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Poly[tetraaquabis(μ-hydrogen maleato)barium(**II**)]

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In the title compound, $[Ba(C_4H_3O_4)_2(H_2O)_4]_n$, the barium(II) cation is coordinated by five O atoms from four different hydrogen maleate ions and four O atoms from water molecules in a tricapped trigonal prismatic geometry. The coordination polyhedra are connected by edge-sharing to form zigzag chains, which are linked by hydrogen bonds into an extended three-dimensional network.

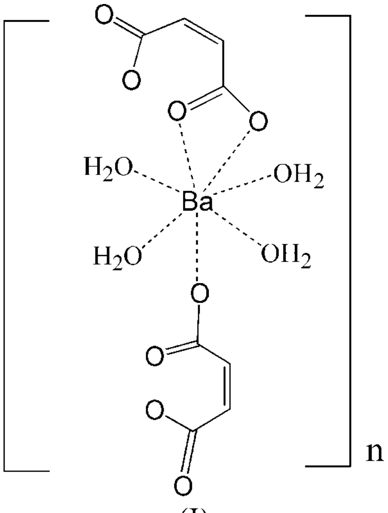
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.037
wR factor = 0.089
Data-to-parameter ratio = 16.5

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

Comment

Recently, salts of dicarboxylic acids, including tris(benzenedicarboxylato)zinc(II) (Li *et al.*, 1999) and tetraaquamesaconatobarium(II) (Briceño *et al.*, 2002), have been found to display porous metal-organic network structures. As part of our ongoing study of the synthesis and structure of new acids salts, we synthesized the title barium compound, (I), and present here its crystal structure.



(I)

In (I), bond lengths and angles within the hydrogen maleate ions are in good agreement with the values reported for other divalent metal derivatives (Diaz de Delgado *et al.*, 1995). The Ba atom is nine-coordinated in a distorted tricapped trigonal prismatic geometry (Table 1) by five O atoms from four different hydrogen maleate ions and four O atoms from water molecules (Fig. 1). The coordination polyhedra are connected by edge-sharing to form zigzag chains running along the b axis, which are linked by intermolecular O—H···O hydrogen-bonding interactions (Table 2) into an extended three-dimensional network (Fig. 2).

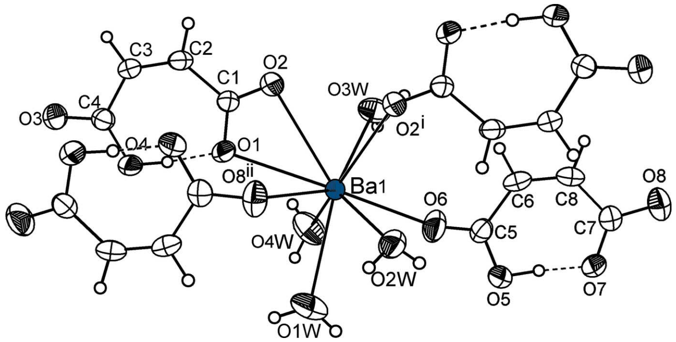


Figure 1
The asymmetric unit of (I), with additional ligands to complete the coordination of Ba. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

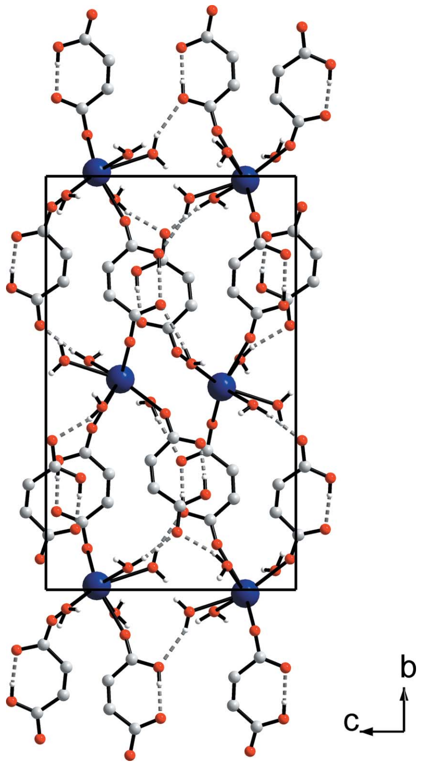


Figure 2
The crystal packing of (I), viewed down the *a* axis, showing the O—H···O hydrogen bonds as dashed lines. H atoms of the CH groups have been omitted for clarity.

Experimental

An mixture of barium carbonate (0.9866 g, 5 mmol) and maleic acid (0.9810 g, 10 mmol) was left to react for 72 h at 318 K with stirring. The solid compound obtained was filtered off and recrystallized several times from aqueous solution to afford the title compound in high yield (nearly 100%) and purity. Single crystals suitable for X-ray analysis were obtained after three weeks by slow evaporation at room temperature of a saturated aqueous solution. The FT–TR spectrum (KBr discs, PE-2000X spectrophotometer) obtained showed the C═C stretch at around 1669 cm^{-1}, the asymmetric stretch of the carboxylate group at 1558 cm^{-1}, and the symmetric stretch at around 1385 cm^{-1}, which are consistent with the expected compound.

Crystal data

$[Ba(C_4H_3O_4)_2(H_2O)_4]$
$M_r = 439.53$
Monoclinic, $P2_1/c$
$a = 6.528$ (2) Å
$b = 19.009$ (7) Å
$c = 11.493$ (5) Å
$\beta = 92.345$ (16)°
$V = 1425.0$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 2.85$ mm^{-1}
$T = 293$ (2) K
0.13 × 0.11 × 0.09 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: none
13762 measured reflections
3263 independent reflections
3054 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.089$
$S = 1.33$
3263 reflections
198 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max} = 1.07$ e Å^{-3}
$\Delta\rho_{\rm min} = -1.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ba1—O6	2.725 (6)	Ba1—O2*W*	2.821 (6)
Ba1—O2^i	2.743 (5)	Ba1—O3*W*	2.877 (6)
Ba1—O4*W*	2.783 (6)	Ba1—O2	2.892 (5)
Ba1—O8^{ii}	2.799 (6)	Ba1—O1	2.927 (5)
Ba1—O1*W*	2.815 (7)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O1	0.82 (4)	1.61 (4)	2.434 (7)	175 (10)
O2*W*—H2*W*1···O4*W*^{iii}	0.85	2.07	2.896 (9)	163
O2*W*—H2*W*2···O3^{iv}	0.85	2.00	2.790 (8)	156
O5—H5···O7	0.83 (5)	1.61 (3)	2.416 (8)	168 (12)
O3*W*—H3*W*1···O2*W*^{v}	0.84	2.08	2.904 (9)	164
O3*W*—H3*W*2···O7^{vi}	0.85	2.30	3.139 (8)	173
O1*W*—H1*W*1···O5^{vii}	0.86	2.17	2.966 (9)	155
O4*W*—H4*W*2···O3^{viii}	0.87	1.96	2.798 (9)	164

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

All H atoms were located in a difference Fourier synthesis. The hydroxyl H atoms were refined isotropically with a distance restraint of 0.82 (1) Å. Water H atoms were refined using the =riding-model approximation, with an O—H distance of 0.86 (1) Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$. The C-bound H atoms were refined in the riding-model approximation, with C—H = 0.93 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The highest peak and the deepest hole in the final difference map are located 0.91 and 0.76 Å from the Ba atom.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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References

Briceño, A., Delgado, J. M. & Díaz de Delgado, G. (2002). *Acta Cryst.* E**58**, m602–m605.

Diaz de Delgado, G., Parra, P. P., Briceño, A. & Delgado, J. M. (1995). *J. Chem. Crystallogr.* **25**, 241–244.

Li, H., Eddaoudi, M., O'Keeffe, M. & Yaghi, O. M. (1999). *Nature (London)*, **402**, 276–279.

McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.

Molecular Structure Corporation (1999). *TEXRAY* (Version 1.10) and *TEXSAN* (Version 1.10). MSC, The Woodlands, Texas, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.