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Polymeric diaqua(μ_6-1,5-naphthalenedisulfonato)barium(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.065
Data-to-parameter ratio = 14.8

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

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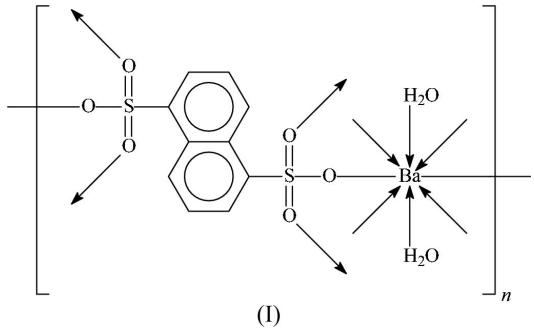
The Ba atom in the title compound, poly[[diaquabarium(II)]-μ_6-1,5-naphthalenedisulfonato], $[Ba(C_{10}H_6S_2O_6)(H_2O)_2]_n$, lies on a special position of site symmetry 2 and the dianion on an inversion centre. The Ba atom interacts with the O atoms of six different dianionic groups in the three-dimensional network and exhibits a square antiprismatic coordination.

Comment

The barium derivative of 1,5-naphthalenedisulfonic acid exists as a monoaqua derivative in which the dianion uses its O atoms to bind to six Ba atoms; the water molecule functions in a bridging mode to two Ba atoms (Cai *et al.*, 2001).



(I)

A slight variation of reaction conditions has led to the isolation of a diaqua analogue, (I) (Fig. 1); the Ba atom, which lies on a special position of site symmetry 2, is linked to the O atoms of six different dianions in a square-antiprismatic environment (Fig. 2). The Ba1—O1w distance [2.720 (2) Å] is

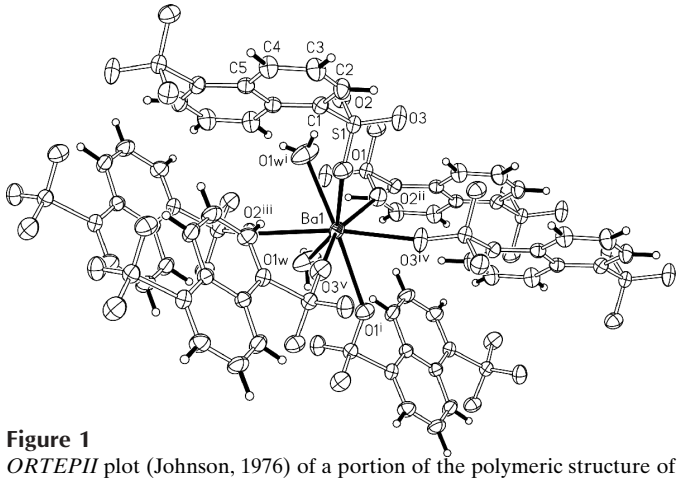


Figure 1
ORTEPII plot (Johnson, 1976) of a portion of the polymeric structure of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii. The symmetry codes are as given in Table 1.

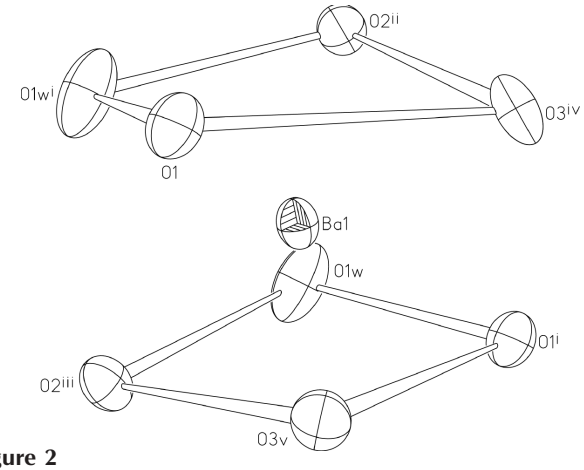


Figure 2
ORTEPII plot (Johnson, 1976), illustrating the square-antiprismatic coordination geometry of the Ba atom in (I). The symmetry codes are as given in Table 1.

significantly shorter than the corresponding distances in the previously reported monoaqua derivative [2.880 (3) and 3.084 (3) Å] where the water molecule serves as a bridge and the geometry of the Ba atom is an unusual bicapped trigonal prism (Fig. 3).

Experimental

To a suspension of barium carbonate (0.58 mg, 3 mmol) in a 50:50 ethanol–water mixture was added 1,5-naphthalenedisulfonic acid (0.66 g, 2 mmol). The mixture was heated to dissolve most of the carbonate; the unchanged reagent was removed by filtration. Colourless prismatic crystals separated after a few days. Analysis calculated for $C_{10}H_{10}BaO_8S_2$: C 26.13, H 2.19%; found: C 26.11, H 2.15%.

Crystal data

$[Ba(C_{10}H_6S_2O_6)(H_2O)_2]$	D_x = 2.299 Mg m^{-3}
M_r = 459.64	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6301 reflections
a = 22.274 (4) Å	θ = 3.7–27.5°
b = 5.715 (1) Å	μ = 3.34 mm^{-1}
c = 10.443 (2) Å	T = 295 (2) K
β = 92.56 (3)°	Prism, colourless
V = 1328.0 (4) Å^3	0.37 × 0.24 × 0.19 mm
Z = 4	

Data collection

Rigaki R-AXIS RAPID IP diffractometer	1525 independent reflections
ω scans	1495 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.045
T_{min} = 0.245, T_{max} = 0.530	θ_{max} = 27.5°
6313 measured reflections	$h = -28 \rightarrow 28$
	$k = -7 \rightarrow 7$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 1.6623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.065	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
S = 1.12	$\Delta\rho_{min}$ = −1.38 e Å^{-3}
1525 reflections	Extinction correction: *SHELXL97*
103 parameters	Extinction coefficient: 0.0071 (6)
H atoms treated by a mixture of independent and constrained refinement	

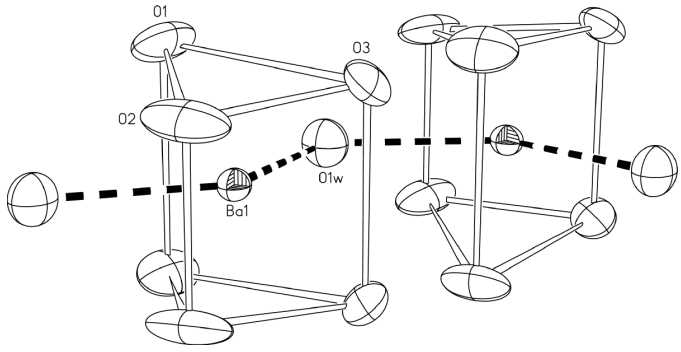


Figure 3
ORTEPII plot (Johnson, 1976), illustrating the bicapped trigonal prismatic geometry of the Ba atom in the monoaqua derivative. Atomic coordinates are taken from the published structure of Cai *et al.* (2001). Atom O1*w* represents the bridging water molecule.

Table 1
Selected geometric parameters (Å, °).

Ba1—O1	2.826 (2)	Ba1—O3^{iv}	2.753 (2)
Ba1—O1^{i}	2.826 (2)	Ba1—O3^{v}	2.752 (2)
Ba1—O2^{ii}	2.783 (2)	Ba1—O1*w*	2.720 (2)
Ba1—O2^{iii}	2.783 (2)	Ba1—O1*w*^{i}	2.720 (2)
O1—Ba1—O1^{i}	137.3 (1)	O2^{ii}—Ba1—O3^{iv}	76.1 (1)
O1—Ba1—O2^{iii}	93.1 (1)	O2^{ii}—Ba1—O3^{v}	160.9 (1)
O1—Ba1—O2^{ii}	107.1 (1)	O2^{ii}—Ba1—O1*w*^{i}	70.4 (1)
O1—Ba1—O3^{iv}	79.8 (1)	O2^{ii}—Ba1—O1*w*	70.7 (1)
O1—Ba1—O3^{v}	68.8 (1)	O3^{iv}—Ba1—O3^{v}	84.7 (1)
O1—Ba1—O1*w*	156.0 (1)	O3^{iv}—Ba1—O1*w*	121.2 (1)
O1—Ba1—O1*w*^{i}	66.1 (1)	O3^{iv}—Ba1—O1*w*^{i}	120.9 (1)
O2^{ii}—Ba1—O2^{iii}	123.0 (1)	O1*w*—Ba1—O1*w*^{i}	91.5 (1)

Symmetry codes: (i) $1-x, y, \frac{3}{2}-z$; (ii) $1-x, 2-y, 1-z$; (iii) $x, 2-y, \frac{1}{2}+z$; (iv) $1-x, 1-y, 1-z$; (v) $x, 1-y, \frac{1}{2}+z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*1···O1^{vi}	0.85 (1)	2.10 (2)	2.889 (3)	155 (5)
O1*w*—H1*w*2···O2^{i}	0.85 (1)	1.98 (1)	2.808 (3)	167 (4)

Symmetry codes: (ii) $1-x, y, \frac{3}{2}-z$; (vi) $1-x, 1+y, \frac{3}{2}-z$.

The water H atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation [U_{iso}(H) = 1.2U_{eq}(C)]. The highest electron-density peak is located about 1 Å from atom Ba1.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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