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Triaquabis[(2-nitrophenylsulfanyl)-acetato-κ^2O,O']cadmium(II) dihydrate

Yan-Jun Hou, Zhi-Zhong Sun,* Ying-Hui Yu, Bai-Yan Li and Guang-Feng Hou

College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: hgf1000@163.com

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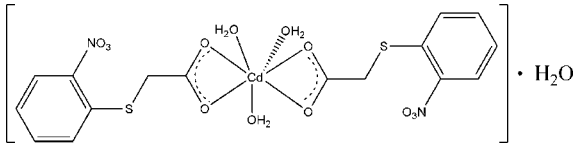
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.030; wR factor = 0.075; data-to-parameter ratio = 17.4.

The title compound, $[Cd(C_8H_6NO_4S)_2(H_2O)_3]\cdot 2H_2O$, has a seven-coordinate Cd^{II} atom in a distorted pentagonal–bipyramidal geometry defined by four carboxylate O atoms from two (2-nitrophenylsulfanyl)acetate groups and three O atoms from three water molecules. The complex molecules are linked together by intermolecular hydrogen bonds involving the uncoordinated water molecules, resulting in a two-dimensional network.

Related literature

For related literature, see: Gao *et al.* (2006); Shi *et al.*, 2007; Nobles & Thompson (1965).



Experimental

Crystal data

$[Cd(C_8H_6NO_4S)_2(H_2O)_3]\cdot 2H_2O$
M_r = 626.91
Monoclinic, $P2_1/c$
a = 19.550 (7) Å
b = 8.216 (3) Å
c = 14.703 (7) Å
β = 97.350 (18)°
V = 2342.3 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 293 (2) K
0.24 × 0.21 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.768, T_{max} = 0.841
21719 measured reflections
5356 independent reflections
3874 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.00
5356 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O9—H13···O13^{i}	0.85	1.84	2.682 (3)	173
O11—H18···O12	0.85	1.83	2.673 (3)	170
O9—H14···O3^{ii}	0.85	1.85	2.688 (2)	168
O10—H15···O11^{i}	0.85	1.94	2.777 (2)	169
O10—H16···O9^{iii}	0.85	1.90	2.738 (2)	171
O11—H17···O8^{i}	0.85	1.85	2.677 (2)	165
O13—H21···O12	0.85	2.53	3.332 (4)	157
O13—H21···O7^{iv}	0.85	2.57	3.204 (3)	132
O12—H19···O7^{iv}	0.85	2.24	2.950 (3)	141
O12—H19···S7^{iv}	0.85	2.57	3.309 (2)	146
O12—H20···O2^{v}	0.85	2.30	3.099 (3)	157
O13—H22···O4^{v}	0.85	2.07	2.879 (3)	160
O13—H22···S1^{v}	0.85	2.97	3.520 (2)	124

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

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*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2254).

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supplementary materials

Acta Cryst. (2007). E**63**, m1506 [**doi:10.1107/S1600536807019472**]

Triaquabis[(2-nitrophenylsulfanyl)acetato-κ^2O,O']cadmium(II) dihydrate

Y.-J. Hou, Z.-Z. Sun, Y.-H. Yu, B.-Y. Li and G.-F. Hou

Comment

The structures of the metal derivative sof 4-nitrophenylsulfanylacetic acid are known for nickel and cobalt (Gao *et al.*, 2006; Shi *et al.*, 2006). The structures of the 2-nitrophenylsulfanylacetic acid analogs are yet unknown.

The asymmetric unit of (I) consists of a cadmium(II) atom, two 2-nitrophenylsulfanylacetate groups, three coordinated water molecules and two uncoordinated water molecules (Fig.1). The CdII atom exists in a pentagonal bipyramidal configuration, with the equatorial plane being defined by the atoms O3, O4, O7, O8 and O10. Atoms O9 and O11 occupy the axial sites.

The structure is stabilized by hydrogen bonding interactions (Table 1) that link the individual components into a two-dimensional layer structure (Fig. 2).

Experimental

2-Nitrophenylsulfanylacetic acid was prepared by nucleophilic reaction of chloroacetic acid and 2-nitrothiophenol under basic conditions. (Nobles *et al.*, 1965). Cadmium(II) nitrate tetrhydrate (0.617 g, 2 mmol) and 2-nitrophenylsulfanylacetic acid (0.394 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01*M* sodium hydroxide; yellow crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with U_{iso}(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5Ueq(O).

Figures

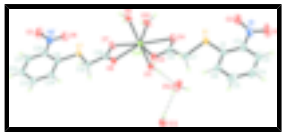

Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate the hydrogen bonding interactions.

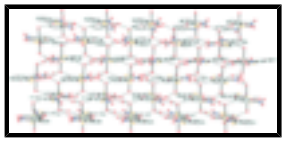

Fig. 2. A partial packing view, showing the two-dimensional hydrogen-bonding plan. Dashed lines indicate the hydrogen-bonding interactions.

Triaquabis[(2-nitrophenylsulfanyl)acetato-κ^2O,O']cadmium(II) dihydrate

Crystal data

$[Cd_1(C_8H_6NO_4S)_2(H_2O)_3]\cdot 2H_2O$	$F_{000} = 1264$
$M_r = 626.91$	$D_x = 1.778$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 16259 reflections
$a = 19.550$ (7) Å	$\theta = 6.2$–55.0º
$b = 8.216$ (3) Å	$\mu = 1.18$ mm^{-1}
$c = 14.703$ (7) Å	$T = 293$ (2) K
$\beta = 97.350$ (18)º	Block, colorless
$V = 2342.3$ (17) Å^3	0.24 × 0.21 × 0.15 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	5356 independent reflections
Radiation source: fine-focus sealed tube	3874 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 293$(2) K	$\theta_{max} = 27.5$º
ω scan	$\theta_{min} = 3.1$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -25\rightarrow25$
$T_{min} = 0.768$, $T_{max} = 0.841$	$k = -9\rightarrow10$
21719 measured reflections	$l = -19\rightarrow19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
5356 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
307 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.30664 (11)	0.4539 (3)	−0.04068 (16)	0.0378 (5)
C2	0.36823 (13)	0.3932 (4)	−0.06608 (19)	0.0489 (7)
C3	0.42292 (14)	0.4928 (5)	−0.0796 (2)	0.0663 (9)
H1	0.4634	0.4478	−0.0957	0.080*
C4	0.41770 (15)	0.6556 (5)	−0.0695 (2)	0.0736 (10)
H2	0.4546	0.7227	−0.0784	0.088*
C5	0.35827 (16)	0.7214 (4)	−0.0462 (2)	0.0620 (8)
H3	0.3547	0.8337	−0.0403	0.074*
C6	0.30320 (13)	0.6233 (3)	−0.03103 (18)	0.0474 (6)
H4	0.2634	0.6704	−0.0142	0.057*
C7	0.18219 (11)	0.4613 (3)	0.02960 (17)	0.0372 (5)
H5A	0.2078	0.5156	0.0819	0.045*
H6B	0.1652	0.5437	−0.0149	0.045*
C8	0.12181 (11)	0.3701 (3)	0.06027 (16)	0.0353 (5)
C9	−0.30084 (11)	0.3969 (3)	0.29923 (16)	0.0351 (5)
C10	−0.36354 (12)	0.3215 (3)	0.30859 (18)	0.0423 (6)
C11	−0.42148 (13)	0.4089 (4)	0.3233 (2)	0.0598 (8)
H7	−0.4626	0.3552	0.3287	0.072*
C12	−0.41807 (15)	0.5750 (4)	0.3297 (2)	0.0649 (9)
H8	−0.4570	0.6346	0.3392	0.078*
C13	−0.35742 (14)	0.6531 (4)	0.3222 (2)	0.0570 (7)
H9	−0.3553	0.7659	0.3269	0.068*
C14	−0.29904 (13)	0.5667 (3)	0.30782 (18)	0.0457 (6)
H10	−0.2580	0.6221	0.3038	0.055*
C15	−0.17024 (11)	0.4421 (3)	0.24590 (17)	0.0360 (5)
H11A	−0.1951	0.5165	0.2023	0.043*
H12B	−0.1521	0.5036	0.2999	0.043*
C16	−0.11144 (11)	0.3636 (3)	0.20362 (16)	0.0356 (5)
Cd4	0.003378 (7)	0.259713 (19)	0.126486 (11)	0.03280 (7)
N1	0.37706 (13)	0.2193 (4)	−0.0799 (2)	0.0645 (7)
N2	−0.37058 (12)	0.1454 (3)	0.30343 (17)	0.0561 (6)
O1	0.43488 (12)	0.1638 (4)	−0.0765 (2)	0.1115 (10)
O2	0.32566 (12)	0.1340 (3)	−0.09545 (19)	0.0847 (8)

O3	0.07383 (8)	0.4577 (2)	0.08316 (12)	0.0436 (4)
O4	0.12048 (9)	0.2188 (2)	0.06435 (14)	0.0498 (5)
O5	−0.42770 (11)	0.0854 (3)	0.3025 (2)	0.1051 (10)
O6	−0.31884 (10)	0.0624 (2)	0.30212 (16)	0.0672 (6)
O7	−0.10346 (9)	0.2133 (2)	0.20501 (14)	0.0531 (5)
O8	−0.07214 (8)	0.4579 (2)	0.16682 (12)	0.0419 (4)
O9	−0.05832 (9)	0.23693 (18)	−0.01830 (12)	0.0393 (4)
H13	−0.0962	0.1894	−0.0130	0.059*
H14	−0.0663	0.3271	−0.0460	0.059*
O10	0.00194 (8)	−0.0128 (2)	0.12473 (11)	0.0482 (5)
H15	−0.0216	−0.0704	0.1574	0.072*
H16	0.0210	−0.0737	0.0886	0.072*
O11	0.06326 (8)	0.26541 (18)	0.27275 (12)	0.0391 (4)
H17	0.0687	0.1752	0.3011	0.059*
H18	0.1021	0.3097	0.2692	0.059*
O12	0.18552 (11)	0.4145 (3)	0.28311 (18)	0.0932 (9)
H19	0.1778	0.5146	0.2712	0.140*
H20	0.2280	0.3976	0.3013	0.140*
O13	0.17204 (9)	0.5729 (2)	0.48872 (14)	0.0618 (5)
H21	0.1670	0.5556	0.4312	0.093*
H22	0.1674	0.4839	0.5167	0.093*
S1	0.23822 (3)	0.32432 (8)	−0.02060 (5)	0.04267 (16)
S7	−0.22770 (3)	0.28581 (7)	0.27683 (5)	0.04085 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0292 (11)	0.0449 (14)	0.0400 (14)	−0.0044 (11)	0.0076 (10)	0.0032 (11)
C2	0.0357 (13)	0.0665 (19)	0.0459 (16)	0.0000 (13)	0.0102 (11)	0.0022 (13)
C3	0.0369 (14)	0.100 (3)	0.064 (2)	−0.0121 (17)	0.0161 (13)	0.0071 (19)
C4	0.0475 (17)	0.099 (3)	0.076 (2)	−0.0333 (19)	0.0151 (15)	0.013 (2)
C5	0.0679 (19)	0.0563 (18)	0.062 (2)	−0.0250 (16)	0.0098 (15)	0.0089 (15)
C6	0.0418 (13)	0.0467 (15)	0.0558 (17)	−0.0100 (12)	0.0140 (12)	0.0055 (12)
C7	0.0323 (12)	0.0354 (12)	0.0463 (14)	−0.0037 (10)	0.0145 (10)	−0.0009 (10)
C8	0.0317 (11)	0.0394 (13)	0.0359 (13)	−0.0035 (10)	0.0089 (10)	0.0036 (10)
C9	0.0299 (11)	0.0399 (13)	0.0368 (13)	0.0039 (10)	0.0093 (9)	0.0012 (10)
C10	0.0341 (12)	0.0477 (14)	0.0467 (16)	−0.0032 (12)	0.0107 (10)	0.0005 (12)
C11	0.0311 (13)	0.083 (2)	0.068 (2)	−0.0007 (15)	0.0155 (13)	−0.0002 (17)
C12	0.0463 (16)	0.069 (2)	0.082 (2)	0.0195 (16)	0.0214 (15)	−0.0056 (17)
C13	0.0546 (17)	0.0488 (16)	0.070 (2)	0.0160 (14)	0.0189 (14)	−0.0064 (15)
C14	0.0386 (13)	0.0402 (14)	0.0606 (17)	0.0036 (11)	0.0145 (12)	−0.0041 (12)
C15	0.0303 (11)	0.0355 (12)	0.0444 (14)	0.0030 (10)	0.0131 (10)	−0.0023 (10)
C16	0.0279 (11)	0.0428 (13)	0.0367 (14)	0.0052 (11)	0.0066 (10)	−0.0057 (11)
Cd4	0.03174 (10)	0.02779 (10)	0.04123 (11)	0.00020 (7)	0.01369 (7)	−0.00157 (7)
N1	0.0470 (14)	0.0758 (19)	0.0743 (19)	0.0177 (14)	0.0217 (12)	−0.0025 (14)
N2	0.0441 (13)	0.0549 (15)	0.0705 (18)	−0.0129 (12)	0.0116 (11)	0.0017 (12)
O1	0.0553 (14)	0.113 (2)	0.172 (3)	0.0363 (15)	0.0375 (16)	−0.003 (2)
O2	0.0604 (14)	0.0629 (15)	0.134 (2)	0.0074 (12)	0.0241 (14)	−0.0206 (14)

O3	0.0363 (9)	0.0424 (10)	0.0559 (11)	0.0021 (8)	0.0209 (8)	0.0063 (8)
O4	0.0513 (11)	0.0340 (10)	0.0687 (13)	−0.0051 (8)	0.0252 (9)	0.0025 (9)
O5	0.0455 (12)	0.0763 (17)	0.196 (3)	−0.0287 (13)	0.0247 (15)	−0.0053 (18)
O6	0.0552 (12)	0.0437 (11)	0.1051 (18)	−0.0057 (10)	0.0193 (12)	0.0036 (11)
O7	0.0490 (10)	0.0401 (10)	0.0753 (14)	0.0072 (8)	0.0272 (9)	−0.0033 (9)
O8	0.0340 (8)	0.0452 (10)	0.0501 (11)	0.0005 (8)	0.0190 (7)	−0.0040 (8)
O9	0.0437 (9)	0.0312 (8)	0.0447 (10)	0.0014 (7)	0.0118 (7)	−0.0014 (7)
O10	0.0691 (13)	0.0251 (8)	0.0578 (12)	0.0010 (7)	0.0365 (10)	−0.0005 (7)
O11	0.0388 (8)	0.0347 (9)	0.0451 (10)	0.0015 (7)	0.0100 (7)	0.0019 (7)
O12	0.0616 (14)	0.0817 (16)	0.132 (2)	−0.0254 (13)	−0.0041 (14)	0.0425 (15)
O13	0.0671 (12)	0.0495 (11)	0.0703 (14)	0.0076 (10)	0.0146 (10)	−0.0037 (10)
S1	0.0346 (3)	0.0338 (3)	0.0629 (4)	−0.0024 (3)	0.0192 (3)	−0.0011 (3)
S7	0.0341 (3)	0.0326 (3)	0.0588 (4)	0.0031 (3)	0.0174 (3)	0.0013 (3)

Geometric parameters (Å, °)

C1—C2	1.398 (3)	C14—H10	0.9300
C1—C6	1.401 (3)	C15—C16	1.519 (3)
C1—S1	1.764 (2)	C15—S7	1.802 (2)
C2—C3	1.381 (4)	C15—H11A	0.9700
C2—N1	1.456 (4)	C15—H12B	0.9700
C3—C4	1.352 (5)	C16—O7	1.244 (3)
C3—H1	0.9300	C16—O8	1.261 (3)
C4—C5	1.364 (4)	Cd4—O10	2.2392 (18)
C4—H2	0.9300	Cd4—O3	2.2743 (17)
C5—C6	1.386 (3)	Cd4—O11	2.314 (2)
C5—H3	0.9300	Cd4—O9	2.316 (2)
C6—H4	0.9300	Cd4—O8	2.3251 (17)
C7—C8	1.515 (3)	Cd4—O7	2.541 (2)
C7—S1	1.794 (2)	Cd4—O4	2.593 (2)
C7—H5A	0.9700	N1—O1	1.214 (3)
C7—H6B	0.9700	N1—O2	1.223 (3)
C8—O4	1.244 (3)	N2—O5	1.219 (3)
C8—O3	1.262 (3)	N2—O6	1.222 (3)
C9—C10	1.396 (3)	O9—H13	0.8501
C9—C14	1.401 (3)	O9—H14	0.8500
C9—S7	1.763 (2)	O10—H15	0.8501
C10—C11	1.381 (4)	O10—H16	0.8499
C10—N2	1.454 (4)	O11—H17	0.8500
C11—C12	1.369 (4)	O11—H18	0.8500
C11—H7	0.9300	O12—H19	0.8500
C12—C13	1.365 (4)	O12—H20	0.8500
C12—H8	0.9300	O13—H21	0.8500
C13—C14	1.383 (3)	O13—H22	0.8500
C13—H9	0.9300		
C2—C1—C6	115.8 (2)	S7—C15—H12B	109.8
C2—C1—S1	121.8 (2)	H11A—C15—H12B	108.3
C6—C1—S1	122.37 (19)	O7—C16—O8	122.3 (2)
C3—C2—C1	122.5 (3)	O7—C16—C15	121.0 (2)

C3—C2—N1	116.9 (3)	O8—C16—C15	116.7 (2)
C1—C2—N1	120.6 (2)	O10—Cd4—O3	135.97 (6)
C4—C3—C2	120.0 (3)	O10—Cd4—O11	92.01 (5)
C4—C3—H1	120.0	O3—Cd4—O11	89.62 (6)
C2—C3—H1	120.0	O10—Cd4—O9	84.51 (6)
C3—C4—C5	119.9 (3)	O3—Cd4—O9	93.62 (6)
C3—C4—H2	120.0	O11—Cd4—O9	176.36 (5)
C5—C4—H2	120.0	O10—Cd4—O8	134.08 (6)
C4—C5—C6	120.9 (3)	O3—Cd4—O8	89.87 (7)
C4—C5—H3	119.5	O11—Cd4—O8	90.64 (6)
C6—C5—H3	119.5	O9—Cd4—O8	91.03 (6)
C5—C6—C1	120.9 (3)	O10—Cd4—O7	81.10 (6)
C5—C6—H4	119.6	O3—Cd4—O7	142.85 (6)
C1—C6—H4	119.6	O11—Cd4—O7	85.89 (7)
C8—C7—S1	110.62 (16)	O9—Cd4—O7	92.51 (7)
C8—C7—H5A	109.5	O8—Cd4—O7	53.39 (6)
S1—C7—H5A	109.5	O10—Cd4—O4	82.92 (5)
C8—C7—H6B	109.5	O3—Cd4—O4	53.15 (6)
S1—C7—H6B	109.5	O11—Cd4—O4	88.02 (7)
H5A—C7—H6B	108.1	O9—Cd4—O4	92.59 (7)
O4—C8—O3	122.4 (2)	O8—Cd4—O4	142.99 (6)
O4—C8—C7	122.0 (2)	O7—Cd4—O4	162.68 (6)
O3—C8—C7	115.6 (2)	O1—N1—O2	122.1 (3)
C10—C9—C14	116.5 (2)	O1—N1—C2	119.3 (3)
C10—C9—S7	122.14 (19)	O2—N1—C2	118.6 (2)
C14—C9—S7	121.40 (18)	O5—N2—O6	122.2 (3)
C11—C10—C9	122.2 (3)	O5—N2—C10	118.9 (2)
C11—C10—N2	116.8 (2)	O6—N2—C10	118.9 (2)
C9—C10—N2	121.0 (2)	C8—O3—Cd4	99.46 (14)
C12—C11—C10	119.7 (3)	C8—O4—Cd4	84.99 (14)
C12—C11—H7	120.2	C16—O7—Cd4	87.26 (14)
C10—C11—H7	120.2	C16—O8—Cd4	96.93 (14)
C13—C12—C11	119.9 (3)	Cd4—O9—H13	108.1
C13—C12—H8	120.1	Cd4—O9—H14	114.3
C11—C12—H8	120.1	H13—O9—H14	109.6
C12—C13—C14	120.9 (3)	Cd4—O10—H15	123.8
C12—C13—H9	119.5	Cd4—O10—H16	126.1
C14—C13—H9	119.5	H15—O10—H16	109.8
C13—C14—C9	120.9 (2)	Cd4—O11—H17	117.1
C13—C14—H10	119.6	Cd4—O11—H18	107.6
C9—C14—H10	119.6	H17—O11—H18	110.2
C16—C15—S7	109.21 (16)	H19—O12—H20	111.3
C16—C15—H11A	109.8	H21—O13—H22	109.4
S7—C15—H11A	109.8	C1—S1—C7	101.89 (11)
C16—C15—H12B	109.8	C9—S7—C15	102.98 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O9—H13···O13^{i}	0.85	1.84	2.682 (3)	173
O11—H18···O12	0.85	1.83	2.673 (3)	170
O9—H14···O3^{ii}	0.85	1.85	2.688 (2)	168
O10—H15···O11^{i}	0.85	1.94	2.777 (2)	169
O10—H16···O9^{iii}	0.85	1.90	2.738 (2)	171
O11—H17···O8^{i}	0.85	1.85	2.677 (2)	165
O13—H21···O12	0.85	2.53	3.332 (4)	157
O13—H21···O7^{iv}	0.85	2.57	3.204 (3)	132
O12—H19···O7^{iv}	0.85	2.24	2.950 (3)	141
O12—H19···S7^{iv}	0.85	2.57	3.309 (2)	146
O12—H20···O2^{v}	0.85	2.30	3.099 (3)	157
O13—H22···O4^{v}	0.85	2.07	2.879 (3)	160
O13—H22···S1^{v}	0.85	2.97	3.520 (2)	124

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

Fig. 1

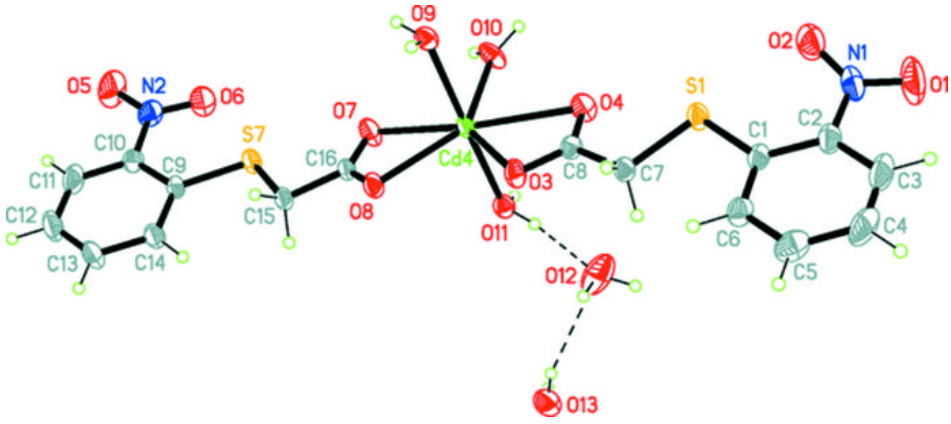
O9
O10
O2
N1
O1
O5
N2
O6
S1
O7
O4
C1
C2
S7
C10
C9
C16
Cd4
C8
C7
C3
C11
O3
C12
C15
O8
O11
C6
C4
C13
C14
O12
C5
O13

Fig. 2