

trans-Tetraaquabis(nicotinamide- κ N)-cadmium(II) biphenyl-4,4'-disulfonate

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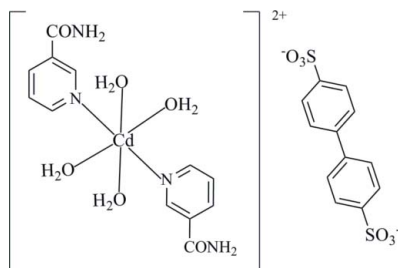
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.031; wR factor = 0.092; data-to-parameter ratio = 14.4.

In the title compound, $[\text{Cd}(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_4](\text{C}_{10}\text{H}_8\text{O}_6\text{S}_2)_2$, the Cd^{II} ion is located on a crystallographic inversion centre. An octahedral coordination geometry is defined by four water molecules in one plane, and two *trans* N-atom donors of the nicotinamide ligands. The biphenyl-4,4'-disulfonate anion also lies on a crystallographic inversion centre. In the crystal structure, the complex cations are connected to the counteranions *via* $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Beatty (2001); Christer *et al.* (2004); Holman *et al.* (2001); Lian & Li (2007*a,b,c,d*).



Experimental

Crystal data

 $[\text{Cd}(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_4] \cdot (\text{C}_{10}\text{H}_8\text{O}_6\text{S}_2)_2$
 $M_r = 741.02$
Monoclinic, $P2_1/c$
 $a = 14.742$ (8) Å
 $b = 6.899$ (4) Å
 $c = 15.292$ (8) Å
 $\beta = 110.980$ (9)°
 $V = 1452.2$ (13) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.96$ mm⁻¹
 $T = 298$ (2) K
 $0.40 \times 0.36 \times 0.31$ mm

Data collection

 Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.682$, $T_{\text{max}} = 0.741$

 7656 measured reflections
2842 independent reflections
2477 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.092$
 $S = 1.07$
2842 reflections

 197 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.57$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.19$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O5}-\text{H5A}\cdots\text{O3}^{\text{i}}$	0.81	2.03	2.832 (3)	171
$\text{O5}-\text{H5B}\cdots\text{O4}^{\text{ii}}$	0.86	1.83	2.676 (2)	172
$\text{O6}-\text{H6A}\cdots\text{O3}$	0.85	1.93	2.777 (3)	178
$\text{O6}-\text{H6B}\cdots\text{O2}^{\text{iii}}$	0.83	1.89	2.716 (3)	171
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{iv}}$	0.86	2.08	2.932 (2)	171
$\text{N2}-\text{H2B}\cdots\text{O2}^{\text{v}}$	0.86	2.17	3.025 (3)	172

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2097).

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supplementary materials

Acta Cryst. (2008). E64, m424 [doi:10.1107/S1600536808002390]

***trans*-Tetraaquabis(nicotinamide- κ N)cadmium(II) biphenyl-4,4'-disulfonate**

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Comment

The strong and directional nature of hydrogen bonds is exploited in the organized self-assembly of molecules in the solid state. Amides are commonly used functional groups in crystal engineering owing to the inherent coordination and hydrogen bonding donor/acceptor functionalities, and were used to construct extended frameworks sustained both by hydrogen bonds and coordination bonds (Beatty 2001; Christer *et al.*, 2004). On the other hand, the sulfonate group is a suitable hydrogen-bond acceptor, and has been used to build extended frameworks. (Holman *et al.*, 2001; Lian & Li, 2007a,b,c,d) In this paper, we report the synthesis and crystal structure of the title compound.

In the title compound, the metal centre, located on a crystallographic inversion centre, is in an octahedral geometry defined by four O atoms from four aqua ligands, respectively, and two *trans*-positioned N-atom donors of the nicotinamide ligands, as shown in Fig 1. The amide substituents are twisted away from the conformation in the pyridine ring plane by 37.6 (6)°. The biphenyl-4,4'-disulfonate anion also lies on a crystallographic inversion centre. The planes through phenyl ring in biphenyl-4,4'-disulfonate are twisted by 28.5 (7)°. In the crystal structure, all the amide groups are involved in amide-amide hydrogen bonded linkage in head to head fashion leading to infinite chains of the cations. These chains are linked by hydrogen bonds formed by the remaining N—H protons on the nicotinamide and sulfonate oxygen atoms, and coordinated water molecules and sulfonate oxygen atoms into three-dimensional networks as shown in Fig 2.

Experimental

Nicotinamide (0.050 g, 0.4 mmol) was added with constant stirring to an aqueous solution (10 mL) of Cd(CH₃COO)₂·2H₂O (0.058 g, 0.2 mmol). The solution was then treated with disodium biphenyl-4,4'-disulfonate (0.070 g, 0.2 mmol). Colourless crystals of the title complex were collected by slow evaporation at room temperature after 7 days, (80% yield based on Cd).

Refinement

All the non-H atoms were refined with anisotropic thermal parameters.

H atoms attached to C or N atoms were placed in geometrically calculated positions (C—H = 0.93 Å, N—H=0.86 Å), and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$.

The O-bound H atoms were located in difference maps and refined as riding on the attached O atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Figures

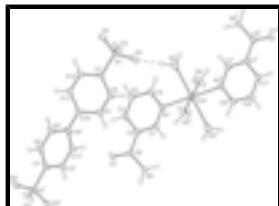


Fig. 1. The molecular structure of (1), with the atom labelling scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms are represented as spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines. Symmetry codes: (i) $-x, y, -z + 1/2$; (ii) $-x + 1, -y, -z + 1$.

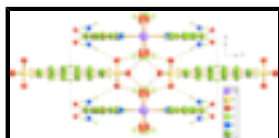


Fig. 2. The three dimensional H-bonded network viewed from b axis direction. Hydrogen bonds are shown as dashed lines.

trans-Tetraaquabis(nicotinamide- κ N)cadmium(II) biphenyl-4,4'-disulfonate

Crystal data

$[\text{Cd}(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_4](\text{C}_{10}\text{H}_8\text{O}_6\text{S}_2)$

$M_r = 741.02$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 14.742\ (8)\ \text{\AA}$

$b = 6.899\ (4)\ \text{\AA}$

$c = 15.292\ (8)\ \text{\AA}$

$\beta = 110.980\ (9)^\circ$

$V = 1452.2\ (13)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 752$

$D_x = 1.695\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Cell parameters from 7656 reflections

$\theta = 12\text{--}18^\circ$

$\mu = 0.97\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, colourless

$0.40 \times 0.36 \times 0.31\ \text{mm}$

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ (2)\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.682, T_{\max} = 0.741$

7656 measured reflections

2842 independent reflections

2477 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 3.3^\circ$

$h = -18 \rightarrow 12$

$k = -8 \rightarrow 7$

$l = -13 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.3728P]$
$wR(F^2) = 0.092$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\max} < 0.001$
2842 reflections	$\Delta\rho_{\max} = 0.58 \text{ e } \text{\AA}^{-3}$
197 parameters	$\Delta\rho_{\min} = -1.19 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.052 (2)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.5000	0.0000	0.5000	0.02772 (14)
S1	0.31842 (5)	0.50038 (6)	0.18505 (5)	0.03230 (18)
O1	0.03394 (9)	0.0836 (3)	0.40310 (11)	0.0485 (4)
O2	0.30985 (11)	0.3259 (3)	0.12698 (14)	0.0544 (5)
O3	0.39387 (14)	0.4851 (2)	0.27876 (16)	0.0462 (5)
O4	0.32299 (12)	0.6768 (3)	0.13379 (15)	0.0582 (5)
O5	0.51977 (12)	-0.2553 (3)	0.41016 (16)	0.0738 (7)
H5A	0.4803	-0.3193	0.3698	0.089*
H5B	0.5698	-0.2876	0.3976	0.089*
O6	0.51991 (12)	0.2033 (3)	0.38506 (14)	0.0657 (6)
H6A	0.4802	0.2889	0.3531	0.079*
H6B	0.5701	0.2527	0.3817	0.079*
N1	0.34204 (14)	-0.00860 (19)	0.41343 (14)	0.0296 (4)
N2	0.12317 (10)	-0.1123 (3)	0.52234 (10)	0.0370 (4)
H2A	0.0802	-0.1148	0.5484	0.044*
H2B	0.1766	-0.1754	0.5469	0.044*
C1	0.27511 (17)	-0.0072 (2)	0.45320 (16)	0.0279 (5)
H1	0.2932	-0.0044	0.5180	0.033*
C2	0.18103 (17)	-0.0100 (2)	0.39791 (17)	0.0277 (5)
C3	0.15424 (17)	-0.0111 (2)	0.29767 (16)	0.0316 (5)
H3	0.0888	-0.0066	0.2600	0.038*
C4	0.22217 (18)	-0.0186 (3)	0.25694 (16)	0.0334 (5)

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H4	0.2057	-0.0249	0.1923	0.040*
C5	0.31554 (17)	-0.0164 (2)	0.31683 (16)	0.0320 (5)
H5	0.3645	-0.0202	0.2919	0.038*
C6	0.10639 (16)	-0.0082 (2)	0.44191 (16)	0.0302 (5)
C7	0.21328 (17)	0.5140 (2)	0.20881 (19)	0.0303 (5)
C8	0.21293 (18)	0.4744 (3)	0.30073 (19)	0.0348 (5)
H8	0.2707	0.4455	0.3494	0.042*
C9	0.12884 (18)	0.4791 (3)	0.31652 (19)	0.0349 (5)
H9	0.1271	0.4538	0.3756	0.042*
C10	0.04503 (16)	0.5228 (2)	0.24163 (18)	0.0311 (5)
C11	0.04791 (14)	0.5662 (3)	0.15037 (15)	0.0353 (4)
H11	-0.0095	0.5976	0.1017	0.042*
C12	0.13142 (14)	0.5621 (3)	0.13407 (14)	0.0342 (4)
H12	0.1338	0.5904	0.0754	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01281 (17)	0.03481 (19)	0.03689 (19)	-0.00051 (5)	0.01054 (11)	-0.00146 (6)
S1	0.0174 (3)	0.0352 (3)	0.0500 (4)	-0.00152 (14)	0.0190 (3)	-0.00351 (17)
O1	0.0210 (7)	0.0697 (11)	0.0582 (9)	0.0136 (8)	0.0181 (6)	0.0197 (9)
O2	0.0275 (8)	0.0627 (11)	0.0810 (11)	-0.0076 (8)	0.0290 (8)	-0.0316 (10)
O3	0.0196 (9)	0.0565 (11)	0.0619 (12)	-0.0001 (5)	0.0136 (8)	-0.0056 (6)
O4	0.0369 (9)	0.0594 (11)	0.0942 (13)	0.0054 (8)	0.0427 (9)	0.0243 (10)
O5	0.0318 (8)	0.0794 (13)	0.1183 (16)	-0.0128 (9)	0.0366 (10)	-0.0596 (13)
O6	0.0289 (8)	0.0791 (13)	0.0921 (13)	0.0042 (8)	0.0254 (8)	0.0459 (11)
N1	0.0152 (9)	0.0393 (10)	0.0338 (9)	-0.0004 (5)	0.0083 (7)	-0.0008 (6)
N2	0.0186 (7)	0.0542 (11)	0.0399 (9)	0.0035 (7)	0.0125 (6)	0.0069 (8)
C1	0.0161 (11)	0.0381 (12)	0.0295 (10)	-0.0004 (6)	0.0082 (8)	0.0001 (6)
C2	0.0189 (11)	0.0288 (10)	0.0353 (12)	0.0000 (6)	0.0095 (9)	-0.0004 (6)
C3	0.0184 (11)	0.0377 (12)	0.0340 (12)	0.0001 (6)	0.0036 (9)	0.0009 (7)
C4	0.0283 (12)	0.0421 (12)	0.0277 (10)	-0.0005 (7)	0.0075 (9)	-0.0006 (7)
C5	0.0228 (11)	0.0398 (11)	0.0362 (11)	0.0007 (7)	0.0139 (9)	-0.0008 (7)
C6	0.0154 (10)	0.0387 (12)	0.0352 (11)	-0.0019 (6)	0.0074 (8)	-0.0013 (7)
C7	0.0183 (11)	0.0288 (10)	0.0499 (13)	-0.0005 (6)	0.0197 (10)	-0.0014 (7)
C8	0.0212 (10)	0.0388 (10)	0.0483 (13)	0.0048 (7)	0.0172 (9)	0.0074 (8)
C9	0.0254 (11)	0.0388 (11)	0.0469 (12)	0.0054 (7)	0.0209 (10)	0.0098 (8)
C10	0.0200 (11)	0.0287 (9)	0.0508 (12)	0.0002 (7)	0.0202 (9)	-0.0007 (8)
C11	0.0195 (9)	0.0427 (11)	0.0454 (11)	0.0000 (9)	0.0139 (8)	-0.0004 (10)
C12	0.0237 (9)	0.0419 (10)	0.0412 (10)	-0.0029 (9)	0.0169 (8)	-0.0012 (10)

Geometric parameters (\AA , $^\circ$)

Cd1—N1 ⁱ	2.230 (2)	C1—C2	1.341 (3)
Cd1—N1	2.230 (2)	C1—H1	0.9300
Cd1—O5 ⁱ	2.316 (2)	C2—C3	1.439 (3)
Cd1—O5	2.316 (2)	C2—C6	1.481 (3)
Cd1—O6 ⁱ	2.3479 (19)	C3—C4	1.357 (4)

Cd1—O6	2.3479 (19)	C3—H3	0.9300
S1—O4	1.463 (2)	C4—C5	1.353 (3)
S1—O3	1.470 (2)	C4—H4	0.9300
S1—O2	1.4742 (19)	C5—H5	0.9300
S1—C7	1.717 (2)	C7—C12	1.373 (3)
O1—C6	1.200 (3)	C7—C8	1.434 (4)
O5—H5A	0.8108	C8—C9	1.346 (3)
O5—H5B	0.8551	C8—H8	0.9300
O6—H6A	0.8517	C9—C10	1.384 (4)
O6—H6B	0.8328	C9—H9	0.9300
N1—C1	1.332 (3)	C10—C10 ⁱⁱ	1.439 (4)
N1—C5	1.387 (3)	C10—C11	1.443 (3)
N2—C6	1.368 (3)	C11—C12	1.341 (3)
N2—H2A	0.8600	C11—H11	0.9300
N2—H2B	0.8600	C12—H12	0.9300
N1 ⁱ —Cd1—N1	180.00 (6)	C2—C1—H1	120.7
N1 ⁱ —Cd1—O5 ⁱ	87.37 (7)	C1—C2—C3	119.9 (2)
N1—Cd1—O5 ⁱ	92.63 (7)	C1—C2—C6	118.8 (2)
N1 ⁱ —Cd1—O5	92.63 (6)	C3—C2—C6	121.2 (2)
N1—Cd1—O5	87.37 (7)	C4—C3—C2	121.5 (2)
O5 ⁱ —Cd1—O5	180.0	C4—C3—H3	119.2
N1 ⁱ —Cd1—O6 ⁱ	87.44 (7)	C2—C3—H3	119.2
N1—Cd1—O6 ⁱ	92.56 (7)	C5—C4—C3	115.4 (2)
O5 ⁱ —Cd1—O6 ⁱ	86.23 (10)	C5—C4—H4	122.3
O5—Cd1—O6 ⁱ	93.77 (10)	C3—C4—H4	122.3
N1 ⁱ —Cd1—O6	92.56 (7)	C4—C5—N1	123.5 (2)
N1—Cd1—O6	87.44 (7)	C4—C5—H5	118.3
O5 ⁱ —Cd1—O6	93.77 (10)	N1—C5—H5	118.3
O5—Cd1—O6	86.23 (10)	O1—C6—N2	124.3 (2)
O6 ⁱ —Cd1—O6	180.0	O1—C6—C2	117.0 (2)
O4—S1—O3	114.71 (11)	N2—C6—C2	118.65 (18)
O4—S1—O2	111.55 (16)	C12—C7—C8	123.5 (2)
O3—S1—O2	113.62 (11)	C12—C7—S1	115.34 (19)
O4—S1—C7	106.64 (9)	C8—C7—S1	121.17 (18)
O3—S1—C7	102.88 (13)	C9—C8—C7	119.9 (2)
O2—S1—C7	106.44 (9)	C9—C8—H8	120.1
Cd1—O5—H5A	131.1	C7—C8—H8	120.1
Cd1—O5—H5B	129.3	C8—C9—C10	117.6 (2)
H5A—O5—H5B	97.4	C8—C9—H9	121.2
Cd1—O6—H6A	126.9	C10—C9—H9	121.2
Cd1—O6—H6B	130.0	C9—C10—C10 ⁱⁱ	117.4 (3)
H6A—O6—H6B	97.1	C9—C10—C11	121.3 (2)
C1—N1—C5	120.96 (19)	C10 ⁱⁱ —C10—C11	121.4 (3)
C1—N1—Cd1	121.05 (16)	C12—C11—C10	121.50 (19)
C5—N1—Cd1	117.99 (15)	C12—C11—H11	119.3
C6—N2—H2A	120.0	C10—C11—H11	119.3

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C6—N2—H2B	120.0	C11—C12—C7	116.2 (2)
H2A—N2—H2B	120.0	C11—C12—H12	121.9
N1—C1—C2	118.7 (2)	C7—C12—H12	121.9
N1—C1—H1	120.7		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D—H\cdotsA</i>	<i>D—H</i>	<i>H\cdotsA</i>	<i>D\cdotsA</i>	<i>D—H\cdotsA</i>
O5—H5A \cdots O3 ⁱⁱⁱ	0.81	2.03	2.832 (3)	171
O5—H5B \cdots O4 ^{iv}	0.86	1.83	2.676 (2)	172
O6—H6A \cdots O3	0.85	1.93	2.777 (3)	178
O6—H6B \cdots O2 ^v	0.83	1.89	2.716 (3)	171
N2—H2A \cdots O1 ^{vi}	0.86	2.08	2.932 (2)	171
N2—H2B \cdots O2 ^{vii}	0.86	2.17	3.025 (3)	172

Symmetry codes: (iii) $x, y-1, z$; (iv) $-x+1, y-1, -z+1/2$; (v) $-x+1, y, -z+1/2$; (vi) $-x, -y, -z+1$; (vii) $x, -y, z+1/2$.

Fig. 1

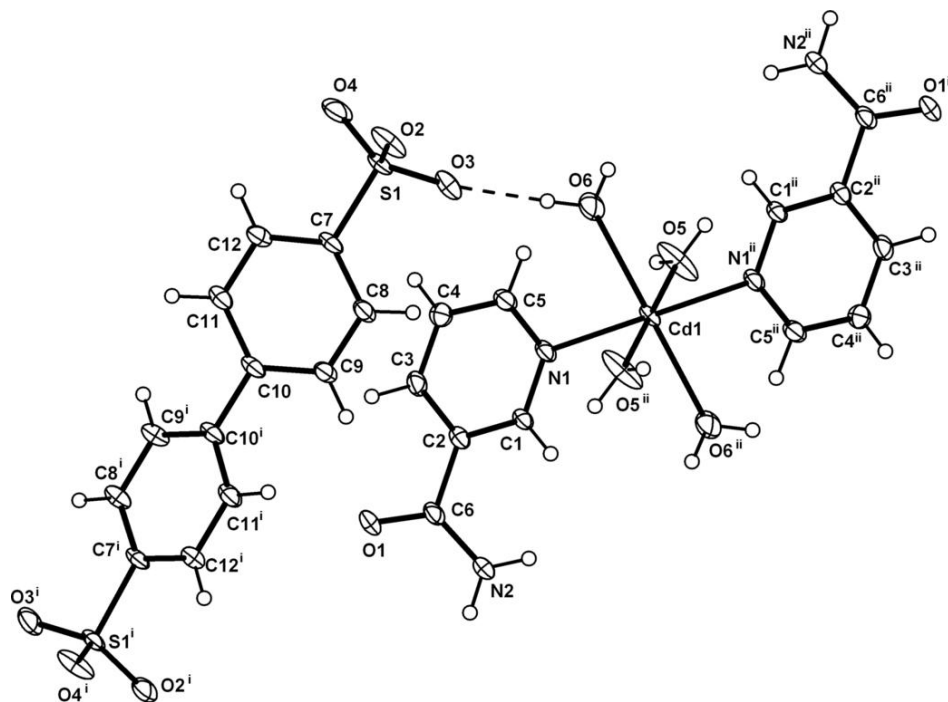


Fig. 2

