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Polymeric diaqua(naphthalene-2,7-disulfonato)-barium(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.028
wR factor = 0.063
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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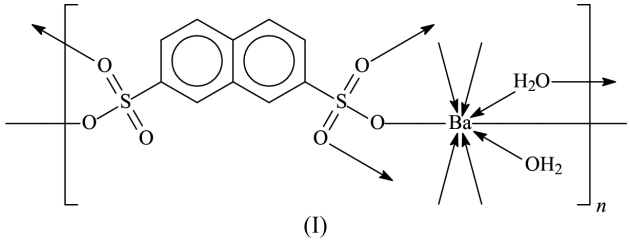
The Ba^{II} ion in the title compound, $[Ba(C_{10}H_6O_6S_2)(H_2O)_2]_n$, is eight-coordinate in a dodecahedral geometry. The coordinated water molecules link the Ba^{II} ion and the dianion into a three-dimensional network structure.

Comment

Organosulfonate anions have recently been examined in the context of extended architectures in their metal derivatives (Côté & Shimizu, 2003). The structural chemistry of the organic salts is also rich; for example, naphthalene disulfonates feature prominently as building blocks in hydrogen-bonded supramolecular architectures (Ng, 2003; Sakwa & Wheeler, 2003). With the main-group derivatives, reports on barium salts are limited (Cai *et al.*, 2001; Chandler *et al.*, 2002; Dalrymple & Shimizu, 2002; Gunderman *et al.*, 1997). Owing to the large size of the Ba^{2+} cation (Shannon, 1976), the coordination geometry is usually not regular.

The title compound, (I), with naphthalene-2,7-disulfonate exists as a diaqua compound (Fig. 1); there are eight O atoms surrounding the Ba^{II} ion, and the geometry is, expectedly, irregular (Fig. 2). The coordinated water molecules link the Ba^{II} ion and the dianion into a three-dimensional network structure. The geometry of monoaqua barium naphthalene-1,5-disulfonate is also irregular; it approximates a square antiprism (Fig. 3).



(I)

Experimental

An aqueous solution (100 ml) of sodium 2,7-naphthanedisulfonate (6.64 g, 20 mmol) was passed through an ion-exchange column. Barium chloride dihydrate (3.66 g, 15 mmol) was added to the filtered solution. The barium salt separated as crystals after more than a week.

Crystal data

$[Ba(C_{10}H_6O_6S_2)(H_2O)_2]$
M_r = 459.64
Orthorhombic, $Pna2_1$
a = 13.298 (1) Å
b = 19.333 (3) Å
c = 5.3590 (5) Å
V = 1377.7 (3) Å^3
Z = 4
D_x = 2.216 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12 090 reflections
θ = 3.7–27.4°
μ = 3.22 mm^{-1}
T = 295 (2) K
Block, colorless
0.38 × 0.26 × 0.18 mm

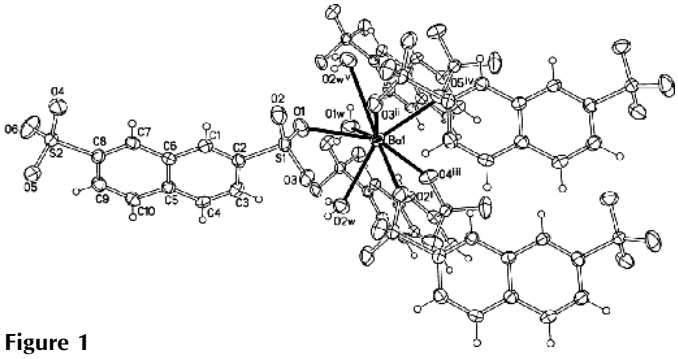


Figure 1
*ORTEP*II (Johnson, 1976) plot of a portion of the structure of $[(C_{10}H_6O_6S_2)(H_2O)_2Ba]_n$. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes are as given in Table 1.

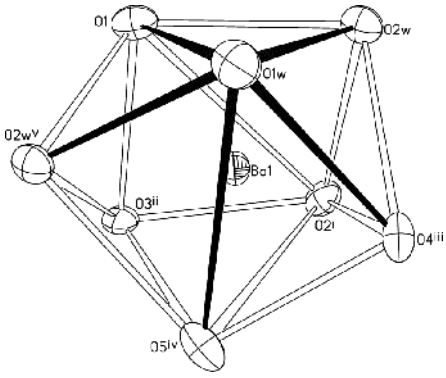


Figure 2
Dodecahedral geometry of the Ba atom in $[(C_{10}H_6O_6S_2)(H_2O)_2Ba]_n$.

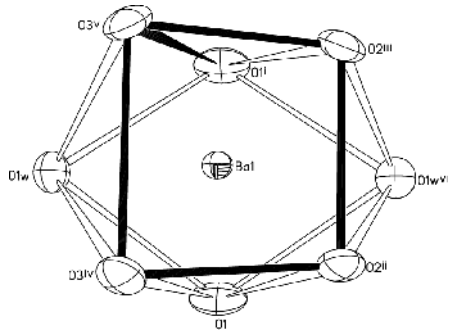


Figure 3
Square antiprismatic geometry of the Ba atom in $[C_{10}H_6$-1,5-$(SO_3)_2](H_2O)$Ba. Atomic coordinates are taken from Cai *et al.* (2001). [Symmetry codes: (i) $x, \frac{3}{2}-y, z$; (ii) $x, y, z-1$; (iii) $x, \frac{3}{2}-y, z-1$; (iv) $x-\frac{1}{2}, y, \frac{3}{2}-z$; (v) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{3}{2}-z$; (vi) $\frac{1}{2}-x, y, \frac{3}{2}-z$.]

Data collection

Rigaku R-AXIS RAPID diffractometer	2993 independent reflections
ω scans	2623 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.038$
$T_{min} = 0.379$, $T_{max} = 0.595$	$\theta_{max} = 27.5^\circ$
12 606 measured reflections	$h = -17 \rightarrow 17$
	$k = -25 \rightarrow 25$
	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.576P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.063$	$\Delta\rho_{max} = 0.99$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
2993 reflections	Absolute structure: Flack (1983), 1265 Friedel pairs
202 parameters	Flack parameter = 0.02 (2)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Ba1—O1	2.794 (3)	Ba1—O5^{iv}	2.736 (4)
Ba1—O2^{i}	2.653 (3)	Ba1—O1*w*	2.801 (3)
Ba1—O3^{ii}	2.792 (3)	Ba1—O2*w*	2.895 (6)
Ba1—O4^{iii}	2.696 (3)	Ba1—O2*w*^{v}	3.029 (6)
O1—Ba1—O2^{i}	105.9 (1)	O3^{ii}—Ba1—O5^{iv}	78.9 (1)
O1—Ba1—O3^{ii}	74.1 (1)	O3^{ii}—Ba1—O1*w*	137.9 (1)
O1—Ba1—O4^{iii}	147.8 (1)	O3^{ii}—Ba1—O2*w*	128.4 (1)
O1—Ba1—O5^{iv}	136.7 (1)	O3^{ii}—Ba1—O2*w*^{v}	64.0 (1)
O1—Ba1—O1*w*	78.6 (1)	O4^{iii}—Ba1—O5^{iv}	72.3 (1)
O1—Ba1—O2*w*	75.3 (1)	O4^{iii}—Ba1—O1*W*	82.3 (1)
O1—Ba1—O2*w*^{v}	61.3 (1)	O4^{iii}—Ba1—O2*w*	74.4 (1)
O2^{i}—Ba1—O3^{ii}	76.1 (1)	O4^{iii}—Ba1—O2*w*^{v}	136.7 (1)
O2^{i}—Ba1—O4^{iii}	75.3 (1)	O5^{iv}—Ba1—O1*w*	101.0 (1)
O2^{i}—Ba1—O5^{iv}	99.7 (1)	O5^{iv}—Ba1—O2*w*	146.6 (1)
O2^{i}—Ba1—O1*w*	143.1 (2)	O5^{iv}—Ba1—O2*w*^{v}	76.5 (1)
O2^{i}—Ba1—O2*w*	73.7 (1)	O1*w*—Ba1—O2*w*	72.2 (1)
O2^{i}—Ba1—O2*w*^{v}	140.0 (1)	O1*w*—Ba1—O2*w*^{v}	74.9 (1)
O3^{ii}—Ba1—O4^{iii}	134.9 (1)	O2*w*—Ba1—O2*w*^{v}	129.5 (1)

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

The water H atoms were located and isotropically refined with the O—H and H···H distances restrained to 0.85 (1) and 1.39 (1) Å, respectively. All other H atoms were placed in calculated positions [aromatic C—H = 0.93 Å], and were included in the refinement in the riding-model approximation. U_{iso} values of all H atoms were set equal to $1.2U_{eq}$(parent atom). The Ba···H distances for each water molecule were restrained to be equal within 0.01 Å. The highest peak in the difference map was located 0.98 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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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