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syn and *anti* conformations in 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid and two related salts

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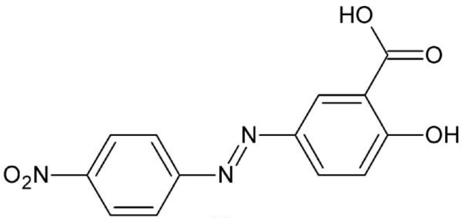
The crystal structures of 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid, $C_{13}H_9N_3O_5$, (I), ammonium 2-hydroxy-5-[(*E*)-phenyldiazenyl]benzoate, $NH_4^+\cdot C_{13}H_9N_2O_3^-$, (II), and sodium 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoate trihydrate, $Na^+\cdot C_{13}H_8N_3O_5^-\cdot 3H_2O$, (III), have been determined using single-crystal X-ray diffraction. In (I) and (III), the phenyldiazenyl and carboxylic acid/carboxylate groups are in an *anti* orientation with respect to each other, which is in accord with the results of density functional theory (DFT) calculations, whereas in (II), the anion adopts a *syn* conformation. In (I), molecules form slanted stacks along the [100] direction. In (II), anions form bilayers parallel to (010), the inner part of the bilayers being formed by the benzene rings, with the –OH and $-COO^-$ substituents on the bilayer surface. The NH_4^+ cations in (II) are located between the bilayers and are engaged in numerous $N-H\cdots O$ hydrogen bonds. In (III), anions form layers parallel to (001). Both Na^+ cations have a distorted octahedral environment, with four octahedra edge-shared by bridging water O atoms, forming $[Na_4(H_2O)_{12}]^{4+}$ units.

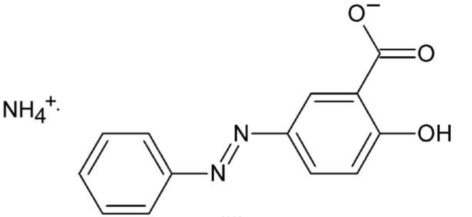
Keywords: crystal structure; *syn*/*anti* conformations; 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid; ammonium salicylate salt; sodium salicylate salt; dyes; DFT calculations.

1. Introduction

Arylazo derivatives of salicylic (2-hydroxybenzoic) acid and their salts have been used as dyes for many years. A search of the Cambridge Structural Database (CSD, Version 5.35; Allen, 2002) for the 5-phenylazosalicylic acid residue yielded 56 hits, including coordination and organometallic compounds and containing 109 such fragments. In particular, organotin(IV) complexes were studied in great detail due to their biological properties (Basu Baul *et al.*, 2007, and references therein). At the same time, only two structures of free acids, namely 5-(4-methoxyphenyldiazenyl)salicylic acid (Basu Baul *et al.*, 2000) and 5-(phenyldiazenyl)salicylic acid (Saikia *et al.*, 2012), and one structure of a molecular complex, that of 5-(phenyldiazenyl)salicylic acid with dimethylpyrazole (Xu *et al.*, 2011), have been reported so far, and no structures of such salts with alkaline metals or ammonium cations have been described.



(I)



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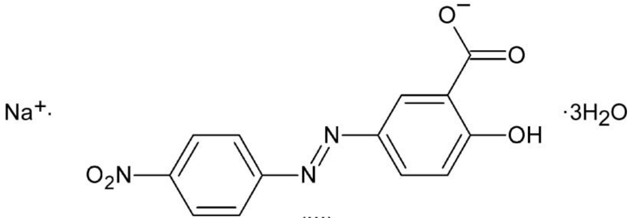

(III)

In the course of our studies on the structures of azo dyes (Aslanov *et al.*, 2009), we have determined the X-ray crystal structures of three compounds, *viz.* 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid (C. I. Mordant Orange 1), (I), the ammonium salt of (I), denoted (II), and the sodium salt trihydrate of (I), denoted (III) (see Scheme above).

2. Experimental

2.1. Synthesis and crystallization

Diazo-coupling of 4-nitroaniline and 2-hydroxybenzoic acid in alkaline solution afforded compound (I) in 48% yield. Recrystallization from a toluene–acetone (3:1 *v*/*v*) mixture gave red–orange crystals (prisms). Dropwise addition of a 10% ammonia solution to a solution of 5-(phenyldiazenyl)salicylic acid in ethanol until a pH of 7–8 was attained afforded compound (II) in 77% yield. Recrystallization from a water–ethanol (3:1 *v*/*v*) mixture gave dark-yellow crystals (plates). Dropwise addition of an NaOH solution to a solution of 5-[(4-nitrophenyl)diazenyl]salicylic acid in ethanol until a pH of 7–8 was attained afforded compound (III) in 72% yield. Recrystallization from water gave dark-yellow crystals (prisms).

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. In all three title compounds,

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Table 1
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{13}H_9N_3O_5$	$NH_4^+ \cdot C_{13}H_9N_2O_3^-$	$Na^+ \cdot C_{13}H_8N_3O_5^- \cdot 3H_2O$
M_r	287.23	259.26	363.26
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$	Triclinic, $P\overline{1}$
Temperature (K)	293	293	293
a, b, c (Å)	4.9319 (5), 11.6649 (14), 21.619 (2)	6.0471 (1), 34.371 (1), 6.2824 (2)	7.2123 (5), 13.0205 (8), 17.0317 (11)
α, β, γ (°)	90, 94.991 (8), 90	90, 103.278 (2), 90	77.185 (6), 80.933 (5), 83.401 (5)
V (Å^3)	1239.0 (2)	1270.85 (6)	1534.76 (17)
Z	4	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.04	0.82	0.16
Crystal size (mm)	0.12 × 0.04 × 0.03	0.08 × 0.05 × 0.05	0.50 × 0.45 × 0.40
Data collection			
Diffractometer	Stoe STADI VARI diffractometer	Stoe STADI VARI diffractometer	Stoe STADI VARI diffractometer
Absorption correction	Multi-scan (Blessing, 1995)	Multi-scan (Blessing, 1995)	Multi-scan (Blessing, 1995)
T_{min}, T_{max}	0.925, 0.979	0.945, 0.960	0.926, 0.952
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14169, 2334, 1804	15094, 2352, 1561	6773, 5936, 3776
R_{int}	0.074	0.052	0.026
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.609	0.605	0.617
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.119, 1.00	0.048, 0.141, 1.04	0.041, 0.120, 0.92
No. of reflections	2334	2352	5936
No. of parameters	199	189	493
No. of restraints	4	12	22
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.18	0.14, −0.16	0.21, −0.27

Computer programs: *X-AREA* (Stoe & Cie, 2012), *X-RED32* (Stoe & Cie, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

O- and N-bound H atoms were located in difference electron-density maps and were refined with restraints. The NH_4^+ cation in (II) was refined with distance restraints N—H = 0.890 (5) Å and H···H = 1.453 (5) Å, and with $U_{iso}(H) = 1.5U_{eq}(N)$, so as to provide the tetrahedral structure of the ammonium cation. The H_2O molecules in (III) were refined with distance restraints O—H = 0.820 (3) Å and H···H = 1.300 (5) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$, so as to provide a H—O—H angle of 105°. The carboxylic acid group in (I) was refined with distance restraints O3—H13 = 0.820 (1) Å and C13···H13 = 1.761 (1) Å so as to reproduce the C—O—H angle of 109° observed in salicylic acid (neutron structure determination; Bacon & Jude, 1973). The phenol groups in (I) and (II) were refined with distance restraints O1—H1 = 0.820 (1) Å and C2···H1 = 1.769 (1) Å so as to reproduce the C—O—H angle of 107° observed in salicylic acid (neutron structure determination; Bacon & Jude, 1973). In (III), the corresponding restraints were O1—H1 = 0.820 (1) Å and C2···H1 = 1.789 (1) Å, and the C—O—H angle was 109°. All C-bound H atoms were placed in idealized positions, with distance restraints of C—H = 0.93 Å (*SHELXL* AFIX 43 instruction; Sheldrick, 2008) and with $U_{iso}(H) = 1.2U_{eq}(C)$.

3. Results and discussion

For neutral salicylic acid (I) (Fig. 1) and its ammonium salt (II) (Fig. 1), there is one formula unit in the asymmetric part of the unit cell, whereas the structure of sodium salt trihydrate (III) (Fig. 2) contains two symmetry-independent cations, two anions and six water molecules. One of these water O atoms has a large anisotropic displacement parameter value and is

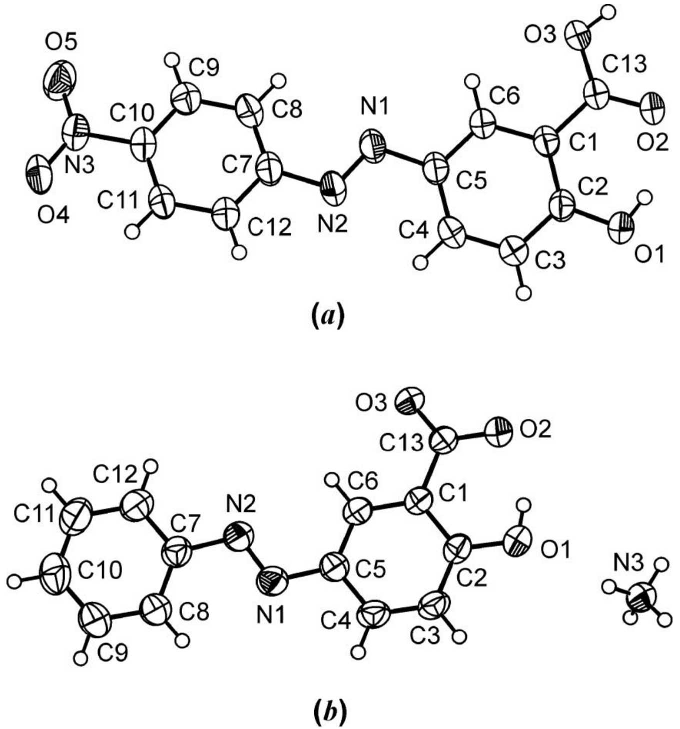

Figure 1
Views of (*a*) (I) and (*b*) (II), showing the atom-numbering schemes. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Selected interatomic distances (Å) in (I)–(III) compared with closely related structures.

Distance	(I)	(II)	(III)	(III)*A*^{a}	ACEFIZ^{b}	FUGYIP^{c}	EXIZUH1^{d,e}	EXIZUH2^{d}
O1—C2	1.3400 (17)	1.350 (3)	1.352 (3)	1.347 (3)	1.354 (3)	1.355 (2)	1.350 (4)	1.362 (4)
C1—C2	1.403 (2)	1.419 (3)	1.399 (2)	1.421 (3)	1.401 (3)	1.403 (3)	1.396 (5)	1.397 (4)
C1—C13	1.4653 (19)	1.500 (3)	1.503 (3)	1.496 (3)	1.454 (3)	1.462 (3)	1.479 (4)	1.482 (5)
C5—N1	1.4213 (19)	1.421 (3)	1.420 (3)	1.405 (3)	1.451 (3)	1.432 (2)	1.413 (4)	1.421 (4)
N1—N2	1.2519 (19)	1.249 (3)	1.266 (3)	1.245 (3)	1.246 (3)	1.260 (2)	1.242 (3)	1.245 (3)
N2—C7	1.4256 (19)	1.428 (3)	1.419 (3)	1.420 (3)	1.431 (3)	1.424 (2)	1.431 (4)	1.437 (4)
O2—C13	1.2290 (17)	1.265 (3)	1.286 (3)	1.281 (3)	1.240 (2)	1.241 (2)	1.229 (4)	1.228 (4)
O3—C13	1.3081 (19)	1.246 (3)	1.257 (3)	1.234 (3)	1.313 (2)	1.311 (2)	1.300 (4)	1.290 (4)
O1···O2	2.619 (2)	2.524 (3)	2.534 (3)	2.532 (2)	2.630 (2)	2.631 (2)	2.574 (3)	2.605 (3)

Notes: (*a*) the second anion in (III) is labelled with the letter '*A*'; (*b*) 5-(phenyldiazenyl)salicylic acid (Saikia *et al.*, 2012); (*c*) 5-(4-methoxyphenyldiazenyl)salicylic acid (Basu Baul *et al.*, 2000); (*d*) the molecular complex of 5-(phenyldiazenyl)salicylic acid with dimethylpyrazole (Xu *et al.*; 2011); (*e*) the structure contains two symmetry-independent molecules.

probably partially disordered. Acid molecule (I) and the related anions in (II) and (III) are basically planar; the r.m.s. deviations from the mean planes are 0.215 and 0.141 Å, respectively, for (I) and (II), and 0.117 and 0.084 Å for the two independent anions of (III). The largest dihedral angle between the mean planes of the two benzene rings is observed in (I) [21.00 (7)°]; this angle is 4.9 (1)° in (II), and 7.5 (1) and 4.7 (1)° in (III). Such an essentially flat geometry is typical for most of the similar azo compounds, because the barrier to rotation about the N—C bond in these compounds is *ca* 40 kJ mol^{-1} (Yazici *et al.*, 2011). All three studied structures contain intramolecular O—H···O hydrogen bonds between the hydroxy and carboxylic acid (or carboxylate) groups, which further contribute to stabilization of the planarity of the molecules and anions (Tables 2 and 3).

Comparison of neutral molecule (I) and 5-(phenyldiazenyl)salicylic acid (CSD refcode ACEFIZ; Saikia *et al.*, 2012) with the anions in (II) and (III) demonstrates that in the anions the C—C bonds between the benzene ring and the carboxylate group are longer by 0.04 Å on average and the C—O bond lengths in the latter group are more equal (Table 2). It should be noted that in the neutral molecules, the shorter C═O bonds are oriented towards the –OH group, whereas in the anions, the C—O bonds adjacent to the –OH groups become longer (by 0.02–0.05 Å) than the C—O bonds not participating in intramolecular hydrogen bonding. Along with this, in the anions in (II) and (III), the O1···O2 distances are on average 0.1 Å shorter than those in neutral molecule (I) and ACEFIZ, that is, the internal hydrogen bonds in the anions are stronger than those in the neutral molecules. Analogous tendencies in bond lengths are also observed in the structures of salts of salicylic acid (Klepeis *et al.*, 2009, and references therein). The nitro groups in (I) and (III) do not cause any noticeable changes in the bond lengths and hydrogen-bonding parameters compared with those in ACEFIZ and (II).

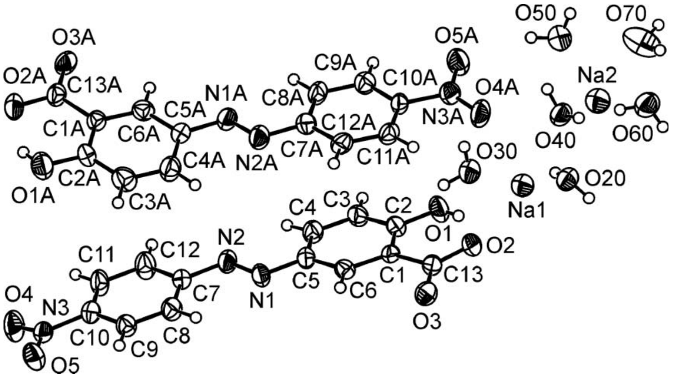

Figure 2
A view of the two symmetry-independent molecules of (III), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

In (I) and (III), the phenyldiazenyl and carboxylic acid/carboxylate groups are positioned *anti* to each other with respect to the C5—N1 bond, whereas in (II), the anion adopts a *syn* conformation. The predominance of *anti* conformers is

Table 3
Hydrogen-bonding geometry (Å, °) in (I)–(III).

D—H···A	D—H	H···A	D···A	D—H···A
(I)				
O1—H1···O2	0.820 (14)	1.895 (14)	2.6189 (16)	146.8 (14)
O1—H1···O4^{a}	0.820 (14)	2.420 (14)	3.0461 (18)	134.0 (13)
O3—H13···O2^{b}	0.820 (13)	1.847 (14)	2.6651 (16)	176.4 (14)
C4—H4···O5^{c}	0.93	2.38	3.202 (2)	147
(II)				
O1—H1···O2	0.82 (2)	1.78 (2)	2.524 (3)	151 (2)
N3—H21···O3^{d}	0.89 (2)	1.99 (2)	2.788 (3)	150 (2)
N3—H22···O2^{e}	0.89 (2)	1.91 (2)	2.779 (3)	164 (2)
N3—H23···O1	0.89 (2)	2.38 (2)	3.052 (3)	132 (2)
N3—H24···O3^{f}	0.89 (2)	1.91 (2)	2.799 (3)	172 (2)
(III)				
O1—H1···O2	0.820 (11)	1.796 (17)	2.534 (3)	148.9 (16)
O1*A*—H1*A*···O2*A*	0.820 (10)	1.804 (18)	2.532 (3)	147.3 (17)
O20—H21···O3*A*^{g}	0.82 (2)	1.93 (2)	2.750 (2)	174 (3)
O20—H22···O2^{h}	0.82 (2)	2.04 (2)	2.862 (2)	173 (2)
O30—H31···O5^{i}	0.82 (2)	2.32 (2)	3.135 (3)	175 (2)
O30—H32···O3*A*^{j}	0.82 (2)	2.14 (3)	2.823 (3)	141 (2)
O40—H41···O2*A*^{j}	0.82 (2)	2.00 (2)	2.819 (3)	172 (2)
O40—H42···O3^{k}	0.82 (2)	2.02 (2)	2.813 (3)	161 (3)
O50—H51···O60^{l}	0.82 (3)	2.04 (2)	2.838 (3)	163 (3)
O50—H52···O5*A*	0.82 (3)	2.18 (2)	2.931 (3)	152 (3)
O60—H61···O3^{h}	0.82 (3)	2.09 (3)	2.828 (3)	150 (3)
O60—H62···O2*A*^{g}	0.82 (2)	2.21 (2)	2.917 (3)	145 (3)
O70—H71···O50^{l}	0.82 (4)	2.19 (5)	2.892 (4)	144 (4)
O70—H72···O1*A*^{m}	0.82 (3)	2.48 (5)	2.972 (4)	119 (4)
C12—H12···O5*A*^{g}	0.93	2.55	3.358 (3)	146
C12*A*—H12*A*···O5^{i}	0.93	2.34	3.125 (3)	141

Symmetry codes: (*a*) $x + 2, -y + \frac{1}{2}, z - \frac{1}{2}$; (*b*) $-x + 3, -y + 1, -z$; (*c*) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (*d*) $x - 1, y, z + 1$; (*e*) $x - 1, y, z$; (*f*) $-x + 1, -y, -z + 2$; (*g*) $-x, -y + 1, -z + 1$; (*h*) $-x, -y + 1, -z$; (*i*) $-x + 1, -y, -z + 1$; (*j*) $-x + 1, -y + 1, -z + 1$; (*k*) $-x + 1, -y + 1, -z$; (*l*) $-x, -y + 2, -z$; (*m*) $x, y + 1, z - 1$.

Table 4
Results of DFT calculations for an isolated molecule of 2-hydroxy-5-(phenyldiazenyl)benzoic acid, for the same molecule placed in a polarizable continuum with parameters simulating acetone, for two molecules bound as a dimer by a pair of hydrogen bonds between the carboxylate groups and for the anion of 2-hydroxy-5-(phenyldiazenyl)benzoic acid placed in a polarizable continuum with parameters simulating acetone.

	E (*anti*) (Hartree)	*E* (*syn*) (Hartree)	*E* (*syn*) − *E* (*anti*) (kJ mol^{-1})
Isolated molecule	−836.78754	−836.78666	2.3
Molecule in a polarizable continuum	−836.79481	−836.79419	1.6
Hydrogen-bonded dimer	−1673.60221	−1673.60034	4.9
Anion in a polarizable continuum	−836.32959	−836.32899	1.6

evident from an analysis of the CSD data: 83 out of 109 5-(phenyldiazenyl)salicylic residues have an *anti* conformation and only 26 adopt a *syn* conformation. In order to rationalize the predominance of the *anti* conformation, we performed DFT calculations of *syn* and *anti* conformers for the following model systems: (i) the isolated molecule of 2-hydroxy-5-(phenyldiazenyl)benzoic acid; (ii) the same molecule placed in a polarizable continuum with parameters simulating acetone; (iii) two molecules bound as a dimer by a pair of hydrogen bonds between the carboxylate groups; (iv) the anion of this acid placed into a polarizable continuum with parameters simulating acetone. Calculations were carried out using *GAUSSIAN98* (Frisch *et al.*, 1998) with a B3LYP exchange-correlation functional (Becke, 1993; Lee *et al.*, 1988) and a 6–311G** basis set (Krishnan *et al.*, 1980). The effect of continuum was accounted for by the PCM (polarizable continuum model) method (Tomasi *et al.*, 2005, and references therein). In all the above-mentioned cases, the energy of the *anti* conformer appeared to be 1.6–2.4 kJ mol^{-1} lower than that of the *syn* conformer (see Table 4). This difference is sufficient for rationalization of the predominance of the *anti* conformation.

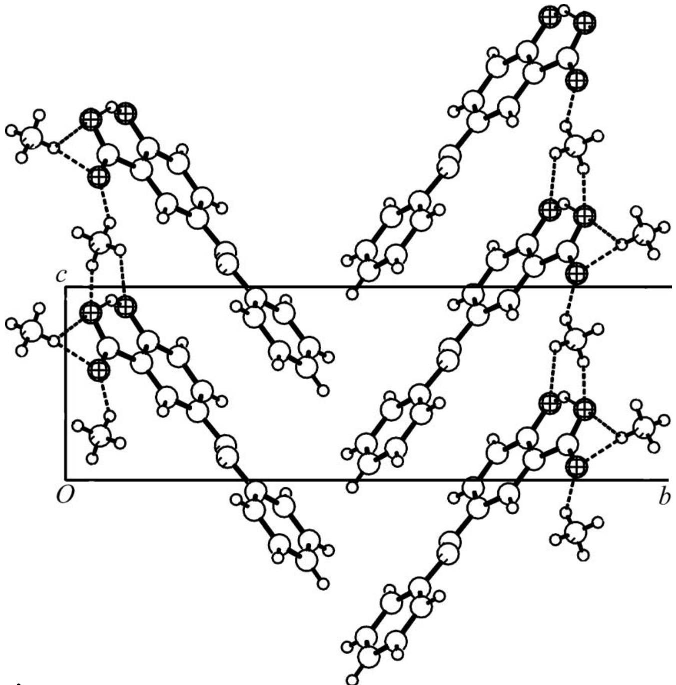

Figure 3
The crystal packing of (II), viewed along [100], showing the bilayered structure. Hydrogen bonds are shown as dashed lines.

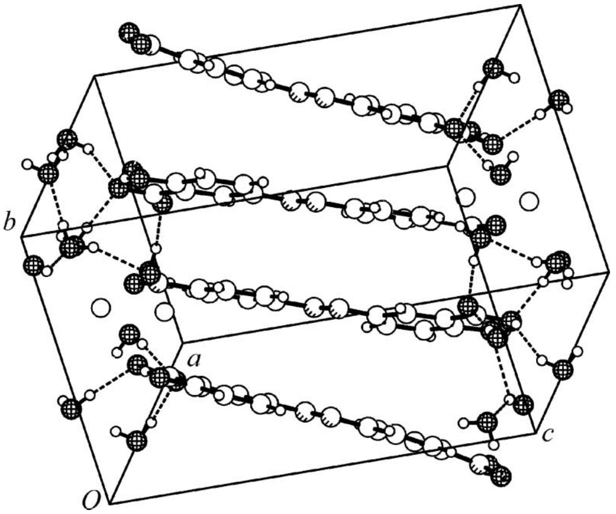

Figure 4
The stacking arrangement of anions in (III). Hydrogen bonds are shown as dashed lines.

In (I), similar to ACEFIZ, molecules are paired into centrosymmetric dimers by two O—H···O hydrogen bonds between the carboxylic acid groups (Table 3). Dimers, related by translation along [100], form slanted stacks; the shortest intermolecular C···C contact in a stack is 3.393 (2) Å [C5···C13(x − 1, y, z)]. In contrast to ACEFIZ, where short contacts between stacks are absent, in (I) neighbouring stacks are connected by weak C—H···O and O—H···O hydrogen bonds (Table 3). These interactions may explain the large torsion angle between the aromatic rings in (I). In the structures of salts (II) and (III), anions also form stacks; in (II), neighbouring anions in a stack are steeply inclined and related by an [001] translation, with the shortest C···C contact being 3.536 (3) Å [C3···C7(x, y, z + 1)] (Fig. 3); in (III), which contains two symmetry-independent anions, *A* and *B*, stacks are formed *via* an ...*AABB*... motif, with two adjacent anions of each type being related by an inversion centre. The stack axes are directed along [110]. The shortest C···C distances in the stacks are 3.415 (3) [C4···C9($-x$, $-y$, $-z + 1$)] and 3.271 (3) Å (C2···C11*A*) between the crystallographically identical anions and between the symmetry-independent anions, respectively (Fig. 4). Thus, there is no evidence for extensive π–π interactions in the three structures.

In (II), stacks of anions form bilayers parallel to (010); the inner part of a bilayer is formed by benzene rings, whereas the –OH and –COO$^-$ groups form the outer layer surface. NH_4^+ cations are located between the bilayers and are engaged in numerous N—H···O hydrogen bonds (Table 3). In (III), stacks also form layers parallel to (001). The –NO_2, –OH and –COO$^-$ groups are located on the layer surface, and Na^+

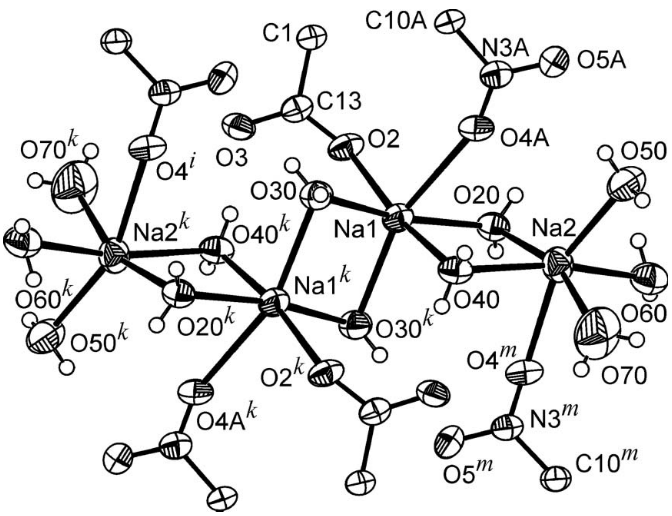

Figure 5
A view of the $[Na_4(H_2O)_{12}]^{4+}$ units in (III). Symmetry codes are as in Table 3. Displacement ellipsoids are drawn at the 50% probability level.

cations and solvent water molecules are located between the layers.

In (III), both Na^+ cations have a distorted octahedral environment. One Na^+ cation is coordinated by four water molecules and two O atoms of two crystallographically independent anions, one of which provides an O atom from the $-COO^-$ group and the other an O atom from the NO_2 group. The second Na^+ cation is coordinated by five water molecules and an O atom of the NO_2 group belonging to the first anion. The Na—O distances are in the range 2.321 (3)–2.680 (2) Å and angle deviations from ideal octahedral values attain a value of 23°. Four octahedra are edge-shared by the bridging O atoms of water molecules, forming $[Na_4(H_2O)_{12}]^{4+}$ units (Fig. 5). Similar although not quite identical $[Na_4(H_2O)_n]^{4+}$ clusters are described in the literature, *e.g.* with $n = 14$ (Dinoi *et al.*, 2007) and $n = 16$ (Elacqua *et al.*, 2012). Water molecules are involved in hydrogen bonds with each other and with the carboxylate O atoms of the anions (Table 3).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: YF3059).

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supplementary materials

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syn and *anti* conformations in 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid and two related salts

Alexandr V. Yatsenko and Ksenia A. Paseshnichenko

Computing details

For all compounds, data collection: *X-AREA* (Stoe & Cie, 2012); cell refinement: *X-AREA* (Stoe & Cie, 2012); data reduction: *X-RED32* (Stoe & Cie, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(I) 2-Hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoic acid

Crystal data

$C_{13}H_9N_3O_5$
M_r = 287.23
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 4.9319 (5) Å
b = 11.6649 (14) Å
c = 21.619 (2) Å
β = 94.991 (8)°
V = 1239.0 (2) Å^3
Z = 4

$F(000)$ = 592.0
D_x = 1.540 Mg m^{-3}
Melting point: 530 K
Cu $K\alpha$ radiation, λ = 1.54186 Å
Cell parameters from 2234 reflections
θ = 3.8–56.3°
μ = 1.04 mm^{-1}
T = 293 K
Needle, red–orange
0.12 × 0.04 × 0.03 mm

Data collection

Stoe STADI VARI diffractometer
Radiation source: microfocus sealed tube
None monochromator
Detector resolution: 5.81 pixels mm^{-1}
rotation method scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.925, T_{max} = 0.979

14169 measured reflections
2334 independent reflections
1804 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 70.0°, θ_{min} = 4.1°
$h = -5 \rightarrow 6$
$k = -14 \rightarrow 13$
$l = -22 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.119
S = 1.00
2334 reflections
199 parameters
4 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0832P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0143 (13)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger. The C-bound H atoms were placed in idealized positions, with constrained distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Phenol and carboxylic H atoms were restrained so that to reproduce the C—O—H angle values observed in salicylic acid (neutron structure determination, Bacon *et al.*, 1973): 107° for phenol and 109° for COOH group.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.1662 (2)	0.16995 (10)	−0.01162 (5)	0.0516 (3)
H1	1.259 (4)	0.2232 (6)	−0.0226 (7)	0.086 (8)*
O2	1.3733 (2)	0.37681 (10)	−0.00850 (5)	0.0529 (3)
O3	1.2554 (2)	0.50125 (10)	0.06235 (6)	0.0559 (3)
H13	1.370 (3)	0.5406 (7)	0.0471 (7)	0.074 (6)*
O4	−0.3794 (3)	0.26095 (12)	0.40909 (6)	0.0658 (4)
O5	−0.3102 (3)	0.44066 (11)	0.39742 (6)	0.0676 (4)
N1	0.5734 (3)	0.30930 (12)	0.18177 (6)	0.0470 (3)
N2	0.4515 (3)	0.22991 (13)	0.20677 (6)	0.0508 (4)
N3	−0.2672 (3)	0.34058 (12)	0.38566 (6)	0.0488 (3)
C1	1.0527 (3)	0.31879 (13)	0.05999 (6)	0.0395 (3)
C2	1.0260 (3)	0.20830 (13)	0.03457 (6)	0.0413 (4)
C3	0.8421 (3)	0.13098 (14)	0.05774 (7)	0.0482 (4)
H3	0.8203	0.0583	0.0404	0.058*
C4	0.6948 (3)	0.16214 (14)	0.10573 (7)	0.0469 (4)
H4	0.5739	0.1101	0.1209	0.056*
C5	0.7233 (3)	0.27134 (13)	0.13239 (7)	0.0423 (4)
C6	0.8975 (3)	0.34931 (13)	0.10875 (7)	0.0417 (4)
H6	0.9122	0.4228	0.1253	0.050*
C7	0.2843 (3)	0.26631 (14)	0.25364 (7)	0.0458 (4)
C8	0.2244 (3)	0.37942 (15)	0.26665 (7)	0.0510 (4)
H8	0.3036	0.4386	0.2457	0.061*
C9	0.0471 (3)	0.40402 (15)	0.31068 (7)	0.0506 (4)
H9	0.0063	0.4796	0.3200	0.061*
C10	−0.0687 (3)	0.31457 (14)	0.34076 (6)	0.0435 (4)
C11	−0.0092 (3)	0.20176 (15)	0.32949 (8)	0.0522 (4)
H11	−0.0872	0.1431	0.3510	0.063*
C12	0.1689 (4)	0.17777 (15)	0.28548 (8)	0.0534 (4)
H12	0.2119	0.1021	0.2771	0.064*
C13	1.2401 (3)	0.40097 (13)	0.03518 (7)	0.0422 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0522 (7)	0.0533 (7)	0.0528 (6)	−0.0086 (5)	0.0242 (5)	−0.0106 (5)
O2	0.0544 (7)	0.0533 (7)	0.0554 (6)	−0.0111 (5)	0.0299 (5)	−0.0075 (5)
O3	0.0622 (7)	0.0464 (6)	0.0640 (7)	−0.0148 (5)	0.0344 (6)	−0.0092 (5)
O4	0.0675 (8)	0.0678 (8)	0.0679 (8)	−0.0032 (6)	0.0393 (6)	0.0040 (6)
O5	0.0713 (9)	0.0625 (8)	0.0725 (8)	0.0196 (6)	0.0272 (6)	0.0011 (6)
N1	0.0430 (7)	0.0571 (8)	0.0426 (7)	−0.0059 (6)	0.0141 (5)	0.0007 (6)
N2	0.0491 (8)	0.0597 (8)	0.0463 (7)	−0.0077 (6)	0.0197 (6)	0.0011 (6)
N3	0.0450 (7)	0.0584 (8)	0.0446 (7)	0.0076 (6)	0.0132 (5)	0.0027 (6)
C1	0.0354 (7)	0.0450 (8)	0.0391 (7)	−0.0024 (6)	0.0092 (6)	0.0013 (6)
C2	0.0364 (7)	0.0495 (8)	0.0390 (7)	−0.0009 (6)	0.0095 (6)	−0.0021 (6)
C3	0.0496 (9)	0.0461 (8)	0.0506 (9)	−0.0083 (7)	0.0146 (7)	−0.0049 (7)
C4	0.0441 (8)	0.0493 (8)	0.0492 (8)	−0.0098 (7)	0.0145 (7)	0.0029 (7)
C5	0.0383 (8)	0.0508 (8)	0.0390 (7)	−0.0031 (6)	0.0107 (6)	0.0003 (6)
C6	0.0409 (8)	0.0444 (8)	0.0415 (7)	−0.0043 (6)	0.0129 (6)	−0.0026 (6)
C7	0.0429 (8)	0.0561 (9)	0.0399 (7)	−0.0042 (7)	0.0118 (6)	0.0009 (6)
C8	0.0534 (9)	0.0538 (9)	0.0479 (8)	−0.0092 (7)	0.0165 (7)	0.0061 (7)
C9	0.0564 (10)	0.0479 (9)	0.0490 (8)	−0.0008 (7)	0.0135 (7)	0.0017 (7)
C10	0.0412 (8)	0.0537 (9)	0.0369 (7)	0.0014 (7)	0.0112 (6)	0.0025 (6)
C11	0.0561 (10)	0.0508 (9)	0.0534 (9)	−0.0038 (7)	0.0255 (7)	0.0051 (7)
C12	0.0603 (10)	0.0487 (9)	0.0546 (9)	−0.0025 (7)	0.0252 (8)	−0.0009 (7)
C13	0.0391 (8)	0.0459 (8)	0.0433 (8)	−0.0035 (6)	0.0134 (6)	−0.0004 (6)

Geometric parameters (Å, º)

O1—C2	1.3400 (17)	C3—H3	0.9300
O1—H1	0.820 (14)	C4—C5	1.400 (2)
O2—C13	1.2290 (17)	C4—H4	0.9300
O3—C13	1.3081 (19)	C5—C6	1.379 (2)
O3—H13	0.820 (13)	C6—H6	0.9300
O4—N3	1.2142 (18)	C7—C8	1.386 (2)
O5—N3	1.2173 (19)	C7—C12	1.390 (2)
N1—N2	1.2519 (19)	C8—C9	1.378 (2)
N1—C5	1.4213 (19)	C8—H8	0.9300
N2—C7	1.4256 (19)	C9—C10	1.379 (2)
N3—C10	1.4691 (19)	C9—H9	0.9300
C1—C6	1.4014 (19)	C10—C11	1.375 (2)
C1—C2	1.403 (2)	C11—C12	1.378 (2)
C1—C13	1.4653 (19)	C11—H11	0.9300
C2—C3	1.402 (2)	C12—H12	0.9300
C3—C4	1.367 (2)		
C2—O1—H1	107.5 (10)	C5—C6—H6	119.7
C13—O3—H13	109.6 (8)	C1—C6—H6	119.7
N2—N1—C5	113.24 (13)	C8—C7—C12	120.18 (14)
N1—N2—C7	114.56 (14)	C8—C7—N2	125.06 (14)
O4—N3—O5	123.55 (13)	C12—C7—N2	114.70 (15)
O4—N3—C10	118.15 (13)	C9—C8—C7	119.86 (15)

O5—N3—C10	118.30 (14)	C9—C8—H8	120.1
C6—C1—C2	119.29 (13)	C7—C8—H8	120.1
C6—C1—C13	120.81 (13)	C8—C9—C10	118.81 (16)
C2—C1—C13	119.89 (12)	C8—C9—H9	120.6
O1—C2—C3	116.31 (13)	C10—C9—H9	120.6
O1—C2—C1	124.17 (13)	C11—C10—C9	122.48 (14)
C3—C2—C1	119.51 (13)	C11—C10—N3	118.66 (14)
C4—C3—C2	120.22 (14)	C9—C10—N3	118.85 (15)
C4—C3—H3	119.9	C10—C11—C12	118.38 (15)
C2—C3—H3	119.9	C10—C11—H11	120.8
C3—C4—C5	120.88 (14)	C12—C11—H11	120.8
C3—C4—H4	119.6	C11—C12—C7	120.26 (16)
C5—C4—H4	119.6	C11—C12—H12	119.9
C6—C5—C4	119.40 (13)	C7—C12—H12	119.9
C6—C5—N1	117.03 (13)	O2—C13—O3	122.43 (13)
C4—C5—N1	123.52 (13)	O2—C13—C1	121.83 (14)
C5—C6—C1	120.64 (14)	O3—C13—C1	115.74 (12)

C5—N1—N2—C7	−175.91 (12)	C12—C7—C8—C9	−0.8 (3)
C6—C1—C2—O1	−179.33 (14)	N2—C7—C8—C9	176.20 (15)
C13—C1—C2—O1	1.1 (2)	C7—C8—C9—C10	−0.4 (3)
C6—C1—C2—C3	0.9 (2)	C8—C9—C10—C11	1.5 (3)
C13—C1—C2—C3	−178.70 (14)	C8—C9—C10—N3	−177.25 (14)
O1—C2—C3—C4	178.64 (14)	O4—N3—C10—C11	−3.1 (2)
C1—C2—C3—C4	−1.6 (2)	O5—N3—C10—C11	176.89 (16)
C2—C3—C4—C5	0.3 (2)	O4—N3—C10—C9	175.76 (15)
C3—C4—C5—C6	1.7 (2)	O5—N3—C10—C9	−4.3 (2)
C3—C4—C5—N1	179.13 (15)	C9—C10—C11—C12	−1.4 (3)
N2—N1—C5—C6	−170.02 (13)	N3—C10—C11—C12	177.42 (15)
N2—N1—C5—C4	12.4 (2)	C10—C11—C12—C7	0.1 (3)
C4—C5—C6—C1	−2.3 (2)	C8—C7—C12—C11	1.0 (3)
N1—C5—C6—C1	−179.96 (13)	N2—C7—C12—C11	−176.32 (16)
C2—C1—C6—C5	1.0 (2)	C6—C1—C13—O2	−178.27 (14)
C13—C1—C6—C5	−179.36 (13)	C2—C1—C13—O2	1.3 (2)
N1—N2—C7—C8	8.5 (2)	C6—C1—C13—O3	1.5 (2)
N1—N2—C7—C12	−174.29 (14)	C2—C1—C13—O3	−178.89 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82 (1)	1.90 (1)	2.6189 (16)	147 (1)
O1—H1···O4^{i}	0.82 (1)	2.42 (1)	3.0461 (18)	134 (1)
O3—H13···O2^{ii}	0.82 (1)	1.85 (1)	2.6651 (16)	176 (1)
C4—H4···O5^{iii}	0.93	2.38	3.202 (2)	147

Symmetry codes: (i) *x*+2, −*y*+1/2, *z*−1/2; (ii) −*x*+3, −*y*+1, −*z*; (iii) −*x*, *y*−1/2, −*z*+1/2.

(II) Ammonium 2-hydroxy-5-[(*E*)-phenyldiazenyl]benzoate

Crystal data

$NH_4^+\cdot C_{13}H_9N_2O_3^-$
$M_r = 259.26$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.0471$ (1) Å
$b = 34.371$ (1) Å
$c = 6.2824$ (2) Å
$\beta = 103.278$ (2)°
$V = 1270.85$ (6) Å^3
$Z = 4$

$F(000) = 544$
$D_x = 1.355$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54186$ Å
Cell parameters from 3698 reflections
$\theta = 5.1$–72.1°
$\mu = 0.82$ mm^{-1}
$T = 293$ K
Irregular block, dark yellow
0.08 × 0.05 × 0.05 mm

Data collection

Stoe STADI VARI diffractometer
Radiation source: microfocus sealed tube
None monochromator
Detector resolution: 5.81 pixels mm^{-1}
rotation method scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.945$, $T_{max} = 0.960$

15094 measured reflections
2352 independent reflections
1561 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 69.0°$, $\theta_{min} = 5.2°$
$h = -7\rightarrow6$
$k = -41\rightarrow41$
$l = -7\rightarrow7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.141$
$S = 1.04$
2352 reflections
189 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.38P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0052 (7)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. The C-bound H atoms were placed in idealized positions, with constrained distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Phenol H atoms were restrained so that to reproduce the C—O—H angle value of 107° observed in salicylic acid (neutron structure determination, Bacon *et al.*, 1973). All N—H distances and tetrahedral environment of the N atom were also restrained.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2531 (3)	0.05503 (5)	0.8971 (3)	0.0534 (5)
H1	0.370 (3)	0.0422 (7)	0.930 (3)	0.087 (12)*
O2	0.6199 (3)	0.02302 (5)	0.8656 (3)	0.0539 (5)
O3	0.7530 (3)	0.03045 (5)	0.5682 (3)	0.0534 (5)
N1	0.2848 (4)	0.14683 (5)	0.1780 (4)	0.0512 (5)
N2	0.4682 (4)	0.14854 (6)	0.1187 (4)	0.0508 (5)
C1	0.4416 (4)	0.06971 (6)	0.6068 (4)	0.0403 (5)
C2	0.2647 (4)	0.07579 (6)	0.7175 (4)	0.0432 (5)
C3	0.0987 (4)	0.10345 (7)	0.6398 (4)	0.0499 (6)
H3	−0.0193	0.1071	0.7101	0.060*
C4	0.1077 (4)	0.12544 (7)	0.4601 (4)	0.0509 (6)
H4	−0.0066	0.1434	0.4072	0.061*
C5	0.2866 (4)	0.12113 (6)	0.3555 (4)	0.0456 (6)
C6	0.4488 (4)	0.09291 (6)	0.4288 (4)	0.0425 (5)
H6	0.5656	0.0894	0.3567	0.051*
C7	0.4620 (4)	0.17474 (7)	−0.0590 (4)	0.0495 (6)
C8	0.2868 (5)	0.20058 (7)	−0.1365 (5)	0.0634 (8)
H8	0.1650	0.2022	−0.0696	0.076*
C9	0.2935 (6)	0.22386 (8)	−0.3135 (6)	0.0771 (10)
H9	0.1763	0.2414	−0.3648	0.093*
C10	0.4716 (6)	0.22141 (8)	−0.4152 (5)	0.0723 (9)
H10	0.4726	0.2367	−0.5373	0.087*
C11	0.6476 (6)	0.19641 (9)	−0.3356 (5)	0.0703 (8)
H11	0.7696	0.1950	−0.4025	0.084*
C12	0.6445 (5)	0.17321 (8)	−0.1560 (5)	0.0619 (7)
H12	0.7655	0.1566	−0.1009	0.074*
C13	0.6177 (4)	0.03893 (6)	0.6836 (4)	0.0421 (5)
N3	−0.0209 (3)	0.03147 (5)	1.2283 (3)	0.0487 (5)
H21	−0.087 (3)	0.0405 (6)	1.331 (2)	0.073*
H22	−0.127 (3)	0.0243 (6)	1.111 (2)	0.073*
H23	0.066 (3)	0.0499 (4)	1.191 (3)	0.073*
H24	0.065 (3)	0.0110 (4)	1.281 (3)	0.073*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0507 (11)	0.0624 (11)	0.0521 (11)	0.0042 (8)	0.0223 (9)	0.0090 (8)
O2	0.0459 (10)	0.0673 (11)	0.0499 (10)	0.0061 (8)	0.0140 (9)	0.0170 (8)
O3	0.0461 (9)	0.0588 (10)	0.0618 (11)	0.0132 (7)	0.0258 (9)	0.0138 (8)
N1	0.0489 (11)	0.0437 (10)	0.0638 (14)	0.0045 (8)	0.0186 (11)	0.0046 (9)
N2	0.0469 (11)	0.0476 (11)	0.0605 (14)	0.0030 (8)	0.0174 (11)	0.0067 (9)
C1	0.0376 (12)	0.0407 (11)	0.0444 (13)	−0.0014 (8)	0.0129 (11)	−0.0016 (9)
C2	0.0442 (12)	0.0410 (12)	0.0481 (14)	−0.0040 (9)	0.0184 (12)	−0.0008 (10)
C3	0.0446 (13)	0.0515 (13)	0.0590 (16)	0.0055 (10)	0.0231 (12)	−0.0027 (11)
C4	0.0459 (13)	0.0425 (12)	0.0680 (17)	0.0072 (10)	0.0206 (13)	0.0005 (11)
C5	0.0460 (13)	0.0398 (11)	0.0521 (15)	0.0018 (9)	0.0136 (12)	0.0034 (10)
C6	0.0384 (12)	0.0443 (12)	0.0468 (13)	−0.0002 (9)	0.0141 (11)	−0.0011 (10)

C7	0.0488 (14)	0.0438 (12)	0.0585 (16)	−0.0022 (10)	0.0178 (13)	0.0029 (11)
C8	0.0599 (16)	0.0523 (15)	0.083 (2)	0.0089 (12)	0.0273 (16)	0.0201 (14)
C9	0.076 (2)	0.0567 (17)	0.103 (3)	0.0123 (14)	0.031 (2)	0.0335 (16)
C10	0.084 (2)	0.0585 (17)	0.078 (2)	−0.0127 (15)	0.0248 (19)	0.0154 (14)
C11	0.0701 (19)	0.0738 (19)	0.076 (2)	−0.0055 (15)	0.0348 (18)	0.0052 (16)
C12	0.0557 (16)	0.0593 (16)	0.077 (2)	0.0044 (12)	0.0273 (16)	0.0078 (13)
C13	0.0355 (11)	0.0444 (12)	0.0463 (13)	−0.0028 (9)	0.0092 (11)	0.0027 (10)
N3	0.0473 (11)	0.0484 (11)	0.0536 (13)	0.0040 (8)	0.0182 (10)	0.0039 (9)

Geometric parameters (Å, º)

O1—C2	1.350 (3)	C6—H6	0.9300
O1—H1	0.82 (2)	C7—C12	1.379 (3)
O2—C13	1.265 (3)	C7—C8	1.383 (4)
O3—C13	1.246 (3)	C8—C9	1.378 (4)
N1—N2	1.249 (3)	C8—H8	0.9300
N1—C5	1.421 (3)	C9—C10	1.375 (4)
N2—C7	1.428 (3)	C9—H9	0.9300
C1—C6	1.382 (3)	C10—C11	1.370 (4)
C1—C2	1.419 (3)	C10—H10	0.9300
C1—C13	1.500 (3)	C11—C12	1.385 (4)
C2—C3	1.387 (3)	C11—H11	0.9300
C3—C4	1.370 (3)	C12—H12	0.9300
C3—H3	0.9300	N3—H21	0.89 (2)
C4—C5	1.397 (3)	N3—H22	0.89 (2)
C4—H4	0.9300	N3—H23	0.89 (2)
C5—C6	1.381 (3)	N3—H24	0.89 (2)

C2—O1—H1	106.6 (14)	C9—C8—C7	119.7 (3)
N2—N1—C5	114.6 (2)	C9—C8—H8	120.2
N1—N2—C7	113.4 (2)	C7—C8—H8	120.2
C6—C1—C2	118.6 (2)	C10—C9—C8	120.7 (3)
C6—C1—C13	121.01 (19)	C10—C9—H9	119.7
C2—C1—C13	120.4 (2)	C8—C9—H9	119.7
O1—C2—C3	119.0 (2)	C11—C10—C9	119.6 (3)
O1—C2—C1	121.4 (2)	C11—C10—H10	120.2
C3—C2—C1	119.6 (2)	C9—C10—H10	120.2
C4—C3—C2	120.4 (2)	C10—C11—C12	120.2 (3)
C4—C3—H3	119.8	C10—C11—H11	119.9
C2—C3—H3	119.8	C12—C11—H11	119.9
C3—C4—C5	120.7 (2)	C7—C12—C11	120.0 (3)
C3—C4—H4	119.6	C7—C12—H12	120.0
C5—C4—H4	119.6	C11—C12—H12	120.0
C6—C5—C4	119.0 (2)	O3—C13—O2	123.6 (2)
C6—C5—N1	125.1 (2)	O3—C13—C1	119.4 (2)
C4—C5—N1	115.9 (2)	O2—C13—C1	117.1 (2)
C5—C6—C1	121.5 (2)	H21—N3—H22	110 (2)
C5—C6—H6	119.2	H21—N3—H23	110 (2)
C1—C6—H6	119.2	H22—N3—H23	109 (2)
C12—C7—C8	119.7 (2)	H21—N3—H24	109 (2)

C12—C7—N2	116.2 (2)	H22—N3—H24	110 (2)
C8—C7—N2	124.1 (2)	H23—N3—H24	109 (2)

C5—N1—N2—C7	−179.7 (2)	C13—C1—C6—C5	179.5 (2)
C6—C1—C2—O1	−177.6 (2)	N1—N2—C7—C12	−169.5 (2)
C13—C1—C2—O1	1.9 (3)	N1—N2—C7—C8	10.1 (4)
C6—C1—C2—C3	2.8 (3)	C12—C7—C8—C9	1.6 (4)
C13—C1—C2—C3	−177.8 (2)	N2—C7—C8—C9	−178.0 (3)
O1—C2—C3—C4	178.9 (2)	C7—C8—C9—C10	0.6 (5)
C1—C2—C3—C4	−1.4 (4)	C8—C9—C10—C11	−2.0 (5)
C2—C3—C4—C5	−1.6 (4)	C9—C10—C11—C12	1.1 (5)
C3—C4—C5—C6	3.3 (4)	C8—C7—C12—C11	−2.5 (4)
C3—C4—C5—N1	−176.8 (2)	N2—C7—C12—C11	177.2 (3)
N2—N1—C5—C6	−15.3 (3)	C10—C11—C12—C7	1.1 (5)
N2—N1—C5—C4	164.9 (2)	C6—C1—C13—O3	−10.1 (3)
C4—C5—C6—C1	−1.9 (4)	C2—C1—C13—O3	170.4 (2)
N1—C5—C6—C1	178.2 (2)	C6—C1—C13—O2	169.6 (2)
C2—C1—C6—C5	−1.1 (3)	C2—C1—C13—O2	−9.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82 (2)	1.78 (2)	2.524 (3)	151 (2)
N3—H21···O3^{i}	0.89 (2)	1.99 (2)	2.788 (3)	150 (2)
N3—H22···O2^{ii}	0.89 (2)	1.91 (2)	2.779 (3)	164 (2)
N3—H23···O1	0.89 (2)	2.38 (2)	3.052 (3)	132 (2)
N3—H24···O3^{iii}	0.89 (2)	1.91 (2)	2.799 (3)	172 (2)

Symmetry codes: (i) $x-1, y, z+1$; (ii) $x-1, y, z$; (iii) $-x+1, -y, -z+2$.

(III) Sodium 2-hydroxy-5-[(*E*)-(4-nitrophenyl)diazenyl]benzoate trihydrate

Crystal data

$Na^+\cdot C_{13}H_8N_3O_5^-\cdot 3H_2O$
$M_r = 363.26$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2123$ (5) Å
$b = 13.0205$ (8) Å
$c = 17.0317$ (11) Å
$\alpha = 77.185$ (6)°
$\beta = 80.933$ (5)°
$\gamma = 83.401$ (5)°
$V = 1534.76$ (17) Å^3

$Z = 4$
$F(000) = 752$
$D_x = 1.572$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5966 reflections
$\theta = 2.4$–30.4°
$\mu = 0.16$ mm^{-1}
$T = 293$ K
Irregular block, dark yellow
0.50 × 0.45 × 0.40 mm

Data collection

Stoe STADI VARI diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 5.81 pixels mm^{-1}
rotation method scans

Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.926$, $T_{max} = 0.952$
6773 measured reflections
5936 independent reflections
3776 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$

θ_{max} = 26.0°, θ_{min} = 2.7°
$h = -4\rightarrow8$
$k = -15\rightarrow16$
$l = -19\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.120$
$S = 0.92$
5936 reflections
493 parameters
22 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. The C-bound H atoms were placed in idealized positions, with constrained distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Phenol H atoms were restrained so that to reproduce the C—O—H angle value of 107° observed in salicylic acid (neutron structure determination, Bacon *et al.*, 1973). For all water molecules, the O—H distances and H—O—H angles of 106° were restrained.

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

	x	y	z	U_{iso}*/U_{eq}
Na1	0.29209 (14)	0.54778 (7)	0.04310 (5)	0.0411 (2)
Na2	0.12688 (15)	0.81138 (8)	−0.01809 (6)	0.0489 (3)
O20	−0.0003 (2)	0.63987 (14)	0.01501 (10)	0.0413 (4)
H21	−0.085 (2)	0.651 (2)	0.0511 (11)	0.062*
H22	−0.055 (3)	0.630 (2)	−0.0212 (11)	0.062*
O30	0.5998 (3)	0.48619 (14)	0.09144 (10)	0.0447 (4)
H31	0.597 (4)	0.4339 (14)	0.1286 (12)	0.067*
H32	0.681 (3)	0.5201 (19)	0.0997 (17)	0.067*
O40	0.4292 (3)	0.71079 (14)	−0.00868 (10)	0.0424 (4)
H41	0.478 (3)	0.742 (2)	0.0187 (13)	0.064*
H42	0.503 (3)	0.713 (2)	−0.0508 (9)	0.064*
O50	0.0461 (4)	0.90808 (16)	0.08695 (13)	0.0630 (6)
H51	0.106 (5)	0.9606 (18)	0.072 (2)	0.095*
H52	0.086 (5)	0.876 (2)	0.1289 (13)	0.095*
O60	−0.1860 (3)	0.88960 (16)	−0.05485 (12)	0.0536 (5)
H61	−0.257 (4)	0.870 (3)	−0.0806 (15)	0.080*
H62	−0.210 (5)	0.856 (2)	−0.0083 (7)	0.080*
O70	0.2955 (5)	0.9520 (2)	−0.0899 (2)	0.1026 (10)
H71	0.236 (7)	1.010 (2)	−0.100 (3)	0.154*

H72	0.360 (7)	0.946 (4)	−0.1331 (16)	0.154*
O1	−0.0793 (3)	0.46163 (13)	0.22701 (10)	0.0473 (4)
H1	−0.018 (3)	0.4605 (14)	0.1823 (4)	0.057*
O2	0.1590 (3)	0.39434 (13)	0.11992 (9)	0.0436 (4)
O3	0.3135 (3)	0.23308 (14)	0.15024 (10)	0.0458 (4)
O4	0.1739 (3)	−0.22444 (16)	0.84208 (10)	0.0604 (6)
O5	0.3900 (3)	−0.29157 (14)	0.76258 (11)	0.0505 (5)
N1	0.1704 (3)	0.12249 (15)	0.45539 (11)	0.0371 (4)
N2	0.1011 (3)	0.12523 (16)	0.52805 (11)	0.0404 (5)
N3	0.2706 (3)	−0.21953 (15)	0.77658 (11)	0.0365 (4)
C1	0.1194 (3)	0.30052 (17)	0.25700 (12)	0.0311 (5)
C2	−0.0165 (3)	0.37726 (17)	0.28110 (14)	0.0362 (5)
C3	−0.0952 (4)	0.36977 (18)	0.36155 (14)	0.0380 (5)
H3	−0.1871	0.4210	0.3761	0.046*
C4	−0.0366 (4)	0.28584 (18)	0.42029 (14)	0.0386 (5)
H4	−0.0902	0.2800	0.4743	0.046*
C5	0.1029 (3)	0.21024 (17)	0.39831 (13)	0.0337 (5)
C6	0.1779 (3)	0.21715 (17)	0.31709 (13)	0.0326 (5)
H6	0.2685	0.1653	0.3027	0.039*
C7	0.1589 (3)	0.03711 (17)	0.58710 (13)	0.0342 (5)
C8	0.2876 (4)	−0.04755 (19)	0.57064 (14)	0.0391 (5)
H8	0.3462	−0.0474	0.5179	0.047*
C9	0.3263 (3)	−0.13020 (18)	0.63268 (13)	0.0364 (5)
H9	0.4103	−0.1870	0.6224	0.044*
C10	0.2389 (3)	−0.12844 (18)	0.71104 (13)	0.0367 (5)
C11	0.1150 (4)	−0.0458 (2)	0.72882 (14)	0.0453 (6)
H11	0.0575	−0.0465	0.7818	0.054*
C12	0.0773 (4)	0.0385 (2)	0.66638 (15)	0.0510 (7)
H12	−0.0029	0.0963	0.6775	0.061*
C13	0.2054 (3)	0.30891 (18)	0.16969 (13)	0.0356 (5)
O1A	0.6032 (3)	0.07174 (15)	0.80581 (11)	0.0539 (5)
H1A	0.560 (4)	0.0856 (15)	0.85009 (16)	0.065*
O2A	0.4361 (3)	0.18204 (14)	0.90509 (10)	0.0493 (5)
O3A	0.2881 (3)	0.33815 (14)	0.86157 (10)	0.0470 (4)
O4A	0.2033 (3)	0.66000 (15)	0.15994 (10)	0.0525 (5)
O5A	0.0646 (3)	0.75726 (14)	0.24188 (11)	0.0526 (5)
N1A	0.3363 (3)	0.38085 (16)	0.55961 (11)	0.0384 (5)
N2A	0.3935 (3)	0.36973 (16)	0.48885 (11)	0.0423 (5)
N3A	0.1545 (3)	0.67607 (16)	0.22755 (12)	0.0399 (5)
C1A	0.4205 (3)	0.23760 (17)	0.76376 (13)	0.0322 (5)
C2A	0.5323 (4)	0.14575 (18)	0.74698 (14)	0.0380 (5)
C3A	0.5708 (4)	0.1304 (2)	0.66745 (16)	0.0482 (6)
H3A	0.6399	0.0691	0.6567	0.058*
C4A	0.5078 (4)	0.2049 (2)	0.60525 (15)	0.0461 (6)
H4A	0.5349	0.1939	0.5524	0.055*
C5A	0.4012 (3)	0.29899 (17)	0.62036 (13)	0.0342 (5)
C6A	0.3575 (3)	0.31237 (18)	0.70010 (14)	0.0367 (5)
H6A	0.2846	0.3727	0.7109	0.044*
C7A	0.3266 (3)	0.45134 (18)	0.42707 (13)	0.0362 (5)

C8A	0.2047 (4)	0.53881 (19)	0.44037 (13)	0.0408 (6)
H8A	0.1622	0.5473	0.4932	0.049*
C9A	0.1465 (4)	0.61303 (19)	0.37529 (14)	0.0395 (5)
H9A	0.0645	0.6714	0.3835	0.047*
C10A	0.2138 (3)	0.59775 (17)	0.29782 (12)	0.0322 (5)
C11A	0.3370 (3)	0.51270 (18)	0.28285 (13)	0.0370 (5)
H11A	0.3811	0.5049	0.2300	0.044*
C12A	0.3923 (4)	0.43972 (19)	0.34866 (14)	0.0395 (5)
H12A	0.4752	0.3818	0.3401	0.047*
C13A	0.3759 (4)	0.2550 (2)	0.84887 (14)	0.0389 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0435 (6)	0.0394 (5)	0.0368 (5)	−0.0051 (4)	−0.0020 (4)	−0.0016 (4)
Na2	0.0520 (6)	0.0389 (5)	0.0562 (6)	−0.0043 (4)	−0.0044 (5)	−0.0123 (5)
O20	0.0436 (10)	0.0475 (10)	0.0345 (9)	−0.0057 (8)	−0.0055 (7)	−0.0112 (8)
O30	0.0524 (11)	0.0462 (10)	0.0351 (9)	−0.0039 (8)	−0.0060 (8)	−0.0076 (7)
O40	0.0480 (11)	0.0491 (10)	0.0319 (9)	−0.0103 (8)	−0.0040 (7)	−0.0103 (8)
O50	0.0938 (17)	0.0480 (12)	0.0484 (12)	−0.0096 (11)	−0.0190 (11)	−0.0041 (9)
O60	0.0611 (13)	0.0582 (12)	0.0440 (10)	−0.0114 (10)	−0.0044 (9)	−0.0149 (9)
O70	0.113 (3)	0.0613 (16)	0.129 (3)	−0.0298 (15)	−0.006 (2)	−0.0059 (16)
O1	0.0568 (12)	0.0376 (9)	0.0408 (10)	0.0063 (8)	−0.0115 (8)	0.0046 (8)
O2	0.0574 (11)	0.0397 (9)	0.0317 (8)	−0.0162 (8)	−0.0054 (8)	0.0024 (7)
O3	0.0586 (12)	0.0470 (10)	0.0308 (8)	−0.0037 (9)	0.0024 (8)	−0.0124 (7)
O4	0.0763 (14)	0.0646 (12)	0.0291 (9)	0.0013 (11)	0.0036 (9)	0.0025 (8)
O5	0.0551 (12)	0.0411 (10)	0.0476 (10)	0.0069 (9)	−0.0087 (9)	0.0028 (8)
N1	0.0443 (12)	0.0340 (10)	0.0290 (10)	−0.0009 (9)	−0.0054 (8)	0.0008 (8)
N2	0.0534 (13)	0.0403 (11)	0.0261 (10)	0.0012 (9)	−0.0065 (9)	−0.0058 (8)
N3	0.0437 (12)	0.0383 (11)	0.0278 (10)	−0.0095 (9)	−0.0046 (8)	−0.0044 (8)
C1	0.0388 (13)	0.0301 (11)	0.0258 (10)	−0.0107 (9)	−0.0052 (9)	−0.0045 (8)
C2	0.0424 (14)	0.0290 (11)	0.0361 (12)	−0.0047 (10)	−0.0103 (10)	0.0000 (9)
C3	0.0485 (14)	0.0289 (11)	0.0349 (12)	0.0060 (10)	−0.0053 (10)	−0.0078 (9)
C4	0.0464 (14)	0.0375 (12)	0.0304 (11)	0.0016 (11)	−0.0019 (10)	−0.0083 (10)
C5	0.0408 (13)	0.0325 (11)	0.0265 (11)	−0.0012 (10)	−0.0064 (9)	−0.0027 (9)
C6	0.0338 (12)	0.0282 (11)	0.0348 (12)	−0.0004 (9)	−0.0042 (9)	−0.0060 (9)
C7	0.0435 (14)	0.0301 (11)	0.0291 (11)	−0.0028 (10)	−0.0089 (10)	−0.0041 (9)
C8	0.0458 (14)	0.0408 (13)	0.0277 (11)	−0.0023 (11)	0.0039 (10)	−0.0078 (10)
C9	0.0402 (13)	0.0353 (12)	0.0312 (11)	−0.0010 (10)	−0.0002 (10)	−0.0061 (9)
C10	0.0415 (14)	0.0398 (13)	0.0273 (11)	−0.0045 (10)	−0.0028 (10)	−0.0046 (9)
C11	0.0633 (18)	0.0424 (13)	0.0237 (11)	0.0081 (12)	−0.0012 (11)	−0.0027 (10)
C12	0.0685 (19)	0.0462 (15)	0.0318 (12)	0.0155 (13)	−0.0023 (12)	−0.0075 (11)
C13	0.0405 (13)	0.0365 (12)	0.0308 (11)	−0.0100 (10)	−0.0085 (10)	−0.0028 (10)
O1A	0.0668 (13)	0.0477 (11)	0.0422 (10)	0.0057 (9)	−0.0099 (9)	−0.0023 (8)
O2A	0.0659 (13)	0.0486 (10)	0.0308 (9)	−0.0013 (9)	−0.0116 (8)	−0.0009 (8)
O3A	0.0658 (12)	0.0454 (10)	0.0319 (9)	0.0063 (9)	−0.0066 (8)	−0.0181 (7)
O4A	0.0711 (13)	0.0586 (11)	0.0258 (9)	0.0027 (10)	−0.0067 (8)	−0.0084 (8)
O5A	0.0676 (13)	0.0427 (10)	0.0413 (10)	0.0097 (9)	−0.0057 (9)	−0.0044 (8)
N1A	0.0431 (12)	0.0428 (11)	0.0300 (10)	−0.0050 (9)	−0.0059 (8)	−0.0078 (8)
N2A	0.0502 (13)	0.0460 (12)	0.0293 (10)	−0.0023 (10)	−0.0035 (9)	−0.0068 (9)

N3A	0.0435 (12)	0.0418 (11)	0.0331 (11)	−0.0092 (9)	−0.0029 (9)	−0.0038 (9)
C1A	0.0330 (12)	0.0345 (12)	0.0292 (11)	−0.0069 (9)	−0.0046 (9)	−0.0044 (9)
C2A	0.0457 (14)	0.0320 (12)	0.0326 (12)	−0.0037 (10)	−0.0079 (10)	0.0029 (9)
C3A	0.0531 (16)	0.0401 (14)	0.0476 (15)	0.0024 (12)	0.0014 (12)	−0.0102 (11)
C4A	0.0563 (17)	0.0477 (14)	0.0334 (13)	0.0055 (12)	−0.0080 (11)	−0.0100 (11)
C5A	0.0396 (13)	0.0348 (12)	0.0295 (11)	−0.0038 (10)	−0.0078 (9)	−0.0071 (9)
C6A	0.0389 (13)	0.0331 (12)	0.0377 (12)	−0.0026 (10)	−0.0011 (10)	−0.0099 (10)
C7A	0.0408 (13)	0.0354 (12)	0.0315 (11)	−0.0058 (10)	−0.0024 (10)	−0.0054 (9)
C8A	0.0554 (16)	0.0429 (13)	0.0241 (11)	0.0016 (11)	−0.0054 (10)	−0.0101 (10)
C9A	0.0441 (14)	0.0389 (13)	0.0351 (12)	−0.0019 (11)	−0.0047 (10)	−0.0081 (10)
C10A	0.0371 (13)	0.0345 (11)	0.0240 (10)	−0.0071 (9)	−0.0063 (9)	−0.0006 (9)
C11A	0.0415 (13)	0.0424 (13)	0.0280 (11)	−0.0034 (10)	−0.0020 (10)	−0.0111 (10)
C12A	0.0472 (15)	0.0414 (13)	0.0316 (12)	−0.0040 (11)	−0.0001 (10)	−0.0148 (10)
C13A	0.0424 (14)	0.0471 (14)	0.0273 (11)	−0.0149 (11)	−0.0052 (10)	−0.0016 (10)

Geometric parameters (Å, º)

Na1—O2	2.3474 (18)	C3—H3	0.9300
Na1—O20	2.366 (2)	C4—C5	1.392 (3)
Na1—O40	2.3743 (19)	C4—H4	0.9300
Na1—O30^{i}	2.4211 (19)	C5—C6	1.391 (3)
Na1—O30	2.474 (2)	C6—H6	0.9300
Na1—O4A	2.679 (2)	C7—C12	1.388 (3)
Na1—Na1^{i}	3.3560 (19)	C7—C8	1.406 (3)
Na1—Na2	3.4857 (14)	C8—C9	1.368 (3)
Na2—O70	2.319 (3)	C8—H8	0.9300
Na2—O50	2.372 (2)	C9—C10	1.387 (3)
Na2—O40	2.420 (2)	C9—H9	0.9300
Na2—O20	2.428 (2)	C10—C11	1.374 (3)
Na2—O60	2.481 (3)	C11—C12	1.384 (3)
Na2—O4^{ii}	2.491 (2)	C11—H11	0.9300
Na2—H21	2.67 (3)	C12—H12	0.9300
Na2—H62	2.42 (3)	O1A—C2A	1.347 (3)
O20—H21	0.821 (3)	O1A—H1A	0.8200 (10)
O20—H22	0.820 (3)	O2A—C13A	1.281 (3)
O30—Na1^{i}	2.4212 (19)	O3A—C13A	1.234 (3)
O30—H31	0.820 (3)	O4A—N3A	1.207 (2)
O30—H32	0.820 (3)	O5A—N3A	1.226 (3)
O40—H41	0.820 (3)	N1A—N2A	1.245 (3)
O40—H42	0.820 (3)	N1A—C5A	1.405 (3)
O50—H51	0.821 (3)	N2A—C7A	1.420 (3)
O50—H52	0.821 (3)	N3A—C10A	1.475 (3)
O60—H61	0.821 (3)	C1A—C6A	1.384 (3)
O60—H62	0.820 (3)	C1A—C2A	1.421 (3)
O70—H71	0.821 (3)	C1A—C13A	1.496 (3)
O70—H72	0.821 (3)	C2A—C3A	1.393 (4)
O1—C2	1.352 (3)	C3A—C4A	1.365 (4)
O1—H1	0.8201 (10)	C3A—H3A	0.9300
O2—C13	1.286 (3)	C4A—C5A	1.421 (3)
O3—C13	1.257 (3)	C4A—H4A	0.9300

O4—N3	1.212 (3)	C5A—C6A	1.390 (3)
O4—Na2^{iii}	2.491 (2)	C6A—H6A	0.9300
O5—N3	1.236 (3)	C7A—C12A	1.380 (3)
N1—N2	1.266 (3)	C7A—C8A	1.394 (3)
N1—C5	1.420 (3)	C8A—C9A	1.384 (3)
N2—C7	1.419 (3)	C8A—H8A	0.9300
N3—C10	1.462 (3)	C9A—C10A	1.382 (3)
C1—C6	1.394 (3)	C9A—H9A	0.9300
C1—C2	1.399 (3)	C10A—C11A	1.381 (3)
C1—C13	1.503 (3)	C11A—C12A	1.379 (3)
C2—C3	1.385 (3)	C11A—H11A	0.9300
C3—C4	1.384 (3)	C12A—H12A	0.9300

O2—Na1—O20	94.62 (7)	C13—O2—Na1	139.59 (16)
O2—Na1—O40	168.45 (7)	N3—O4—Na2^{iii}	149.03 (19)
O20—Na1—O40	87.33 (7)	N2—N1—C5	112.87 (19)
O2—Na1—O30^{i}	106.34 (7)	N1—N2—C7	114.96 (19)
O20—Na1—O30^{i}	97.26 (7)	O4—N3—O5	121.8 (2)
O40—Na1—O30^{i}	84.66 (7)	O4—N3—C10	119.2 (2)
O2—Na1—O30	91.35 (7)	O5—N3—C10	118.96 (18)
O20—Na1—O30	165.76 (7)	C6—C1—C2	117.82 (19)
O40—Na1—O30	84.32 (7)	C6—C1—C13	120.6 (2)
O30^{i}—Na1—O30	93.44 (6)	C2—C1—C13	121.53 (19)
O2—Na1—O4A	95.53 (7)	O1—C2—C3	116.7 (2)
O20—Na1—O4A	76.60 (6)	O1—C2—C1	121.8 (2)
O40—Na1—O4A	73.82 (6)	C3—C2—C1	121.5 (2)
O30^{i}—Na1—O4A	157.77 (7)	C4—C3—C2	119.8 (2)
O30—Na1—O4A	89.97 (7)	C4—C3—H3	120.1
O2—Na1—Na1^{i}	102.72 (6)	C2—C3—H3	120.1
O20—Na1—Na1^{i}	143.67 (6)	C3—C4—C5	119.8 (2)
O40—Na1—Na1^{i}	81.95 (6)	C3—C4—H4	120.1
O30^{i}—Na1—Na1^{i}	47.38 (5)	C5—C4—H4	120.1
O30—Na1—Na1^{i}	46.07 (5)	C6—C5—C4	119.9 (2)
O4A—Na1—Na1^{i}	131.87 (7)	C6—C5—N1	117.2 (2)
O2—Na1—Na2	135.26 (6)	C4—C5—N1	122.8 (2)
O20—Na1—Na2	44.06 (5)	C5—C6—C1	121.0 (2)
O40—Na1—Na2	43.88 (5)	C5—C6—H6	119.5
O30^{i}—Na1—Na2	97.02 (5)	C1—C6—H6	119.5
O30—Na1—Na2	125.25 (6)	C12—C7—C8	120.0 (2)
O4A—Na1—Na2	63.55 (5)	C12—C7—N2	114.8 (2)
Na1^{i}—Na1—Na2	120.90 (4)	C8—C7—N2	125.2 (2)
O70—Na2—O50	86.84 (11)	C9—C8—C7	119.6 (2)
O70—Na2—O40	86.28 (11)	C9—C8—H8	120.2
O50—Na2—O40	111.51 (8)	C7—C8—H8	120.2
O70—Na2—O20	159.68 (11)	C8—C9—C10	119.3 (2)
O50—Na2—O20	113.44 (8)	C8—C9—H9	120.3
O40—Na2—O20	84.92 (7)	C10—C9—H9	120.3
O70—Na2—O60	96.60 (11)	C11—C10—C9	122.2 (2)
O50—Na2—O60	82.84 (8)	C11—C10—N3	118.3 (2)

O40—Na2—O60	165.54 (8)
O20—Na2—O60	87.70 (7)
O70—Na2—O4^{ii}	78.88 (11)
O50—Na2—O4^{ii}	158.56 (8)
O40—Na2—O4^{ii}	83.66 (7)
O20—Na2—O4^{ii}	81.96 (7)
O60—Na2—O4^{ii}	83.01 (7)
O70—Na2—Na1	128.35 (10)
O50—Na2—Na1	115.65 (6)
O40—Na2—Na1	42.85 (5)
O20—Na2—Na1	42.65 (5)
O60—Na2—Na1	130.21 (6)
O4^{ii}—Na2—Na1	85.78 (6)
O70—Na2—H21	174.1 (5)
O50—Na2—H21	96.7 (3)
O40—Na2—H21	96.7 (5)
O20—Na2—H21	17.7 (3)
O60—Na2—H21	79.3 (5)
O4^{ii}—Na2—H21	96.4 (3)
Na1—Na2—H21	54.0 (5)
O70—Na2—H62	112.2 (5)
O50—Na2—H62	73.5 (7)
O40—Na2—H62	161.3 (6)
O20—Na2—H62	76.8 (6)
O60—Na2—H62	19.22 (10)
O4^{ii}—Na2—H62	97.0 (5)
Na1—Na2—H62	118.5 (6)
H21—Na2—H62	64.7 (7)
Na1—O20—Na2	93.28 (7)
Na1—O20—H21	122.3 (19)
Na2—O20—H21	98 (2)
Na1—O20—H22	122.5 (19)
Na2—O20—H22	112 (2)
H21—O20—H22	105 (2)
Na1^{i}—O30—Na1	86.56 (6)
Na1^{i}—O30—H31	116 (2)
Na1—O30—H31	114 (2)
Na1^{i}—O30—H32	104 (2)
Na1—O30—H32	130 (2)
H31—O30—H32	105 (3)
Na1—O40—Na2	93.27 (7)
Na1—O40—H41	124 (2)
Na2—O40—H41	102 (2)
Na1—O40—H42	115 (2)
Na2—O40—H42	117 (2)
H41—O40—H42	105 (3)
Na2—O50—H51	106 (3)
Na2—O50—H52	111 (3)
H51—O50—H52	105 (3)

C9—C10—N3	119.5 (2)
C10—C11—C12	118.7 (2)
C10—C11—H11	120.7
C12—C11—H11	120.7
C11—C12—C7	120.2 (2)
C11—C12—H12	119.9
C7—C12—H12	119.9
O3—C13—O2	124.9 (2)
O3—C13—C1	118.8 (2)
O2—C13—C1	116.3 (2)
C2A—O1A—H1A	108.9 (14)
N3A—O4A—Na1	157.52 (16)
N2A—N1A—C5A	114.6 (2)
N1A—N2A—C7A	115.0 (2)
O4A—N3A—O5A	123.8 (2)
O4A—N3A—C10A	119.3 (2)
O5A—N3A—C10A	116.80 (19)
C6A—C1A—C2A	119.2 (2)
C6A—C1A—C13A	120.2 (2)
C2A—C1A—C13A	120.5 (2)
O1A—C2A—C3A	118.2 (2)
O1A—C2A—C1A	122.1 (2)
C3A—C2A—C1A	119.7 (2)
C4A—C3A—C2A	120.4 (2)
C4A—C3A—H3A	119.8
C2A—C3A—H3A	119.8
C3A—C4A—C5A	120.8 (2)
C3A—C4A—H4A	119.6
C5A—C4A—H4A	119.6
C6A—C5A—N1A	117.0 (2)
C6A—C5A—C4A	118.7 (2)
N1A—C5A—C4A	124.3 (2)
C1A—C6A—C5A	121.2 (2)
C1A—C6A—H6A	119.4
C5A—C6A—H6A	119.4
C12A—C7A—C8A	119.8 (2)
C12A—C7A—N2A	114.9 (2)
C8A—C7A—N2A	125.2 (2)
C9A—C8A—C7A	120.3 (2)
C9A—C8A—H8A	119.9
C7A—C8A—H8A	119.9
C10A—C9A—C8A	118.0 (2)
C10A—C9A—H9A	121.0
C8A—C9A—H9A	121.0
C9A—C10A—C11A	122.9 (2)
C9A—C10A—N3A	119.0 (2)
C11A—C10A—N3A	118.11 (19)
C12A—C11A—C10A	118.0 (2)
C12A—C11A—H11A	121.0

Na2—O60—H61	130 (3)	C10A—C11A—H11A	121.0
Na2—O60—H62	76 (2)	C11A—C12A—C7A	121.0 (2)
H61—O60—H62	105 (3)	C11A—C12A—H12A	119.5
Na2—O70—H71	117 (4)	C7A—C12A—H12A	119.5
Na2—O70—H72	118 (4)	O3A—C13A—O2A	123.4 (2)
H71—O70—H72	105 (5)	O3A—C13A—C1A	119.5 (2)
C2—O1—H1	108.3 (13)	O2A—C13A—C1A	117.1 (2)

O2—Na1—Na2—O70	176.45 (14)	C6—C1—C2—C3	−1.8 (3)
O20—Na1—Na2—O70	−154.96 (15)	C13—C1—C2—C3	−179.7 (2)
O40—Na1—Na2—O70	12.97 (14)	O1—C2—C3—C4	−179.6 (2)
O30^{i}—Na1—Na2—O70	−61.76 (14)	C1—C2—C3—C4	1.3 (4)
O30—Na1—Na2—O70	37.51 (15)	C2—C3—C4—C5	0.8 (4)
O4A—Na1—Na2—O70	106.88 (14)	C3—C4—C5—C6	−2.3 (4)
Na1^{i}—Na1—Na2—O70	−17.94 (15)	C3—C4—C5—N1	179.6 (2)
O2—Na1—Na2—O50	68.87 (11)	N2—N1—C5—C6	176.9 (2)
O20—Na1—Na2—O50	97.46 (10)	N2—N1—C5—C4	−5.0 (3)
O40—Na1—Na2—O50	−94.61 (10)	C4—C5—C6—C1	1.7 (4)
O30^{i}—Na1—Na2—O50	−169.34 (9)	N1—C5—C6—C1	179.9 (2)
O30—Na1—Na2—O50	−70.07 (10)	C2—C1—C6—C5	0.3 (3)
O4A—Na1—Na2—O50	−0.69 (9)	C13—C1—C6—C5	178.2 (2)
Na1^{i}—Na1—Na2—O50	−125.52 (9)	N1—N2—C7—C12	−177.8 (2)
O2—Na1—Na2—O40	163.48 (10)	N1—N2—C7—C8	2.1 (4)
O20—Na1—Na2—O40	−167.93 (9)	C12—C7—C8—C9	2.5 (4)
O30^{i}—Na1—Na2—O40	−74.73 (8)	N2—C7—C8—C9	−177.4 (2)
O30—Na1—Na2—O40	24.54 (8)	C7—C8—C9—C10	−0.6 (4)
O4A—Na1—Na2—O40	93.92 (8)	C8—C9—C10—C11	−0.4 (4)
Na1^{i}—Na1—Na2—O40	−30.91 (7)	C8—C9—C10—N3	176.2 (2)
O2—Na1—Na2—O20	−28.60 (10)	O4—N3—C10—C11	7.3 (3)
O40—Na1—Na2—O20	167.93 (9)	O5—N3—C10—C11	−175.7 (2)
O30^{i}—Na1—Na2—O20	93.20 (8)	O4—N3—C10—C9	−169.4 (2)
O30—Na1—Na2—O20	−167.53 (9)	O5—N3—C10—C9	7.6 (3)
O4A—Na1—Na2—O20	−98.16 (8)	C9—C10—C11—C12	−0.4 (4)
Na1^{i}—Na1—Na2—O20	137.02 (8)	N3—C10—C11—C12	−177.0 (3)
O2—Na1—Na2—O60	−34.14 (12)	C10—C11—C12—C7	2.2 (4)
O20—Na1—Na2—O60	−5.54 (9)	C8—C7—C12—C11	−3.3 (4)
O40—Na1—Na2—O60	162.38 (10)	N2—C7—C12—C11	176.6 (3)
O30^{i}—Na1—Na2—O60	87.65 (9)	Na1—O2—C13—O3	−71.7 (3)
O30—Na1—Na2—O60	−173.08 (9)	Na1—O2—C13—C1	109.3 (2)
O4A—Na1—Na2—O60	−103.70 (9)	C6—C1—C13—O3	8.7 (3)
Na1^{i}—Na1—Na2—O60	131.48 (8)	C2—C1—C13—O3	−173.5 (2)
O2—Na1—Na2—O4^{ii}	−111.30 (10)	C6—C1—C13—O2	−172.3 (2)
O20—Na1—Na2—O4^{ii}	−82.71 (8)	C2—C1—C13—O2	5.6 (3)
O40—Na1—Na2—O4^{ii}	85.22 (8)	O2—Na1—O4A—N3A	15.2 (5)
O30^{i}—Na1—Na2—O4^{ii}	10.49 (8)	O20—Na1—O4A—N3A	108.6 (5)
O30—Na1—Na2—O4^{ii}	109.76 (8)	O40—Na1—O4A—N3A	−160.3 (5)
O4A—Na1—Na2—O4^{ii}	179.14 (8)	O30^{i}—Na1—O4A—N3A	−175.2 (4)
Na1^{i}—Na1—Na2—O4^{ii}	54.31 (8)	O30—Na1—O4A—N3A	−76.2 (5)
O2—Na1—O20—Na2	160.25 (7)	Na1^{i}—Na1—O4A—N3A	−97.4 (5)

O40—Na1—O20—Na2	−8.34 (6)	Na2—Na1—O4A—N3A	153.7 (5)
O30^{i}—Na1—O20—Na2	−92.61 (7)	C5A—N1A—N2A—C7A	179.2 (2)
O30—Na1—O20—Na2	45.8 (3)	Na1—O4A—N3A—O5A	−148.3 (3)
O4A—Na1—O20—Na2	65.65 (6)	Na1—O4A—N3A—C10A	35.5 (6)
Na1^{i}—Na1—O20—Na2	−80.88 (12)	C6A—C1A—C2A—O1A	177.8 (2)
O70—Na2—O20—Na1	72.9 (3)	C13A—C1A—C2A—O1A	−0.5 (4)
O50—Na2—O20—Na1	−103.05 (9)	C6A—C1A—C2A—C3A	−2.4 (4)
O40—Na2—O20—Na1	8.21 (6)	C13A—C1A—C2A—C3A	179.4 (2)
O60—Na2—O20—Na1	175.77 (7)	O1A—C2A—C3A—C4A	−177.7 (3)
O4^{ii}—Na2—O20—Na1	92.50 (7)	C1A—C2A—C3A—C4A	2.5 (4)
O2—Na1—O30—Na1^{i}	106.46 (7)	C2A—C3A—C4A—C5A	−0.3 (4)
O20—Na1—O30—Na1^{i}	−138.7 (3)	N2A—N1A—C5A—C6A	173.7 (2)
O40—Na1—O30—Na1^{i}	−84.28 (6)	N2A—N1A—C5A—C4A	−6.1 (3)
O30^{i}—Na1—O30—Na1^{i}	0.0	C3A—C4A—C5A—C6A	−1.9 (4)
O4A—Na1—O30—Na1^{i}	−158.02 (7)	C3A—C4A—C5A—N1A	177.9 (3)
Na2—Na1—O30—Na1^{i}	−101.09 (7)	C2A—C1A—C6A—C5A	0.2 (4)
O2—Na1—O40—Na2	−91.7 (4)	C13A—C1A—C6A—C5A	178.4 (2)
O20—Na1—O40—Na2	8.37 (6)	N1A—C5A—C6A—C1A	−177.9 (2)
O30^{i}—Na1—O40—Na2	105.92 (7)	C4A—C5A—C6A—C1A	1.9 (4)
O30—Na1—O40—Na2	−160.07 (7)	N1A—N2A—C7A—C12A	179.1 (2)
O4A—Na1—O40—Na2	−68.45 (7)	N1A—N2A—C7A—C8A	−0.6 (4)
Na1^{i}—Na1—O40—Na2	153.57 (6)	C12A—C7A—C8A—C9A	1.2 (4)
O70—Na2—O40—Na1	−169.84 (11)	N2A—C7A—C8A—C9A	−179.1 (2)
O50—Na2—O40—Na1	105.03 (8)	C7A—C8A—C9A—C10A	−0.4 (4)
O20—Na2—O40—Na1	−8.18 (6)	C8A—C9A—C10A—C11A	−0.6 (4)
O60—Na2—O40—Na1	−67.7 (3)	C8A—C9A—C10A—N3A	−179.7 (2)
O4^{ii}—Na2—O40—Na1	−90.63 (7)	O4A—N3A—C10A—C9A	−175.5 (2)
O20—Na1—O2—C13	−165.9 (2)	O5A—N3A—C10A—C9A	8.1 (3)
O40—Na1—O2—C13	−66.6 (5)	O4A—N3A—C10A—C11A	5.3 (3)
O30^{i}—Na1—O2—C13	95.1 (2)	O5A—N3A—C10A—C11A	−171.1 (2)
O30—Na1—O2—C13	1.2 (2)	C9A—C10A—C11A—C12A	0.8 (4)
O4A—Na1—O2—C13	−88.9 (2)	N3A—C10A—C11A—C12A	179.9 (2)
Na1^{i}—Na1—O2—C13	46.2 (2)	C10A—C11A—C12A—C7A	0.0 (4)
Na2—Na1—O2—C13	−146.4 (2)	C8A—C7A—C12A—C11A	−1.0 (4)
C5—N1—N2—C7	177.7 (2)	N2A—C7A—C12A—C11A	179.3 (2)
Na2^{iii}—O4—N3—O5	90.3 (4)	C6A—C1A—C13A—O3A	−2.5 (4)
Na2^{iii}—O4—N3—C10	−92.8 (3)	C2A—C1A—C13A—O3A	175.7 (2)
C6—C1—C2—O1	179.0 (2)	C6A—C1A—C13A—O2A	179.0 (2)
C13—C1—C2—O1	1.1 (3)	C2A—C1A—C13A—O2A	−2.8 (3)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, y+1, z-1$; (iii) $x, y-1, z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82 (1)	1.80 (2)	2.534 (3)	149 (2)
O1*A*—H1*A*···O2*A*	0.82 (1)	1.80 (2)	2.532 (3)	147 (2)
O20—H21···O3*A*^{iv}	0.82 (2)	1.93 (2)	2.750 (2)	174 (3)
O20—H22···O2^{v}	0.82 (2)	2.04 (2)	2.862 (2)	173 (2)
O30—H31···O5^{vi}	0.82 (2)	2.32 (2)	3.135 (3)	175 (2)

O30—H32···O3*A*$^{\text{vii}}$	0.82 (2)	2.14 (3)	2.823 (3)	141 (2)
O40—H41···O2*A*$^{\text{vii}}$	0.82 (2)	2.00 (2)	2.819 (3)	172 (2)
O40—H42···O3$^{\text{i}}$	0.82 (2)	2.02 (2)	2.813 (3)	161 (3)
O50—H51···O60$^{\text{viii}}$	0.82 (3)	2.04 (2)	2.838 (3)	163 (3)
O50—H52···O5*A*	0.82 (3)	2.18 (2)	2.931 (3)	152 (3)
O60—H61···O3$^{\text{v}}$	0.82 (3)	2.09 (3)	2.828 (3)	150 (3)
O60—H62···O2*A*$^{\text{iv}}$	0.82 (2)	2.21 (3)	2.917 (3)	145 (3)
O70—H71···O50$^{\text{viii}}$	0.82 (4)	2.19 (5)	2.892 (4)	144 (4)
O70—H72···O1*A*$^{\text{ii}}$	0.82 (3)	2.48 (5)	2.972 (4)	119 (4)
C12—H12···O5*A*$^{\text{iv}}$	0.93	2.55	3.358 (3)	146
C12*A*—H12*A*···O5$^{\text{vi}}$	0.93	2.34	3.125 (3)	141

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) *x*, *y*+1, *z*−1; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*, −*y*+1, −*z*; (vi) −*x*+1, −*y*, −*z*+1; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) −*x*, −*y*+2, −*z*.

Selected interatomic distances (Å) in (I)–(III) compared with closely related structures

Distance	(I)	(II)	(III)	(III)*A*[d]	ACEFIZ	FUGYIP	EXIZUH1[e]	EXIZUH2
O1—C2	1.3400 (17)	1.350 (3)	1.352 (3)	1.347 (3)	1.354 (3)	1.355 (2)	1.350 (4)	1.362 (4)
C1—C2	1.403 (2)	1.419 (3)	1.399 (2)	1.421 (3)	1.401 (3)	1.403 (3)	1.396 (5)	1.397 (4)
C1—C13	1.4653 (19)	1.500 (3)	1.503 (3)	1.496 (3)	1.454 (3)	1.462 (3)	1.479 (4)	1.482 (5)
C5—N1	1.4213 (19)	1.421 (3)	1.420 (3)	1.405 (3)	1.451 (3)	1.432 (2)	1.413 (4)	1.421 (4)
N1—N2	1.2519 (19)	1.249 (3)	1.266 (3)	1.245 (3)	1.246 (3)	1.260 (2)	1.242 (3)	1.245 (3)
N2—C7	1.4256 (19)	1.428 (3)	1.419 (3)	1.420 (3)	1.431 (3)	1.424 (2)	1.431 (4)	1.437 (4)
O2—C13	1.2290 (17)	1.265 (3)	1.286 (3)	1.281 (3)	1.240 (2)	1.241 (2)	1.229 (4)	1.228 (4)
O3—C13	1.3081 (19)	1.246 (3)	1.257 (3)	1.234 (3)	1.313 (2)	1.311 (2)	1.300 (4)	1.290 (4)
O1···O2	2.619 (2)	2.524 (3)	2.534 (3)	2.532 (2)	2.630 (2)	2.631 (2)	2.574 (3)	2.605 (3)

Notes: (*a*) 5-(phenyldiazenyl)salicylic acid (Saikia *et al.*, 2012); (*b*) 5-(4-methoxyphenyldiazenyl)salicylic acid (Basu Baul *et al.*, 2000); (*c*) the molecular complex of 5-(phenyldiazenyl)salicylic acid with dimethylpyrazole (Xu *et al.*; 2011); (*d*) the second anion in (III) is labelled with the letter `*A*'; (*e*) the structure contains two symmetry-independent molecules.

Hydrogen-bonding geometry (Å, °) in (I)–(III)

D—H···A	D—H	H···A	D···A	D—H···A
(I)				
O1—H1···O2	0.820 (14)	1.895 (14)	2.6189 (16)	146.8 (14)
O1—H1···O4^{a}	0.820 (14)	2.420 (14)	3.0461 (18)	134.0 (13)
O3—H13···O2^{b}	0.820 (13)	1.847 (14)	2.6651 (16)	176.4 (14)
C4—H4···O5^{c}	0.93	2.38	3.202 (2)	147
(II)				
O1—H1···O2	0.82 (2)	1.78 (2)	2.524 (3)	151 (2)
N3—H21···O3^{d}	0.89 (2)	1.99 (2)	2.788 (3)	150 (2)
N3—H22···O2^{e}	0.89 (2)	1.91 (2)	2.779 (3)	164 (2)
N3—H23···O1	0.89 (2)	2.38 (2)	3.052 (3)	132 (2)
N3—H24···O3^{f}	0.89 (2)	1.91 (2)	2.799 (3)	172 (2)
(III)				
O1—H1···O2	0.820 (11)	1.796 (17)	2.534 (3)	148.9 (16)
O1A—H1A···O2A	0.820 (10)	1.804 (18)	2.532 (3)	147.3 (17)
O20—H21···O3A^{g}	0.82 (2)	1.93 (2)	2.750 (2)	174 (3)

O20—H22···O2^h	0.82 (2)	2.04 (2)	2.862 (2)	173 (2)
O30—H31···O5^i	0.82 (2)	2.32 (2)	3.135 (3)	175 (2)
O30—H32···O3A^j	0.82 (2)	2.14 (3)	2.823 (3)	141 (2)
O40—H41···O2A^j	0.82 (2)	2.00 (2)	2.819 (3)	172 (2)
O40—H42···O3^k	0.82 (2)	2.02 (2)	2.813 (3)	161 (3)
O50—H51···O60^l	0.82 (3)	2.04 (2)	2.838 (3)	163 (3)
O50—H52···O5A	0.82 (3)	2.18 (2)	2.931 (3)	152 (3)
O60—H61···O3^h	0.82 (3)	2.09 (3)	2.828 (3)	150 (3)
O60—H62···O2A^g	0.82 (2)	2.21 (2)	2.917 (3)	145 (3)
O70—H71···O50^l	0.82 (4)	2.19 (5)	2.892 (4)	144 (4)
O70—H72···O1A^m	0.82 (3)	2.48 (5)	2.972 (4)	119 (4)
C12—H12···O5A^g	0.93	2.55	3.358 (3)	146
C12A—H12A···O5^i	0.93	2.34	3.125 (3)	141

Symmetry codes: (*a*) *x*+2, -*y*+1/2, *z*-1/2; (*b*) -*x*+3, -*y*+1, -*z*; (*c*) -*x*, *y*-1/2, -*z*+1/2; (*d*) *x*-1, *y*, *z*+1; (*e*) *x*-1, *y*, *z*; (*f*) -*x*+1, -*y*, -*z*+2; (*g*) -*x*, -*y*+1, -*z*+1; (*h*) -*x*, -*y*+1, -*z*; (*i*) -*x*+1, -*y*, -*z*+1; (*j*) -*x*+1, -*y*+1, -*z*+1; (*k*) -*x*+1, -*y*+1, -*z*; (*l*) -*x*, -*y*+2, -*z*; (*m*) *x*, *y*+1, *z*-1.

Results of DFT calculations for an isolated molecule of 2-hydroxy-5-(phenyldiazenyl)benzoic acid, for the same molecule placed in a polarizable continuum with parameters simulating acetone, for two molecules bound as a dimer by a pair of hydrogen bonds between the carboxylate groups and for the anion of 2-hydroxy-5-(phenyldiazenyl)benzoic acid placed in a polarizable continuum with parameters simulating acetone

	E (*anti*) (Hartree)	*E* (*syn*) (Hartree)	*E* (*syn*) – *E* (*anti*) (kJ mol^{-1})
Isolated molecule	-836.78754	-836.78666	2.3
Molecule in a polarizable continuum	-836.79481	-836.79419	1.6
Hydrogen-bonded dimer	-1673.60221	-1673.60034	4.9
Anion in a polarizable continuum	-836.32959	-836.32899	1.6