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Bis(μ-3,5-dinitropyridin-2-olato)bis[tetraaqua(3,5-dinitropyridin-2-olato)barium(II)]

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The barium cation in the centrosymmetric title compound, $[Ba_2(C_5H_2N_3O_5)_4(H_2O)_8]$, is in a ten-coordinate environment with two anionic ligands and four water molecules. The Ba—O bond distances lie in the range 2.723 (2)–3.260 (2) Å. The deprotonated O atom of the ligand bridges the Ba atoms to form a dimeric unit, forming an approximately regular parallelogram Ba_2O_2 motif. The dimeric units are linked in a three-dimensional network by hydrogen bonds.

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.016
wR factor = 0.039
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

3,5-Dinitropyridine exists as a monomeric molecule whose aromatic ring is delocalized (Destro *et al.*, 1974). Pyridone and hydroxypyridine are tautomeric organic molecules. A calculation of the two tautomeric forms of unsubstituted hydroxypyridine, benzenoid and quinonoid structures, judged that the benzenoid form is slightly more preferable than the quinonoid form (Kuz'mina *et al.*, 1999). 3,5-Dinitropyridine and its derivatives have received much attention owing to their practical applications. Indeed, the number of patent claims and publications related to 2-hydroxy-3,5-dinitropyridine show it to be extremely important as an intermediate for oxidative dyestuffs, medicines or agrochemicals (Tanogaki *et al.*, 1994). In addition, some derivatives of 3,5-dinitripyridine have nonlinear optical properties (Twieg *et al.*, 1982), and a variety of substituted 3,5-dinitropyridine compounds are used as herbicidal chemicals (Driscoll, 1970). 2-Hydroxyl-3,5-dinitropyridine and its metal complexes are explosive and are used as energetic catalysts for solid propellants in order to adjust and improve their trajectory properties (Zhao *et al.*, 2003). The crystal structure of the ligand 2-hydroxy-3,5-dinitropyridine was reported last year (Zhang *et al.*, 2006).

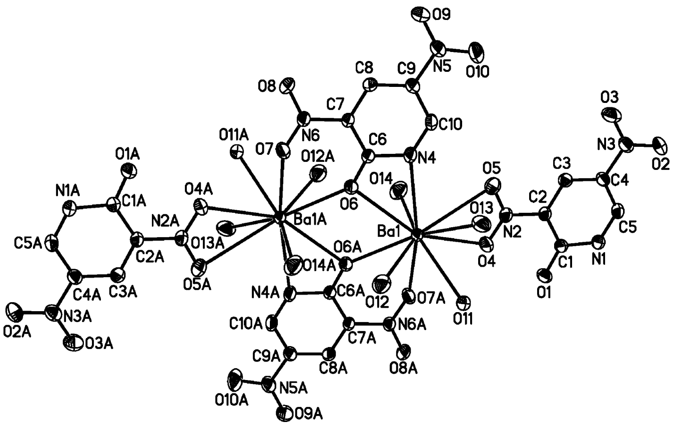
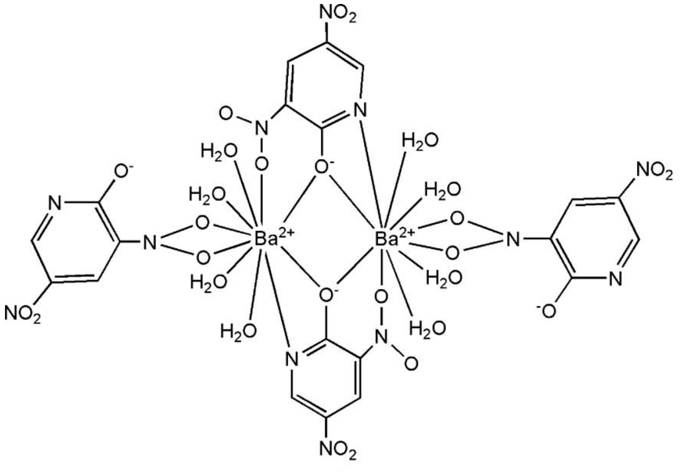


Figure 1
The molecular structure, showing the atom-numbering scheme and displacement ellipsoids at the 40% probability level. Hydrogen atoms have been omitted for clarity. [Symmetry code: (A) $-x, 1 - y, 2 - z$.]

In the centrosymmetric title compound, (I) (Fig. 1), the barium cation is in a ten-coordinate environment with two anionic ligands and four water molecules. The Ba—O bond distances lie in the range 2.723 (2)–3.260 (2) Å (Table 1), which is well within the ranges reported for comparable barium complexes (Otway & Rees, 2000; Pan *et al.*, 2001; Hancock *et al.*, 2004). The deprotonated O atom of the ligand bridges the Ba atoms to form a dimeric unit. The bridging Ba—O bonds in the Ba_2O_2 motif make an approximately regular parallelogram of the Ba and bridging O atoms, with a Ba···Ba distance of 4.677 (2) Å. The mean C—O distance is slightly longer than that in the free ligand 1.223 (3) Å (Zhang *et al.*, 2006), and indicative of the weakening of the carbonyl bond strength after coordination. The dimeric units are linked into a three-dimensional network by hydrogen bonds.



(I)

Experimental

Barium hydroxide (0.77 g, 0.5 mmol) was added to 2-hydroxy-3,5-dinitropyridine (1.85 g, 10 mmol) suspended in water (20 ml). The suspension was heated to 343 K until it had dissolved completely. The solution was concentrated and then set aside for the growth of crystals. Yellow crystals were isolated after several weeks.

Crystal data

$[Ba_2(C_5H_2N_3O_5)_4(H_2O)_8]$
M_r = 1155.17
Triclinic, $P\overline{1}$
a = 8.2036 (8) Å
b = 10.6875 (11) Å
c = 10.8308 (11) Å
α = 93.150 (1)°
β = 92.219 (1)°
γ = 96.027 (1)°
V = 941.98 (16) $Å^3$
Z = 1
Mo *Kα* radiation
μ = 2.20 mm^{-1}
T = 291 (2) K
0.42 × 0.31 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.457, T_{max} = 0.567 (expected range = 0.426–0.529)
8122 measured reflections
4239 independent reflections
4071 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.039
S = 1.06
4239 reflections
313 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.55 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Ba1—O14	2.7232 (18)	Ba1—O6	2.8651 (13)
Ba1—$O6^i$	2.7644 (13)	Ba1—$O7^i$	2.9204 (13)
Ba1—O13	2.7819 (16)	Ba1—N4	2.9426 (16)
Ba1—O11	2.8029 (14)	Ba1—O4	3.0060 (14)
Ba1—O12	2.8604 (17)	Ba1—O5	3.2602 (15)
O14—Ba1—$O6^i$	76.86 (5)	O13—Ba1—N4	69.78 (5)
O14—Ba1—O13	127.73 (5)	O11—Ba1—N4	132.55 (5)
$O6^i$—Ba1—O13	153.82 (5)	O12—Ba1—N4	98.33 (5)
O14—Ba1—O11	139.34 (5)	O6—Ba1—N4	45.52 (4)
$O6^i$—Ba1—O11	104.69 (4)	$O7^i$—Ba1—N4	160.93 (5)
O13—Ba1—O11	63.92 (5)	O14—Ba1—O4	78.47 (5)
O14—Ba1—O12	142.48 (5)	$O6^i$—Ba1—O4	120.41 (4)
$O6^i$—Ba1—O12	69.67 (5)	O13—Ba1—O4	77.99 (5)
O13—Ba1—O12	84.16 (5)	O11—Ba1—O4	65.65 (4)
O11—Ba1—O12	67.86 (4)	O12—Ba1—O4	133.44 (4)
O14—Ba1—O6	75.81 (5)	O6—Ba1—O4	150.19 (4)
$O6^i$—Ba1—O6	67.64 (4)	$O7^i$—Ba1—O4	67.02 (4)
O13—Ba1—O6	106.48 (5)	N4—Ba1—O4	114.60 (4)
O11—Ba1—O6	143.33 (4)	O14—Ba1—O5	69.37 (5)
O12—Ba1—O6	76.17 (4)	$O6^i$—Ba1—O5	143.47 (5)
O14—Ba1—$O7^i$	82.94 (5)	O13—Ba1—O5	62.66 (5)
$O6^i$—Ba1—$O7^i$	56.74 (4)	O11—Ba1—O5	92.48 (4)
O13—Ba1—$O7^i$	127.38 (5)	O12—Ba1—O5	146.60 (5)
O11—Ba1—$O7^i$	66.26 (4)	O6—Ba1—O5	115.14 (4)
O12—Ba1—$O7^i$	92.30 (5)	$O7^i$—Ba1—O5	104.47 (4)
O6—Ba1—$O7^i$	123.57 (4)	N4—Ba1—O5	74.74 (4)
O14—Ba1—N4	78.98 (6)	O4—Ba1—O5	39.86 (4)
$O6^i$—Ba1—N4	112.52 (4)		

Symmetry code: (i) $-x, -y+1, -z+2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H1*W*···$O7^{ii}$	0.811 (16)	2.273 (17)	3.0752 (19)	170 (3)
O11—H1*W*···$O8^{ii}$	0.811 (16)	2.53 (2)	3.125 (2)	131 (2)
O11—H2*W*···$O1^{iii}$	0.826 (16)	1.946 (17)	2.7234 (19)	156 (3)
O11—H2*W*···$O4^{iii}$	0.826 (16)	2.46 (2)	3.046 (2)	129 (2)
O14—H8*W*···$N1^{iv}$	0.814 (16)	2.062 (18)	2.833 (2)	158 (3)
O12—H3*W*···$O1^{iii}$	0.842 (17)	2.03 (2)	2.828 (2)	159 (4)
O13—H5*W*···$O2^{v}$	0.811 (17)	2.091 (17)	2.897 (2)	172 (3)
O14—H7*W*···$O12^{i}$	0.794 (17)	2.132 (18)	2.908 (2)	166 (3)
O13—H6*W*···O11	0.805 (17)	2.52 (3)	2.956 (2)	115 (3)
O13—H6*W*···$O8^{ii}$	0.805 (17)	2.71 (3)	3.230 (2)	124 (3)
O13—H6*W*···$O3^{vi}$	0.805 (17)	2.57 (3)	3.203 (3)	137 (3)
O12—H4*W*···$O9^{vii}$	0.811 (17)	2.35 (2)	3.114 (3)	158 (3)

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

Aryl H atoms were treated as riding, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map and refined freely.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine

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structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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