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(Phenylmethanethiolato)(1,5,9-triazacyclododecane)zinc(II) thiocyanate

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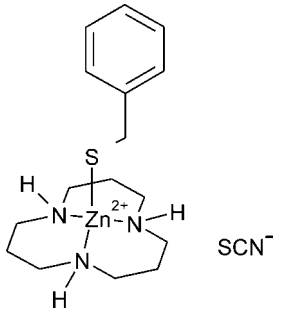
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.007 Å; R factor = 0.036; wR factor = 0.077; data-to-parameter ratio = 18.0.

The title compound, $[Zn(C_7H_7S)(C_9H_{21}N_3)]SCN$, features a cationic Zn complex with the metal atom in a distorted tetrahedral environment. The crystal packing is stabilized by N—H···N and N—H···S hydrogen bonds. However, one of the amino H atoms is not involved in hydrogen bonding.

Related literature

A series of related complexes has been prepared and characterized structurally (Notni, Görls & Anders, 2006). The complexes react with carbon disulfide to give trithiocarbonates (Notni, Schenk *et al.*, 2006; Schenk *et al.*, 2006), and with methyl iodide to give thioethers (Notni *et al.*, 2007). The complexes are of importance as biomimetics for a sulfur analogue of carbonic anhydrase (Schenk *et al.*, 2006).

For related literature, see: Börzel *et al.* (2003); Brand *et al.* (2001).



Experimental

Crystal data

$[Zn(C_7H_7S)(C_9H_{21}N_3)]SCN$
M_r = 417.92
Monoclinic, *Cc*
a = 15.6005 (7) Å
b = 8.8031 (4) Å
c = 16.2518 (6) Å
β = 117.777 (2)°
V = 1974.72 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 183 (2) K
0.04 × 0.04 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
6436 measured reflections
4132 independent reflections
3636 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.077
S = 1.01
4132 reflections
229 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), 1885 Friedel pairs
Flack parameter: 0.020 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1*N2*···N1*T*^{i}	0.89 (4)	2.06 (5)	2.875 (6)	150.00
N3—H1*N3*···S1*T*^{ii}	0.81 (5)	2.75 (5)	3.536 (3)	165.00

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Siemens, 1990); 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: BT2510).

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supplementary materials

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(Phenylmethanethiolato)(1,5,9-triazacyclododecane)zinc(II) thiocyanate

H. Görls, J. Notni and E. Anders

Comment

The title compound belongs to a series of cationic zinc thiolate complexes with azamacrocyclic ligands (Notni, Görls & Anders, 2006), where the crystal structure of the corresponding perchlorate salt has been published. These complexes have shown to react with heterocumulenes (COS, CS_2) to give di- and trithiocarbonato complexes, respectively (Notni, Schenk *et al.*, 2006), In the course of our efforts to elucidate the reactivity towards other heterocumulenes we also investigated the reaction with thiocyanate anion. However, no reaction was observed, but the complex precipitated as thiocyanate salt whose crystal structure is reported herein. The crystal structure of (1) consists of a Zn-complex-monocation and a discrete thiocyanato anion as shown in Fig. 1. Within the Zn-cation, the Zn atom is coordinated by three nitrogen atoms and one sulfur atom in a distorted tetrahedral arrangement, the Zn—S bond length being 2.2497 (8) Å and the Zn—N bond lengths 2.054 (3), 2.046 (3) and 2.050 (3) Å. The bond angles around Zn range from 112.04 (9) to 119.65 (9)° for S–Zn–N angles and from 101.86 (13) to 102.86 (12)° for N–Zn–N angles. The Zn–N and Zn–S distances are in accord with the corresponding distances in the other Zn complexes reported in the literature (Notni, Görls & Anders, 2006; Börzel *et al.*, 2003; Brand *et al.*, 2001). There are no unexpected geometrical features associated with the coordination structure of zinc ion. The hydrogen atoms of the amine-groups are all in *cis*-position and found on the side of the complex that bears the thiolate.

Experimental

A sample of {(phenylmethylthiolato)(1,5,9-triazacyclododecane)}zinc(II) perchlorate (0.5 mmol, 23 mg) was placed in an NMR tube and dissolved in acetonitrile-D_3 (0.5 ml) Then tetrabutylammonium thiocyanate (0.5 mmol, 15.5 mg) was added. The signals of the complex cation in the NMR spectra showed no alteration, even after prolonged standing at r. t.. After one week, a precipitate had formed, which was subjected to X-ray structural analysis.

Refinement

The hydrogen atoms of the tree amines groups at N1, N2 and N3 were located by difference Fourier synthesis and refined isotropically. All other hydrogen atoms were calculated into idealized positions and were refined with 1.5 times the isotropic displacement parameter of the corresponding carbon atom.

Figures

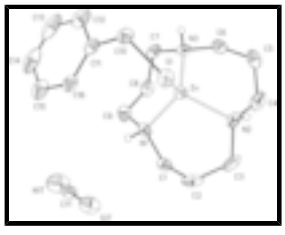


Fig. 1. Molecular structure of **1**. Displacement ellipsoids are drawn at the 40% probability level. H atoms bonded to C omitted.

(Phenylmethanethiolato)(1,5,9-triazacyclododecane)zinc(II) thiocyanate

Crystal data

$[Zn(C_7H_7S)(C_9H_{21}N_3)]SCN$	$Z = 4$
$M_r = 417.92$	$F_{000} = 880$
Monoclinic, *Cc*	$D_x = 1.406$ Mg m^{-3}
Hall symbol: C-2yc	Mo *K*α radiation λ = 0.71073 Å
a = 15.6005 (7) Å	μ = 1.46 mm^{-1}
b = 8.8031 (4) Å	*T* = 183 (2) K
c = 16.2518 (6) Å	Prism, colourless
β = 117.777 (2)º	0.04 × 0.04 × 0.03 mm
V = 1974.72 (15) Å^3	

Data collection

KappaCCD diffractometer	3636 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.034$
Monochromator: graphite	$\theta_{max} = 27.5$º
T = 183(2) K	$\theta_{min} = 2.8$º
φ and ω scan	*h* = −18→20
Absorption correction: none	*k* = −10→11
6436 measured reflections	*l* = −21→19
4132 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 0.6448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.077$	$(\Delta/\sigma)_{max} = 0.005$
S = 1.01	$\Delta\rho_{max} = 0.33$ e Å^{-3}
4132 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
229 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), 1885 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.020 (14)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Zn	0.19047 (2)	0.28977 (4)	0.83730 (2)	0.02175 (10)
S1	0.10003 (7)	0.33403 (10)	0.68420 (6)	0.0312 (2)
N1	0.1643 (2)	0.0879 (3)	0.8850 (2)	0.0279 (7)
N2	0.1642 (2)	0.4447 (3)	0.9167 (2)	0.0294 (7)
N3	0.3386 (2)	0.2917 (3)	0.8947 (2)	0.0268 (6)
C1	0.1251 (3)	0.1120 (4)	0.9516 (2)	0.0317 (8)
H1A	0.1793	0.1341	1.0140	0.038*
H1B	0.0930	0.0177	0.9562	0.038*
C2	0.0534 (3)	0.2409 (5)	0.9225 (3)	0.0442 (10)
H2A	0.0164	0.2422	0.8538	0.053*
H2B	0.0069	0.2217	0.9469	0.053*
C3	0.0981 (4)	0.3935 (5)	0.9550 (3)	0.0514 (12)
H3A	0.1352	0.3919	1.0237	0.062*
H3B	0.0456	0.4693	0.9377	0.062*
C4	0.2507 (3)	0.5225 (5)	0.9887 (3)	0.0483 (11)
H4A	0.2774	0.4614	1.0465	0.058*
H4B	0.2310	0.6222	1.0025	0.058*
C5	0.3288 (3)	0.5468 (5)	0.9605 (3)	0.0447 (10)
H5A	0.3723	0.6285	0.9996	0.054*
H5B	0.2984	0.5821	0.8952	0.054*
C6	0.3890 (3)	0.4068 (4)	0.9692 (2)	0.0358 (9)
H6A	0.4492	0.4387	0.9678	0.043*
H6B	0.4078	0.3587	1.0303	0.043*
C7	0.3846 (3)	0.1394 (4)	0.9263 (2)	0.0329 (8)
H7A	0.4552	0.1530	0.9654	0.039*
H7B	0.3746	0.0788	0.8712	0.039*
C8	0.3443 (3)	0.0521 (4)	0.9813 (2)	0.0343 (9)
H8A	0.3915	−0.0275	1.0181	0.041*
H8B	0.3380	0.1226	1.0257	0.041*
C9	0.2468 (3)	−0.0225 (4)	0.9227 (3)	0.0356 (9)
H9A	0.2488	−0.0764	0.8701	0.043*
H9B	0.2351	−0.0990	0.9610	0.043*
C10	0.1668 (3)	0.2321 (4)	0.6338 (2)	0.0316 (8)

H10A	0.1272	0.2338	0.5653	0.038*
H10B	0.2270	0.2894	0.6491	0.038*
C11	0.1941 (3)	0.0699 (4)	0.6634 (2)	0.0304 (8)
C12	0.2855 (3)	0.0175 (5)	0.6836 (2)	0.0454 (11)
H12A	0.3323	0.0862	0.6833	0.054*
C13	0.3096 (4)	−0.1364 (7)	0.7047 (3)	0.0615 (16)
H13A	0.3726	−0.1712	0.7186	0.074*
C14	0.2424 (5)	−0.2363 (6)	0.7051 (3)	0.0629 (16)
H14A	0.2588	−0.3404	0.7188	0.076*
C15	0.1516 (4)	−0.1863 (5)	0.6857 (3)	0.0472 (11)
H15A	0.1053	−0.2559	0.6862	0.057*
C16	0.1273 (3)	−0.0342 (4)	0.6652 (2)	0.0336 (9)
H16A	0.0645	−0.0004	0.6523	0.040*
S1T	−0.08174 (7)	−0.05941 (12)	0.73994 (7)	0.0424 (3)
C1T	−0.0051 (3)	−0.1944 (4)	0.7955 (3)	0.0338 (9)
N1T	0.0514 (3)	−0.2856 (5)	0.8386 (4)	0.0685 (13)
H1N2	0.132 (3)	0.517 (5)	0.875 (3)	0.036 (11)*
H1N1	0.121 (3)	0.043 (5)	0.843 (3)	0.042 (13)*
H1N3	0.347 (3)	0.317 (5)	0.851 (3)	0.046 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.02147 (17)	0.02404 (17)	0.01877 (15)	0.0013 (2)	0.00856 (12)	0.00112 (19)
S1	0.0325 (5)	0.0335 (5)	0.0197 (4)	0.0069 (4)	0.0056 (3)	0.0045 (4)
N1	0.0302 (17)	0.0282 (16)	0.0213 (14)	−0.0070 (13)	0.0085 (13)	0.0004 (13)
N2	0.0345 (17)	0.0281 (16)	0.0270 (14)	0.0100 (14)	0.0155 (13)	0.0022 (13)
N3	0.0234 (15)	0.0374 (17)	0.0220 (14)	−0.0005 (13)	0.0126 (12)	0.0012 (13)
C1	0.032 (2)	0.037 (2)	0.0276 (17)	−0.0069 (16)	0.0153 (16)	0.0040 (16)
C2	0.027 (2)	0.065 (3)	0.049 (2)	0.0055 (19)	0.0239 (19)	0.017 (2)
C3	0.071 (3)	0.045 (2)	0.068 (3)	0.025 (2)	0.057 (3)	0.015 (2)
C4	0.044 (3)	0.056 (3)	0.040 (2)	0.010 (2)	0.0161 (19)	−0.015 (2)
C5	0.042 (2)	0.036 (2)	0.044 (2)	−0.0128 (19)	0.0099 (18)	−0.0110 (18)
C6	0.0219 (18)	0.042 (2)	0.036 (2)	−0.0085 (17)	0.0076 (16)	−0.0062 (17)
C7	0.0274 (19)	0.042 (2)	0.0266 (17)	0.0092 (17)	0.0103 (15)	−0.0024 (16)
C8	0.035 (2)	0.0323 (19)	0.0262 (18)	0.0118 (16)	0.0064 (16)	0.0037 (15)
C9	0.044 (2)	0.0254 (17)	0.0331 (19)	0.0054 (16)	0.0145 (17)	0.0060 (15)
C10	0.036 (2)	0.039 (2)	0.0193 (16)	−0.0017 (17)	0.0120 (15)	−0.0016 (15)
C11	0.035 (2)	0.041 (2)	0.0138 (15)	0.0026 (17)	0.0095 (14)	−0.0029 (15)
C12	0.033 (2)	0.073 (3)	0.0224 (18)	0.007 (2)	0.0064 (16)	−0.008 (2)
C13	0.054 (3)	0.091 (4)	0.022 (2)	0.043 (3)	0.003 (2)	−0.007 (2)
C14	0.103 (5)	0.055 (3)	0.027 (2)	0.037 (3)	0.027 (3)	0.009 (2)
C15	0.075 (3)	0.038 (2)	0.033 (2)	0.009 (2)	0.029 (2)	0.0042 (18)
C16	0.042 (2)	0.037 (2)	0.0252 (17)	0.0004 (17)	0.0182 (16)	−0.0029 (15)
S1T	0.0311 (5)	0.0466 (6)	0.0440 (5)	0.0053 (5)	0.0127 (4)	0.0154 (5)
C1T	0.031 (2)	0.0298 (19)	0.048 (2)	−0.0014 (17)	0.0250 (19)	0.0028 (17)
N1T	0.061 (3)	0.054 (3)	0.099 (3)	0.019 (2)	0.045 (3)	0.030 (2)

Geometric parameters (Å, °)

Zn—N2	2.046 (3)	C5—H5B	0.9900
Zn—N3	2.050 (3)	C6—H6A	0.9900
Zn—N1	2.054 (3)	C6—H6B	0.9900
Zn—S1	2.2497 (8)	C7—C8	1.520 (5)
S1—C10	1.831 (4)	C7—H7A	0.9900
N1—C1	1.487 (5)	C7—H7B	0.9900
N1—C9	1.497 (5)	C8—C9	1.517 (5)
N1—H1N1	0.81 (4)	C8—H8A	0.9900
N2—C4	1.479 (5)	C8—H8B	0.9900
N2—C3	1.501 (5)	C9—H9A	0.9900
N2—H1N2	0.89 (4)	C9—H9B	0.9900
N3—C6	1.491 (5)	C10—C11	1.504 (5)
N3—C7	1.493 (5)	C10—H10A	0.9900
N3—H1N3	0.81 (4)	C10—H10B	0.9900
C1—C2	1.506 (6)	C11—C12	1.384 (5)
C1—H1A	0.9900	C11—C16	1.398 (5)
C1—H1B	0.9900	C12—C13	1.405 (7)
C2—C3	1.492 (7)	C12—H12A	0.9500
C2—H2A	0.9900	C13—C14	1.371 (8)
C2—H2B	0.9900	C13—H13A	0.9500
C3—H3A	0.9900	C14—C15	1.372 (8)
C3—H3B	0.9900	C14—H14A	0.9500
C4—C5	1.502 (6)	C15—C16	1.390 (5)
C4—H4A	0.9900	C15—H15A	0.9500
C4—H4B	0.9900	C16—H16A	0.9500
C5—C6	1.516 (6)	S1T—C1T	1.628 (4)
C5—H5A	0.9900	C1T—N1T	1.156 (5)
N2—Zn—N3	102.86 (12)	C4—C5—H5B	108.7
N2—Zn—N1	101.86 (13)	C6—C5—H5B	108.7
N3—Zn—N1	102.44 (12)	H5A—C5—H5B	107.6
N2—Zn—S1	112.04 (9)	N3—C6—C5	114.1 (3)
N3—Zn—S1	119.65 (9)	N3—C6—H6A	108.7
N1—Zn—S1	115.75 (9)	C5—C6—H6A	108.7
C10—S1—Zn	102.43 (12)	N3—C6—H6B	108.7
C1—N1—C9	111.2 (3)	C5—C6—H6B	108.7
C1—N1—Zn	111.9 (2)	H6A—C6—H6B	107.6
C9—N1—Zn	115.6 (2)	N3—C7—C8	113.1 (3)
C1—N1—H1N1	104 (3)	N3—C7—H7A	109.0
C9—N1—H1N1	104 (3)	C8—C7—H7A	109.0
Zn—N1—H1N1	109 (3)	N3—C7—H7B	109.0
C4—N2—C3	111.2 (3)	C8—C7—H7B	109.0
C4—N2—Zn	115.5 (2)	H7A—C7—H7B	107.8
C3—N2—Zn	116.1 (2)	C9—C8—C7	114.7 (3)
C4—N2—H1N2	105 (3)	C9—C8—H8A	108.6
C3—N2—H1N2	106 (3)	C7—C8—H8A	108.6
Zn—N2—H1N2	101 (3)	C9—C8—H8B	108.6

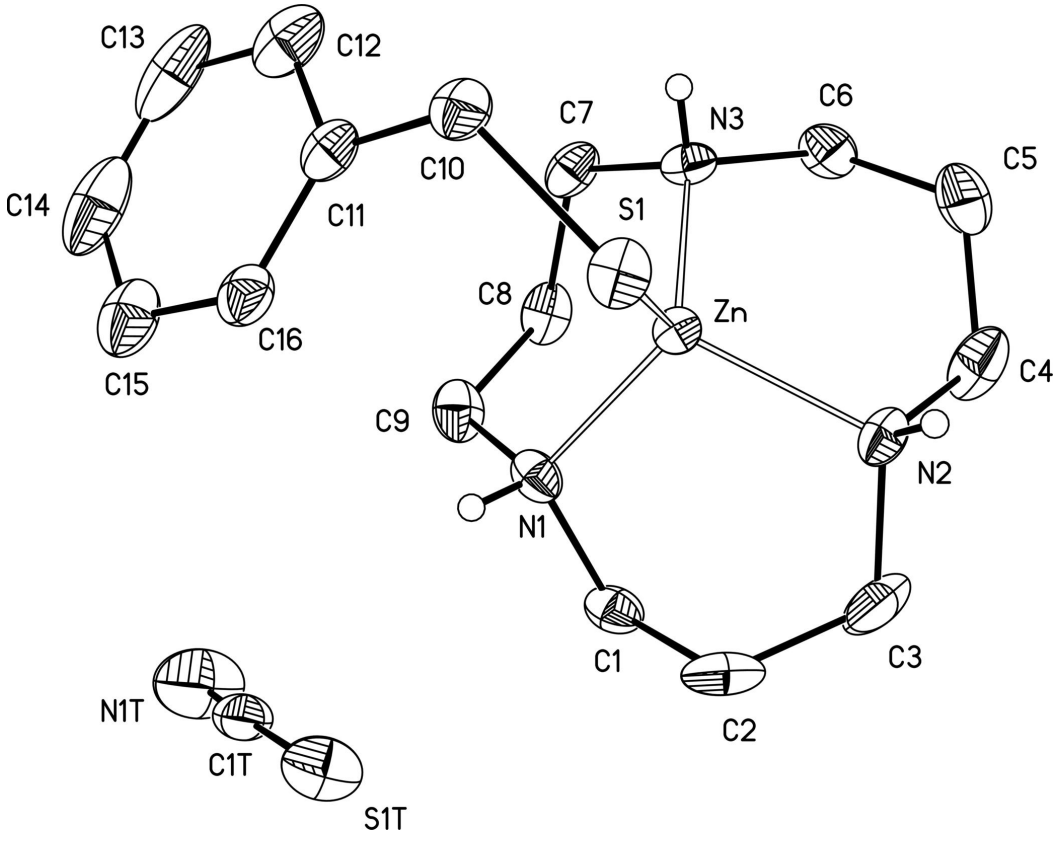
C6—N3—C7	110.1 (3)	C7—C8—H8B	108.6
C6—N3—Zn	115.5 (2)	H8A—C8—H8B	107.6
C7—N3—Zn	114.1 (2)	N1—C9—C8	113.3 (3)
C6—N3—H1N3	106 (3)	N1—C9—H9A	108.9
C7—N3—H1N3	107 (3)	C8—C9—H9A	108.9
Zn—N3—H1N3	103 (3)	N1—C9—H9B	108.9
N1—C1—C2	112.1 (3)	C8—C9—H9B	108.9
N1—C1—H1A	109.2	H9A—C9—H9B	107.7
C2—C1—H1A	109.2	C11—C10—S1	117.3 (3)
N1—C1—H1B	109.2	C11—C10—H10A	108.0
C2—C1—H1B	109.2	S1—C10—H10A	108.0
H1A—C1—H1B	107.9	C11—C10—H10B	108.0
C3—C2—C1	114.3 (4)	S1—C10—H10B	108.0
C3—C2—H2A	108.7	H10A—C10—H10B	107.2
C1—C2—H2A	108.7	C12—C11—C16	118.1 (4)
C3—C2—H2B	108.7	C12—C11—C10	120.0 (4)
C1—C2—H2B	108.7	C16—C11—C10	121.7 (3)
H2A—C2—H2B	107.6	C11—C12—C13	120.6 (5)
C2—C3—N2	114.9 (3)	C11—C12—H12A	119.7
C2—C3—H3A	108.5	C13—C12—H12A	119.7
N2—C3—H3A	108.5	C14—C13—C12	120.0 (5)
C2—C3—H3B	108.5	C14—C13—H13A	120.0
N2—C3—H3B	108.5	C12—C13—H13A	120.0
H3A—C3—H3B	107.5	C13—C14—C15	120.2 (5)
N2—C4—C5	113.3 (3)	C13—C14—H14A	119.9
N2—C4—H4A	108.9	C15—C14—H14A	119.9
C5—C4—H4A	108.9	C14—C15—C16	120.0 (5)
N2—C4—H4B	108.9	C14—C15—H15A	120.0
C5—C4—H4B	108.9	C16—C15—H15A	120.0
H4A—C4—H4B	107.7	C15—C16—C11	121.0 (4)
C4—C5—C6	114.3 (4)	C15—C16—H16A	119.5
C4—C5—H5A	108.7	C11—C16—H16A	119.5
C6—C5—H5A	108.7	N1T—C1T—S1T	176.7 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1N2···N1T^{i}	0.89 (4)	2.06 (5)	2.875 (6)	150.00
N3—H1N3···S1T^{ii}	0.81 (5)	2.75 (5)	3.536 (3)	165.00

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

Fig. 1


C13
C12
C7
N3
C6
C5
C10
C14
C11
S1
C8
Zn
C16
C4
C15
C9
N2
N1
C1
C3
C2
N1T
C1T
S1T