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(*p*-Methylbenzenethiolato)[tris(3-phenyl-5-methylpyrazolyl)borato]zinc(II)

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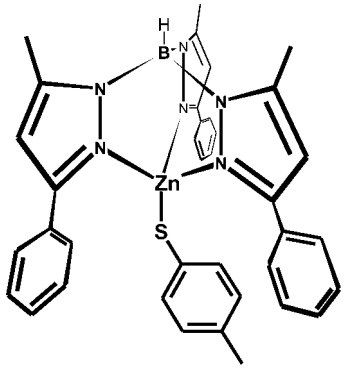
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.087; data-to-parameter ratio = 18.1.

The crystal structure of the title compound, [Zn($C_{30}H_{28}BN_6$)(C_7H_7S)], is closely related to a series of other tripod zinc thiolates. The Zn atom adopts a very distorted tetrahedral coordination geometry. In addition to the crystallographic data, ^{11}B NMR as well as ^{11}B-decoupled ^{1}H NMR data are provided. A proton shift for the boron-bound hydride (5.15 p.p.m.) of a pyrazolylborato ligand is reported for the first time.

Related literature

Tris(pyrazolyl)borato zinc thiolates and their reactions have been studied by Brand *et al.* (2001). A comparative kinetic study on thiolate alkylation in tripodal zinc complexes with N_3S, N_2S_2, NS_3 and S_4 donor sets has been published by Tekeste & Vahrenkamp (2006). For related literature, see: Börzel *et al.* (2003); Rombach *et al.* (2002).



Experimental

Crystal data

[Zn($C_{30}H_{28}BN_6$)(C_7H_7S)]
M_r = 671.95
Monoclinic, $P2_1/n$
a = 16.2448 (7) Å
b = 12.3442 (3) Å
c = 17.3988 (7) Å
β = 101.675 (1)°
V = 3416.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 183 (2) K
0.18 × 0.12 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
13913 measured reflections
7635 independent reflections
4579 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.087
S = 0.87
7635 reflections
422 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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* (Siemens, 1990); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2507).

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supplementary materials

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(*p*-Methylbenzenethiolato)[tris(3-phenyl-5-methylpyrazolyl)borato]zinc(II)

H. Görls, W. Günther, J. Notni and E. Anders

Comment

The title compound is closely related to a class of complexes synthesized by Tekeste and Vahrenkamp (2006), which are useful model compounds for thiolate alkylating enzymes. Thus, their structural chemistry and reactivity has been extensively studied by these authors. However, to the best of our knowledge, no comment on the chemical shift of the single hydride ion at the boron atom can be found in the literature. In routine ^{1}H spectra, this signal is usually not detected due to ^{11}B-^{1}H coupling: Natural boron isotopes are ^{10}B (19.9%, spin 3/2) and ^{11}B (80.1%, spin 3), both of them possessing large quadrupol moments. This causes the signal of the hydride to exhibit a large multiplicity and increased band width. As a result, the detected signal appears in the spectra as a slight elevation of the baseline, which normally is not considered a real peak by most processing software. Nonetheless, in a ^{11}B decoupled ^{1}H NMR, a slightly broadened singlet at 5.15 p.p.m. with a relative intensity of 0.8 protons is found which corresponds to the hydride. The unusual intensity is a result of the natural abundance of the ^{11}B nucleus of ~80%, since only this portion of the signal experiences line width reduction by decoupling. The moleculare structure of (1) is shown in Fig. 1. The Zn atom is coordinated by three N atoms and one sulfur atom in a distorted tetrahedral arrangement. The Zn–S bond length is 2.2289 (6) Å and the Zn—N bond lengths are 2.038 (2), 2.058 (2) and 2.088 (2) Å, respectively. The bond angles around Zn range from 120.98 (5) to 127.46 (5)° for S–Zn–N angles and from 91.59 (7) to 94.66 (7)° for N–Zn–N angles. The Zn–N and Zn–S distances are in agreement with the corresponding distances in the other Zn complexes reported in the literature (Rombach *et al.*, 2002; Börzel *et al.*, 2003; Brand *et al.*, 2001). There are no unexpected geometrical features associated with the coordination structure of zinc.

Experimental

To a solution of $Tp^{(Ph,Me)}$ZnOH (1 mmol, 561 mg) in methylene chloride (20 ml) 4-methylthiophenol (1 mmol, 124 mg) were added. The mixture was stirred for 1 h, and methanol (10 ml) was added. The methylene chloride was evaporated, and the complex was allowed to precipitate at −20 °C. Obtained were colourless prisms, m. p. 230 °C, yield 640 mg (95%). Anal. calcd. for $C_{37}H_{35}BN_6SZn$: C, 66.14, H, 5.25, N, 12.50, S, 4.77. Found C, 66.74, H, 5.02, N, 12.69, S, 4.89. NMR (^{1}H, 400 MHz, $CDCl_3$,^{11}B-decoupled): 1.95 (s, 3H), 2.55 (s, 9H), 5.15 (s, 0.8H) 6.12 (d, 2H), 6.26 (d, 2H), 7.11 (m, 9H), 7.59 (m, 6H) p.p.m.. NMR (^{11}B, 128.4 MHz, $CDCl_3$): −6.3 p.p.m.. NMR (^{13}C, 100 MHz, $CDCl_3$): 12.9, 20.5, 105.5, 127.5, 127.8, 128.1, 128.5, 129.7, 131.0, 131.2, 136.9, 145.7, 154.5 p.p.m..

Refinement

The hydrogen atom bonded to B was located by difference Fourier synthesis and freely refined. All other hydrogen atoms were set to idealized positions and were refined with 1.2 times (1.5 for methyl groups) the isotropic displacement parameter of the corresponding carbon atom. The methyl groups were allowed to rotate but not to tip.

Figures

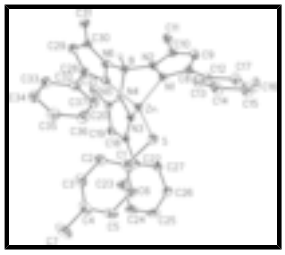


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level.

(*p*-Methylbenzenethiolato)[tris(3-phenyl-5-methylpyrazolyl)borato]zinc(II)

Crystal data

$[Zn(C_{30}H_{28}BN_6)(C_7H_7S)]$	$Z = 4$
$M_r = 671.95$	$F_{000} = 1400$
Monoclinic, $P2_1/n$	$D_x = 1.306$ Mg m^{-3}
Hall symbol: -P2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 16.2448$ (7) Å	$\mu = 0.82$ mm^{-1}
$b = 12.3442$ (3) Å	$T = 183$ (2) K
$c = 17.3988$ (7) Å	Prism, colourless
$\beta = 101.675$ (1)º	0.18 × 0.12 × 0.10 mm
$V = 3416.8$ (2) Å^3	

Data collection

Nonius KappaCCD diffractometer	4579 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.040$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 183(2)$ K	$\theta_{min} = 2.5$º
phi– + ω–scan	$h = -21 \rightarrow 21$
Absorption correction: none	$k = -14 \rightarrow 13$
13913 measured reflections	$l = -22 \rightarrow 22$
7635 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.087$	$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.87$	$(\Delta/\sigma)_{max} = 0.001$

7635 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
422 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ 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	0.829763 (16)	0.72798 (2)	0.034357 (14)	0.03008 (9)
S	0.70537 (4)	0.66651 (5)	−0.02881 (3)	0.03546 (15)
N1	0.93538 (11)	0.70497 (13)	−0.00994 (11)	0.0314 (4)
N2	1.00753 (11)	0.72512 (14)	0.04482 (10)	0.0325 (4)
N3	0.88773 (11)	0.66740 (14)	0.14189 (10)	0.0306 (4)
N4	0.95800 (11)	0.72717 (13)	0.17318 (10)	0.0297 (4)
N5	0.86364 (11)	0.88850 (13)	0.06250 (10)	0.0315 (4)
N6	0.94927 (11)	0.89614 (13)	0.09183 (10)	0.0312 (4)
C1	0.64030 (15)	0.68671 (18)	0.04035 (14)	0.0368 (6)
C2	0.66207 (16)	0.75162 (19)	0.10691 (14)	0.0440 (6)
H2A	0.7139	0.7898	0.1160	0.053*
C3	0.60969 (19)	0.7614 (2)	0.15993 (16)	0.0540 (7)
H3A	0.6266	0.8056	0.2051	0.065*
C4	0.53267 (19)	0.7081 (2)	0.14872 (18)	0.0581 (8)
C5	0.51059 (17)	0.6458 (2)	0.0817 (2)	0.0581 (8)
H5A	0.4580	0.6095	0.0720	0.070*
C6	0.56291 (15)	0.63468 (19)	0.02811 (16)	0.0467 (7)
H6A	0.5456	0.5911	−0.0173	0.056*
C7	0.4756 (2)	0.7200 (3)	0.2067 (2)	0.0938 (12)
H7A	0.5088	0.7145	0.2602	0.141*
H7B	0.4331	0.6625	0.1979	0.141*
H7C	0.4477	0.7907	0.1996	0.141*
C8	0.95876 (15)	0.64799 (17)	−0.06788 (13)	0.0343 (5)
C9	1.04514 (15)	0.63145 (18)	−0.05002 (14)	0.0402 (6)
H9A	1.0777	0.5938	−0.0811	0.048*
C10	1.07439 (15)	0.68013 (18)	0.02127 (14)	0.0364 (6)
C11	1.16243 (15)	0.6886 (2)	0.06763 (15)	0.0476 (7)
H11A	1.1651	0.6586	0.1202	0.071*

H11B	1.1795	0.7648	0.0719	0.071*
H11C	1.2003	0.6478	0.0411	0.071*
C12	0.89822 (15)	0.61680 (17)	−0.13931 (13)	0.0348 (6)
C13	0.82745 (15)	0.6780 (2)	−0.16843 (14)	0.0416 (6)
H13A	0.8155	0.7398	−0.1401	0.050*
C14	0.77392 (17)	0.6506 (2)	−0.23795 (15)	0.0544 (7)
H14A	0.7254	0.6932	−0.2571	0.065*
C15	0.79142 (18)	0.5604 (3)	−0.27977 (16)	0.0640 (8)
H15A	0.7548	0.5411	−0.3276	0.077*
C16	0.8614 (2)	0.4994 (2)	−0.25188 (16)	0.0611 (8)
H16A	0.8736	0.4382	−0.2808	0.073*
C17	0.91456 (17)	0.52619 (19)	−0.18201 (15)	0.0480 (7)
H17A	0.9626	0.4827	−0.1628	0.058*
C18	0.86601 (14)	0.61354 (16)	0.20231 (13)	0.0300 (5)
C19	0.92140 (14)	0.64100 (18)	0.27169 (13)	0.0346 (5)
H19A	0.9202	0.6148	0.3228	0.042*
C20	0.97809 (14)	0.71310 (16)	0.25209 (13)	0.0323 (5)
C21	1.04815 (15)	0.77291 (19)	0.30342 (14)	0.0431 (6)
H21A	1.0385	0.8510	0.2969	0.065*
H21B	1.1015	0.7539	0.2888	0.065*
H21C	1.0504	0.7530	0.3583	0.065*
C22	0.79528 (14)	0.53684 (16)	0.18952 (13)	0.0318 (5)
C23	0.75279 (17)	0.5145 (2)	0.24959 (16)	0.0481 (6)
H23A	0.7696	0.5486	0.2992	0.058*
C24	0.68578 (18)	0.4423 (2)	0.23680 (17)	0.0600 (8)
H24A	0.6570	0.4270	0.2780	0.072*
C25	0.66086 (18)	0.3931 (2)	0.16536 (17)	0.0547 (7)
H25A	0.6144	0.3447	0.1568	0.066*
C26	0.70296 (16)	0.41381 (18)	0.10604 (16)	0.0442 (6)
H26A	0.6858	0.3792	0.0566	0.053*
C27	0.77029 (14)	0.48485 (17)	0.11794 (14)	0.0351 (6)
H27A	0.7996	0.4981	0.0768	0.042*
C28	0.83466 (15)	0.99171 (17)	0.05226 (12)	0.0330 (5)
C29	0.90126 (15)	1.06349 (18)	0.07509 (13)	0.0379 (6)
H29A	0.8981	1.1403	0.0744	0.046*
C30	0.97251 (15)	1.00187 (17)	0.09878 (13)	0.0348 (6)
C31	1.06169 (15)	1.03660 (19)	0.12619 (15)	0.0446 (6)
H31A	1.0975	0.9725	0.1386	0.067*
H31B	1.0662	1.0817	0.1732	0.067*
H31C	1.0799	1.0784	0.0847	0.067*
C32	0.74580 (14)	1.02015 (17)	0.02264 (13)	0.0335 (5)
C33	0.71553 (16)	1.11925 (18)	0.04451 (14)	0.0410 (6)
H33A	0.7523	1.1667	0.0782	0.049*
C34	0.63253 (16)	1.14877 (19)	0.01753 (15)	0.0465 (7)
H34A	0.6131	1.2168	0.0322	0.056*
C35	0.57777 (16)	1.08049 (18)	−0.03043 (15)	0.0451 (7)
H35A	0.5206	1.1004	−0.0484	0.054*
C36	0.60729 (16)	0.98283 (19)	−0.05190 (15)	0.0476 (7)
H36A	0.5701	0.9351	−0.0850	0.057*

C37	0.69034 (15)	0.95342 (19)	−0.02595 (14)	0.0422 (6)
H37A	0.7095	0.8860	−0.0419	0.051*
B	1.00221 (17)	0.79415 (19)	0.11767 (16)	0.0327 (6)
H1BO	1.0673 (11)	0.8177 (13)	0.1481 (10)	0.044 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.02610 (15)	0.03474 (14)	0.02890 (15)	−0.00106 (11)	0.00439 (11)	0.00005 (11)
S	0.0285 (3)	0.0434 (3)	0.0332 (3)	−0.0023 (3)	0.0032 (3)	−0.0030 (3)
N1	0.0259 (11)	0.0359 (10)	0.0330 (11)	−0.0001 (8)	0.0072 (9)	−0.0008 (8)
N2	0.0249 (11)	0.0376 (10)	0.0343 (11)	−0.0019 (9)	0.0043 (9)	0.0007 (9)
N3	0.0252 (11)	0.0363 (10)	0.0297 (11)	−0.0036 (8)	0.0038 (9)	−0.0004 (8)
N4	0.0238 (10)	0.0344 (9)	0.0295 (10)	−0.0002 (8)	0.0020 (8)	−0.0010 (8)
N5	0.0276 (11)	0.0346 (10)	0.0320 (11)	0.0010 (8)	0.0052 (9)	0.0027 (8)
N6	0.0263 (11)	0.0344 (10)	0.0323 (11)	−0.0034 (8)	0.0048 (9)	−0.0003 (8)
C1	0.0306 (14)	0.0379 (12)	0.0428 (15)	0.0074 (11)	0.0096 (11)	0.0087 (11)
C2	0.0381 (16)	0.0530 (15)	0.0410 (15)	0.0025 (12)	0.0084 (12)	0.0014 (12)
C3	0.060 (2)	0.0594 (16)	0.0454 (16)	0.0136 (15)	0.0175 (15)	0.0050 (13)
C4	0.061 (2)	0.0556 (18)	0.066 (2)	0.0213 (15)	0.0344 (17)	0.0220 (15)
C5	0.0377 (17)	0.0513 (16)	0.091 (2)	0.0055 (13)	0.0265 (17)	0.0224 (16)
C6	0.0357 (16)	0.0387 (13)	0.0659 (19)	−0.0008 (12)	0.0107 (14)	0.0036 (12)
C7	0.092 (3)	0.109 (3)	0.102 (3)	0.025 (2)	0.070 (2)	0.030 (2)
C8	0.0358 (15)	0.0338 (12)	0.0345 (14)	0.0019 (10)	0.0103 (11)	0.0050 (10)
C9	0.0363 (15)	0.0444 (14)	0.0417 (15)	0.0078 (11)	0.0124 (12)	−0.0018 (11)
C10	0.0304 (14)	0.0390 (12)	0.0409 (15)	0.0030 (11)	0.0097 (12)	0.0060 (11)
C11	0.0315 (15)	0.0624 (16)	0.0493 (17)	0.0065 (12)	0.0094 (13)	−0.0028 (13)
C12	0.0364 (15)	0.0364 (12)	0.0338 (14)	−0.0027 (10)	0.0124 (11)	−0.0007 (10)
C13	0.0375 (16)	0.0542 (14)	0.0350 (14)	0.0051 (12)	0.0118 (12)	−0.0039 (11)
C14	0.0362 (17)	0.091 (2)	0.0363 (16)	0.0083 (14)	0.0070 (13)	−0.0078 (14)
C15	0.050 (2)	0.096 (2)	0.0432 (17)	−0.0062 (17)	0.0027 (15)	−0.0202 (16)
C16	0.072 (2)	0.0587 (17)	0.0509 (19)	0.0013 (15)	0.0087 (16)	−0.0222 (14)
C17	0.0527 (18)	0.0462 (15)	0.0446 (16)	0.0072 (13)	0.0086 (14)	−0.0065 (12)
C18	0.0293 (13)	0.0301 (11)	0.0311 (13)	0.0045 (9)	0.0069 (11)	0.0014 (9)
C19	0.0322 (14)	0.0423 (13)	0.0293 (13)	0.0028 (10)	0.0061 (11)	0.0029 (10)
C20	0.0293 (13)	0.0358 (13)	0.0306 (13)	0.0046 (10)	0.0029 (10)	−0.0015 (10)
C21	0.0378 (15)	0.0543 (14)	0.0349 (13)	−0.0027 (12)	0.0016 (11)	−0.0046 (12)
C22	0.0300 (14)	0.0297 (11)	0.0361 (14)	0.0050 (9)	0.0072 (11)	0.0059 (10)
C23	0.0513 (17)	0.0565 (15)	0.0390 (15)	−0.0075 (13)	0.0148 (13)	0.0028 (12)
C24	0.056 (2)	0.0752 (19)	0.0548 (19)	−0.0224 (16)	0.0263 (16)	0.0071 (16)
C25	0.0493 (18)	0.0542 (16)	0.063 (2)	−0.0186 (13)	0.0170 (16)	0.0051 (14)
C26	0.0434 (16)	0.0395 (13)	0.0492 (16)	−0.0076 (11)	0.0086 (13)	−0.0031 (12)
C27	0.0337 (14)	0.0338 (12)	0.0392 (14)	0.0007 (10)	0.0108 (11)	0.0024 (10)
C28	0.0391 (15)	0.0337 (12)	0.0277 (13)	0.0012 (11)	0.0105 (11)	0.0026 (9)
C29	0.0434 (16)	0.0303 (12)	0.0403 (14)	−0.0030 (11)	0.0090 (12)	0.0022 (10)
C30	0.0392 (15)	0.0363 (13)	0.0299 (13)	−0.0080 (11)	0.0094 (11)	0.0014 (10)
C31	0.0413 (16)	0.0392 (13)	0.0525 (17)	−0.0104 (11)	0.0078 (13)	−0.0012 (12)
C32	0.0368 (15)	0.0354 (12)	0.0289 (13)	−0.0001 (10)	0.0080 (11)	0.0075 (10)

C33	0.0419 (16)	0.0341 (13)	0.0462 (16)	0.0004 (11)	0.0069 (13)	−0.0016 (11)
C34	0.0484 (18)	0.0363 (13)	0.0550 (17)	0.0051 (12)	0.0110 (14)	−0.0009 (12)
C35	0.0389 (16)	0.0427 (14)	0.0521 (17)	0.0064 (12)	0.0055 (13)	0.0129 (12)
C36	0.0420 (17)	0.0438 (14)	0.0514 (17)	0.0013 (12)	−0.0036 (13)	−0.0043 (12)
C37	0.0417 (17)	0.0380 (14)	0.0435 (15)	0.0060 (11)	0.0006 (13)	−0.0036 (11)
B	0.0286 (16)	0.0336 (15)	0.0353 (16)	−0.0014 (11)	0.0049 (12)	0.0018 (11)

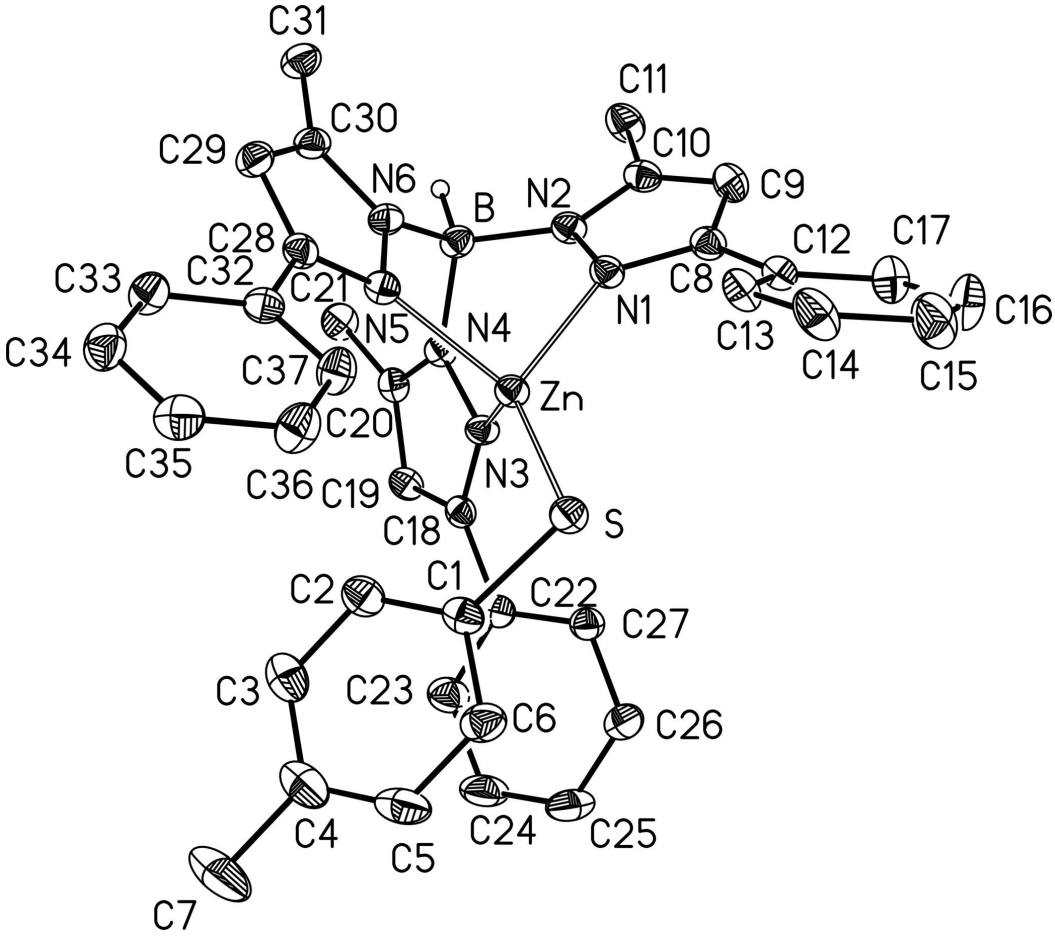
Geometric parameters (Å, °)

Zn—N1	2.0380 (19)	C15—C16	1.368 (4)
Zn—N3	2.0575 (17)	C15—H15A	0.9500
Zn—N5	2.0880 (17)	C16—C17	1.381 (3)
Zn—S	2.2289 (6)	C16—H16A	0.9500
S—C1	1.773 (2)	C17—H17A	0.9500
N1—C8	1.345 (3)	C18—C19	1.394 (3)
N1—N2	1.375 (2)	C18—C22	1.471 (3)
N2—C10	1.355 (3)	C19—C20	1.372 (3)
N2—B	1.544 (3)	C19—H19A	0.9500
N3—C18	1.350 (3)	C20—C21	1.492 (3)
N3—N4	1.376 (2)	C21—H21A	0.9800
N4—C20	1.357 (3)	C21—H21B	0.9800
N4—B	1.553 (3)	C21—H21C	0.9800
N5—C28	1.357 (3)	C22—C27	1.387 (3)
N5—N6	1.385 (2)	C22—C23	1.392 (3)
N6—C30	1.357 (3)	C23—C24	1.389 (3)
N6—B	1.540 (3)	C23—H23A	0.9500
C1—C6	1.389 (3)	C24—C25	1.369 (4)
C1—C2	1.394 (3)	C24—H24A	0.9500
C2—C3	1.381 (3)	C25—C26	1.372 (3)
C2—H2A	0.9500	C25—H25A	0.9500
C3—C4	1.392 (4)	C26—C27	1.384 (3)
C3—H3A	0.9500	C26—H26A	0.9500
C4—C5	1.381 (4)	C27—H27A	0.9500
C4—C7	1.509 (4)	C28—C29	1.393 (3)
C5—C6	1.390 (4)	C28—C32	1.474 (3)
C5—H5A	0.9500	C29—C30	1.377 (3)
C6—H6A	0.9500	C29—H29A	0.9500
C7—H7A	0.9800	C30—C31	1.493 (3)
C7—H7B	0.9800	C31—H31A	0.9800
C7—H7C	0.9800	C31—H31B	0.9800
C8—C9	1.390 (3)	C31—H31C	0.9800
C8—C12	1.472 (3)	C32—C37	1.377 (3)
C9—C10	1.374 (3)	C32—C33	1.400 (3)
C9—H9A	0.9500	C33—C34	1.384 (3)
C10—C11	1.497 (3)	C33—H33A	0.9500
C11—H11A	0.9800	C34—C35	1.377 (3)
C11—H11B	0.9800	C34—H34A	0.9500
C11—H11C	0.9800	C35—C36	1.377 (3)
C12—C13	1.383 (3)	C35—H35A	0.9500

C12—C17	1.398 (3)	C36—C37	1.382 (3)
C13—C14	1.381 (3)	C36—H36A	0.9500
C13—H13A	0.9500	C37—H37A	0.9500
C14—C15	1.391 (4)	B—H1BO	1.120 (17)
C14—H14A	0.9500		
N1—Zn—N3	91.59 (7)	C15—C16—H16A	119.8
N1—Zn—N5	91.08 (7)	C17—C16—H16A	119.8
N3—Zn—N5	94.66 (7)	C16—C17—C12	120.5 (2)
N1—Zn—S	120.98 (5)	C16—C17—H17A	119.8
N3—Zn—S	121.81 (5)	C12—C17—H17A	119.8
N5—Zn—S	127.46 (5)	N3—C18—C19	109.28 (19)
C1—S—Zn	102.89 (8)	N3—C18—C22	121.24 (19)
C8—N1—N2	106.47 (18)	C19—C18—C22	129.5 (2)
C8—N1—Zn	137.99 (16)	C20—C19—C18	106.9 (2)
N2—N1—Zn	112.18 (13)	C20—C19—H19A	126.6
C10—N2—N1	109.83 (18)	C18—C19—H19A	126.6
C10—N2—B	130.98 (19)	N4—C20—C19	107.37 (19)
N1—N2—B	119.15 (18)	N4—C20—C21	122.7 (2)
C18—N3—N4	106.42 (16)	C19—C20—C21	129.9 (2)
C18—N3—Zn	138.04 (15)	C20—C21—H21A	109.5
N4—N3—Zn	110.82 (12)	C20—C21—H21B	109.5
C20—N4—N3	110.01 (17)	H21A—C21—H21B	109.5
C20—N4—B	130.59 (18)	C20—C21—H21C	109.5
N3—N4—B	119.37 (17)	H21A—C21—H21C	109.5
C28—N5—N6	106.28 (17)	H21B—C21—H21C	109.5
C28—N5—Zn	142.37 (15)	C27—C22—C23	118.9 (2)
N6—N5—Zn	110.39 (12)	C27—C22—C18	120.8 (2)
C30—N6—N5	109.81 (17)	C23—C22—C18	120.3 (2)
C30—N6—B	129.15 (19)	C24—C23—C22	119.9 (3)
N5—N6—B	120.81 (17)	C24—C23—H23A	120.1
C6—C1—C2	117.6 (2)	C22—C23—H23A	120.1
C6—C1—S	118.4 (2)	C25—C24—C23	120.5 (3)
C2—C1—S	123.99 (19)	C25—C24—H24A	119.7
C3—C2—C1	121.2 (3)	C23—C24—H24A	119.7
C3—C2—H2A	119.4	C24—C25—C26	120.0 (2)
C1—C2—H2A	119.4	C24—C25—H25A	120.0
C2—C3—C4	121.5 (3)	C26—C25—H25A	120.0
C2—C3—H3A	119.3	C25—C26—C27	120.3 (2)
C4—C3—H3A	119.3	C25—C26—H26A	119.9
C5—C4—C3	117.0 (3)	C27—C26—H26A	119.9
C5—C4—C7	121.9 (3)	C26—C27—C22	120.4 (2)
C3—C4—C7	121.1 (3)	C26—C27—H27A	119.8
C4—C5—C6	122.1 (3)	C22—C27—H27A	119.8
C4—C5—H5A	118.9	N5—C28—C29	109.3 (2)
C6—C5—H5A	118.9	N5—C28—C32	123.96 (19)
C5—C6—C1	120.6 (3)	C29—C28—C32	126.7 (2)
C5—C6—H6A	119.7	C30—C29—C28	106.94 (19)
C1—C6—H6A	119.7	C30—C29—H29A	126.5
C4—C7—H7A	109.5	C28—C29—H29A	126.5

C4—C7—H7B	109.5	N6—C30—C29	107.6 (2)
H7A—C7—H7B	109.5	N6—C30—C31	122.6 (2)
C4—C7—H7C	109.5	C29—C30—C31	129.8 (2)
H7A—C7—H7C	109.5	C30—C31—H31A	109.5
H7B—C7—H7C	109.5	C30—C31—H31B	109.5
N1—C8—C9	109.5 (2)	H31A—C31—H31B	109.5
N1—C8—C12	121.9 (2)	C30—C31—H31C	109.5
C9—C8—C12	128.5 (2)	H31A—C31—H31C	109.5
C10—C9—C8	106.7 (2)	H31B—C31—H31C	109.5
C10—C9—H9A	126.7	C37—C32—C33	117.9 (2)
C8—C9—H9A	126.7	C37—C32—C28	123.0 (2)
N2—C10—C9	107.5 (2)	C33—C32—C28	119.1 (2)
N2—C10—C11	123.1 (2)	C34—C33—C32	120.6 (2)
C9—C10—C11	129.4 (2)	C34—C33—H33A	119.7
C10—C11—H11A	109.5	C32—C33—H33A	119.7
C10—C11—H11B	109.5	C35—C34—C33	120.7 (2)
H11A—C11—H11B	109.5	C35—C34—H34A	119.7
C10—C11—H11C	109.5	C33—C34—H34A	119.7
H11A—C11—H11C	109.5	C36—C35—C34	118.8 (2)
H11B—C11—H11C	109.5	C36—C35—H35A	120.6
C13—C12—C17	118.4 (2)	C34—C35—H35A	120.6
C13—C12—C8	122.0 (2)	C35—C36—C37	120.8 (2)
C17—C12—C8	119.5 (2)	C35—C36—H36A	119.6
C14—C13—C12	121.1 (2)	C37—C36—H36A	119.6
C14—C13—H13A	119.4	C32—C37—C36	121.2 (2)
C12—C13—H13A	119.4	C32—C37—H37A	119.4
C13—C14—C15	119.6 (3)	C36—C37—H37A	119.4
C13—C14—H14A	120.2	N6—B—N2	109.41 (18)
C15—C14—H14A	120.2	N6—B—N4	108.39 (19)
C16—C15—C14	119.9 (3)	N2—B—N4	109.04 (17)
C16—C15—H15A	120.1	N6—B—H1BO	110.1 (9)
C14—C15—H15A	120.1	N2—B—H1BO	109.1 (9)
C15—C16—C17	120.5 (3)	N4—B—H1BO	110.8 (9)

Fig. 1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