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Crystal structure of (4,4′-bipyridyl-κN)bis[*N*-(2-hydroxyethyl)-*N*-isopropyldithiocarbamato-$\kappa^2 S,S'$]-zinc(II)–4,4′-bipyridyl (2/1) and its isostructural cadmium(II) analogue

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The title structures, $[M(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot 0.5C_{10}H_8N_2$, for M = Zn, (I), and Cd, (II), feature terminally bound 4,4′-bipyridyl ligands and non-coordinating 4,4′-bipyridyl molecules, with the latter disposed about a centre of inversion. The coordination geometry about the metal atom is defined by two non-symmetrically chelating dithiocarbamate ligands and a pyridyl N atom. The NS_4 donor sets are distorted but, approximate to trigonal bipyramidal in each case. In the crystal, hydroxy-O—H···O(hydroxy) and hydroxy-O—H···N(pyridyl) hydrogen bonds between the zinc-containing molecules lead to a supramolecular layer parallel to (100). The three-dimensional architecture arises as the layers are linked *via* methine-C—H···S, pyridyl-C—H···O(hydroxy) and π–π [inter-centroid distance between coordinated pyridyl rings = 3.6246 (18) Å] interactions. Channels along the *c*-axis direction are occupied by the non-coordinating 4,4′-bipyridine molecules, which are held in place by C—H···π(chelate ring) contacts.

1. Chemical context

The ditopic ligand 4,4′-bipyridyl is ubiquitous in coordination chemistry, usually providing bridges between metal centres to generate coordination polymers. While bidentate bridging is normally observed in the structural chemistry of zinc(II) bis(*N*,*N*′-dialkyldithiocarbamate)s, these more often than not lead to binuclear species of the general formula $[Zn(S_2CNRR')_2]_2$(4,4′-bipyridyl) as first observed in the archetypal compound $[Zn(S_2CNEt_2)_2]_2$(4,4′-bipyridyl) (Zemskova *et al.*, 1994) and in other compounds relevant to the present study, such as $\{Zn[S_2CN(R)CH_2CH_2OH]_2\}_2$(4,4′-bipyridyl) for R = Me, Et and CH_2CH_2OH (Benson *et al.*, 2007). The exceptional structure is that of $Zn[S_2CN(n\text{-}Pr)_2]_2$-(4,4′-bipyridyl), which features a relatively rare monodentate coordination mode for the 4,4′-bipyridyl molecule (Klevtsova *et al.*, 2001). The analogous chemistry for cadmium(II) bis-(*N*,*N*′-dialkyldithiocarbamate)s is considerably less explored with the only example in the Cambridge Structural Database (Groom *et al.*, 2016) being a linear coordination polymer in the crystal of $\{Cd[S_2CN(CH_2Ph)_2]_2$(4,4′-bipyridyl)$\}_n$ (Fan *et al.*, 2007). The difference in chemistry between zinc and cadmium dithiocarbamates can be rationalized in terms of the larger size of cadmium *versus* zinc but, also in terms of the reduced Lewis acidity of the zinc atom owing to the strong chelation mode of the dithiocarbamate ligand. This is also true for cadmium whereby unusual coordination modes are found for

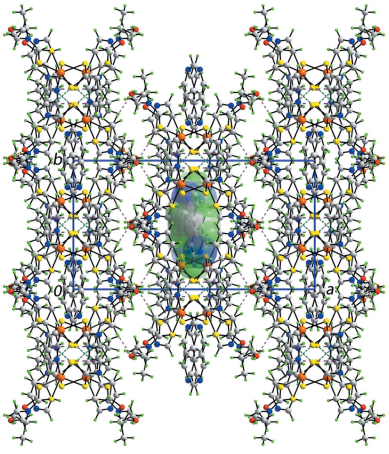


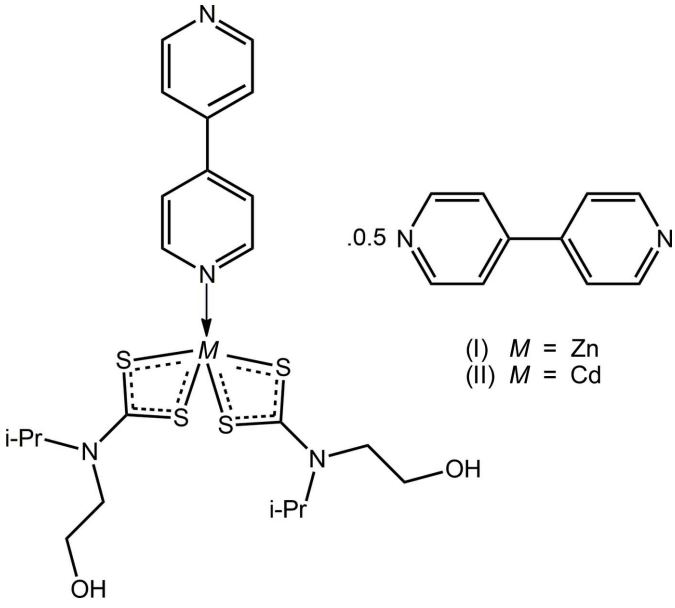
Table 1
Selected geometric parameters (Å, °) for (I).

Zn—N3	2.077 (2)	C1—S1	1.733 (3)
Zn—S1	2.3540 (10)	C1—S2	1.715 (3)
Zn—S2	2.5366 (9)	C7—S3	1.735 (3)
Zn—S3	2.3541 (9)	C7—S4	1.714 (3)
Zn—S4	2.5904 (9)		
S1—Zn—S3	124.19 (3)	S2—Zn—S4	162.87 (3)

Table 2
Selected geometric parameters (Å, °) for (II).

Cd—N3	2.3011 (11)	C1—S1	1.7310 (12)
Cd—S1	2.5547 (3)	C1—S2	1.7218 (12)
Cd—S2	2.6500 (3)	C7—S3	1.7328 (13)
Cd—S3	2.5620 (4)	C7—S4	1.7257 (13)
Cd—S4	2.6696 (4)		
S1—Cd—S3	125.725 (11)	S2—Cd—S4	165.865 (11)

related pyridyl-containing molecules that might otherwise be expected to be bridging. This is discussed further below in *Database survey*. In the present report, the crystal and molecular structures of two compounds, formulated as $Zn[S_2CN(i\text{-}Pr)CH_2CH_2OH]_2(4,4'\text{-bipyridyl})\cdot 0.5(4,4'\text{-bipyridyl})$ (I) and the cadmium analogue (II), are described, *i.e.* featuring monodentate and non-coordinating 4,4′-bipyridine molecules.



2. Structural commentary

The molecular structure of the constituents of (I) are shown in Fig. 1*a* and selected geometric parameters are collected in Table 1. The asymmetric unit comprises an entire molecule of $Zn[S_2CN(i\text{-}Pr)CH_2CH_2OH]_2(4,4'\text{-bipyridyl})$ and half a molecule of 4,4′-bipyridine, the latter being disposed about a centre of inversion. The zinc atom is coordinated by two dithiocarbamate ligands that form disparate Zn—S bond lengths. This is seen in the values of $\Delta(Zn-S) = Zn-S_{long} - Zn-S_{short}$, which compute to 0.19 and 0.23 Å for the S1- and S3-dithiocarbamate ligands, respectively. The fifth position in the coordination geometry is occupied by a pyridyl-N atom. Based on the value of τ (Addison *et al.*, 1984), which equals to 0.0 and 1.0 for ideal square-pyramidal and trigonal–bipyramidal geometries, respectively, it is possible to assign a coordination geometry based on the NS_4 donor set. In (I), τ = 0.64 indicating a highly distorted coordination geometry but, one approximating a trigonal bipyramid. In this description, the less tightly bound S2 and S4 atoms define the axial positions, Table 1. The coordinated 4,4′-bipyridyl molecule is non-planar with the dihedral angle between the two residues being 28.12 (14)°.

Crystals of (II) are isostructural to those of (I), Fig. 1*b* and Table 2. Some differences in molecular geometry are apparent, most notably in the degree of symmetry in the Cd—

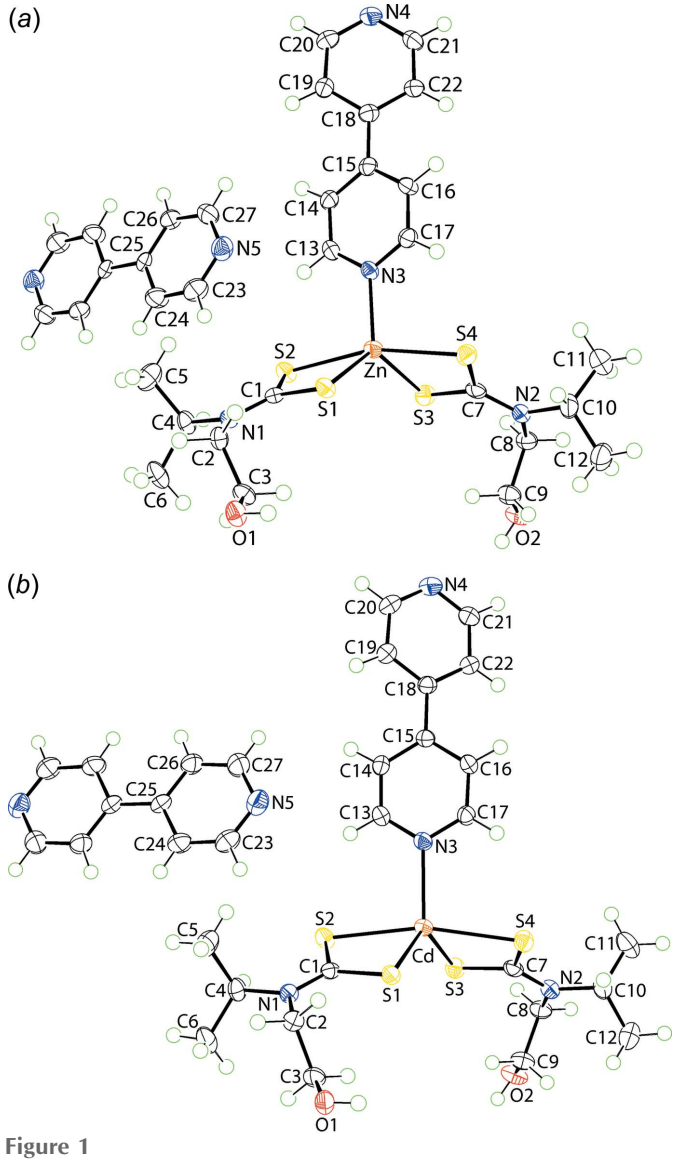


Figure 1
The molecular structures of the constituents of (*a*) (I) and (*b*) (II) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level. For each of (I) and (II), the 4,4′-bipyridine molecule has been expanded to show the entire molecule; unlabelled atoms are related by the symmetry operation $-x, 2-y, -z$.

Table 3
Hydrogen-bond geometry (Å, °) for (II).

*Cg*1 is the centroid of the Zn/S3/S4/C7 chelate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N4^{i}	0.83 (2)	1.88 (2)	2.7085 (15)	176 (1)
O2—H2*O*···O1^{ii}	0.83 (1)	1.89 (1)	2.7162 (14)	173 (2)
C4—H4···S2^{iii}	1.00	2.68	3.5395 (14)	144
C22—H22···O2^{iv}	0.95	2.40	3.3473 (17)	174
C26—H26···*Cg*1^{v}	0.95	3.00	3.776 (3)	140

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

Table 4
Hydrogen-bond geometry (Å, °) for (I).

*Cg*1 is the centroid of the Cd/S3/S4/C7 chelate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N4^{i}	0.85 (2)	1.85 (2)	2.697 (3)	179 (3)
O2—H2*O*···O1^{ii}	0.84 (2)	1.88 (2)	2.718 (3)	176 (4)
C4—H4···S2^{iii}	1.00	2.67	3.515 (3)	142
C22—H22···O2^{iv}	0.95	2.36	3.300 (3)	170
C26—H26···*Cg*1^{v}	0.95	3.04	3.7943 (15)	138

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

S bond lengths, *i.e.* Δ(Cd—S) = 0.09 and 0.11 Å for the S1- and S3-dithiocarbamate ligands, respectively. This is reflected in the narrower ranges in the C—S bond lengths in (II) *cf.* (I), Tables 1 and 2. The value of τ = 0.67 suggests a coordination geometry marginally closer to trigonal bipyramidal in (II) than for (I). The dihedral angle between the two rings comprising the coordinated 4,4′-bipyridyl molecule is 28.86 (7)°.

3. Supramolecular features

The molecular packing of (I) comprises conventional hydrogen bonding as well as a number of weaker, non-covalent interactions, Table 3. The presence of hydroxy-O—H···O(hydroxy) hydrogen bonds leads to the formation of a centrosymmetric, 28-membered $\{\cdots HOC_2NCSZnSCNC_2O\}_2$ synthon. This ring contains two additional hydroxy-O—H H atoms and these form hydroxy-O—H···N(pyridyl) hydrogen bonds with the non-coordinating end of the monodentate 4,4′-bipyridyl molecules. This network of hydrogen bonds leads to the formation of a two-dimensional array lying parallel to (100), Fig. 2*a*. These layers are connected into double-layers *via* methine-C—H···S and π–π interactions involving the coordinated pyridyl ring [inter-centroid distance between the (N3/C13–C17) and (N3/C13–C17)^{i} rings = 3.6246 (18) Å and angle of inclination = 0.46 (13)° for symmetry code (i): $-x, y, \frac{1}{2}-z$]. The double-layers are connected into a three-dimensional architecture *via* 4,4′-bipyridyl-C—H···O(hydroxy) interactions, involving an H atom from the non-coordinating ring of the coordinated 4,4′-bipyridyl molecule. This architecture defines channels parallel to the *c* axis in which residue the non-coordinating 4,4′-bipyridine molecules. The closest interaction between the host and guests are of the type pyridine-C—H···π(Zn/S3/S4/C7), *i.e.* C—H···π(chelate ring), a supramolecular synthon gaining prominence in the structural chemistry of metal-containing species (Tiekink, 2017), especially for dithiocarbamates (Tiekink & Zukerman-Schpector, 2011) owing to

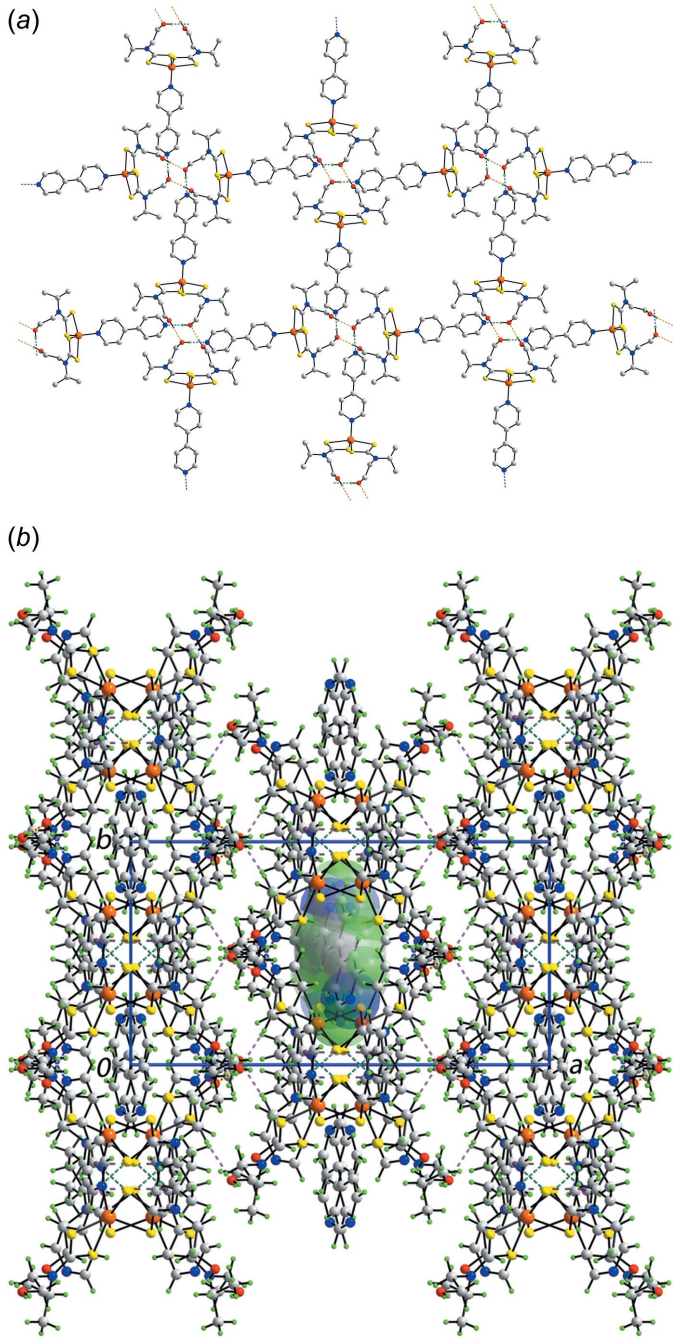


Figure 2
Molecular packing in (I): (*a*) view of two-dimensional supramolecular array sustained by hydroxy-O—H···O(hydroxy) and hydroxy-O–H···N(pyridyl) hydrogen bonding with all but the acidic H atoms removed and (*b*) a view of the unit-cell contents in projection down the *c* axis, with the non-coordinating 4,4′-bipyridine molecules in one channel highlighted in space-filling mode. The O—H···O, O—H···N, C—H···O, C—H···S and π–π interactions are shown as orange, blue, pink, sea-blue and purple dashed lines, respectively.

Table 5
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[Zn(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot0.5C_{10}H_8N_2$	$[Cd(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot0.5C_{10}H_8N_2$
M_r	656.22	703.25
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	100	100
a, *b*, *c* (Å)	22.418 (5), 11.501 (2), 25.094 (5)	22.7028 (12), 11.5950 (6), 24.8196 (13)
β (°)	105.50 (3)	103.385 (1)
V (Å^3)	6235 (2)	6356.0 (6)
Z	8	8
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	1.09	0.98
Crystal size (mm)	0.30 × 0.20 × 0.20	0.04 × 0.04 × 0.03
Data collection		
Diffractometer	Bruker SMART APEX CCD	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.968, 0.979	0.962, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31204, 7738, 5204	41284, 7847, 7204
R_{int}	0.082	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667	0.667
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.096, 1.00	0.019, 0.049, 0.99
No. of reflections	7738	7847
No. of parameters	358	358
No. of restraints	2	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.46	0.46, −0.24

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

the ability of the dithiocarbamate ligand to form strong chelating interactions (see above).

The molecular packing for isostructural (II) follows that just described for (I), Table 4. However, in this case, the putative pyridyl-C—H$\cdots\pi$(Cd/S3/S4/C7) interaction is just beyond the sum of the van der Waals radii for this type of contact (Spek, 2009).

4. Database survey

As mentioned in the *Chemical context*, ditopic ligands such as 4,4′-bipyridyl are normally observed providing bridges between metal centres. Thus, the structures of (I) and (II) are doubly curious as not only is the 4,4′-bipyridyl ligand coordinating in a monodentate fashion, there is a non-coordinating 4,4′-bipyridine molecule in the crystal. Recent reports confirm these interesting observations with related bipyridyl-type molecules of both the zinc(II) and, especially, cadmium(II) dithiocarbamates. Thus, just as for the 4,4′-bipyridyl structures mentioned in the *Chemical context*, *i.e.* $[Zn(S_2CNEt_2)_2]_2$(4,4′-bipyridyl) (Zemskova *et al.*, 1994) and $Zn[S_2CN(n\text{-}Pr)_2]_2$(4,4′-bipyridyl) (Klevtsova *et al.*, 2001), with the anticipated bidentate, bridging and non-anticipated terminal coordination, respectively, similar chemistry occurs for the ditopic ligand with an ethylene space, *i.e. trans*-bis(4-pyridyl)ethylene (bpe) where structures of both bridging, *i.e.* $[Zn(S_2CNEt_2)_2]_2$(bpe) (Arman *et al.*, 2009), and terminal, *i.e.* $Zn[S_2CN(n\text{-}Pr)_2]_2$(bpe) (Lai & Tiekink, 2003), coordination modes are known. Very recently, terminal coordination was found for 4-pyridinealdazine in the structure of $Zn[S_2CN(Me)CH_2CH_2OH_2]_2$(4-pyridinealdazine) (Broker *et al.*, 2017). In the realm of cadmium dithiocarbamates, the potentially bridging ligand just mentioned occurs in the structure of $Cd[S_2CN(n\text{-}Pr)CH_2CH_2OH_2]_2$(4-pyridinealdazine)$_2$ with both being terminally bound (Broker & Tiekink, 2011). The ditopic ligand bpe was mentioned above. In the case of cadmium dithiocarbamates, a bidentate, bridging mode is seen in the crystal of $[Cd(S_2CNEt_2)_2(bpe)]_n$ (Chai *et al.*, 2003). However, in another example both bridging and terminal modes, in a 1:2 ratio, are seen in the structure of $Cd[S_2CN(i\text{-}Pr)CH_2CH_2OH_2]_2(bpe)_3$ (Jotani *et al.*, 2016). The occurrence of unusual coordination modes for these bipyridyl-type ligands indicate additional factors are coming into play, often a competition between hydrogen bonding and *M*←N donor interactions but, not always as seen in the structure of $Zn[S_2CN(n\text{-}Pr)_2]_2$(4,4′-bipyridyl) (Klevtsova *et al.*, 2001).

5. Synthesis and crystallization

All chemicals and solvents were used as purchased without purification·The melting point was determined using an Krüss KSP1N melting point meter. The IR spectra were obtained by the attenuated total reflectance (ATR) technique on a Perkin Elmer RX1 FTIR spectrophotometer from 4000 to 400 cm^{-1}.

^{1}H and ^{13}C NMR spectra were recorded at room temperature in DMSO-d_6 solution on a Bruker Avance 400MHz NMR spectrometer.

Synthesis of (I): 4,4′-bipyridine (1.79 mmol, 0.28 g) in ethanol (25 ml) was added dropwise to bis(*N*-2-hydroxyethyl,*N*-isopropyldithiocarbamato)zinc(II) (1.21 mmol, 0.51 g) in ethanol (25 ml). The resulting mixture was stirred for 0.5 h follow by filtration. After a week of slow evaporation of the filtrate, yellow blocks precipitated (yield: 0.698 g, 88%; m.p. 445.6 K). IR (cm^{-1}): 1467 (*m*) [ν(C—N)], 1175 (*m*) [ν(C—S)] cm$^{-1.}$ ^{1}H NMR: δ 8.78–7.83 (*m*, 12H, aromatic H), 5.14 (*sept*, 2H, NCH, 6.63 Hz), 4.90 (*t*, 2H, OH, 5.38 Hz), 3.78–3.64 (*m*, 8H, NCH_2CH_2O), 1.18 (*d*, 12H, CH_3, 6.72 Hz). ^{13}C NMR: δ 204.15 (CS_2), 150.53, 144.65, 121.58 (aromatic-C), 58.21 (CH_2O), 55.53 (NCH_2), 49.80 (NCH), 19.88 (CH_3).

Synthesis of (II): 4,4′-bipyridine (1.61 mmol, 0.25 g) in ethanol (25 ml) was added dropwise to bis(*N*-2-hydroxyethyl,*N*-isopropyldithiocarbamato)cadmium(II) (1.07 mmol, 0.50 g) in ethanol (25 ml). The resulting mixture was stirred for 0.5 h follow by filtration. A week of slow evaporation of the filtrate yielded yellow blocks (yield: 0.652 g, 87%; m.p. 438.7 K). IR (cm^{-1}): 1467 (*m*) [ν(C—N)], 1174 (*m*) [ν(C—S)] cm$^{-1.}$ ^{1}H NMR: δ 8.79–7.80 (*m*, 12H, aromatic H), 5.22 (*sept*, 2H, NCH, 6.63 Hz), 4.84 (*t*, 2H, OH, 5.52 Hz), 3.80–3.64 (*m*, 8H, NCH_2CH_2O), 1.17 (*d*, 12H, CH_3, 6.72 Hz). ^{13}C NMR: δ 205.29 (CS_2), 150.57, 144.46, 121.41 (aromatic-C), 58.26 (CH_2O), 56.62 (NCH_2), 50.47 (NCH), 19.91 (CH_3).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. For each of (I) and (II), carbon-bound H atoms were placed in calculated positions (C—H = 0.95–1.00 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) set to 1.2–1.5U_{eq}(C). The O-bound H atoms were located in difference-Fourier maps but were refined with a distance restraint of O—H = 0.84±0.01 Å, and with U_{iso}(H) set to 1.5U_{eq}(O). For (I), owing to poor agreement, two reflections, *i.e.* (0 0 6) and (27 3 4), were omitted from the final cycles of refinement. For (II), one reflection, *i.e.* ($\overline{27}$ 7 7), was omitted for the same reason.

Acknowledgements

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References

Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
Arman, H. D., Poplaukhin, P. & Tiekink, E. R. T. (2009). *Acta Cryst.* E**65**, m1472–m1473.
Benson, R. E., Ellis, C. A., Lewis, C. E. & Tiekink, E. R. T. (2007). *CrystEngComm*, **9**, 930–941.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Broker, G. A., Jotani, M. M. & Tiekink, E. R. T. (2017). *Acta Cryst.* E**73**, 1458–1464.
Broker, G. A. & Tiekink, E. R. T. (2011). *Acta Cryst.* E**67**, m320–m321.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chai, J., Lai, C. S., Yan, J. & Tiekink, E. R. T. (2003). *Appl. Organomet. Chem.* **17**, 249–250.
Fan, J., Wei, F.-X., Zhang, W.-G., Yin, X., Lai, C.-S. & Tiekink, E. R. T. (2007). *Acta Chim. Sinica*, **65**, 2014–2018.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Jotani, M. M., Arman, H. D., Poplaukhin, P. & Tiekink, E. R. T. (2016). *Acta Cryst.* E**72**, 1700–1709.
Klevtsova, R. F., Glinskaya, L. A., Berus, E. I. & Larionov, S. V. (2001). *J. Struct. Chem.* **42**, 639–647.
Lai, C. S. & Tiekink, E. R. T. (2003). *Appl. Organomet. Chem.* **17**, 251–252.
Sheldrick, G. M. (1996). *SADABS* University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tiekink, E. R. T. (2017). *Coord. Chem. Rev.* **345**, 209–228.
Tiekink, E. R. T. & Zukerman-Schpector, J. (2011). *Chem. Commun.* **47**, 6623–6625.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zemskova, S. M., Glinskaya, L. A., Durasov, V. B., Klevtsova, R. F. & Larionov, S. V. (1994). *J. Struct. Chem.* **34**, 794–802.

supporting information

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Crystal structure of (4,4′-bipyridyl-κN)bis[*N*-(2-hydroxyethyl)-*N*-isopropyldithiocarbamato-$\kappa^2 S,S'$]zinc(II)–4,4′-bipyridyl (2/1) and its isostructural cadmium(II) analogue

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(4,4′-Bipyridyl-κN)bis[*N*-(2-hydroxyethyl)-*N*-isopropyldithiocarbamato-$\kappa^2 S,S'$]zinc(II)–4,4′-bipyridyl (2/1) (I)

Crystal data

$[Zn(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot 0.5C_{10}H_8N_2$
M_r = 656.22
Monoclinic, $C2/c$
a = 22.418 (5) Å
b = 11.501 (2) Å
c = 25.094 (5) Å
β = 105.50 (3)°
V = 6235 (2) Å^3
Z = 8
$F(000)$ = 2744
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3045 reflections
θ = 2.3–25.2°
μ = 1.09 mm^{-1}
T = 100 K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.979
31204 measured reflections
7738 independent reflections
5204 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −27→29
k = −15→15
l = −33→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
S = 1.00
7738 reflections
358 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.48 e Å^{-3} $\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.05280 (2)	0.31725 (3)	0.16518 (2)	0.01632 (9)
S1	−0.04838 (3)	0.24709 (6)	0.12760 (3)	0.01626 (15)
S2	0.00828 (3)	0.43350 (6)	0.07767 (3)	0.01723 (15)
S3	0.14139 (3)	0.24004 (6)	0.14471 (3)	0.01887 (16)
S4	0.09136 (3)	0.14774 (6)	0.23371 (3)	0.01927 (16)
O1	−0.20135 (9)	0.08393 (16)	0.01233 (8)	0.0200 (4)
H1O	−0.1869 (13)	0.034 (2)	0.0372 (9)	0.030*
O2	0.25910 (9)	−0.01819 (18)	0.09286 (8)	0.0250 (5)
H2O	0.2425 (14)	−0.036 (3)	0.0599 (6)	0.038*
N1	−0.10592 (10)	0.35160 (18)	0.03253 (9)	0.0138 (5)
N2	0.18772 (10)	0.05318 (19)	0.20497 (9)	0.0162 (5)
N3	0.06894 (10)	0.45571 (18)	0.22034 (9)	0.0147 (5)
N4	0.15344 (12)	0.9270 (2)	0.40786 (10)	0.0240 (6)
N5	0.02413 (12)	0.7932 (2)	0.11006 (10)	0.0260 (6)
C1	−0.05450 (12)	0.3457 (2)	0.07419 (11)	0.0140 (5)
C2	−0.15890 (12)	0.2760 (2)	0.03229 (11)	0.0157 (6)
H2A	−0.1974	0.3119	0.0093	0.019*
H2B	−0.1630	0.2682	0.0704	0.019*
C3	−0.15066 (13)	0.1563 (2)	0.00952 (11)	0.0180 (6)
H3A	−0.1488	0.1632	−0.0293	0.022*
H3B	−0.1114	0.1214	0.0314	0.022*
C4	−0.11249 (13)	0.4398 (2)	−0.01199 (11)	0.0183 (6)
H4	−0.0699	0.4635	−0.0129	0.022*
C5	−0.14485 (14)	0.5472 (2)	0.00182 (13)	0.0280 (7)
H5A	−0.1490	0.6049	−0.0277	0.042*
H5B	−0.1860	0.5258	0.0052	0.042*
H5C	−0.1204	0.5802	0.0369	0.042*
C6	−0.14513 (14)	0.3914 (3)	−0.06898 (11)	0.0265 (7)
H6A	−0.1484	0.4524	−0.0969	0.040*
H6B	−0.1213	0.3259	−0.0776	0.040*
H6C	−0.1867	0.3647	−0.0691	0.040*
C7	0.14472 (13)	0.1375 (2)	0.19613 (11)	0.0167 (6)
C8	0.23385 (12)	0.0495 (2)	0.17274 (11)	0.0185 (6)
H8A	0.2719	0.0110	0.1950	0.022*
H8B	0.2448	0.1300	0.1650	0.022*
C9	0.21025 (13)	−0.0148 (3)	0.11867 (11)	0.0208 (6)
H9A	0.1976	−0.0947	0.1255	0.025*
H9B	0.1740	0.0259	0.0947	0.025*

C10	0.19577 (13)	−0.0287 (2)	0.25202 (11)	0.0216 (6)
H10	0.1560	−0.0303	0.2629	0.026*
C11	0.24603 (15)	0.0160 (3)	0.30141 (12)	0.0342 (8)
H11A	0.2511	−0.0384	0.3324	0.051*
H11B	0.2852	0.0227	0.2912	0.051*
H11C	0.2341	0.0925	0.3124	0.051*
C12	0.20898 (15)	−0.1525 (2)	0.23619 (13)	0.0294 (7)
H12A	0.2140	−0.2037	0.2683	0.044*
H12B	0.1744	−0.1801	0.2061	0.044*
H12C	0.2471	−0.1532	0.2241	0.044*
C13	0.06136 (13)	0.5664 (2)	0.20303 (11)	0.0190 (6)
H13	0.0458	0.5809	0.1645	0.023*
C14	0.07504 (12)	0.6604 (2)	0.23849 (11)	0.0182 (6)
H14	0.0692	0.7373	0.2242	0.022*
C15	0.09742 (12)	0.6424 (2)	0.29521 (11)	0.0158 (6)
C16	0.10366 (12)	0.5272 (2)	0.31327 (11)	0.0165 (6)
H16	0.1175	0.5102	0.3517	0.020*
C17	0.08975 (12)	0.4380 (2)	0.27525 (11)	0.0169 (6)
H17	0.0951	0.3602	0.2884	0.020*
C18	0.11560 (13)	0.7408 (2)	0.33461 (11)	0.0172 (6)
C19	0.08885 (13)	0.8507 (2)	0.32338 (12)	0.0208 (6)
H19	0.0571	0.8641	0.2903	0.025*
C20	0.10898 (14)	0.9398 (2)	0.36078 (12)	0.0235 (7)
H20	0.0902	1.0141	0.3526	0.028*
C21	0.17857 (14)	0.8211 (2)	0.41830 (12)	0.0251 (7)
H21	0.2101	0.8102	0.4517	0.030*
C22	0.16164 (13)	0.7269 (2)	0.38367 (11)	0.0192 (6)
H22	0.1811	0.6536	0.3932	0.023*
C23	−0.00233 (15)	0.7643 (2)	0.05770 (13)	0.0277 (7)
H23	−0.0148	0.6858	0.0501	0.033*
C24	−0.01294 (14)	0.8414 (2)	0.01340 (12)	0.0256 (7)
H24	−0.0318	0.8151	−0.0231	0.031*
C25	0.00438 (12)	0.9574 (2)	0.02306 (11)	0.0152 (6)
C26	0.03155 (13)	0.9879 (2)	0.07766 (11)	0.0218 (6)
H26	0.0444	1.0658	0.0868	0.026*
C27	0.03987 (14)	0.9051 (3)	0.11860 (12)	0.0260 (7)
H27	0.0581	0.9292	0.1556	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.01770 (18)	0.01443 (16)	0.01542 (16)	−0.00168 (14)	0.00199 (13)	−0.00196 (13)
S1	0.0195 (4)	0.0144 (3)	0.0137 (3)	−0.0037 (3)	0.0024 (3)	0.0018 (3)
S2	0.0190 (4)	0.0162 (3)	0.0149 (3)	−0.0062 (3)	0.0019 (3)	0.0018 (3)
S3	0.0212 (4)	0.0169 (3)	0.0191 (4)	−0.0009 (3)	0.0062 (3)	0.0018 (3)
S4	0.0232 (4)	0.0183 (3)	0.0172 (4)	0.0032 (3)	0.0071 (3)	0.0019 (3)
O1	0.0201 (11)	0.0164 (10)	0.0207 (11)	−0.0046 (8)	0.0006 (9)	0.0059 (8)
O2	0.0193 (11)	0.0349 (12)	0.0216 (11)	−0.0052 (9)	0.0066 (9)	−0.0113 (10)

N1	0.0157 (12)	0.0126 (11)	0.0126 (11)	−0.0023 (9)	0.0031 (9)	0.0012 (8)
N2	0.0159 (12)	0.0178 (12)	0.0139 (11)	0.0007 (10)	0.0020 (9)	−0.0006 (9)
N3	0.0134 (12)	0.0159 (11)	0.0134 (11)	−0.0017 (9)	0.0010 (9)	−0.0001 (9)
N4	0.0313 (15)	0.0186 (12)	0.0204 (13)	0.0010 (11)	0.0039 (11)	−0.0049 (10)
N5	0.0279 (15)	0.0205 (13)	0.0284 (14)	0.0004 (11)	0.0055 (12)	0.0037 (11)
C1	0.0161 (14)	0.0120 (12)	0.0146 (13)	−0.0001 (11)	0.0050 (11)	−0.0028 (10)
C2	0.0113 (14)	0.0175 (13)	0.0176 (14)	−0.0014 (11)	0.0025 (11)	0.0039 (11)
C3	0.0165 (15)	0.0202 (14)	0.0163 (14)	−0.0059 (11)	0.0026 (11)	−0.0010 (11)
C4	0.0195 (15)	0.0186 (14)	0.0150 (14)	−0.0025 (12)	0.0014 (11)	0.0064 (11)
C5	0.0345 (19)	0.0170 (15)	0.0354 (18)	0.0029 (13)	0.0142 (15)	0.0076 (13)
C6	0.0271 (18)	0.0318 (17)	0.0162 (15)	−0.0034 (14)	−0.0020 (13)	0.0073 (13)
C7	0.0175 (15)	0.0154 (13)	0.0147 (14)	−0.0044 (11)	0.0003 (11)	−0.0047 (10)
C8	0.0153 (15)	0.0213 (14)	0.0189 (14)	−0.0005 (12)	0.0044 (12)	−0.0045 (11)
C9	0.0166 (15)	0.0242 (15)	0.0216 (15)	−0.0037 (12)	0.0047 (12)	−0.0049 (12)
C10	0.0215 (16)	0.0227 (15)	0.0200 (15)	0.0053 (13)	0.0046 (12)	0.0054 (12)
C11	0.039 (2)	0.0365 (19)	0.0228 (17)	0.0076 (16)	0.0007 (15)	0.0012 (14)
C12	0.0344 (19)	0.0234 (16)	0.0299 (18)	0.0057 (14)	0.0076 (15)	0.0068 (13)
C13	0.0201 (15)	0.0198 (14)	0.0143 (14)	0.0016 (12)	−0.0002 (12)	0.0007 (11)
C14	0.0198 (15)	0.0136 (13)	0.0195 (14)	0.0014 (11)	0.0022 (12)	−0.0002 (11)
C15	0.0115 (14)	0.0179 (14)	0.0181 (14)	0.0011 (11)	0.0042 (11)	−0.0021 (11)
C16	0.0193 (15)	0.0183 (14)	0.0115 (13)	−0.0017 (12)	0.0035 (11)	−0.0010 (11)
C17	0.0191 (15)	0.0138 (13)	0.0179 (14)	−0.0003 (11)	0.0050 (12)	0.0010 (11)
C18	0.0200 (16)	0.0154 (13)	0.0172 (14)	−0.0008 (11)	0.0067 (12)	−0.0008 (11)
C19	0.0212 (16)	0.0180 (14)	0.0206 (15)	0.0032 (12)	0.0012 (12)	−0.0015 (11)
C20	0.0289 (17)	0.0160 (14)	0.0250 (16)	0.0019 (13)	0.0065 (13)	−0.0040 (12)
C21	0.0324 (18)	0.0223 (15)	0.0161 (14)	0.0017 (14)	−0.0013 (13)	−0.0025 (12)
C22	0.0239 (16)	0.0163 (14)	0.0166 (14)	0.0008 (12)	0.0042 (12)	−0.0023 (11)
C23	0.0342 (19)	0.0154 (14)	0.0330 (18)	−0.0033 (13)	0.0077 (15)	−0.0007 (13)
C24	0.0342 (19)	0.0179 (15)	0.0233 (16)	−0.0031 (13)	0.0051 (14)	−0.0013 (12)
C25	0.0120 (14)	0.0135 (13)	0.0203 (14)	0.0026 (11)	0.0049 (11)	0.0014 (11)
C26	0.0270 (17)	0.0109 (13)	0.0255 (16)	−0.0030 (12)	0.0035 (13)	−0.0013 (11)
C27	0.0295 (18)	0.0244 (16)	0.0208 (16)	−0.0003 (14)	0.0009 (13)	−0.0022 (13)

Geometric parameters (Å, º)

Zn—N3	2.077 (2)	C8—H8A	0.9900
Zn—S1	2.3540 (10)	C8—H8B	0.9900
Zn—S2	2.5366 (9)	C9—H9A	0.9900
Zn—S3	2.3541 (9)	C9—H9B	0.9900
Zn—S4	2.5904 (9)	C10—C11	1.525 (4)
C1—S1	1.733 (3)	C10—C12	1.529 (4)
C1—S2	1.715 (3)	C10—H10	1.0000
C7—S3	1.735 (3)	C11—H11A	0.9800
C7—S4	1.714 (3)	C11—H11B	0.9800
O1—C3	1.426 (3)	C11—H11C	0.9800
O1—H1O	0.843 (10)	C12—H12A	0.9800
O2—C9	1.414 (3)	C12—H12B	0.9800
O2—H2O	0.837 (10)	C12—H12C	0.9800

N1—C1	1.335 (3)	C13—C14	1.381 (4)
N1—C2	1.471 (3)	C13—H13	0.9500
N1—C4	1.486 (3)	C14—C15	1.392 (4)
N2—C7	1.343 (3)	C14—H14	0.9500
N2—C8	1.474 (3)	C15—C16	1.396 (4)
N2—C10	1.483 (3)	C15—C18	1.486 (4)
N3—C13	1.341 (3)	C16—C17	1.378 (4)
N3—C17	1.347 (3)	C16—H16	0.9500
N4—C20	1.335 (4)	C17—H17	0.9500
N4—C21	1.338 (3)	C18—C22	1.388 (4)
N5—C23	1.331 (4)	C18—C19	1.395 (4)
N5—C27	1.337 (4)	C19—C20	1.381 (4)
C2—C3	1.520 (4)	C19—H19	0.9500
C2—H2A	0.9900	C20—H20	0.9500
C2—H2B	0.9900	C21—C22	1.377 (4)
C3—H3A	0.9900	C21—H21	0.9500
C3—H3B	0.9900	C22—H22	0.9500
C4—C5	1.519 (4)	C23—C24	1.391 (4)
C4—C6	1.527 (4)	C23—H23	0.9500
C4—H4	1.0000	C24—C25	1.393 (4)
C5—H5A	0.9800	C24—H24	0.9500
C5—H5B	0.9800	C25—C26	1.388 (4)
C5—H5C	0.9800	C25—C25^{i}	1.489 (5)
C6—H6A	0.9800	C26—C27	1.377 (4)
C6—H6B	0.9800	C26—H26	0.9500
C6—H6C	0.9800	C27—H27	0.9500
C8—C9	1.512 (4)		

N3—Zn—S1	120.49 (7)	O2—C9—C8	107.2 (2)
N3—Zn—S3	115.32 (7)	O2—C9—H9A	110.3
S1—Zn—S3	124.19 (3)	C8—C9—H9A	110.3
N3—Zn—S2	97.53 (6)	O2—C9—H9B	110.3
S1—Zn—S2	73.73 (3)	C8—C9—H9B	110.3
S3—Zn—S2	99.76 (3)	H9A—C9—H9B	108.5
N3—Zn—S4	99.60 (6)	N2—C10—C11	109.8 (2)
S1—Zn—S4	97.06 (3)	N2—C10—C12	112.1 (2)
S3—Zn—S4	73.12 (3)	C11—C10—C12	111.9 (2)
S2—Zn—S4	162.87 (3)	N2—C10—H10	107.6
C1—S1—Zn	87.38 (9)	C11—C10—H10	107.6
C1—S2—Zn	82.03 (9)	C12—C10—H10	107.6
C7—S3—Zn	88.01 (10)	C10—C11—H11A	109.5
C7—S4—Zn	81.07 (10)	C10—C11—H11B	109.5
C3—O1—H1O	106 (2)	H11A—C11—H11B	109.5
C9—O2—H2O	105 (2)	C10—C11—H11C	109.5
C1—N1—C2	120.0 (2)	H11A—C11—H11C	109.5
C1—N1—C4	121.0 (2)	H11B—C11—H11C	109.5
C2—N1—C4	118.8 (2)	C10—C12—H12A	109.5
C7—N2—C8	120.5 (2)	C10—C12—H12B	109.5

C7—N2—C10	121.3 (2)	H12A—C12—H12B	109.5
C8—N2—C10	117.7 (2)	C10—C12—H12C	109.5
C13—N3—C17	117.0 (2)	H12A—C12—H12C	109.5
C13—N3—Zn	121.84 (18)	H12B—C12—H12C	109.5
C17—N3—Zn	121.11 (17)	N3—C13—C14	123.2 (2)
C20—N4—C21	116.7 (2)	N3—C13—H13	118.4
C23—N5—C27	115.3 (3)	C14—C13—H13	118.4
N1—C1—S2	122.3 (2)	C13—C14—C15	120.0 (2)
N1—C1—S1	120.8 (2)	C13—C14—H14	120.0
S2—C1—S1	116.84 (15)	C15—C14—H14	120.0
N1—C2—C3	111.0 (2)	C14—C15—C16	116.8 (2)
N1—C2—H2A	109.4	C14—C15—C18	121.8 (2)
C3—C2—H2A	109.4	C16—C15—C18	121.4 (2)
N1—C2—H2B	109.4	C17—C16—C15	119.8 (2)
C3—C2—H2B	109.4	C17—C16—H16	120.1
H2A—C2—H2B	108.0	C15—C16—H16	120.1
O1—C3—C2	109.4 (2)	N3—C17—C16	123.2 (2)
O1—C3—H3A	109.8	N3—C17—H17	118.4
C2—C3—H3A	109.8	C16—C17—H17	118.4
O1—C3—H3B	109.8	C22—C18—C19	117.4 (2)
C2—C3—H3B	109.8	C22—C18—C15	120.6 (2)
H3A—C3—H3B	108.2	C19—C18—C15	121.9 (2)
N1—C4—C5	109.9 (2)	C20—C19—C18	119.4 (3)
N1—C4—C6	112.4 (2)	C20—C19—H19	120.3
C5—C4—C6	111.8 (2)	C18—C19—H19	120.3
N1—C4—H4	107.5	N4—C20—C19	123.4 (3)
C5—C4—H4	107.5	N4—C20—H20	118.3
C6—C4—H4	107.5	C19—C20—H20	118.3
C4—C5—H5A	109.5	N4—C21—C22	124.2 (3)
C4—C5—H5B	109.5	N4—C21—H21	117.9
H5A—C5—H5B	109.5	C22—C21—H21	117.9
C4—C5—H5C	109.5	C21—C22—C18	118.9 (3)
H5A—C5—H5C	109.5	C21—C22—H22	120.6
H5B—C5—H5C	109.5	C18—C22—H22	120.6
C4—C6—H6A	109.5	N5—C23—C24	124.5 (3)
C4—C6—H6B	109.5	N5—C23—H23	117.8
H6A—C6—H6B	109.5	C24—C23—H23	117.8
C4—C6—H6C	109.5	C23—C24—C25	119.4 (3)
H6A—C6—H6C	109.5	C23—C24—H24	120.3
H6B—C6—H6C	109.5	C25—C24—H24	120.3
N2—C7—S4	122.3 (2)	C26—C25—C24	116.3 (2)
N2—C7—S3	120.0 (2)	C26—C25—C25^{i}	122.2 (3)
S4—C7—S3	117.69 (16)	C24—C25—C25^{i}	121.5 (3)
N2—C8—C9	112.2 (2)	C27—C26—C25	119.9 (3)
N2—C8—H8A	109.2	C27—C26—H26	120.1
C9—C8—H8A	109.2	C25—C26—H26	120.1
N2—C8—H8B	109.2	N5—C27—C26	124.7 (3)
C9—C8—H8B	109.2	N5—C27—H27	117.7

H8A—C8—H8B	107.9	C26—C27—H27	117.7
C2—N1—C1—S2	−178.61 (19)	C17—N3—C13—C14	1.4 (4)
C4—N1—C1—S2	−3.1 (3)	Zn—N3—C13—C14	−176.2 (2)
C2—N1—C1—S1	1.6 (3)	N3—C13—C14—C15	−0.5 (4)
C4—N1—C1—S1	177.10 (19)	C13—C14—C15—C16	−1.3 (4)
Zn—S2—C1—N1	−178.6 (2)	C13—C14—C15—C18	177.0 (3)
Zn—S2—C1—S1	1.23 (13)	C14—C15—C16—C17	2.1 (4)
Zn—S1—C1—N1	178.5 (2)	C18—C15—C16—C17	−176.2 (3)
Zn—S1—C1—S2	−1.31 (14)	C13—N3—C17—C16	−0.5 (4)
C1—N1—C2—C3	−83.1 (3)	Zn—N3—C17—C16	177.1 (2)
C4—N1—C2—C3	101.3 (3)	C15—C16—C17—N3	−1.2 (4)
N1—C2—C3—O1	177.3 (2)	C14—C15—C18—C22	−150.2 (3)
C1—N1—C4—C5	−93.7 (3)	C16—C15—C18—C22	28.0 (4)
C2—N1—C4—C5	81.8 (3)	C14—C15—C18—C19	27.9 (4)
C1—N1—C4—C6	141.0 (3)	C16—C15—C18—C19	−153.9 (3)
C2—N1—C4—C6	−43.5 (3)	C22—C18—C19—C20	0.2 (4)
C8—N2—C7—S4	−178.27 (18)	C15—C18—C19—C20	−178.0 (3)
C10—N2—C7—S4	−6.7 (3)	C21—N4—C20—C19	−0.4 (4)
C8—N2—C7—S3	2.4 (3)	C18—C19—C20—N4	0.2 (5)
C10—N2—C7—S3	173.96 (19)	C20—N4—C21—C22	0.4 (5)
Zn—S4—C7—N2	−176.4 (2)	N4—C21—C22—C18	−0.1 (5)
Zn—S4—C7—S3	2.93 (13)	C19—C18—C22—C21	−0.2 (4)
Zn—S3—C7—N2	176.2 (2)	C15—C18—C22—C21	177.9 (3)
Zn—S3—C7—S4	−3.19 (14)	C27—N5—C23—C24	1.1 (5)
C7—N2—C8—C9	−86.4 (3)	N5—C23—C24—C25	−0.4 (5)
C10—N2—C8—C9	101.7 (3)	C23—C24—C25—C26	−0.1 (4)
N2—C8—C9—O2	−176.9 (2)	C23—C24—C25—C25^{i}	178.3 (3)
C7—N2—C10—C11	−94.0 (3)	C24—C25—C26—C27	−0.1 (4)
C8—N2—C10—C11	77.8 (3)	C25^{i}—C25—C26—C27	−178.5 (3)
C7—N2—C10—C12	140.9 (3)	C23—N5—C27—C26	−1.3 (5)
C8—N2—C10—C12	−47.3 (3)	C25—C26—C27—N5	0.8 (5)

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

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the Cd/S3/S4/C7 chelate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N4^{ii}	0.85 (2)	1.85 (2)	2.697 (3)	179 (3)
O2—H2*O*···O1^{iii}	0.84 (2)	1.88 (2)	2.718 (3)	176 (4)
C4—H4···S2^{iv}	1.00	2.67	3.515 (3)	142
C22—H22···O2^{v}	0.95	2.36	3.300 (3)	170
C26—H26···*Cg*1^{vi}	0.95	3.04	3.7943 (15)	138

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

(4,4′-Bipyridyl-κN)bis(*N*-2-hydroxyethyl-*N*-isopropyldithiocarbamato-κ²*S*,*S*′)cadmium(II)–4,4′-bipyridyl (2/1) (II)

Crystal data

$[Cd(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot 0.5C_{10}H_8N_2$
$M_r = 703.25$
Monoclinic, *C*2/*c*
$a = 22.7028$ (12) Å
$b = 11.5950$ (6) Å
$c = 24.8196$ (13) Å
$\beta = 103.385$ (1)°
$V = 6356.0$ (6) Å^3
$Z = 8$
$F(000) = 2888$
$D_x = 1.470$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 24754 reflections
$\theta = 2.2$–$28.3°$
$\mu = 0.98$ mm^{-1}
$T = 100$ K
Block, yellow
0.04 × 0.04 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.962$, $T_{max} = 0.971$
41284 measured reflections
7847 independent reflections
7204 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.7°$
$h = -30 \rightarrow 30$
$k = -15 \rightarrow 15$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.049$
$S = 0.99$
7847 reflections
358 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0249P)^2 + 6.291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd	0.04996 (2)	0.31263 (2)	0.16486 (2)	0.01723 (3)
S1	−0.05744 (2)	0.24286 (3)	0.12217 (2)	0.01723 (6)
S2	0.00085 (2)	0.43727 (3)	0.07636 (2)	0.01907 (7)
S3	0.14726 (2)	0.23031 (3)	0.14448 (2)	0.02008 (7)
S4	0.09406 (2)	0.14429 (3)	0.23619 (2)	0.02109 (7)
O1	−0.20171 (4)	0.08734 (8)	0.00837 (4)	0.02070 (19)
H1O	−0.1878 (8)	0.0408 (13)	0.0337 (6)	0.031*
O2	0.26295 (4)	−0.02139 (9)	0.09436 (4)	0.0253 (2)
H2O	0.2468 (8)	−0.0409 (17)	0.0620 (5)	0.038*

N1	−0.10858 (5)	0.35363 (9)	0.02905 (4)	0.0151 (2)
N2	0.19087 (5)	0.05102 (10)	0.20849 (4)	0.0180 (2)
N3	0.06811 (5)	0.46557 (9)	0.22553 (4)	0.0166 (2)
N4	0.15540 (6)	0.92852 (10)	0.41323 (5)	0.0257 (2)
N5	0.02716 (6)	0.79642 (11)	0.11132 (6)	0.0294 (3)
C1	−0.05999 (5)	0.34592 (10)	0.07123 (5)	0.0146 (2)
C2	−0.16139 (5)	0.27871 (11)	0.02738 (5)	0.0169 (2)
H2A	−0.1980	0.3156	0.0045	0.020*
H2B	−0.1676	0.2693	0.0653	0.020*
C3	−0.15277 (6)	0.16054 (11)	0.00341 (5)	0.0189 (2)
H3A	−0.1516	0.1683	−0.0360	0.023*
H3B	−0.1139	0.1266	0.0237	0.023*
C4	−0.11285 (6)	0.44310 (11)	−0.01475 (5)	0.0187 (2)
H4	−0.0706	0.4674	−0.0149	0.022*
C5	−0.14574 (7)	0.54876 (13)	−0.00028 (7)	0.0298 (3)
H5A	−0.1484	0.6072	−0.0293	0.045*
H5B	−0.1866	0.5269	0.0025	0.045*
H5C	−0.1234	0.5803	0.0352	0.045*
C6	−0.14156 (7)	0.39715 (14)	−0.07228 (6)	0.0269 (3)
H6A	−0.1434	0.4589	−0.0996	0.040*
H6B	−0.1172	0.3332	−0.0811	0.040*
H6C	−0.1826	0.3698	−0.0732	0.040*
C7	0.14824 (6)	0.13339 (11)	0.19783 (5)	0.0176 (2)
C8	0.23758 (6)	0.04441 (12)	0.17638 (5)	0.0198 (3)
H8A	0.2740	0.0063	0.1990	0.024*
H8B	0.2491	0.1234	0.1677	0.024*
C9	0.21556 (6)	−0.02239 (12)	0.12279 (6)	0.0216 (3)
H9A	0.2055	−0.1027	0.1309	0.026*
H9B	0.1788	0.0143	0.0999	0.026*
C10	0.19723 (6)	−0.02799 (12)	0.25659 (6)	0.0235 (3)
H10	0.1579	−0.0276	0.2682	0.028*
C11	0.24587 (8)	0.01794 (16)	0.30508 (6)	0.0369 (4)
H11A	0.2500	−0.0343	0.3368	0.055*
H11B	0.2846	0.0229	0.2941	0.055*
H11C	0.2342	0.0948	0.3154	0.055*
C12	0.20978 (7)	−0.15172 (13)	0.24188 (7)	0.0302 (3)
H12A	0.2136	−0.2008	0.2747	0.045*
H12B	0.1763	−0.1796	0.2124	0.045*
H12C	0.2475	−0.1544	0.2291	0.045*
C13	0.06012 (6)	0.57559 (11)	0.20834 (5)	0.0184 (2)
H13	0.0437	0.5903	0.1702	0.022*
C14	0.07479 (6)	0.66804 (11)	0.24394 (5)	0.0182 (2)
H14	0.0688	0.7446	0.2301	0.022*
C15	0.09848 (5)	0.64880 (11)	0.30033 (5)	0.0153 (2)
C16	0.10526 (6)	0.53450 (11)	0.31809 (5)	0.0168 (2)
H16	0.1201	0.5173	0.3562	0.020*
C17	0.09027 (6)	0.44634 (11)	0.27985 (5)	0.0172 (2)
H17	0.0959	0.3689	0.2925	0.021*

C18	0.11718 (6)	0.74550 (11)	0.33969 (5)	0.0167 (2)
C19	0.08995 (6)	0.85379 (12)	0.33087 (6)	0.0226 (3)
H19	0.0577	0.8671	0.2995	0.027*
C20	0.11034 (7)	0.94170 (12)	0.36829 (6)	0.0263 (3)
H20	0.0914	1.0150	0.3617	0.032*
C21	0.18115 (7)	0.82418 (12)	0.42167 (6)	0.0241 (3)
H21	0.2131	0.8134	0.4535	0.029*
C22	0.16396 (6)	0.73140 (11)	0.38674 (5)	0.0196 (2)
H22	0.1837	0.6590	0.3946	0.024*
C23	−0.00188 (8)	0.76757 (13)	0.05982 (7)	0.0323 (3)
H23	−0.0154	0.6902	0.0533	0.039*
C24	−0.01356 (7)	0.84325 (12)	0.01538 (6)	0.0288 (3)
H24	−0.0343	0.8172	−0.0203	0.035*
C25	0.00530 (6)	0.95788 (11)	0.02321 (5)	0.0188 (2)
C26	0.03523 (7)	0.98828 (12)	0.07680 (6)	0.0258 (3)
H26	0.0490	1.0651	0.0848	0.031*
C27	0.04485 (7)	0.90635 (13)	0.11837 (7)	0.0299 (3)
H27	0.0655	0.9299	0.1545	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01892 (5)	0.01605 (5)	0.01519 (5)	−0.00140 (3)	0.00083 (3)	−0.00184 (3)
S1	0.02100 (15)	0.01453 (14)	0.01510 (14)	−0.00512 (11)	0.00201 (11)	0.00145 (11)
S2	0.02016 (15)	0.01946 (15)	0.01593 (14)	−0.00819 (12)	0.00078 (11)	0.00279 (11)
S3	0.02200 (15)	0.02007 (15)	0.01891 (15)	−0.00138 (12)	0.00624 (12)	0.00193 (12)
S4	0.02419 (16)	0.02194 (16)	0.01883 (15)	0.00403 (12)	0.00847 (12)	0.00277 (12)
O1	0.0189 (4)	0.0182 (4)	0.0216 (5)	−0.0049 (4)	−0.0023 (4)	0.0050 (4)
O2	0.0196 (5)	0.0355 (6)	0.0214 (5)	−0.0060 (4)	0.0062 (4)	−0.0109 (4)
N1	0.0155 (5)	0.0150 (5)	0.0151 (5)	−0.0024 (4)	0.0041 (4)	0.0010 (4)
N2	0.0174 (5)	0.0204 (5)	0.0158 (5)	−0.0001 (4)	0.0028 (4)	−0.0006 (4)
N3	0.0167 (5)	0.0170 (5)	0.0150 (5)	−0.0016 (4)	0.0016 (4)	−0.0009 (4)
N4	0.0340 (7)	0.0196 (6)	0.0230 (6)	−0.0005 (5)	0.0057 (5)	−0.0054 (5)
N5	0.0313 (7)	0.0235 (6)	0.0328 (7)	0.0015 (5)	0.0061 (5)	0.0050 (5)
C1	0.0170 (6)	0.0129 (5)	0.0146 (5)	−0.0020 (4)	0.0052 (4)	−0.0016 (4)
C2	0.0135 (5)	0.0172 (6)	0.0198 (6)	−0.0028 (4)	0.0036 (5)	0.0001 (5)
C3	0.0172 (6)	0.0188 (6)	0.0192 (6)	−0.0040 (5)	0.0015 (5)	−0.0023 (5)
C4	0.0186 (6)	0.0207 (6)	0.0167 (6)	−0.0018 (5)	0.0036 (5)	0.0054 (5)
C5	0.0379 (8)	0.0205 (7)	0.0345 (8)	0.0032 (6)	0.0156 (7)	0.0084 (6)
C6	0.0281 (7)	0.0324 (8)	0.0175 (6)	−0.0029 (6)	−0.0002 (5)	0.0056 (6)
C7	0.0188 (6)	0.0182 (6)	0.0146 (5)	−0.0037 (5)	0.0014 (4)	−0.0033 (5)
C8	0.0168 (6)	0.0228 (6)	0.0197 (6)	−0.0019 (5)	0.0038 (5)	−0.0047 (5)
C9	0.0192 (6)	0.0248 (7)	0.0211 (6)	−0.0047 (5)	0.0055 (5)	−0.0067 (5)
C10	0.0236 (7)	0.0269 (7)	0.0191 (6)	0.0044 (5)	0.0031 (5)	0.0046 (5)
C11	0.0408 (9)	0.0442 (10)	0.0199 (7)	0.0038 (8)	−0.0047 (6)	0.0004 (7)
C12	0.0320 (8)	0.0254 (7)	0.0336 (8)	0.0054 (6)	0.0087 (6)	0.0083 (6)
C13	0.0188 (6)	0.0203 (6)	0.0149 (6)	0.0009 (5)	0.0013 (5)	0.0010 (5)
C14	0.0192 (6)	0.0159 (6)	0.0182 (6)	0.0024 (5)	0.0018 (5)	0.0019 (5)

C15	0.0131 (5)	0.0164 (6)	0.0160 (6)	0.0000 (4)	0.0028 (4)	−0.0020 (4)
C16	0.0175 (6)	0.0187 (6)	0.0136 (5)	−0.0006 (5)	0.0026 (4)	0.0011 (4)
C17	0.0184 (6)	0.0158 (6)	0.0166 (6)	−0.0018 (5)	0.0025 (5)	0.0015 (5)
C18	0.0187 (6)	0.0158 (6)	0.0164 (6)	−0.0008 (5)	0.0055 (5)	−0.0009 (5)
C19	0.0254 (7)	0.0199 (6)	0.0213 (6)	0.0050 (5)	0.0032 (5)	−0.0009 (5)
C20	0.0337 (8)	0.0170 (6)	0.0273 (7)	0.0053 (6)	0.0055 (6)	−0.0029 (5)
C21	0.0283 (7)	0.0224 (7)	0.0188 (6)	−0.0006 (5)	−0.0005 (5)	−0.0034 (5)
C22	0.0228 (6)	0.0166 (6)	0.0188 (6)	0.0019 (5)	0.0036 (5)	−0.0012 (5)
C23	0.0436 (9)	0.0152 (6)	0.0365 (8)	−0.0051 (6)	0.0062 (7)	0.0002 (6)
C24	0.0392 (8)	0.0171 (6)	0.0284 (7)	−0.0059 (6)	0.0045 (6)	−0.0032 (6)
C25	0.0169 (6)	0.0146 (6)	0.0256 (7)	0.0011 (5)	0.0067 (5)	−0.0018 (5)
C26	0.0272 (7)	0.0182 (6)	0.0291 (7)	−0.0026 (5)	0.0010 (6)	−0.0026 (5)
C27	0.0328 (8)	0.0253 (7)	0.0284 (7)	−0.0006 (6)	0.0003 (6)	0.0005 (6)

Geometric parameters (Å, º)

Cd—N3	2.3011 (11)	C8—H8A	0.9900
Cd—S1	2.5547 (3)	C8—H8B	0.9900
Cd—S2	2.6500 (3)	C9—H9A	0.9900
Cd—S3	2.5620 (4)	C9—H9B	0.9900
Cd—S4	2.6696 (4)	C10—C12	1.523 (2)
C1—S1	1.7310 (12)	C10—C11	1.528 (2)
C1—S2	1.7218 (12)	C10—H10	1.0000
C7—S3	1.7328 (13)	C11—H11A	0.9800
C7—S4	1.7257 (13)	C11—H11B	0.9800
O1—C3	1.4259 (15)	C11—H11C	0.9800
O1—H1O	0.833 (9)	C12—H12A	0.9800
O2—C9	1.4168 (16)	C12—H12B	0.9800
O2—H2O	0.832 (9)	C12—H12C	0.9800
N1—C1	1.3364 (16)	C13—C14	1.3801 (18)
N1—C2	1.4733 (15)	C13—H13	0.9500
N1—C4	1.4895 (16)	C14—C15	1.3960 (17)
N2—C7	1.3416 (17)	C14—H14	0.9500
N2—C8	1.4688 (16)	C15—C16	1.3940 (17)
N2—C10	1.4851 (17)	C15—C18	1.4832 (17)
N3—C13	1.3441 (16)	C16—C17	1.3827 (17)
N3—C17	1.3441 (16)	C16—H16	0.9500
N4—C20	1.3363 (19)	C17—H17	0.9500
N4—C21	1.3389 (18)	C18—C19	1.3942 (18)
N5—C27	1.3356 (19)	C18—C22	1.3944 (18)
N5—C23	1.338 (2)	C19—C20	1.3846 (19)
C2—C3	1.5242 (18)	C19—H19	0.9500
C2—H2A	0.9900	C20—H20	0.9500
C2—H2B	0.9900	C21—C22	1.3801 (18)
C3—H3A	0.9900	C21—H21	0.9500
C3—H3B	0.9900	C22—H22	0.9500
C4—C5	1.520 (2)	C23—C24	1.386 (2)
C4—C6	1.5220 (19)	C23—H23	0.9500

C4—H4	1.0000	C24—C25	1.3960 (18)
C5—H5A	0.9800	C24—H24	0.9500
C5—H5B	0.9800	C25—C26	1.3917 (19)
C5—H5C	0.9800	C25—C25^{i}	1.487 (3)
C6—H6A	0.9800	C26—C27	1.382 (2)
C6—H6B	0.9800	C26—H26	0.9500
C6—H6C	0.9800	C27—H27	0.9500
C8—C9	1.5202 (18)		

N3—Cd—S1	121.64 (3)	O2—C9—C8	107.32 (10)
N3—Cd—S3	112.61 (3)	O2—C9—H9A	110.3
S1—Cd—S3	125.725 (11)	C8—C9—H9A	110.3
N3—Cd—S2	95.71 (3)	O2—C9—H9B	110.3
S1—Cd—S2	69.571 (10)	C8—C9—H9B	110.3
S3—Cd—S2	104.839 (11)	H9A—C9—H9B	108.5
N3—Cd—S4	98.43 (3)	N2—C10—C12	112.15 (11)
S1—Cd—S4	102.645 (11)	N2—C10—C11	109.64 (12)
S3—Cd—S4	69.533 (10)	C12—C10—C11	112.07 (13)
S2—Cd—S4	165.865 (11)	N2—C10—H10	107.6
C1—S1—Cd	87.22 (4)	C12—C10—H10	107.6
C1—S2—Cd	84.39 (4)	C11—C10—H10	107.6
C7—S3—Cd	87.13 (4)	C10—C11—H11A	109.5
C7—S4—Cd	83.88 (5)	C10—C11—H11B	109.5
C3—O1—H1O	106.5 (13)	H11A—C11—H11B	109.5
C9—O2—H2O	105.2 (13)	C10—C11—H11C	109.5
C1—N1—C2	120.10 (10)	H11A—C11—H11C	109.5
C1—N1—C4	121.37 (10)	H11B—C11—H11C	109.5
C2—N1—C4	118.36 (10)	C10—C12—H12A	109.5
C7—N2—C8	120.56 (11)	C10—C12—H12B	109.5
C7—N2—C10	121.95 (11)	H12A—C12—H12B	109.5
C8—N2—C10	117.13 (11)	C10—C12—H12C	109.5
C13—N3—C17	117.88 (11)	H12A—C12—H12C	109.5
C13—N3—Cd	122.21 (8)	H12B—C12—H12C	109.5
C17—N3—Cd	119.83 (8)	N3—C13—C14	122.62 (12)
C20—N4—C21	117.14 (12)	N3—C13—H13	118.7
C27—N5—C23	115.51 (13)	C14—C13—H13	118.7
N1—C1—S2	121.29 (9)	C13—C14—C15	119.85 (12)
N1—C1—S1	120.01 (9)	C13—C14—H14	120.1
S2—C1—S1	118.69 (7)	C15—C14—H14	120.1
N1—C2—C3	111.34 (10)	C16—C15—C14	117.23 (11)
N1—C2—H2A	109.4	C16—C15—C18	121.11 (11)
C3—C2—H2A	109.4	C14—C15—C18	121.64 (11)
N1—C2—H2B	109.4	C17—C16—C15	119.62 (11)
C3—C2—H2B	109.4	C17—C16—H16	120.2
H2A—C2—H2B	108.0	C15—C16—H16	120.2
O1—C3—C2	109.17 (10)	N3—C17—C16	122.77 (12)
O1—C3—H3A	109.8	N3—C17—H17	118.6
C2—C3—H3A	109.8	C16—C17—H17	118.6

O1—C3—H3B	109.8	C19—C18—C22	117.47 (12)
C2—C3—H3B	109.8	C19—C18—C15	121.90 (12)
H3A—C3—H3B	108.3	C22—C18—C15	120.62 (11)
N1—C4—C5	109.96 (11)	C20—C19—C18	119.37 (13)
N1—C4—C6	112.47 (11)	C20—C19—H19	120.3
C5—C4—C6	112.12 (12)	C18—C19—H19	120.3
N1—C4—H4	107.3	N4—C20—C19	123.24 (13)
C5—C4—H4	107.3	N4—C20—H20	118.4
C6—C4—H4	107.3	C19—C20—H20	118.4
C4—C5—H5A	109.5	N4—C21—C22	123.81 (13)
C4—C5—H5B	109.5	N4—C21—H21	118.1
H5A—C5—H5B	109.5	C22—C21—H21	118.1
C4—C5—H5C	109.5	C21—C22—C18	118.98 (12)
H5A—C5—H5C	109.5	C21—C22—H22	120.5
H5B—C5—H5C	109.5	C18—C22—H22	120.5
C4—C6—H6A	109.5	N5—C23—C24	124.26 (14)
C4—C6—H6B	109.5	N5—C23—H23	117.9
H6A—C6—H6B	109.5	C24—C23—H23	117.9
C4—C6—H6C	109.5	C23—C24—C25	119.73 (14)
H6A—C6—H6C	109.5	C23—C24—H24	120.1
H6B—C6—H6C	109.5	C25—C24—H24	120.1
N2—C7—S4	121.13 (10)	C26—C25—C24	116.13 (13)
N2—C7—S3	119.58 (10)	C26—C25—C25^{i}	121.98 (15)
S4—C7—S3	119.30 (8)	C24—C25—C25^{i}	121.88 (15)
N2—C8—C9	111.65 (10)	C27—C26—C25	119.81 (13)
N2—C8—H8A	109.3	C27—C26—H26	120.1
C9—C8—H8A	109.3	C25—C26—H26	120.1
N2—C8—H8B	109.3	N5—C27—C26	124.56 (14)
C9—C8—H8B	109.3	N5—C27—H27	117.7
H8A—C8—H8B	108.0	C26—C27—H27	117.7

C2—N1—C1—S2	−176.55 (9)	C17—N3—C13—C14	1.25 (19)
C4—N1—C1—S2	−1.29 (16)	Cd—N3—C13—C14	−175.45 (10)
C2—N1—C1—S1	3.28 (16)	N3—C13—C14—C15	−0.6 (2)
C4—N1—C1—S1	178.54 (9)	C13—C14—C15—C16	−1.00 (19)
Cd—S2—C1—N1	−176.80 (10)	C13—C14—C15—C18	177.49 (12)
Cd—S2—C1—S1	3.36 (6)	C14—C15—C16—C17	1.82 (18)
Cd—S1—C1—N1	176.69 (10)	C18—C15—C16—C17	−176.68 (12)
Cd—S1—C1—S2	−3.48 (7)	C13—N3—C17—C16	−0.37 (19)
C1—N1—C2—C3	−83.28 (14)	Cd—N3—C17—C16	176.41 (9)
C4—N1—C2—C3	101.32 (13)	C15—C16—C17—N3	−1.19 (19)
N1—C2—C3—O1	173.57 (10)	C16—C15—C18—C19	−152.60 (13)
C1—N1—C4—C5	−93.77 (14)	C14—C15—C18—C19	28.96 (19)
C2—N1—C4—C5	81.57 (14)	C16—C15—C18—C22	28.66 (18)
C1—N1—C4—C6	140.52 (12)	C14—C15—C18—C22	−149.77 (13)
C2—N1—C4—C6	−44.15 (15)	C22—C18—C19—C20	0.4 (2)
C8—N2—C7—S4	−178.55 (9)	C15—C18—C19—C20	−178.33 (13)
C10—N2—C7—S4	−5.59 (17)	C21—N4—C20—C19	−0.3 (2)

C8—N2—C7—S3	1.70 (16)	C18—C19—C20—N4	−0.1 (2)
C10—N2—C7—S3	174.65 (10)	C20—N4—C21—C22	0.3 (2)
Cd—S4—C7—N2	−176.04 (10)	N4—C21—C22—C18	0.1 (2)
Cd—S4—C7—S3	3.71 (7)	C19—C18—C22—C21	−0.45 (19)
Cd—S3—C7—N2	175.91 (10)	C15—C18—C22—C21	178.35 (12)
Cd—S3—C7—S4	−3.85 (7)	C27—N5—C23—C24	0.4 (2)
C7—N2—C8—C9	−84.72 (15)	N5—C23—C24—C25	−0.2 (3)
C10—N2—C8—C9	102.00 (13)	C23—C24—C25—C26	−0.1 (2)
N2—C8—C9—O2	178.55 (11)	C23—C24—C25—C25^{i}	179.10 (16)
C7—N2—C10—C12	138.65 (13)	C24—C25—C26—C27	0.3 (2)
C8—N2—C10—C12	−48.17 (16)	C25^{i}—C25—C26—C27	−178.94 (16)
C7—N2—C10—C11	−96.19 (15)	C23—N5—C27—C26	−0.2 (2)
C8—N2—C10—C11	76.99 (15)	C25—C26—C27—N5	−0.1 (2)

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

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the Zn/S3/S4/C7 chelate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N4^{ii}	0.83 (2)	1.88 (2)	2.7085 (15)	176 (1)
O2—H2*O*···O1^{iii}	0.83 (1)	1.89 (1)	2.7162 (14)	173 (2)
C4—H4···S2^{iv}	1.00	2.68	3.5395 (14)	144
C22—H22···O2^{v}	0.95	2.40	3.3473 (17)	174
C26—H26···*Cg*1^{vi}	0.95	3.00	3.776 (3)	140

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