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Bis(benzylammonium) tetraaqua[bis(sulfato)cadmate(II)]

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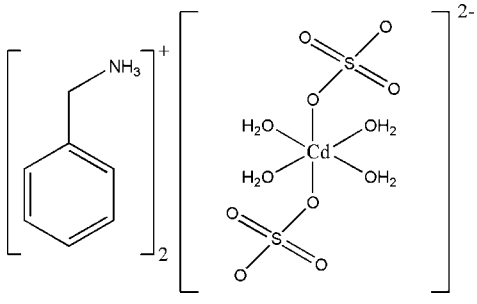
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.052; data-to-parameter ratio = 12.6.

In the crystal structure of the title compound, $(C_7H_7NH_3)_2[Cd(SO_4)_2(H_2O)_4]$, the Cd atom of the complex anion is located on a center of inversion and exhibits a slightly distorted octahedral coordination by six O atoms which belong to four water molecules and two sulfate ligands. Intermolecular hydrogen bonding between the cations and the anions consolidates the monomeric units into a three-dimensional network structure. The title compound is isotypic with its Cu^{II} and Mn^{II} analogues.

Related literature

The formula of the title compound resembles the general formula of Tutton's salts, $M^I_2M^{II}(SO_4)_2\cdot6H_2O$ (Mahadevan Pillai *et al.*, 1997), but with only four water molecules and benzylammonium instead of ammonium. For the isotypic Cu and Mn analogues, see Rademeyer (2004) and Naumov *et al.* (2005), respectively. The preparation of the title compound was described by Jordanovska *et al.* (2000).



Experimental

Crystal data

$(C_7H_{10}N)_2[Cd(SO_4)_2(H_2O)_4]$
M_r = 592.93
Triclinic, $P\overline{1}$
a = 6.6361 (14) Å
b = 8.1378 (18) Å
c = 11.087 (3) Å
α = 81.246 (18)°
β = 80.320 (18)°
γ = 76.302 (18)°
V = 569.5 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.20 mm^{-1}
T = 120 (2) K
0.40 × 0.35 × 0.18 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: numerical [*X-RED* and *X-SHAPE* (Stoe & Cie, 2005)]
T_{min} = 0.620, T_{max} = 0.840
5164 measured reflections
2502 independent reflections
2498 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.052
S = 1.09
2502 reflections
198 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1*W*	2.2453 (13)	S1—O5	1.4731 (12)
Cd1—O2*W*	2.2718 (12)	S1—O3	1.4843 (10)
Cd1—O3	2.3257 (11)	S1—O6	1.4968 (11)
S1—O4	1.4615 (12)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O6^{i}	0.79 (2)	2.04 (2)	2.817 (2)	167 (3)
N1—H1*D*···O3^{ii}	0.89 (3)	2.02 (3)	2.890 (2)	168 (2)
N1—H1*D*···O4^{ii}	0.89 (3)	2.44 (3)	2.990 (2)	120 (3)
N1—H1*E*···O5	0.93 (3)	1.89 (3)	2.808 (2)	175 (3)
O1*W*—H1*W*···O6^{iii}	0.83 (3)	1.90 (3)	2.728 (2)	179 (3)
O1*W*—H2*W*···O4^{iv}	0.86 (3)	1.85 (3)	2.708 (2)	176 (3)
O2*W*—H3*W*···O6^{v}	0.80 (3)	1.95 (3)	2.734 (2)	170 (3)
O2*W*—H4*W*···O5^{iii}	0.88 (3)	1.85 (3)	2.718 (2)	172 (3)

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2138).

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  doi:10.1107/S1600536807043504

supplementary materials

Acta Cryst. (2007). E**63**, m2516 [**doi:10.1107/S1600536807043504**]

Bis(benzylammonium) tetraaqua[bis(sulfato)cadmate(II)]

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Comment

Tutton's salts with general formula $M^{I}_2M^{II}(SO_4)_2{\cdot}6H_2O$, where M^{I} is a monovalent metal or ammonium, and M^{II} is a divalent transition metal, are a well know class of compounds (Mahadevan Pillai *et al.*, 1997). Replacing ammonium with alkylammonium cations leads to different structures. In this communication we report on the crystal structure of the title compound, (I), where the ammonium cations are replaced with benzylammonium.

The molecular geometry and atom labelling of (I) are shown in Fig. 1. In the crystal structure, the Cd atom is located on a centre of inversion and shows a slightly distorted octahedral coordination of oxygen atoms belonging to four water molecules and to two sulfate ligands. Intermolecular hydrogen bonding between the complex anion and the cation leads to a formation of a tightly bonded 3-D network structure. The crystal structure of (I) is isotypic with the Cu^{II} (Rademeyer, 2004) and the Mn^{II} analogue (Naumov *et al.*, 2005).

Experimental

(I) was crystallized as described previously (Jordanovska *et al.*, 2000) by evaporation of an aqueous mixture of Cd(II) sulfate and benzylammonium sulfate in the molar ratio 1:2 at room temperature and in the presence of sulfuric acid. Suitable colorless crystals with block-like habit were obtained by slow evaporation.

Refinement

The H atoms were located in a difference Fourier map and were refined freely.

Figures

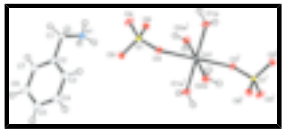


Fig. 1. The cation and anion of (I), displayed at the 30% probability level. [Symmetry operator: i) $-x+2, -y+2, -z$]. H atoms are given as spheres of arbitrary radius.

Bis(benzylammonium) tetraaqua[bis(sulfato)cadmate(II)]

Crystal data

$(C_7H_{10}N)_2[Cd(SO_4)_2(H_2O)_4]$	$Z = 1$
$M_r = 592.93$	$F_{000} = 302$
Triclinic, $P\overline{1}$	$D_x = 1.729$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation

	λ = 0.71073 Å
a = 6.6361 (14) Å	Cell parameters from 2000 reflections
b = 8.1378 (18) Å	θ = 2.6–28.9º
c = 11.087 (3) Å	μ = 1.20 mm^{-1}
α = 81.246 (18)º	*T* = 120 (2) K
β = 80.320 (18)º	Block, colorless
γ = 76.302 (18)º	0.40 × 0.35 × 0.18 mm
V = 569.5 (2) Å^3	

Data collection

Stoe IPDS II diffractometer	R_{int} = 0.034
ω–scans	θ_{max} = 27.9º
Absorption correction: numerical [X-RED and X-SHAPE (Stoe & Cie, 2005)]	θ_{min} = 2.6º
T_{min} = 0.620, T_{max} = 0.840	*h* = −8→8
5164 measured reflections	*k* = −9→10
2502 independent reflections	*l* = −13→14
2498 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	All H-atom parameters refined
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.2838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.020	$(\Delta/\sigma)_{max}$ = 0.011
$wR(F^2)$ = 0.052	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
S = 1.09	$\Delta\rho_{min}$ = −0.55 e Å^{-3}
2502 reflections	Extinction correction: none
198 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	1	1	0	0.01113 (7)
C1	0.3326 (3)	0.5167 (2)	−0.30551 (14)	0.0207 (3)
H1A	0.479 (4)	0.460 (3)	−0.314 (2)	0.026 (5)*
H1B	0.237 (4)	0.434 (3)	−0.291 (2)	0.026 (6)*
C2	0.2858 (3)	0.64749 (19)	−0.41469 (13)	0.0183 (3)
C3	0.4280 (3)	0.7478 (2)	−0.46858 (14)	0.0218 (3)

H3	0.556 (4)	0.741 (3)	−0.437 (2)	0.034 (7)*
C4	0.3845 (3)	0.8656 (2)	−0.57095 (15)	0.0267 (4)
H4	0.488 (4)	0.929 (3)	−0.609 (2)	0.032 (6)*
C5	0.2018 (4)	0.8822 (2)	−0.62017 (15)	0.0298 (4)
H5	0.174 (5)	0.962 (4)	−0.687 (3)	0.049 (8)*
C6	0.0586 (3)	0.7838 (3)	−0.56597 (17)	0.0322 (4)
H6	−0.073 (5)	0.794 (4)	−0.605 (3)	0.042 (7)*
C7	0.1004 (3)	0.6673 (2)	−0.46258 (16)	0.0257 (3)
H7	0.003 (4)	0.599 (3)	−0.424 (2)	0.037 (7)*
N1	0.2975 (2)	0.59854 (16)	−0.18991 (11)	0.0142 (2)
H1C	0.319 (4)	0.523 (3)	−0.136 (2)	0.029 (6)*
H1D	0.172 (4)	0.667 (3)	−0.179 (2)	0.024 (5)*
H1E	0.394 (4)	0.665 (3)	−0.193 (2)	0.028 (6)*
S1	0.74925 (5)	0.71887 (4)	−0.10746 (3)	0.01189 (8)
O1W	1.22112 (19)	0.76313 (15)	0.06889 (12)	0.0221 (2)
H1W	1.351 (5)	0.743 (4)	0.056 (2)	0.035 (7)*
H2W	1.195 (5)	0.665 (4)	0.096 (2)	0.041 (7)*
O2W	1.25772 (18)	1.06754 (15)	−0.14851 (10)	0.0184 (2)
H3W	1.296 (4)	1.136 (4)	−0.119 (2)	0.035 (7)*
H4W	1.372 (5)	0.988 (4)	−0.161 (2)	0.036 (7)*
O3	0.90400 (16)	0.82761 (13)	−0.11968 (9)	0.01422 (19)
O4	0.85681 (18)	0.55127 (14)	−0.14329 (11)	0.0212 (2)
O5	0.58598 (18)	0.79984 (14)	−0.18596 (10)	0.0169 (2)
O6	0.64769 (17)	0.70174 (14)	0.02367 (9)	0.0166 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.00982 (9)	0.00915 (8)	0.01465 (9)	−0.00280 (5)	−0.00174 (5)	−0.00085 (5)
C1	0.0318 (9)	0.0134 (7)	0.0165 (7)	−0.0041 (6)	−0.0032 (6)	−0.0017 (5)
C2	0.0272 (8)	0.0137 (6)	0.0142 (6)	−0.0048 (6)	−0.0021 (5)	−0.0023 (5)
C3	0.0273 (8)	0.0212 (7)	0.0176 (7)	−0.0077 (6)	−0.0013 (6)	−0.0027 (6)
C4	0.0413 (11)	0.0203 (8)	0.0185 (7)	−0.0116 (8)	0.0014 (7)	−0.0005 (6)
C5	0.0511 (12)	0.0194 (8)	0.0170 (7)	−0.0040 (8)	−0.0082 (7)	0.0022 (6)
C6	0.0389 (10)	0.0311 (9)	0.0281 (9)	−0.0059 (8)	−0.0154 (8)	0.0005 (7)
C7	0.0315 (9)	0.0243 (8)	0.0241 (7)	−0.0118 (7)	−0.0069 (7)	0.0009 (6)
N1	0.0138 (6)	0.0141 (6)	0.0146 (5)	−0.0041 (5)	−0.0023 (4)	0.0006 (4)
S1	0.01048 (16)	0.00978 (15)	0.01586 (16)	−0.00383 (12)	−0.00262 (12)	0.00054 (11)
O1W	0.0127 (5)	0.0132 (5)	0.0374 (6)	−0.0028 (4)	−0.0045 (4)	0.0070 (4)
O2W	0.0158 (5)	0.0188 (5)	0.0204 (5)	−0.0060 (4)	0.0008 (4)	−0.0019 (4)
O3	0.0130 (5)	0.0143 (5)	0.0171 (5)	−0.0071 (4)	−0.0018 (4)	−0.0010 (4)
O4	0.0193 (5)	0.0106 (5)	0.0332 (6)	−0.0040 (4)	0.0004 (4)	−0.0037 (4)
O5	0.0146 (5)	0.0184 (5)	0.0189 (5)	−0.0048 (4)	−0.0062 (4)	0.0009 (4)
O6	0.0138 (5)	0.0188 (5)	0.0166 (5)	−0.0063 (4)	−0.0014 (4)	0.0034 (4)

Geometric parameters (Å, °)

Cd1—O1W^{i}	2.2453 (13)	C5—C6	1.388 (3)

Cd1—O1W	2.2453 (13)	C5—H5	0.92 (3)
Cd1—O2W^{i}	2.2718 (12)	C6—C7	1.393 (3)
Cd1—O2W	2.2718 (12)	C6—H6	1.02 (3)
Cd1—O3^{i}	2.3257 (11)	C7—H7	0.96 (3)
Cd1—O3	2.3257 (11)	N1—H1C	0.80 (3)
C1—N1	1.4922 (19)	N1—H1D	0.89 (3)
C1—C2	1.507 (2)	N1—H1E	0.92 (3)
C1—H1A	0.97 (3)	S1—O4	1.4615 (12)
C1—H1B	1.01 (2)	S1—O5	1.4731 (12)
C2—C7	1.386 (2)	S1—O3	1.4843 (10)
C2—C3	1.393 (2)	S1—O6	1.4968 (11)
C3—C4	1.392 (2)	O1W—H1W	0.83 (3)
C3—H3	0.95 (3)	O1W—H2W	0.85 (3)
C4—C5	1.382 (3)	O2W—H3W	0.79 (3)
C4—H4	0.96 (3)	O2W—H4W	0.88 (3)
O1W^{i}—Cd1—O1W	180.00 (6)	C3—C4—H4	118.3 (15)
O1W^{i}—Cd1—O2W^{i}	90.41 (5)	C4—C5—C6	120.02 (16)
O1W—Cd1—O2W^{i}	89.59 (5)	C4—C5—H5	119 (2)
O1W^{i}—Cd1—O2W	89.59 (5)	C6—C5—H5	121 (2)
O1W—Cd1—O2W	90.41 (5)	C5—C6—C7	119.90 (18)
O2W^{i}—Cd1—O2W	180.00 (6)	C5—C6—H6	119.3 (17)
O1W^{i}—Cd1—O3^{i}	85.87 (5)	C7—C6—H6	120.8 (17)
O1W—Cd1—O3^{i}	94.13 (5)	C2—C7—C6	120.24 (17)
O2W^{i}—Cd1—O3^{i}	93.16 (4)	C2—C7—H7	118.6 (16)
O2W—Cd1—O3^{i}	86.84 (4)	C6—C7—H7	121.1 (16)
O1W^{i}—Cd1—O3	94.13 (5)	C1—N1—H1C	106.3 (18)
O1W—Cd1—O3	85.87 (5)	C1—N1—H1D	111.8 (14)
O2W^{i}—Cd1—O3	86.84 (4)	H1C—N1—H1D	114 (2)
O2W—Cd1—O3	93.16 (4)	C1—N1—H1E	110.1 (15)
O3^{i}—Cd1—O3	180.0000 (10)	H1C—N1—H1E	108 (2)
N1—C1—C2	111.17 (13)	H1D—N1—H1E	107 (2)
N1—C1—H1A	104.4 (14)	O4—S1—O5	110.57 (7)
C2—C1—H1A	111.0 (14)	O4—S1—O3	109.17 (7)
N1—C1—H1B	105.9 (13)	O5—S1—O3	109.64 (6)
C2—C1—H1B	111.5 (13)	O4—S1—O6	110.00 (7)
H1A—C1—H1B	113 (2)	O5—S1—O6	108.46 (7)
C7—C2—C3	119.64 (15)	O3—S1—O6	108.97 (6)
C7—C2—C1	119.73 (15)	Cd1—O1W—H1W	127 (2)
C3—C2—C1	120.63 (15)	Cd1—O1W—H2W	128 (2)
C4—C3—C2	119.93 (16)	H1W—O1W—H2W	103 (3)
C4—C3—H3	117.5 (16)	Cd1—O2W—H3W	102.1 (19)
C2—C3—H3	122.5 (16)	Cd1—O2W—H4W	117.0 (18)
C5—C4—C3	120.25 (16)	H3W—O2W—H4W	103 (3)
C5—C4—H4	121.3 (15)	S1—O3—Cd1	137.75 (6)
N1—C1—C2—C7	−103.32 (17)	C5—C6—C7—C2	−0.9 (3)
N1—C1—C2—C3	77.17 (19)	O4—S1—O3—Cd1	−129.45 (9)

C7—C2—C3—C4	−0.8 (2)	O5—S1—O3—Cd1	109.29 (10)
C1—C2—C3—C4	178.68 (15)	O6—S1—O3—Cd1	−9.29 (11)
C2—C3—C4—C5	−0.7 (3)	O1W^{i}—Cd1—O3—S1	−91.15 (10)
C3—C4—C5—C6	1.4 (3)	O1W—Cd1—O3—S1	88.85 (10)
C4—C5—C6—C7	−0.6 (3)	O2W^{i}—Cd1—O3—S1	−0.96 (9)
C3—C2—C7—C6	1.6 (3)	O2W—Cd1—O3—S1	179.04 (9)
C1—C2—C7—C6	−177.88 (17)	O3^{i}—Cd1—O3—S1	12E1(10)

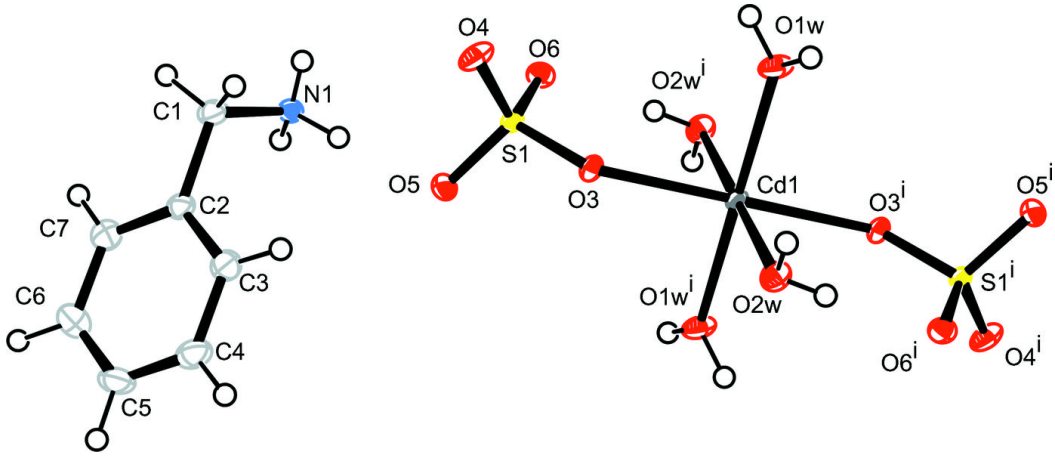
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···O6^{ii}	0.79 (2)	2.04 (2)	2.817 (2)	167 (3)
N1—H1D···O3^{iii}	0.89 (3)	2.02 (3)	2.890 (2)	168 (2)
N1—H1D···O4^{iii}	0.89 (3)	2.44 (3)	2.990 (2)	120 (3)
N1—H1E···O5	0.93 (3)	1.89 (3)	2.808 (2)	175 (3)
O1W—H1W···O6^{iv}	0.83 (3)	1.90 (3)	2.728 (2)	179 (3)
O1W—H2W···O4^{v}	0.86 (3)	1.85 (3)	2.708 (2)	176 (3)
O2W—H3W···O6^{i}	0.80 (3)	1.95 (3)	2.734 (2)	170 (3)
O2W—H4W···O5^{iv}	0.88 (3)	1.85 (3)	2.718 (2)	172 (3)

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

Fig. 1


O4
O6
O1w
O2w^{i}
N1
C1
S1
O5
O3
Cd1
O3^{i}
O5^{i}
C2
C7
C3
C6
O1w^{i}
O2w
S1^{i}
C4
O6^{i}
O4^{i}
C5