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# Di-$\mu$-thiocyanato-$\kappa^2N$:$S$;$\kappa^2S$:$N$-bis[bis(2-methyl-1*H*-benzimidazole-$\kappa N^3$)-(thiocyanato-$\kappa N$)cadmium(II)]

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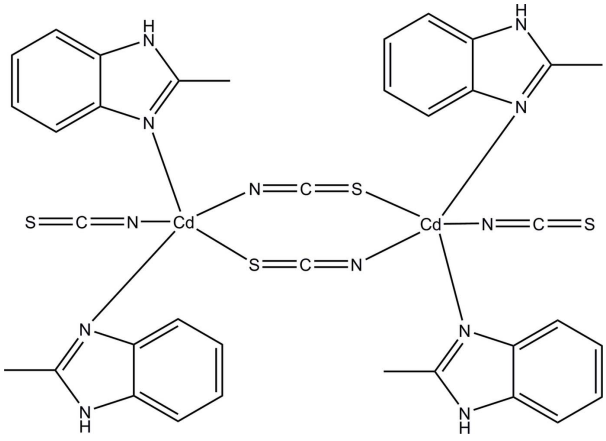
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.021; $wR$ factor = 0.047; data-to-parameter ratio = 14.2.

The title compound, $[Cd_2(NCS)_4(C_8H_8N_2)_4]$, is a centrosymmetric dinuclear cadmium(II) complex in which each two metal ions are linked by a pair of thiocyanate $N$:$S$-bridges. Two 2-methylbenzimidazole N-atom donors and one terminal thiocyanate N atom complete a highly distorted square-pyramidal geometry around the Cd atom. In the crystal structure, two N—H···S hydrogen-bonding interactions occur, resulting in a three-dimensional polymeric structure. The apical 2-methylbenzimidazole ring and its symmetry-related counterpart are arranged in an antiparallel manner with a centroid–centroid separation of 3.6050 (14) Å, indicative of a $\pi$–$\pi$ interaction.

## Related literature

For cadmium complexes having a $[Cd_2(\mu_2\text{-NCS})_2(NCS)_2]$ unit, see: Gou *et al.* (2008); Govor *et al.* (2008); Shi *et al.* (2004).




## Experimental

### Crystal data

$[Cd_2(NCS)_4(C_8H_8N_2)_4]$
$M_r$ = 985.78
Monoclinic, $C2/c$
$a$ = 18.1519 (11) Å
$b$ = 10.2098 (6) Å
$c$ = 21.7385 (13) Å
$\beta$ = 97.864 (1)°
$V$ = 3990.8 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.32 mm$^{-1}$
$T$ = 100 K
0.38 × 0.20 × 0.13 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.634, $T_{max}$ = 0.847
9361 measured reflections
3593 independent reflections
3213 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.047
$S$ = 1.03
3593 reflections
253 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 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···$A$ |
|---|---|---|---|---|
| N2—H2*N*···S1$^{i}$ | 0.86 (2) | 2.45 (2) | 3.273 (2) | 163 (2) |
| N4—H4*N*···S1$^{ii}$ | 0.84 (2) | 2.48 (2) | 3.281 (2) | 159 (2) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2278).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m1464 [ **doi:10.1107/S1600536810042443** ]

# Di-$\mu$-thiocyanato-$\kappa^2N$:$S$;$\kappa^2S$:$N$-bis[bis(2-methyl-1*H*-benzimidazole-$\kappa N^3$)(thiocyanato-$\kappa N$)cadmium(II)]

**S. A. Shaker, H. Khaledi and H. Mohd Ali**

## Comment

The title compound is a mixed-ligand cadmium(II) complex with thiocyanate and 2-methylbenzimidazole. The thiocyanate ions act as either bridging or terminal ligands. The pairs of the former, link each two metal ions into a centrosymmetric dinuclear complex. The resulting eight-membered $Cd_2(\mu_2\text{-NCS})_2$ ring is almost planar (r.m.s = 0.015), unlike the chair conformation observed in most of the similar structures (Gou *et al.* 2008; Govor *et al.* 2008; Shi *et al.* 2004). The terminal thiocyanate ligand forms two types of hydrogen bond with the amine hydrogen atoms (Fig. 2), leading to an infinite three-dimensional network. Two 2-methylbenzimidazole ligands, one in the apical position and the other one equatorially positioned, complete the penta-coordinate cadmium(II) complex in a highly distorted square pyramidal geometry ($\tau = 0.26$). The apical 2-methylbenzimidazole ring and its symmetry related counterpart at (-x+1, -y, -z+1) are arranged in an antiparallel manner with separation of 3.6050 (14) Å, indicative of a $\pi$-$\pi$ interaction.

## Experimental

An ethanolic solution (15 ml) of 2-methylbenzimidazole (1.32 g, 10 mmol) was added to an aqueous solution (20 ml) of $CdCl_2$. $H_2O$ (0.5 g, 2.5 mmol) followed by addition of an aqueous solution (15 ml) of KSCN (0.49 g, 5 mmol). The mixture was heated in a water bath for 30 min with constant stirring. The resulting precipitate was filtered off and recrystallized from ethanol to give the colorless crystals of the title cadmium(II) complex.

## Refinement

The C-bound hydrogen atoms were placed in idealized locations (C—H = 0.95–0.98 Å) and refined as riding on their parent carbon atoms. The N-bound hydrogen atoms were located in a difference Fourier map and were refined with distance restraints of N—H 0.88 (2) Å. *U*(H) were set to either 1.2 *U*eq of the parent atom, or 1.5 *U*eq(C) for methyl H. An additional rigid-bond type restraint (DELU in SHELXL97) was placed on the displacement parameters of S1 and C17.

## Figures

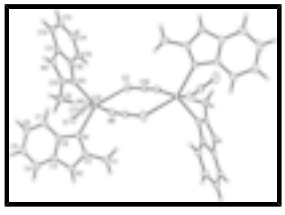

Fig. 1. The molecular structure of the title compound showing displacement ellipsoids at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. The unlabelled atoms are generated by the symmetry operation (–*x* + 1, –*y* + 1, –*z* + 1).

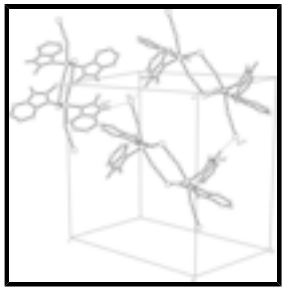

Fig. 2. A view of the hydrogen bonding interactions (dashed lines). C-bound hydrogen atoms have been omitted for clarity. Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z* + 1; (ii) *x* + 1/2, *y* + 1/2, *z*; (iii) -*x* + 3/2, -*y* + 3/2, -*z* + 1/2; (iv) -*x*+3/2, *y* - 1/2, - *z*+3/2.

**Di-μ-thiocyanato-κ$^2$*N*:*S*;κ$^2$*S*:*N*- bis[bis(2-methyl-1*H*-benzimidazole-κ*N*$^3$)(thiocyanato- κ*N*)cadmium(II)]**

*Crystal data*

| | |
|---|---|
| $[Cd_2(NCS)_4(C_8H_8N_2)_4]$ | $F(000) = 1968$ |
| $M_r = 985.78$ | $D_x = 1.641$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 4666 reflections |
| *a* = 18.1519 (11) Å | θ = 2.3–30.1° |
| *b* = 10.2098 (6) Å | μ = 1.32 mm$^{-1}$ |
| *c* = 21.7385 (13) Å | *T* = 100 K |
| β = 97.864 (1)° | Block, colorless |
| *V* = 3990.8 (4) Å$^3$ | 0.38 × 0.20 × 0.13 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 3593 independent reflections |
| Radiation source: fine-focus sealed tube | 3213 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.022$ |
| φ and ω scans | $\theta_{max} = 25.2°$, $\theta_{min} = 2.3°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | *h* = −21→21 |
| $T_{min} = 0.634$, $T_{max} = 0.847$ | *k* = −12→8 |
| 9361 measured reflections | *l* = −26→26 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.021$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.047$ | H atoms treated by a mixture of independent and constrained refinement |
| *S* = 1.03 | $w = 1/[\sigma^2(F_o^2) + (0.0169P)^2 + 6.0676P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3593 reflections | $(\Delta/\sigma)_{max} = 0.003$ |

| | |
|---|---|
| 253 parameters | $\Delta\rho_{max} = 0.35$ e Å$^{-3}$ |
| 3 restraints | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.611050 (9) | 0.354819 (16) | 0.590885 (7) | 0.01561 (6) |
| S1 | 0.88100 (3) | 0.33657 (6) | 0.67126 (3) | 0.02608 (15) |
| S2 | 0.63546 (3) | 0.42113 (7) | 0.47897 (3) | 0.02741 (16) |
| N1 | 0.62322 (10) | 0.41831 (19) | 0.69141 (9) | 0.0181 (4) |
| N2 | 0.63781 (11) | 0.5391 (2) | 0.77688 (9) | 0.0211 (5) |
| H2N | 0.6364 (14) | 0.609 (2) | 0.7982 (11) | 0.025* |
| N3 | 0.57608 (10) | 0.14637 (19) | 0.58946 (8) | 0.0166 (4) |
| N4 | 0.50684 (11) | −0.0294 (2) | 0.59628 (9) | 0.0193 (4) |
| H4N | 0.4715 (12) | −0.075 (2) | 0.6062 (11) | 0.023* |
| N5 | 0.73824 (11) | 0.3290 (2) | 0.60377 (10) | 0.0258 (5) |
| N6 | 0.49556 (11) | 0.4528 (2) | 0.57293 (9) | 0.0227 (5) |
| C1 | 0.57531 (15) | 0.6482 (2) | 0.68162 (12) | 0.0279 (6) |
| H1A | 0.5852 | 0.6462 | 0.6384 | 0.042* |
| H1B | 0.5953 | 0.7293 | 0.7014 | 0.042* |
| H1C | 0.5215 | 0.6444 | 0.6826 | 0.042* |
| C2 | 0.61150 (12) | 0.5342 (2) | 0.71553 (11) | 0.0195 (5) |
| C3 | 0.67023 (13) | 0.4198 (2) | 0.79411 (11) | 0.0199 (5) |
| C4 | 0.70777 (13) | 0.3741 (3) | 0.85017 (11) | 0.0256 (6) |
| H4 | 0.7157 | 0.4277 | 0.8862 | 0.031* |
| C5 | 0.73278 (13) | 0.2465 (3) | 0.85032 (11) | 0.0267 (6) |
| H5 | 0.7590 | 0.2115 | 0.8875 | 0.032* |
| C6 | 0.72085 (13) | 0.1674 (3) | 0.79777 (11) | 0.0244 (6) |
| H6 | 0.7376 | 0.0791 | 0.8004 | 0.029* |
| C7 | 0.68519 (13) | 0.2141 (2) | 0.74170 (11) | 0.0207 (5) |
| H7 | 0.6782 | 0.1606 | 0.7056 | 0.025* |
| C8 | 0.66004 (12) | 0.3433 (2) | 0.74051 (10) | 0.0180 (5) |
| C9 | 0.47424 (14) | 0.1670 (2) | 0.65538 (11) | 0.0235 (6) |
| H9A | 0.5070 | 0.1980 | 0.6921 | 0.035* |
| H9B | 0.4369 | 0.1074 | 0.6683 | 0.035* |
| H9C | 0.4493 | 0.2419 | 0.6333 | 0.035* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.51909 (12) | 0.0964 (2) | 0.61350 (10) | 0.0180 (5) |
| C11 | 0.55900 (12) | −0.0656 (2) | 0.55862 (10) | 0.0179 (5) |
| C12 | 0.57193 (13) | −0.1818 (2) | 0.52880 (11) | 0.0215 (5) |
| H12 | 0.5417 | −0.2570 | 0.5316 | 0.026* |
| C13 | 0.63096 (14) | −0.1828 (2) | 0.49486 (11) | 0.0224 (5) |
| H13 | 0.6421 | −0.2610 | 0.4743 | 0.027* |
| C14 | 0.67477 (13) | −0.0712 (2) | 0.49010 (11) | 0.0221 (5) |
| H14 | 0.7146 | −0.0752 | 0.4660 | 0.027* |
| C15 | 0.66144 (13) | 0.0441 (2) | 0.51961 (10) | 0.0191 (5) |
| H15 | 0.6914 | 0.1194 | 0.5164 | 0.023* |
| C16 | 0.60252 (12) | 0.0460 (2) | 0.55436 (10) | 0.0162 (5) |
| C17 | 0.79736 (13) | 0.3327 (2) | 0.63127 (11) | 0.0190 (5) |
| C18 | 0.55777 (13) | 0.4945 (2) | 0.44892 (10) | 0.0181 (5) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.01419 (9) | 0.01624 (10) | 0.01592 (9) | −0.00017 (7) | 0.00037 (6) | −0.00061 (7) |
| S1 | 0.0177 (3) | 0.0296 (4) | 0.0292 (3) | −0.0058 (3) | −0.0026 (3) | 0.0120 (3) |
| S2 | 0.0179 (3) | 0.0383 (4) | 0.0273 (3) | 0.0099 (3) | 0.0080 (3) | 0.0139 (3) |
| N1 | 0.0166 (10) | 0.0187 (11) | 0.0187 (10) | 0.0004 (8) | 0.0009 (8) | −0.0010 (9) |
| N2 | 0.0222 (11) | 0.0219 (12) | 0.0193 (11) | 0.0006 (9) | 0.0026 (9) | −0.0070 (9) |
| N3 | 0.0148 (9) | 0.0179 (10) | 0.0169 (9) | −0.0008 (8) | 0.0016 (8) | 0.0001 (8) |
| N4 | 0.0176 (10) | 0.0214 (11) | 0.0190 (10) | −0.0059 (8) | 0.0024 (8) | 0.0023 (9) |
| N5 | 0.0183 (11) | 0.0351 (13) | 0.0245 (11) | 0.0003 (9) | 0.0043 (9) | 0.0033 (10) |
| N6 | 0.0210 (11) | 0.0283 (12) | 0.0188 (10) | 0.0040 (9) | 0.0031 (9) | −0.0008 (9) |
| C1 | 0.0305 (14) | 0.0229 (14) | 0.0288 (13) | 0.0028 (11) | −0.0010 (12) | −0.0035 (12) |
| C2 | 0.0150 (11) | 0.0213 (13) | 0.0223 (12) | −0.0009 (10) | 0.0027 (10) | −0.0012 (11) |
| C3 | 0.0160 (12) | 0.0262 (14) | 0.0181 (12) | −0.0029 (10) | 0.0043 (10) | −0.0003 (11) |
| C4 | 0.0209 (13) | 0.0399 (17) | 0.0162 (12) | −0.0057 (11) | 0.0033 (10) | −0.0021 (11) |
| C5 | 0.0186 (13) | 0.0414 (17) | 0.0202 (13) | 0.0015 (11) | 0.0023 (10) | 0.0108 (12) |
| C6 | 0.0185 (12) | 0.0260 (14) | 0.0298 (14) | 0.0029 (10) | 0.0071 (11) | 0.0095 (11) |
| C7 | 0.0177 (12) | 0.0222 (14) | 0.0222 (12) | 0.0005 (10) | 0.0027 (10) | 0.0000 (11) |
| C8 | 0.0138 (11) | 0.0215 (13) | 0.0185 (12) | −0.0012 (10) | 0.0018 (9) | 0.0018 (10) |
| C9 | 0.0232 (13) | 0.0284 (15) | 0.0197 (12) | −0.0038 (11) | 0.0061 (10) | −0.0028 (11) |
| C10 | 0.0164 (12) | 0.0220 (13) | 0.0148 (11) | −0.0014 (10) | −0.0002 (10) | 0.0035 (10) |
| C11 | 0.0178 (12) | 0.0211 (13) | 0.0139 (11) | −0.0015 (10) | −0.0016 (9) | 0.0039 (10) |
| C12 | 0.0248 (13) | 0.0182 (13) | 0.0198 (12) | −0.0046 (10) | −0.0025 (10) | 0.0013 (10) |
| C13 | 0.0256 (13) | 0.0197 (13) | 0.0206 (12) | 0.0024 (10) | −0.0010 (11) | −0.0029 (10) |
| C14 | 0.0194 (12) | 0.0262 (14) | 0.0208 (12) | 0.0011 (10) | 0.0032 (10) | −0.0010 (11) |
| C15 | 0.0174 (12) | 0.0184 (13) | 0.0210 (12) | −0.0023 (10) | 0.0002 (10) | 0.0004 (10) |
| C16 | 0.0156 (11) | 0.0176 (12) | 0.0141 (11) | 0.0004 (9) | −0.0023 (9) | 0.0016 (10) |
| C17 | 0.0201 (12) | 0.0184 (13) | 0.0193 (12) | −0.0006 (10) | 0.0061 (10) | 0.0050 (10) |
| C18 | 0.0177 (12) | 0.0207 (13) | 0.0164 (12) | −0.0015 (10) | 0.0048 (10) | 0.0004 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cd1—N3 | 2.2199 (19) | C3—C8 | 1.394 (3) |
| Cd1—N1 | 2.2611 (19) | C4—C5 | 1.379 (4) |

| | | | |
|---|---|---|---|
| Cd1—N5 | 2.302 (2) | C4—H4 | 0.9500 |
| Cd1—N6 | 2.307 (2) | C5—C6 | 1.392 (4) |
| Cd1—S2 | 2.6207 (7) | C5—H5 | 0.9500 |
| S1—C17 | 1.644 (2) | C6—C7 | 1.385 (3) |
| S2—C18 | 1.651 (2) | C6—H6 | 0.9500 |
| N1—C2 | 1.323 (3) | C7—C8 | 1.394 (3) |
| N1—C8 | 1.406 (3) | C7—H7 | 0.9500 |
| N2—C2 | 1.355 (3) | C9—C10 | 1.488 (3) |
| N2—C3 | 1.382 (3) | C9—H9A | 0.9800 |
| N2—H2N | 0.856 (17) | C9—H9B | 0.9800 |
| N3—C10 | 1.323 (3) | C9—H9C | 0.9800 |
| N3—C16 | 1.401 (3) | C11—C12 | 1.388 (3) |
| N4—C10 | 1.347 (3) | C11—C16 | 1.396 (3) |
| N4—C11 | 1.384 (3) | C12—C13 | 1.382 (3) |
| N4—H4N | 0.844 (16) | C12—H12 | 0.9500 |
| N5—C17 | 1.155 (3) | C13—C14 | 1.401 (3) |
| N6—C18$^{i}$ | 1.152 (3) | C13—H13 | 0.9500 |
| C1—C2 | 1.482 (3) | C14—C15 | 1.378 (3) |
| C1—H1A | 0.9800 | C14—H14 | 0.9500 |
| C1—H1B | 0.9800 | C15—C16 | 1.391 (3) |
| C1—H1C | 0.9800 | C15—H15 | 0.9500 |
| C3—C4 | 1.393 (3) | C18—N6$^{i}$ | 1.152 (3) |
| N3—Cd1—N1 | 106.16 (7) | C4—C5—H5 | 118.9 |
| N3—Cd1—N5 | 99.90 (7) | C6—C5—H5 | 118.9 |
| N1—Cd1—N5 | 87.22 (7) | C7—C6—C5 | 121.6 (2) |
| N3—Cd1—N6 | 99.32 (7) | C7—C6—H6 | 119.2 |
| N1—Cd1—N6 | 90.32 (7) | C5—C6—H6 | 119.2 |
| N5—Cd1—N6 | 160.55 (7) | C6—C7—C8 | 117.1 (2) |
| N3—Cd1—S2 | 108.61 (5) | C6—C7—H7 | 121.5 |
| N1—Cd1—S2 | 144.74 (5) | C8—C7—H7 | 121.5 |
| N5—Cd1—S2 | 81.28 (5) | C3—C8—C7 | 120.6 (2) |
| N6—Cd1—S2 | 89.77 (5) | C3—C8—N1 | 108.9 (2) |
| C18—S2—Cd1 | 103.94 (8) | C7—C8—N1 | 130.5 (2) |
| C2—N1—C8 | 105.77 (19) | C10—C9—H9A | 109.5 |
| C2—N1—Cd1 | 129.77 (16) | C10—C9—H9B | 109.5 |
| C8—N1—Cd1 | 123.42 (15) | H9A—C9—H9B | 109.5 |
| C2—N2—C3 | 108.3 (2) | C10—C9—H9C | 109.5 |
| C2—N2—H2N | 122.1 (18) | H9A—C9—H9C | 109.5 |
| C3—N2—H2N | 129.4 (18) | H9B—C9—H9C | 109.5 |
| C10—N3—C16 | 106.11 (19) | N3—C10—N4 | 111.5 (2) |
| C10—N3—Cd1 | 126.99 (16) | N3—C10—C9 | 125.3 (2) |
| C16—N3—Cd1 | 126.17 (15) | N4—C10—C9 | 123.2 (2) |
| C10—N4—C11 | 108.57 (19) | N4—C11—C12 | 132.7 (2) |
| C10—N4—H4N | 123.9 (18) | N4—C11—C16 | 105.1 (2) |
| C11—N4—H4N | 127.4 (18) | C12—C11—C16 | 122.2 (2) |
| C17—N5—Cd1 | 154.70 (19) | C13—C12—C11 | 116.7 (2) |
| C18$^{i}$—N6—Cd1 | 164.86 (18) | C13—C12—H12 | 121.7 |
| C2—C1—H1A | 109.5 | C11—C12—H12 | 121.7 |

| | | | |
|---|---|---|---|
| C2—C1—H1B | 109.5 | C12—C13—C14 | 121.5 (2) |
| H1A—C1—H1B | 109.5 | C12—C13—H13 | 119.2 |
| C2—C1—H1C | 109.5 | C14—C13—H13 | 119.2 |
| H1A—C1—H1C | 109.5 | C15—C14—C13 | 121.5 (2) |
| H1B—C1—H1C | 109.5 | C15—C14—H14 | 119.2 |
| N1—C2—N2 | 111.7 (2) | C13—C14—H14 | 119.2 |
| N1—C2—C1 | 126.1 (2) | C14—C15—C16 | 117.5 (2) |
| N2—C2—C1 | 122.2 (2) | C14—C15—H15 | 121.2 |
| N2—C3—C4 | 132.2 (2) | C16—C15—H15 | 121.2 |
| N2—C3—C8 | 105.3 (2) | C15—C16—C11 | 120.5 (2) |
| C4—C3—C8 | 122.4 (2) | C15—C16—N3 | 130.7 (2) |
| C5—C4—C3 | 116.1 (2) | C11—C16—N3 | 108.8 (2) |
| C5—C4—H4 | 121.9 | N5—C17—S1 | 179.1 (2) |
| C3—C4—H4 | 121.9 | N6$^{i}$—C18—S2 | 178.5 (2) |
| C4—C5—C6 | 122.2 (2) | | |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2N···S1$^{ii}$ | 0.86 (2) | 2.44 (2) | 3.273 (2) | 163 (2) |
| N4—H4N···S1$^{iii}$ | 0.84 (2) | 2.48 (2) | 3.281 (2) | 159 (2) |

Symmetry codes: (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iii) *x*−1/2, *y*−1/2, *z*.

**Fig. 1**

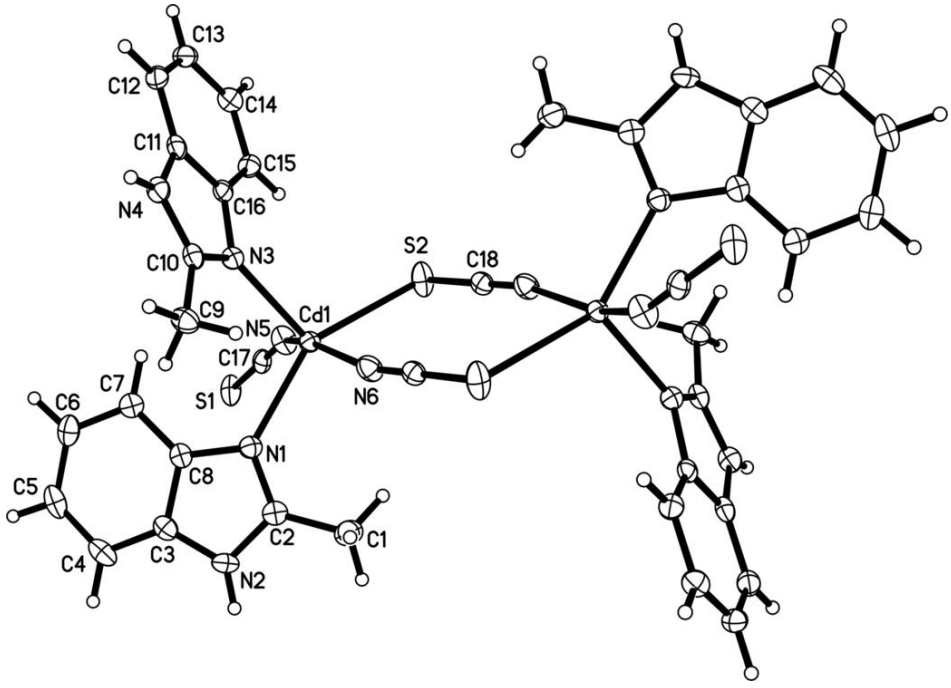
C13
C12
C14
C11
C15
N4
C16
C10
N3
S2
C18
C9
N5
Cd1
C17
S1
N6
C7
C6
N1
C8
C5
C2
C1
C3
C4
N2

**Fig. 2**