

O4—Ti4—I4	99.7 (5)	X1D—Ti4—O3	114.6
Ti1—O1—Ti2	155.9 (9)	X1D—Ti4—O4	119.1
Ti3—O2—Ti2	168.2 (7)	X1D—Ti4—I4	114.2

An attempt was made to perform an absorption correction based on ψ scans, but the weak diffraction caused too few suitable reflections to be available. Accordingly, recourse to a ΔF correction had to be made. The transmission factors are somewhat higher than expected. The number of least-squares parameters was artificially increased by 18 to allow for the extra (hidden) parameters introduced. The structure was refined as a racemic twin with components 0.67, 0.33 (11); the origin was fixed by the method of Flack & Schwarzenbach (1988). The high R values are associated with broad reflection profiles, weak diffraction from a thin plate and (probably) residual absorption errors. To improve the refinement stability, a system of restraints (695 in all) to light-atom temperature-factor components and local Cp-ring symmetry was employed.

Data collection: *DIF4* (Stoe & Cie, 1992a). Cell refinement: *DIF4*. Data reduction: *REDU4* (Stoe & Cie, 1992b). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993b). Molecular graphics: *XP* (Siemens, 1994). Software used to prepare material for publication: *SHELXL93*.

The authors thank the Fonds der Chemischen Industrie for financial support and Mr A. Weinkauff for technical assistance.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1201). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). **C53**, 845–848

Polysulfonylamines. LXXXIII. Heptaaquacalcium 1,2-Benzenedisulfonimide†

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(Received 13 December 1996; accepted 3 February 1997)

Abstract

In heptaaquacalcium bis[1,3,2-benzodithiazole 1,1,3,3-tetroxide(1–)], $[\text{Ca}(\text{H}_2\text{O})_7](\text{C}_6\text{H}_4\text{NO}_4\text{S}_2)_2$, the calcium ion is surrounded by the O atoms of seven water molecules in a distorted pentagonal bipyramidal geometry. The structure displays layers of anions, with the calcium cations and water molecules between these layers. The layers are held together by an extensive network of hydrogen bonds involving the water molecules and the $(\text{SO}_2)_2\text{N}^-$ subunits of the anions.

Comment

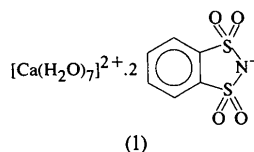
Calcium ions in crystal structures generally bind to O atoms in ligands and their preferred coordination numbers range from 6 to 8 (Katz, Glusker, Beebe & Bock, 1996). However, in hydrated compounds containing six or more water molecules per calcium ion, exclusive hydration of the metal to form $[\text{Ca}(\text{H}_2\text{O})_n]^{2+}$ ($n \geq 6$) is rare; in most of these compounds, the coordination polyhedra involve ligands other than water molecules. It was shown by *ab initio* molecular orbital calculations *in vacuo* that the net energy penalty for changing the number of water molecules in the first coordination shell of Ca^{2+} between 6 and 8 is extremely small (Katz *et al.*, 1996).

The heptahydrated calcium ion has been observed in $\text{CaCr}_2\text{O}_7 \cdot 2[(\text{CH}_2)_6\text{N}_4] \cdot 7\text{H}_2\text{O}$ (Dahan, 1975),

† Part LXXXII: Dalluhn, Henschel, Blaschette & Jones (1997).

in Ca[Bi(edta)]₂·9H₂O (Shkol'nikova, Porai-Koshits & Poznyak, 1993) and in a number of inorganic structures (*e.g.* Thomas & Moore, 1981; Leligny & Monier, 1983; Takagi, Mathew & Brown, 1984; Thiele, Rotter & Faller, 1984; Faggiani, Vilella & Brown, 1986). On the other hand, a search of the Cambridge Structural Database (Allen & Kennard, 1993) located only two structures displaying [Ca(H₂O)₇]²⁺ associated with a purely organic counterion, *viz.* Ca(naphthionate)₂·8H₂O (Brown, Ehrenberg & Yadav, 1984), and CaA·9H₂O, where H₂A is 7-hydroxy-8-(phenylazo)-1,3-naphthalene-disulfonic acid (Ojala *et al.*, 1994). It is interesting that these compounds both contain arene-sulfonate anions, which are obviously suited for stabilizing the heptaquacalcium complex by incorporation into an extended hydrogen-bond network. It should be noted, however, that in the closely related compound [Ca(HA)(H₂O)₆](HA)·6H₂O, where H₂A is *o*-tolidine-6,6'-disulfonic acid, Ca²⁺ attains the coordination number seven by bonding to six water molecules and one sulfonate O atom of an anion (Gunderman & Squatrito, 1996). We now report the first structure exhibiting a [Ca(H₂O)₇]²⁺ cation stabilized by a disulfonimide anion.

The asymmetric unit (Fig. 1) of the title compound, (1), consists of one [Ca(H₂O)₇]²⁺ cation and two 1,2-benzenedisulfonimide anions, henceforth denoted as Z⁻ and Z'⁻ (Z⁻ referring to the lower-numbered anion).



The calcium coordination is sevenfold, the O atoms forming a severely distorted pentagonal bipyramid with a mean Ca—O distance of 2.391 (3) Å (individual values *cf.* Table 1). The apices are occupied by O1_w and O5_w, with the angle O1_w—Ca—O5_w 163.57 (12)°. The equatorial atoms are O2_w, O3_w, O7_w, O4_w and O6_w, subtending angles at Ca of 72.64 (12), 72.81 (11), 75.25 (12), 81.85 (13) and 73.83 (12)°, respectively, a total of 376.38° compared with 360° expected for exact coplanarity of the Ca and five O atoms. The mean deviation of the six atoms from their least-squares plane is 0.47 Å, the largest deviation pertaining to O3_w [0.760 (2) Å] and the smallest to Ca [0.057 (1) Å].

The independent anions are almost identical as regards their bond lengths and interbond angles. Selected geometric data for the five-membered ring of Z⁻ are given in Table 1. Including both anions, the C—C distances range from 1.368 (5) to 1.391 (5) Å and the C—C—C angles from 117.3 (3) to 121.9 (3)°. In Z⁻ and Z'⁻, the C and S atoms are effectively coplanar, the greatest deviations from their mean planes and their mean out-of-plane distances being 0.024 (1) and 0.015 Å

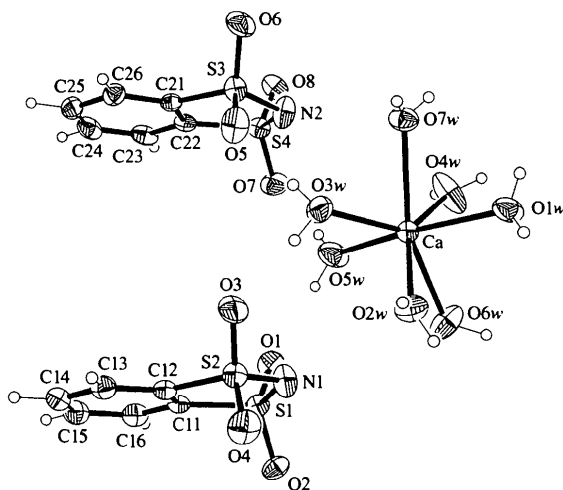


Fig. 1. The formula unit of the title compound in the crystal. Ellipsoids represent 50% probability levels and H-atom radii are arbitrary.

for Z⁻, and 0.009 (3) and 0.005 Å for Z'⁻; N1 and N2 are 0.149 (3) and 0.131 (4) Å out of the reference plane as defined above. The anion was previously characterized in the structure of [(CH₃)₂Sn(H₂O)₄]²⁺·2Z⁻, where it forms interionic hydrogen bonds (Hippel, Jones & Blaschette, 1993), and in the coordination compounds [AgZ(CH₃CN)] (Blaschette *et al.*, 1993) and [AgZ(H₂O)] (Jones, Hamann, Blaschette, Cammenga & Epple, 1993).

As shown in the packing diagram (Fig. 2), the anions are stacked in double layers in which half have the (SO₂)₂N⁻ groups directed towards the next layer up and half towards the layer below. The dihedral angle between the mean C₆S₂ planes of Z⁻ and Z'⁻ is only 4.88 (4)°. Surrounding and connecting the hydrophobic regions are hydrophilic layers composed of water molecules and cations. The (SO₂)₂N⁻ groups of the anions project into the polar regions. Similar stackings were observed for the calcium sulfonate hydrates mentioned

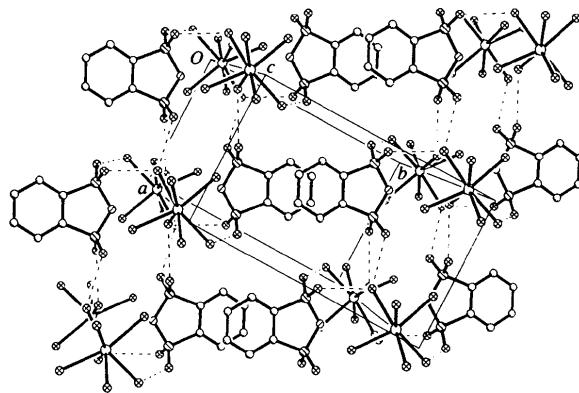


Fig. 2. Packing diagram of the title compound viewed perpendicular to the *ab* plane. Hydrogen bonds are indicated by dashed lines and H atoms have been omitted for clarity.

above. The structure is extensively hydrogen bonded (Table 2). There are 15 independent hydrogen bonds originating from the 14 water O—H groups, O2w—H03 being involved in a three-centre bond. One branch of the latter connects $[\text{Ca}(\text{H}_2\text{O})_7]^{2+}$ cations. The other O—H...A interactions exhaustively use the N and O atoms of the anions as acceptors; O1, O2, O7 and O8 act as bifunctional acceptors in bifurcated hydrogen bonds, with the N atoms and the remaining O atoms acting as monofunctional acceptors.

Experimental

Crystals of (1) were obtained in 85% yield by adding 0.17 g (2.3 mmol) $\text{Ca}(\text{OH})_2$ dissolved in 20 ml deionized water to 1.00 g (4.56 mmol) 1,2-benzenedisulfonimide (Hendrickson, Okano & Bloom, 1969; Blaschette *et al.*, 1993) in 100 ml deionized water, stirring the resulting solution for 3 h, evaporating the heated solution to 3 ml and storing at ambient temperature. The crystals deliquesce at 333 K. Elemental analysis: found C 23.94, H 3.67, N 4.68, S 21.23%; $\text{C}_{12}\text{H}_{22}\text{CaN}_2\text{O}_{15}\text{S}_4$ requires C 23.92, H 3.68, N 4.65, S 21.28%.

Crystal data

$[\text{Ca}(\text{H}_2\text{O})_7](\text{C}_6\text{H}_4\text{NO}_4\text{S}_2)_2$

$M_r = 602.64$

Triclinic

$P\bar{1}$

$a = 7.520(3) \text{ \AA}$

$b = 12.030(3) \text{ \AA}$

$c = 13.789(5) \text{ \AA}$

$\alpha = 73.25(3)^\circ$

$\beta = 89.47(2)^\circ$

$\gamma = 89.82(2)^\circ$

$V = 1194.3(7) \text{ \AA}^3$

$Z = 2$

$D_x = 1.676 \text{ Mg m}^{-3}$

D_m not measured

Data collection

Stoe Stadi-4 diffractometer

ω/θ scans

Absorption correction: none

4552 measured reflections

4201 independent reflections

3239 reflections with

$I > 2\sigma(I)$

$R_{\text{int}} = 0.0176$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 52 reflections

$\theta = 10.0\text{--}11.5^\circ$

$\mu = 0.686 \text{ mm}^{-1}$

$T = 143(2) \text{ K}$

Needle

$0.7 \times 0.2 \times 0.1 \text{ mm}$

Colourless

$\theta_{\text{max}} = 25.02^\circ$

$h = 0 \rightarrow 8$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

3 standard reflections

frequency: 60 min

intensity decay: none

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.0424$

$wR(F^2) = 0.1068$

$S = 1.045$

4201 reflections

363 parameters

H atoms: see below

$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 1.2979P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.415 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.384 \text{ e \AA}^{-3}$

Extinction correction: none

Scattering factors from

International Tables for Crystallography (Vol. C)

Table 1. Selected geometric parameters (\AA , $^\circ$)

S1—O1	1.442 (2)	Ca—O4w	2.346 (3)
S1—O2	1.449 (2)	Ca—O3w	2.349 (3)
S1—N1	1.581 (3)	Ca—O6w	2.385 (3)
S1—C11	1.770 (3)	Ca—O1w	2.391 (3)
S2—O3	1.438 (3)	Ca—O2w	2.417 (3)
S2—O4	1.442 (3)	Ca—O5w	2.422 (3)
S2—N1	1.587 (3)	Ca—O7w	2.428 (3)
S2—C12	1.762 (3)		
O1—S1—O2	113.7 (2)	O3—S2—C12	109.3 (2)
O1—S1—N1	110.2 (2)	O4—S2—C12	109.2 (2)
O2—S1—N1	112.0 (2)	N1—S2—C12	100.8 (2)
O1—S1—C11	110.7 (2)	S1—N1—S2	114.9 (2)
O2—S1—C11	108.8 (2)	C16—C11—S1	127.7 (3)
N1—S1—C11	100.8 (2)	C12—C11—S1	111.1 (2)
O3—S2—O4	113.8 (2)	C13—C12—S2	126.5 (3)
O3—S2—N1	111.0 (2)	C11—C12—S2	111.6 (2)
O4—S2—N1	112.0 (2)		

Table 2. Hydrogen-bonding geometry (\AA , $^\circ$)

D—H...A	D—H	H...A	D...A	D—H...A
O1w—H01...O8 ⁱ	0.80 (5)	2.14 (5)	2.935 (4)	172 (5)
O1w—H02...O2 ⁱⁱ	0.75 (5)	2.19 (5)	2.935 (4)	172 (5)
O2w—H03...N1 ⁱⁱⁱ	0.81 (6)	2.56 (6)	3.262 (5)	146 (5)
O2w—H03...O6w ⁱⁱⁱ	0.81 (6)	2.73 (5)	3.156 (5)	115 (4)
O2w—H04...O1 ⁱⁱⁱ	0.71 (5)	2.22 (5)	2.931 (4)	174 (5)
O3w—H05...O5	0.84 (5)	1.92 (5)	2.763 (4)	175 (5)
O3w—H06...O3	0.83 (4)	1.95 (4)	2.782 (4)	175 (4)
O4w—H07...O8 ^{iv}	0.80 (5)	2.03 (5)	2.812 (4)	166 (5)
O4w—H08...O6 ⁱ	0.80 (5)	1.94 (5)	2.733 (4)	170 (5)
O ^v —H09...O7	0.72 (5)	2.33 (5)	3.041 (5)	170 (6)
O5w—H010...O1	0.84 (5)	2.15 (5)	2.983 (4)	169 (4)
O6w—H011...O2 ⁱ	0.70 (5)	2.18 (5)	2.846 (4)	160 (6)
O6w—H012...O4 ⁱⁱ	0.91 (6)	1.87 (6)	2.776 (4)	170 (5)
O7w—H013...O7 ⁱⁱⁱ	0.70 (5)	2.21 (5)	2.901 (4)	170 (5)
O7w—H014...N2 ⁱ	0.82 (5)	2.36 (5)	3.126 (4)	155 (4)

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

Water H atoms were refined freely, while the other H atoms were refined as riding.

Data collection: *DIF4* (Stoe & Cie, 1992a). Cell refinement: *DIF4*. Data reduction: *REDU4* (Stoe & Cie, 1992b). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XP* (Siemens, 1994). Software used to prepare material for publication: *SHELXL93*.

The authors thank the Fonds der Chemischen Industrie for financial support, and Mr A. Weinkauff for technical assistance.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1272). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). **C53**, 848–850

[*N,N'*-Bis(salicylidene)-1,2-diimino-2-methylpropane]copper(II) †

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(Received 27 September 1996; accepted 10 February 1997)

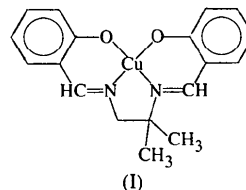
Abstract

In the title compound, [Cu(C₁₈H₁₈N₂O₂)], the coordination geometry about the Cu atom is a 6–5–6 chelate ring structure, with a tetrahedrally distorted square plane composed of two imine N atoms and two phenol O atoms. The angle between the two planes, which each contain the donor atoms of a salicylaldiminato residue, and the central Cu atom is 15.8(2)°.

† Alternative name: {2,2'-[2-methyl-1,2-propanediylbis(nitriolomethylidyne)]diphenolato-*N,N',O,O'*}copper(II).

Comment

Copper(II) complexes with tetradentate imine–phenols have been extensively investigated for their colour isomerism (Llewellyn & Waters, 1960; Hall & Waters, 1960), conformational influences (Clark, Hall & Waters, 1969; Baker, Hall & Waters, 1970*a,b*) and potential as radiopharmaceuticals (John, Bott & Green, 1994). We describe here the synthesis and characterization of the title complex, (I).



The Cu atom is four-coordinated by an N₂O₂ donor set from the imine–phenol ligand in a tetrahedrally distorted square-planar coordination geometry with the two phenolate O atoms being deprotonated. The donor atoms do not form a perfect plane but deviate by 0.190(4) Å from their best plane. The ethylenediamine C15 and C16 atoms are displaced by 0.308(4) and 0.289(4) Å, respectively, in opposite directions from the CuN₂ plane. The Cu–N and Cu–O bond lengths are similar to those found in analogous structures (1.904–2.000 Å for Cu–N and 1.886–1.945 Å for Cu–O; Baker, Hall & Waters, 1970*a*; Cheeseman, Hall & Waters, 1966; Bhadbhade & Srinivas, 1993).

Perhaps the most interesting comparative aspect of copper(II) complexes with tetradentate imine–phenols involves the steric influence of (i) the length of the alkylene backbone, (ii) substitution in the alkylene bridge, and (iii) substitution in the aromatic rings upon the molecular structure. The title compound displays monomeric and four-coordinate geometry which is consistent with that of copper(II)–imine–phenols with a four-coordinate structure (Baker, Hall & Waters, 1970*a*; Bhadbhade & Srinivas, 1993; Cheeseman, Hall & Waters, 1966; Lu, Yao, Lo & Tung, 1997; Yao, Lo, Chen & Lu, 1997). This configuration is significantly distinct from monomeric Cu^{II}–*N,N'*-bis(salicylidene)-1,2-diiminopropane–H₂O (Llewellyn & Waters, 1960) and other dimeric copper(II)–imine–phenols with five-coordinate structures (see Table 2).

The distortion of the inner coordination sphere can be recognized by the dihedral angles between the planes defined by Cu1, N1, O1 and Cu1, N2, O2. It is seen that the dihedral angle for (I), 15.8(2)°, is much larger than that of monomeric Cu^{II}–*N,N'*-bis(salicylidene)di-iminoethane [5.3(2)°; Baker, Hall & Waters, 1970*a*] and that of Cu^{II}–*N,N'*-bis(5-chlorosalicylidene)-1,2-di-iminoethane [9.2(3)°; Bhadbhade & Srinivas, 1993] with substitution of Cl atoms in the aromatic rings. The effect of dimethyl substitution in the ethylene