comment

2,4-Dinitrophenolate is a versatile ligand for crystal engineering, which is able to coordinate with phenoxy or nitro groups to metal centers, yielding different metal complexes (Prondzinski *et al.*, 2007; Zaderenko *et al.*, 1997). It is known that nitrophenols not only form various π-stacking complexes with other aromatic molecules but also form salts through specific electrostatic or hydrogen-bonding interactions (In *et al.*, 1997). The bonding of electron-donor-acceptor complexes depends strongly on the substitution pattern of nitro and hydroxy groups on the benzene ring.

The asymmetric unit of (I) is shown in Fig. 1, where Na atoms and water molecules each lies on a twofold rotation axis. The crystal packing of (I) shows a laminated structure with intercalated coordinated 2,4-dinitrophenolate spacer (Fig. 2). The laminated structure consists of NaO_6 chains linked by 2,4-dinitrophenolate ligands. Each Na atom exhibits a distorted octahedral geometry. The Na1 atom is surrounded by four water molecules and two O atoms from two *para*-nitro groups. The Na2 atom is surrounded by two O atoms from two *ortho*-nitro groups and four phenolate O atoms.

Experimental

Compound (I) was obtained as the product of the reaction of sodium hydroxide (0.20 g, 5 mmol) with 2,4-dinitrophenol (0.70 g, 3.8 mmol) in water (10 ml) (yield 0.66 g).

Refinement

H atoms on water molecules were located in a difference map and refined isotropically. The other H atoms were positioned geometrically and refined as riding, with C—H = 0.94 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

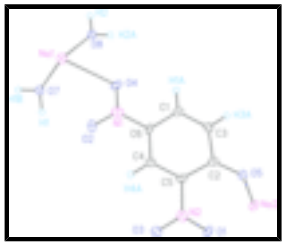

Fig. 1. The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level.

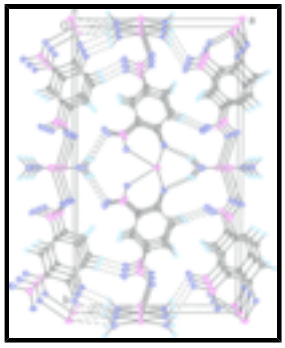

Fig. 2. The crystal packing of (I). Dashed lines denote hydrogen bonds.

Sodium 2,4-dinitrophenolate Monohydrate

Crystal data

$Na^{+}.C_6H_3NO_5^{-}.H_2O$	F_{000} = 456
M_r = 224.11	D_x = 1.851 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 3132 reflections
a = 19.962 (3) Å	θ = 3.2–27.0º
b = 11.4615 (17) Å	μ = 0.21 mm^{-1}
c = 3.5291 (5) Å	*T* = 203 (2) K
β = 95.136 (12)º	Needle, yellow
V = 804.2 (2) Å^3	0.20 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	971 independent reflections
Radiation source: fine-focus sealed tube	716 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.066
Detector resolution: 8.192 pixels mm^{-1}	θ_{max} = 27.5º
T = 203(2) K	θ_{min} = 3.6º
φ and ω scan	*h* = −25→25
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*k* = −14→14
T_{min} = 0.959, T_{max} = 0.979	*l* = −4→4
5696 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.0097P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.040$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.90$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
971 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
145 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	−0.5000	−0.10008 (15)	0.0000	0.0181 (4)
Na2	0.0000	−0.00873 (14)	0.0000	0.0166 (5)
O5	−0.07595 (10)	0.03588 (16)	0.4527 (6)	0.0149 (5)
N1	−0.34206 (13)	−0.1025 (2)	0.1758 (7)	0.0173 (7)
O1	−0.06035 (10)	−0.18077 (16)	0.7752 (6)	0.0187 (6)
O4	−0.38225 (10)	−0.03559 (17)	−0.0055 (6)	0.0200 (6)
O3	−0.12530 (9)	−0.3073 (2)	0.4714 (5)	0.0207 (5)
N2	−0.11202 (13)	−0.2052 (2)	0.5748 (7)	0.0152 (6)
O2	−0.35961 (10)	−0.19710 (18)	0.3024 (6)	0.0210 (6)
C1	−0.25320 (16)	0.0447 (3)	0.1392 (8)	0.0139 (8)
H1A	−0.2852	0.0976	0.0281	0.017*
C2	−0.13592 (15)	0.0009 (3)	0.3809 (8)	0.0120 (7)
C3	−0.18714 (15)	0.0772 (3)	0.2110 (9)	0.0132 (7)
H3A	−0.1748	0.1533	0.1457	0.016*
C4	−0.22575 (15)	−0.1487 (3)	0.3777 (8)	0.0122 (8)
H4A	−0.2387	−0.2256	0.4282	0.015*
C5	−0.15992 (15)	−0.1149 (3)	0.4466 (8)	0.0123 (7)
C6	−0.27234 (15)	−0.0690 (3)	0.2343 (9)	0.0117 (7)
O7	−0.5000	−0.2456 (3)	−0.5000	0.0178 (8)
O8	−0.5000	0.0418 (3)	−0.5000	0.0181 (8)
H2	−0.5300 (14)	0.088 (3)	−0.511 (10)	0.022 (10)*
H1	−0.4654 (15)	−0.298 (3)	−0.498 (9)	0.051 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0162 (11)	0.0180 (10)	0.0203 (11)	0.000	0.0020 (8)	0.000
Na2	0.0116 (10)	0.0212 (11)	0.0167 (11)	0.000	0.0002 (8)	0.000
O5	0.0122 (13)	0.0141 (12)	0.0178 (13)	−0.0009 (10)	−0.0013 (10)	−0.0014 (10)
N1	0.0212 (18)	0.0185 (16)	0.0129 (16)	0.0039 (15)	0.0055 (13)	−0.0065 (14)
O1	0.0119 (13)	0.0183 (14)	0.0236 (13)	−0.0022 (11)	−0.0113 (11)	−0.0010 (10)
O4	0.0094 (13)	0.0237 (14)	0.0258 (15)	0.0054 (10)	−0.0052 (11)	0.0030 (11)
O3	0.0187 (12)	0.0143 (12)	0.0288 (14)	0.0007 (12)	−0.0004 (10)	−0.0036 (13)
N2	0.0171 (17)	0.0168 (16)	0.0128 (15)	0.0001 (13)	0.0073 (13)	−0.0014 (13)
O2	0.0166 (13)	0.0165 (14)	0.0298 (14)	−0.0059 (11)	0.0012 (11)	0.0006 (11)

C1	0.0128 (19)	0.0193 (19)	0.010 (2)	0.0038 (15)	0.0013 (15)	0.0007 (15)
C2	0.0126 (19)	0.0153 (18)	0.0087 (18)	0.0033 (16)	0.0046 (15)	−0.0018 (14)
C3	0.0162 (19)	0.0113 (18)	0.0127 (18)	−0.0015 (15)	0.0054 (15)	0.0026 (14)
C4	0.0145 (19)	0.0124 (17)	0.0098 (18)	0.0024 (14)	0.0013 (14)	−0.0006 (13)
C5	0.0108 (18)	0.0160 (18)	0.0096 (18)	0.0045 (16)	−0.0012 (13)	0.0002 (15)
C6	0.0077 (19)	0.017 (2)	0.0101 (17)	−0.0032 (13)	−0.0011 (13)	−0.0018 (14)
O7	0.016 (2)	0.0138 (19)	0.024 (2)	0.000	0.0046 (17)	0.000
O8	0.012 (2)	0.013 (2)	0.029 (2)	0.000	−0.0019 (18)	0.000

Geometric parameters (Å, °)

Na1—O8^{i}	2.400 (3)	N1—O4	1.245 (3)
Na1—O8	2.400 (3)	N1—C6	1.441 (4)
Na1—O7	2.428 (2)	O1—N2	1.230 (3)
Na1—O7^{i}	2.428 (2)	O3—N2	1.247 (3)
Na1—O4	2.466 (2)	N2—C5	1.454 (4)
Na1—O4^{ii}	2.466 (2)	C1—C3	1.372 (4)
Na1—Na1^{i}	3.5291 (5)	C1—C6	1.407 (4)
Na2—O5^{iii}	2.355 (2)	C1—H1A	0.9400
Na2—O5	2.355 (2)	C2—C5	1.436 (4)
Na2—O5^{iv}	2.401 (2)	C2—C3	1.435 (4)
Na2—O5^{v}	2.401 (2)	C3—H3A	0.9400
Na2—O1^{v}	2.408 (2)	C4—C5	1.371 (4)
Na2—O1^{iv}	2.408 (2)	C4—C6	1.368 (4)
Na2—Na2^{i}	3.5291 (5)	C4—H4A	0.9400
O5—C2	1.267 (3)	O7—H1	0.92 (3)
N1—O2	1.235 (3)	O8—H2	0.80 (3)
O8^{i}—Na1—O8	94.67 (14)	O5^{v}—Na2—Na2^{i}	138.40 (5)
O8^{i}—Na1—O7	179.28 (11)	O1^{v}—Na2—Na2^{i}	106.54 (5)
O8—Na1—O7	86.05 (7)	O1^{iv}—Na2—Na2^{i}	73.46 (5)
O8^{i}—Na1—O7^{i}	86.05 (7)	O5^{iii}—Na2—Na2^{v}	42.60 (5)
O8—Na1—O7^{i}	179.28 (11)	O5—Na2—Na2^{v}	137.40 (5)
O7—Na1—O7^{i}	93.23 (12)	O5^{iv}—Na2—Na2^{v}	138.40 (5)
O8^{i}—Na1—O4	82.26 (6)	O5^{v}—Na2—Na2^{v}	41.60 (5)
O8—Na1—O4	74.23 (6)	O1^{v}—Na2—Na2^{v}	73.46 (5)
O7—Na1—O4	97.94 (5)	O1^{iv}—Na2—Na2^{v}	106.54 (5)
O7^{i}—Na1—O4	105.88 (5)	Na2^{i}—Na2—Na2^{v}	180.00 (5)
O8^{i}—Na1—O4^{ii}	74.23 (6)	C2—O5—Na2	116.73 (18)
O8—Na1—O4^{ii}	82.26 (6)	C2—O5—Na2^{i}	127.66 (19)
O7—Na1—O4^{ii}	105.88 (5)	Na2—O5—Na2^{i}	95.80 (7)
O7^{i}—Na1—O4^{ii}	97.94 (5)	O2—N1—O4	122.4 (3)
O4—Na1—O4^{ii}	145.11 (12)	O2—N1—C6	118.9 (3)
O8^{i}—Na1—Na1^{i}	42.67 (7)	O4—N1—C6	118.6 (3)

O8—Na1—Na1^{i}	137.33 (7)	N2—O1—Na2^{i}	138.17 (18)
O7—Na1—Na1^{i}	136.61 (6)	N1—O4—Na1	112.46 (18)
O7^{i}—Na1—Na1^{i}	43.39 (6)	O1—N2—O3	121.8 (2)
O4—Na1—Na1^{i}	95.35 (5)	O1—N2—C5	120.8 (3)
O4^{ii}—Na1—Na1^{i}	84.65 (5)	O3—N2—C5	117.4 (2)
O8^{i}—Na1—Na1^{v}	137.33 (7)	C3—C1—C6	119.0 (3)
O8—Na1—Na1^{v}	42.67 (7)	C3—C1—H1A	120.5
O7—Na1—Na1^{v}	43.39 (6)	C6—C1—H1A	120.5
O7^{i}—Na1—Na1^{v}	136.61 (6)	O5—C2—C5	125.7 (3)
O4—Na1—Na1^{v}	84.65 (5)	O5—C2—C3	121.0 (3)
O4^{ii}—Na1—Na1^{v}	95.35 (5)	C5—C2—C3	113.3 (3)
Na1^{i}—Na1—Na1^{v}	180.00 (6)	C1—C3—C2	123.3 (3)
O5^{iii}—Na2—O5	154.92 (12)	C1—C3—H3A	118.4
O5^{iii}—Na2—O5^{iv}	95.80 (7)	C2—C3—H3A	118.4
O5—Na2—O5^{iv}	78.85 (8)	C5—C4—C6	119.1 (3)
O5^{iii}—Na2—O5^{v}	78.85 (8)	C5—C4—H4A	120.4
O5—Na2—O5^{v}	95.80 (7)	C6—C4—H4A	120.4
O5^{iv}—Na2—O5^{v}	155.41 (11)	C4—C5—C2	124.1 (3)
O5^{iii}—Na2—O1^{v}	106.72 (7)	C4—C5—N2	116.6 (3)
O5—Na2—O1^{v}	93.89 (8)	C2—C5—N2	119.2 (3)
O5^{iv}—Na2—O1^{v}	134.48 (8)	C4—C6—C1	121.1 (3)
O5^{v}—Na2—O1^{v}	69.40 (7)	C4—C6—N1	119.4 (3)
O5^{iii}—Na2—O1^{iv}	93.89 (8)	C1—C6—N1	119.5 (3)
O5—Na2—O1^{iv}	106.72 (7)	Na1—O7—Na1^{v}	93.23 (12)
O5^{iv}—Na2—O1^{iv}	69.40 (7)	Na1—O7—H1	120 (2)
O5^{v}—Na2—O1^{iv}	134.48 (8)	Na1^{v}—O7—H1	114 (2)
O1^{v}—Na2—O1^{iv}	70.04 (10)	Na1^{v}—O8—Na1	94.67 (14)
O5^{iii}—Na2—Na2^{i}	137.40 (5)	Na1^{v}—O8—H2	118 (2)
O5—Na2—Na2^{i}	42.60 (5)	Na1—O8—H2	116 (2)
O5^{iv}—Na2—Na2^{i}	41.60 (5)		

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*−1, *y*, −*z*; (iii) −*x*, *y*, −*z*; (iv) −*x*, *y*, −*z*+1; (v) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H2···O3^{vi}	0.80 (3)	2.25 (3)	3.035 (3)	171 (3)
O7—H1···O5^{vii}	0.92 (3)	2.07 (3)	2.925 (3)	154 (3)

Symmetry codes: (vi) *x*−1/2, *y*+1/2, *z*−1; (vii) −*x*−1/2, *y*−1/2, −*z*.

Fig. 1

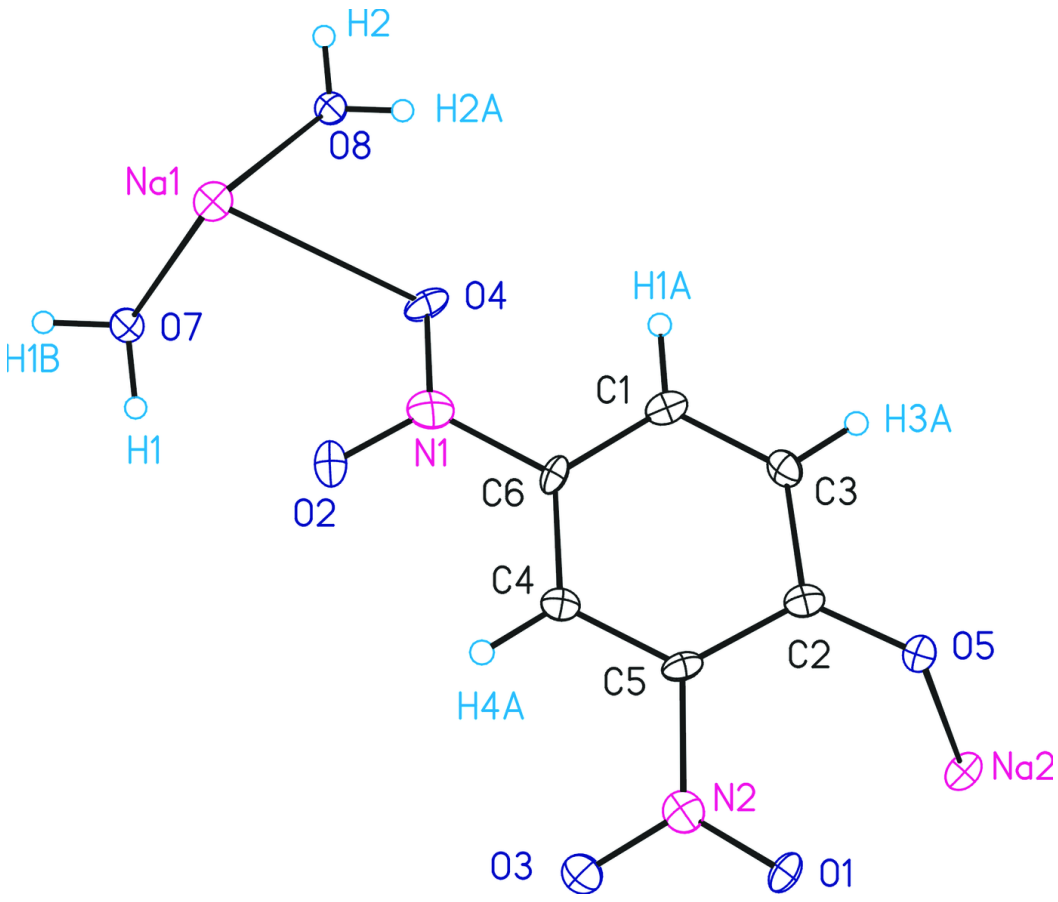
H2
H2A
O8
Na1
O4
H1A
O7
H1B
C1
H3A
H1
N1
C6
C3
O2
C4
C2
O5
H4A
C5
Na2
N2
O3
O1

Fig. 2