Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{*S*-benzyl 3-[(phenyl)(pyridin-2-yl)methylidene]dithiocarbazato}zinc acetonitrile monosolvate

Thahira B. S. A. Ravoof,* Siti Aminah Omar, Mohamed Ibrahim Mohamed Tahir and Karen A. Crouse

Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM, Serdang, Selangor, Malaysia
Correspondence e-mail: thahira.begum@science.upm.edu.my

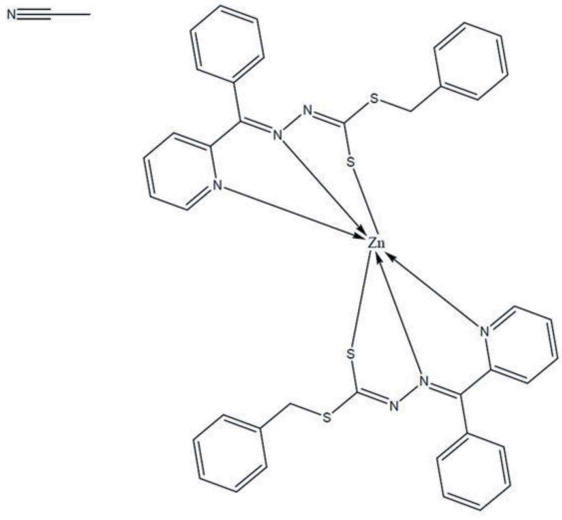
Received 24 February 2012; accepted 5 March 2012

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.081; data-to-parameter ratio = 17.8.

In the title compound, $[Zn(C_{20}H_{16}N_3S_2)_2]\cdot CH_3CN$, two different Schiff base moieties coordinate to the central Zn^{II} ion as tridentate *N*,*N*′,*S*-chelating ligands, creating a distorted octahedral environment [the smallest angle being 73.24 (6)° and the widest angle being 155.73 (7)°], with the two S atoms in *cis* positions. The dihedral angle between the mean planes of the two coordinating ligands is 83.65 (5)°. The crystal packing is consolidated by weak C—H···N hydrogen-bonding interactions.

Related literature

For background to the coordination chemistry of hydrazine carbodithioates, see: Ravoof *et al.* (2010). For the synthesis, see: Ravoof *et al.* (2004). For related structures, see: Hossain *et al.* (1996); Paulus *et al.* (2011). For H-atom treatment in the refinement, see: Cooper *et al.* (2010).



Experimental

Crystal data

$[Zn(C_{20}H_{16}N_3S_2)_2]\cdot C_2H_3N$
M_r = 831.43
Monoclinic, $P2_1/n$
a = 12.5918 (3) Å
b = 14.0025 (3) Å
c = 22.2129 (5) Å
β = 100.429 (2)°
V = 3851.79 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 150 K
0.27 × 0.18 × 0.04 mm

Data collection

Oxford Diffraction Gemini CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.85, T_{max} = 0.96
17196 measured reflections
8678 independent reflections
7022 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.081
S = 0.99
8677 reflections
487 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N102	2.1346 (17)	Zn1—N202	2.1160 (17)
Zn1—S105	2.4403 (6)	Zn1—S205	2.4516 (6)
Zn1—N115	2.2288 (17)	Zn1—N215	2.3188 (17)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C216—H2161···N103	0.95	2.62	3.285 (3)	127

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

Support for this project came from Universiti Putra Malaysia (UPM) under the research University Grant Scheme (RUGS No. 05–01-11–1243RU) and the Malaysian Fundamental Research Grant Scheme (FRGS No: 01–03-11–986FR). SAO wishes to thank UPM for a Graduate Research Fellowship award.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2598).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.

Cooper, R. I., Thompson, A. L. & Watkin, D. J. (2010). *J. Appl. Cryst.* **43**, 1100–1107.
Hossain, M. E., Alam, M. N., Begum, J., Ali, M. A., Nazimuddin, M., Smith, F. E. & Hynes, R. C. (1996). *Inorg. Chim. Acta*, **249**, 207–213.
Oxford Diffraction (2006). *CrysAlis CCD*. Oxford Diffraction Ltd, Abingdon, England.
Paulus, G., Crouse, K. A., Mohamed Tahir, M. I. & Tiekink, E. R. T. (2011). *Acta Cryst.* E**67**, o1370–o1371.
Ravoof, T. B. S. A., Crouse, K. A., Tahir, M. I. M., Cowley, A. R. & Ali, M. A. (2004). *Polyhedron*, **23**, 2491–2498.
Ravoof, T. B. S. A., Crouse, K. A., Tahir, M. I. M., How, F. N. F., Rosli, R. & Watkins, D. J. (2010). *Transition Met. Chem.* **35**, 871–876.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, Oxford, England.

supplementary materials

Acta Cryst. (2012). E**68**, m390–m391 [doi:10.1107/S1600536812009592]

Bis{*S*-benzyl 3-[(phenyl)(pyridin-2-yl)methylidene]dithiocarbazato}zinc acetonitrile monosolvate

Thahira B. S. A. Ravoof, Siti Aminah Omar, Mohamed Ibrahim Mohamed Tahir and Karen A. Crouse

Comment

The title compound was preferentially formed during the synthesis of the tridentate Schiff base with zinc saccharinate, by eliminating the saccharinate anion and instead coordinating one metal ion with two tridentate deprotonated Schiff base moieties. Background on the coordination chemistry of hydrazine carbodithioates is given by Ravoof *et al.* (2010). Similar Cu(II) complexes have been previously synthesized by Hossain *et al.* (1996).

There is one independent molecule in the asymmetric unit which contains the Zn^{II} ion coordinated to two tridentate Schiff bases *via* the pyridyl nitrogen (N115, N215), azomethine nitrogen (N102, N202) and thiolate sulfur (S105, S205) atoms (Fig. 1). A solvent acetonitrile molecule in also present in the lattice. The coordination of the metal ion is distorted octahedral with equatorial angles ranging from 73.24 (6)° to 120.54 (5)°. The angle between the planes containing the atoms of the tridentate chelating rings is 83.65 (5). The planes containing the benzyl rings attached to the sulfur atom on both Schiff bases are almost parallel to each other with an angle of 16.41 (10). Similarly, the benzyl rings on the ketone moiety of the two Schiff bases are also almost parallel with an angle of 11.69 (9)°. However, the pyridine rings of the ketone moiety of the two Schiff bases are at an angle of 66.52 (10)°.

The packing diagram viewed along the *b* axis shows an arrangement where the benzyl ring of the ketone moiety of Schiff base 2 are arranged in such a way that it is facing each other between molecules. The crystal packing is consolidated by weak C—H···N hydrogen bonding interactions (Table 2).

For related structures, see: Hossain *et al.* (1996); Ravoof *et al.* (2010); Paulus *et al.* (2011).

Experimental

Zinc saccharinate, $[Zn(sac)_2(H_2O)_4]$. $2H_2O$ was prepared according to the method outlined in Ravoof *et al.* (2004). The 2-benzoylpyridine Schiff base of *S*-benzyldithiocarbazate was prepared following the method by Hossain *et al.* (1996). The Schiff base was dissolved in acetonitrile (50 ml) and mixed with an equimolar quantity of zinc saccharinate in acetonitrile (25 ml). The resulting mixture was heated on a water bath until the volume reduced to about 30 ml. On standing overnight, the mixture yielded orange crystals which were filtered off, washed with acetonitrile and dried in a desiccator over anhydrous silica gel, overnight. Crystals of the zinc complex suitable for X-ray diffraction analysis were obtained by recrystallisation from a mixture of acetonitrile, THF and chloroform. Slow evaporation over 3 weeks yielded crystals suitable for diffraction experiments.

Refinement

H atoms were all located in difference maps, but those attached to C atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range

0.93–0.98, N—H in the range 0.86–0.89 Å) and U_{iso}(H) (in the range 1.2–1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints (Cooper *et al.*, 2010).

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS* (Betteridge *et al.*, 2003).

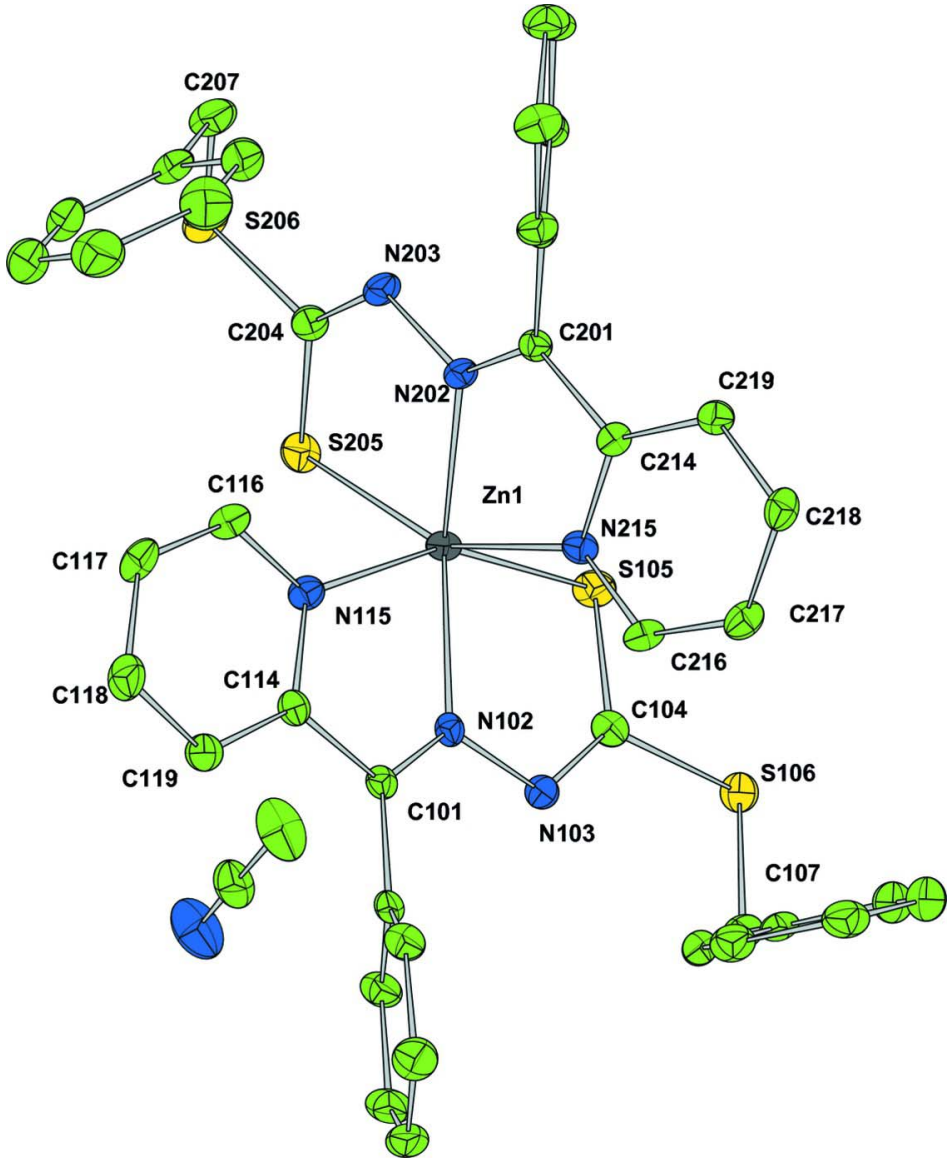


Figure 1

The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

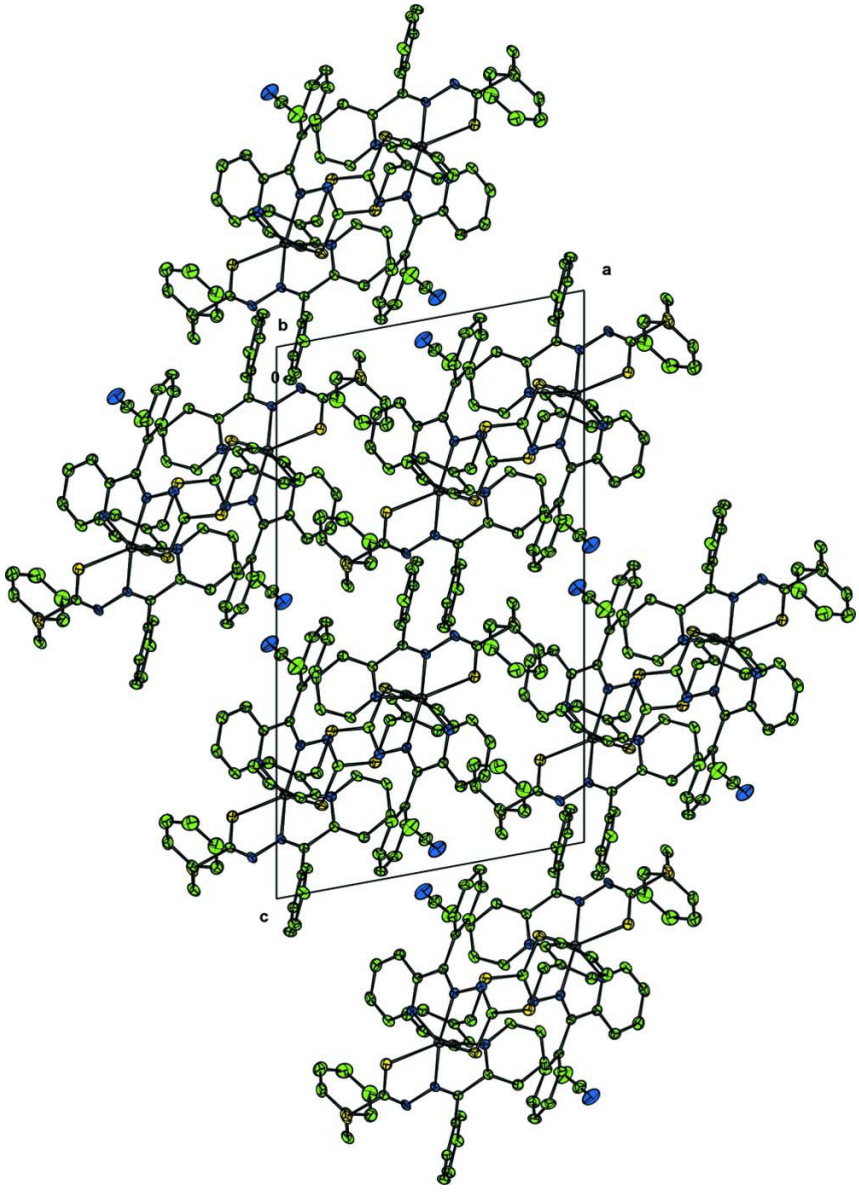


Figure 2

Molecular packing diagram of the title compound viewed along the *b* axis. Hydrogen atoms are omitted for clarity.

Bis{*S*-benzyl 3-[(phenyl)(pyridin-2-yl)methylidene]dithiocarbazato}zinc acetonitrile monosolvate

Crystal data

$[Zn(C_{20}H_{16}N_3S_2)_2]\cdot C_2H_3N$
$M_r = 831.43$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.5918$ (3) Å
$b = 14.0025$ (3) Å
$c = 22.2129$ (5) Å
$\beta = 100.429$ (2)°
$V = 3851.79$ (14) Å^3
$Z = 4$
$F(000) = 1720$
$D_x = 1.434$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6190 reflections
$\theta = 2$–29°
$\mu = 0.90$ mm^{-1}
$T = 150$ K
Prismatic, yellow
0.27 × 0.18 × 0.04 mm

Data collection

Oxford Diffraction Gemini CCD diffractometer
Radiation source: sealed X-ray tube, Oxford Diffraction Enhance X-ray
Graphite monochromator
φ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.85, T_{max} = 0.96

17196 measured reflections
8678 independent reflections
7022 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.032
θ_{max} = 28.8°, θ_{min} = 2.2°
h = −12→17
k = −17→17
l = −28→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.081
S = 0.99
8677 reflections
487 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained
Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.03P)^2 + 2.81P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1 K.
Cosier, J. & Glazer, A.*M*., 1986. J. Appl. Cryst. 105–107.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.52827 (2)	0.992001 (17)	0.315553 (11)	0.0157
C101	0.54238 (16)	0.96909 (14)	0.18279 (9)	0.0151
N102	0.57756 (13)	1.02145 (12)	0.23042 (8)	0.0145
N103	0.66583 (14)	1.07951 (12)	0.22781 (8)	0.0165
C104	0.69996 (17)	1.12459 (14)	0.27968 (9)	0.0170
S105	0.64556 (5)	1.12917 (4)	0.34537 (3)	0.0223
S106	0.82077 (5)	1.18896 (4)	0.28549 (3)	0.0218
C107	0.86887 (19)	1.16235 (16)	0.21458 (10)	0.0227
C108	0.92336 (18)	1.06688 (16)	0.21381 (10)	0.0201
C109	1.02461 (19)	1.04967 (18)	0.24911 (11)	0.0271
C110	1.0748 (2)	0.96228 (19)	0.24752 (11)	0.0306
C111	1.0238 (2)	0.88970 (18)	0.21068 (11)	0.0276
C112	0.92326 (19)	0.90545 (17)	0.17534 (10)	0.0257
C113	0.87376 (18)	0.99394 (16)	0.17643 (10)	0.0212
C114	0.45800 (16)	0.89875 (15)	0.19093 (9)	0.0160
N115	0.43995 (14)	0.88792 (12)	0.24871 (8)	0.0173
C116	0.36456 (17)	0.82562 (16)	0.25873 (10)	0.0211
C117	0.30530 (18)	0.77079 (16)	0.21274 (11)	0.0247
C118	0.32364 (19)	0.78172 (17)	0.15367 (11)	0.0264
C119	0.40036 (18)	0.84708 (16)	0.14234 (10)	0.0220
C120	0.58251 (17)	0.97419 (15)	0.12405 (9)	0.0169

C121	0.62547 (18)	0.89391 (16)	0.10049 (10)	0.0218
C122	0.6655 (2)	0.90042 (18)	0.04628 (11)	0.0288
C123	0.6611 (2)	0.98605 (18)	0.01499 (10)	0.0289
C124	0.6161 (2)	1.06568 (18)	0.03757 (10)	0.0281
C125	0.57791 (19)	1.06006 (16)	0.09211 (10)	0.0223
C201	0.59004 (16)	0.84982 (14)	0.41713 (9)	0.0150
N202	0.51528 (13)	0.90998 (12)	0.39390 (8)	0.0157
N203	0.42040 (14)	0.90721 (13)	0.41716 (8)	0.0193
C204	0.34919 (17)	0.96989 (16)	0.39193 (10)	0.0189
S205	0.35673 (4)	1.05422 (4)	0.33664 (3)	0.0213
S206	0.22568 (5)	0.96742 (5)	0.41839 (3)	0.0309
C207	0.2312 (2)	0.85102 (19)	0.45623 (11)	0.0322
C208	0.22822 (18)	0.76718 (18)	0.41302 (11)	0.0276
C209	0.14642 (19)	0.7582 (2)	0.36166 (12)	0.0346
C210	0.1418 (2)	0.6803 (2)	0.32314 (12)	0.0394
C211	0.2202 (2)	0.6104 (2)	0.33423 (13)	0.0409
C212	0.3031 (2)	0.61924 (19)	0.38429 (13)	0.0391
C213	0.3062 (2)	0.69618 (18)	0.42340 (11)	0.0310
C214	0.68809 (17)	0.85023 (14)	0.38898 (9)	0.0155
N215	0.67706 (14)	0.89154 (12)	0.33326 (8)	0.0163
C216	0.76099 (17)	0.88769 (15)	0.30420 (10)	0.0192
C217	0.85827 (18)	0.84506 (16)	0.32896 (10)	0.0220
C218	0.87086 (17)	0.80787 (15)	0.38733 (10)	0.0208
C219	0.78445 (17)	0.81014 (15)	0.41769 (10)	0.0192
C220	0.58100 (16)	0.77931 (15)	0.46577 (9)	0.0157
C221	0.59856 (18)	0.68281 (16)	0.45448 (10)	0.0204
C222	0.58656 (19)	0.61414 (16)	0.49780 (11)	0.0245
C223	0.55935 (19)	0.64118 (17)	0.55269 (10)	0.0260
C224	0.54377 (18)	0.73704 (17)	0.56474 (10)	0.0237
C225	0.55425 (17)	0.80586 (16)	0.52144 (9)	0.0189
C301	0.5638 (2)	0.54258 (19)	0.08460 (13)	0.0421
C302	0.5150 (2)	0.63022 (19)	0.05801 (11)	0.0308
N303	0.4777 (2)	0.69814 (17)	0.03609 (10)	0.0421
H1071	0.9213	1.2132	0.2111	0.0279*
H1072	0.8069	1.1671	0.1809	0.0280*
H1091	1.0597	1.0995	0.2750	0.0331*
H1101	1.1443	0.9511	0.2701	0.0389*
H1111	1.0583	0.8288	0.2094	0.0346*
H1121	0.8877	0.8560	0.1500	0.0322*
H1131	0.8041	1.0054	0.1510	0.0267*
H1161	0.3528	0.8199	0.3002	0.0264*
H1171	0.2530	0.7272	0.2224	0.0297*
H1181	0.2835	0.7452	0.1212	0.0328*
H1191	0.4138	0.8567	0.1019	0.0273*
H1211	0.6288	0.8342	0.1222	0.0266*
H1221	0.6965	0.8447	0.0307	0.0360*
H1231	0.6890	0.9897	−0.0220	0.0349*
H1241	0.6106	1.1255	0.0160	0.0344*
H1251	0.5479	1.1150	0.1079	0.0278*

H2071	0.2968	0.8479	0.4886	0.0407*
H2072	0.1655	0.8490	0.4758	0.0406*
H2091	0.0920	0.8079	0.3527	0.0422*
H2101	0.0845	0.6752	0.2897	0.0485*
H2111	0.2179	0.5566	0.3074	0.0489*
H2121	0.3592	0.5728	0.3916	0.0497*
H2131	0.3634	0.7018	0.4592	0.0396*
H2161	0.7536	0.9149	0.2645	0.0237*
H2171	0.9146	0.8431	0.3063	0.0266*
H2181	0.9384	0.7810	0.4067	0.0256*
H2191	0.7890	0.7845	0.4586	0.0233*
H2211	0.6186	0.6641	0.4165	0.0255*
H2221	0.5970	0.5479	0.4891	0.0300*
H2231	0.5512	0.5940	0.5829	0.0323*
H2241	0.5264	0.7553	0.6038	0.0282*
H2251	0.5427	0.8719	0.5299	0.0240*
H3012	0.5394	0.5297	0.1234	0.0643*
H3011	0.6406	0.5507	0.0906	0.0637*
H3013	0.5432	0.4920	0.0566	0.0642*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01798 (13)	0.01668 (12)	0.01312 (12)	0.00072 (10)	0.00433 (10)	0.00122 (10)
C101	0.0149 (10)	0.0139 (10)	0.0156 (10)	0.0010 (8)	0.0004 (8)	0.0023 (8)
N102	0.0142 (8)	0.0126 (8)	0.0155 (8)	−0.0019 (7)	−0.0003 (7)	0.0011 (7)
N103	0.0180 (9)	0.0146 (9)	0.0167 (9)	−0.0030 (7)	0.0022 (7)	0.0005 (7)
C104	0.0204 (11)	0.0111 (10)	0.0189 (11)	0.0026 (8)	0.0023 (9)	0.0022 (8)
S105	0.0278 (3)	0.0216 (3)	0.0190 (3)	−0.0035 (2)	0.0079 (2)	−0.0067 (2)
S106	0.0242 (3)	0.0198 (3)	0.0209 (3)	−0.0079 (2)	0.0026 (2)	−0.0038 (2)
C107	0.0239 (12)	0.0229 (12)	0.0221 (11)	−0.0070 (10)	0.0060 (10)	0.0035 (9)
C108	0.0207 (11)	0.0233 (12)	0.0178 (11)	−0.0053 (9)	0.0077 (9)	0.0037 (9)
C109	0.0259 (12)	0.0316 (13)	0.0232 (12)	−0.0078 (11)	0.0029 (10)	−0.0008 (10)
C110	0.0218 (12)	0.0416 (15)	0.0280 (13)	0.0016 (11)	0.0032 (11)	0.0045 (11)
C111	0.0287 (13)	0.0325 (14)	0.0241 (12)	0.0064 (11)	0.0113 (11)	0.0029 (10)
C112	0.0284 (13)	0.0291 (13)	0.0215 (12)	−0.0023 (11)	0.0101 (10)	−0.0046 (10)
C113	0.0178 (11)	0.0282 (12)	0.0181 (11)	−0.0031 (9)	0.0044 (9)	−0.0012 (9)
C114	0.0156 (10)	0.0150 (10)	0.0166 (10)	0.0012 (8)	0.0009 (9)	−0.0003 (8)
N115	0.0180 (9)	0.0168 (9)	0.0178 (9)	−0.0003 (7)	0.0050 (8)	−0.0008 (7)
C116	0.0220 (11)	0.0205 (11)	0.0227 (11)	−0.0017 (9)	0.0098 (10)	−0.0003 (9)
C117	0.0195 (11)	0.0230 (12)	0.0333 (13)	−0.0069 (10)	0.0091 (10)	−0.0027 (10)
C118	0.0226 (12)	0.0273 (12)	0.0283 (13)	−0.0085 (10)	0.0019 (11)	−0.0059 (10)
C119	0.0224 (11)	0.0243 (12)	0.0190 (11)	−0.0057 (10)	0.0031 (10)	−0.0012 (9)
C120	0.0163 (10)	0.0204 (11)	0.0128 (10)	−0.0057 (9)	−0.0007 (8)	−0.0006 (8)
C121	0.0255 (12)	0.0211 (11)	0.0185 (11)	−0.0004 (9)	0.0031 (10)	−0.0003 (9)
C122	0.0303 (13)	0.0330 (14)	0.0243 (12)	−0.0030 (11)	0.0082 (11)	−0.0088 (11)
C123	0.0296 (13)	0.0420 (15)	0.0164 (11)	−0.0131 (12)	0.0077 (10)	−0.0047 (11)
C124	0.0373 (14)	0.0281 (13)	0.0182 (11)	−0.0119 (11)	0.0035 (11)	0.0046 (10)
C125	0.0290 (12)	0.0214 (11)	0.0156 (11)	−0.0047 (10)	0.0021 (10)	−0.0004 (9)
C201	0.0161 (10)	0.0152 (10)	0.0137 (10)	−0.0003 (8)	0.0028 (9)	−0.0009 (8)

N202	0.0144 (8)	0.0188 (9)	0.0151 (9)	0.0016 (7)	0.0056 (7)	−0.0001 (7)
N203	0.0153 (9)	0.0253 (10)	0.0192 (9)	0.0040 (8)	0.0083 (8)	0.0017 (8)
C204	0.0176 (10)	0.0238 (11)	0.0164 (10)	0.0037 (9)	0.0058 (9)	−0.0041 (9)
S205	0.0210 (3)	0.0203 (3)	0.0225 (3)	0.0064 (2)	0.0035 (2)	0.0022 (2)
S206	0.0202 (3)	0.0392 (4)	0.0365 (3)	0.0097 (3)	0.0140 (3)	0.0043 (3)
C207	0.0254 (13)	0.0447 (16)	0.0299 (13)	0.0013 (12)	0.0136 (11)	0.0072 (12)
C208	0.0206 (12)	0.0377 (14)	0.0267 (12)	−0.0046 (11)	0.0101 (10)	0.0079 (11)
C209	0.0185 (12)	0.0499 (17)	0.0352 (14)	−0.0056 (12)	0.0048 (11)	0.0121 (13)
C210	0.0319 (15)	0.0522 (18)	0.0321 (14)	−0.0204 (14)	0.0006 (12)	0.0077 (13)
C211	0.0484 (17)	0.0385 (16)	0.0355 (15)	−0.0211 (14)	0.0063 (14)	0.0019 (12)
C212	0.0406 (16)	0.0307 (14)	0.0448 (16)	−0.0017 (12)	0.0051 (14)	0.0070 (12)
C213	0.0270 (13)	0.0353 (14)	0.0298 (13)	−0.0052 (11)	0.0028 (11)	0.0077 (11)
C214	0.0160 (10)	0.0133 (10)	0.0177 (10)	0.0007 (8)	0.0047 (9)	−0.0003 (8)
N215	0.0184 (9)	0.0145 (9)	0.0159 (9)	0.0017 (7)	0.0029 (8)	0.0022 (7)
C216	0.0216 (11)	0.0183 (11)	0.0200 (11)	0.0002 (9)	0.0098 (9)	0.0024 (9)
C217	0.0183 (11)	0.0235 (12)	0.0263 (12)	0.0019 (9)	0.0094 (10)	0.0000 (10)
C218	0.0146 (10)	0.0190 (11)	0.0286 (12)	0.0032 (9)	0.0033 (10)	0.0020 (9)
C219	0.0193 (11)	0.0200 (11)	0.0184 (11)	−0.0004 (9)	0.0037 (9)	0.0031 (9)
C220	0.0119 (10)	0.0192 (10)	0.0161 (10)	0.0022 (8)	0.0027 (8)	0.0030 (8)
C221	0.0215 (11)	0.0228 (11)	0.0187 (11)	0.0015 (9)	0.0085 (10)	−0.0004 (9)
C222	0.0295 (13)	0.0168 (11)	0.0295 (12)	0.0035 (10)	0.0114 (11)	0.0027 (9)
C223	0.0283 (12)	0.0268 (12)	0.0245 (12)	0.0029 (10)	0.0089 (11)	0.0099 (10)
C224	0.0274 (12)	0.0286 (12)	0.0166 (11)	0.0044 (10)	0.0083 (10)	0.0022 (9)
C225	0.0184 (11)	0.0206 (11)	0.0176 (11)	0.0024 (9)	0.0030 (9)	0.0000 (9)
C301	0.0438 (17)	0.0337 (15)	0.0425 (16)	0.0025 (13)	−0.0089 (14)	−0.0034 (13)
C302	0.0297 (13)	0.0346 (14)	0.0253 (13)	−0.0064 (12)	−0.0024 (11)	−0.0048 (11)
N303	0.0498 (15)	0.0334 (13)	0.0372 (13)	−0.0009 (11)	−0.0082 (12)	−0.0027 (11)

Geometric parameters (Å, º)

Zn1—N102	2.1346 (17)	C201—N202	1.299 (3)
Zn1—S105	2.4403 (6)	C201—C214	1.481 (3)
Zn1—N115	2.2288 (17)	C201—C220	1.483 (3)
Zn1—N202	2.1160 (17)	N202—N203	1.385 (2)
Zn1—S205	2.4516 (6)	N203—C204	1.306 (3)
Zn1—N215	2.3188 (17)	C204—S205	1.719 (2)
C101—N102	1.297 (3)	C204—S206	1.760 (2)
C101—C114	1.484 (3)	S206—C207	1.829 (3)
C101—C120	1.484 (3)	C207—C208	1.512 (4)
N102—N103	1.387 (2)	C207—H2071	0.994
N103—C104	1.316 (3)	C207—H2072	1.002
C104—S105	1.722 (2)	C208—C209	1.397 (3)
C104—S106	1.753 (2)	C208—C213	1.387 (3)
S106—C107	1.825 (2)	C209—C210	1.382 (4)
C107—C108	1.504 (3)	C209—H2091	0.971
C107—H1071	0.984	C210—C211	1.381 (4)
C107—H1072	0.982	C210—H2101	0.939
C108—C109	1.392 (3)	C211—C212	1.386 (4)
C108—C113	1.391 (3)	C211—H2111	0.957
C109—C110	1.380 (4)	C212—C213	1.380 (4)

C109—H1091	0.960	C212—H2121	0.952
C110—C111	1.387 (3)	C213—H2131	0.974
C110—H1101	0.940	C214—N215	1.350 (3)
C111—C112	1.382 (3)	C214—C219	1.383 (3)
C111—H1111	0.960	N215—C216	1.335 (3)
C112—C113	1.389 (3)	C216—C217	1.384 (3)
C112—H1121	0.952	C216—H2161	0.949
C113—H1131	0.967	C217—C218	1.379 (3)
C114—N115	1.352 (3)	C217—H2171	0.942
C114—C119	1.390 (3)	C218—C219	1.380 (3)
N115—C116	1.337 (3)	C218—H2181	0.958
C116—C117	1.383 (3)	C219—H2191	0.970
C116—H1161	0.961	C220—C221	1.399 (3)
C117—C118	1.381 (3)	C220—C225	1.390 (3)
C117—H1171	0.950	C221—C222	1.388 (3)
C118—C119	1.386 (3)	C221—H2211	0.960
C118—H1181	0.952	C222—C223	1.378 (3)
C119—H1191	0.954	C222—H2221	0.961
C120—C121	1.390 (3)	C223—C224	1.389 (3)
C120—C125	1.392 (3)	C223—H2231	0.959
C121—C122	1.390 (3)	C224—C225	1.385 (3)
C121—H1211	0.962	C224—H2241	0.967
C122—C123	1.382 (3)	C225—H2251	0.961
C122—H1221	0.964	C301—C302	1.449 (4)
C123—C124	1.385 (3)	C301—H3012	0.983
C123—H1231	0.951	C301—H3011	0.958
C124—C125	1.384 (3)	C301—H3013	0.947
C124—H1241	0.962	C302—N303	1.131 (3)
C125—H1251	0.951		

N102—Zn1—S105	80.19 (5)	C120—C125—C124	120.4 (2)
N102—Zn1—N115	74.11 (6)	C120—C125—H1251	119.5
S105—Zn1—N115	154.15 (5)	C124—C125—H1251	120.0
N102—Zn1—N202	155.73 (7)	N202—C201—C214	115.42 (18)
S105—Zn1—N202	109.70 (5)	N202—C201—C220	125.14 (19)
N115—Zn1—N202	95.14 (6)	C214—C201—C220	119.33 (17)
N102—Zn1—S205	120.54 (5)	Zn1—N202—C201	121.37 (14)
S105—Zn1—S205	100.33 (2)	Zn1—N202—N203	121.48 (13)
N115—Zn1—S205	90.52 (5)	C201—N202—N203	116.47 (17)
N202—Zn1—S205	80.43 (5)	N202—N203—C204	113.11 (17)
N102—Zn1—N215	84.94 (6)	N203—C204—S205	130.23 (17)
S105—Zn1—N215	90.04 (5)	N203—C204—S206	115.02 (16)
N115—Zn1—N215	90.39 (6)	S205—C204—S206	114.75 (12)
N202—Zn1—N215	73.24 (6)	C204—S205—Zn1	93.26 (7)
S205—Zn1—N215	153.63 (5)	C204—S206—C207	102.05 (11)
N102—C101—C114	114.98 (18)	S206—C207—C208	113.92 (17)
N102—C101—C120	124.71 (19)	S206—C207—H2071	109.2
C114—C101—C120	120.29 (17)	C208—C207—H2071	110.3
Zn1—N102—C101	120.13 (14)	S206—C207—H2072	105.1

Zn1—N102—N103	120.93 (12)	C208—C207—H2072	109.0
C101—N102—N103	117.09 (17)	H2071—C207—H2072	109.1
N102—N103—C104	112.46 (17)	C207—C208—C209	121.2 (2)
N103—C104—S105	130.01 (17)	C207—C208—C213	121.0 (2)
N103—C104—S106	116.92 (16)	C209—C208—C213	117.8 (2)
S105—C104—S106	113.05 (12)	C208—C209—C210	121.2 (3)
C104—S105—Zn1	93.14 (7)	C208—C209—H2091	119.4
C104—S106—C107	104.51 (10)	C210—C209—H2091	119.4
S106—C107—C108	114.49 (15)	C209—C210—C211	120.1 (3)
S106—C107—H1071	104.6	C209—C210—H2101	119.3
C108—C107—H1071	109.2	C211—C210—H2101	120.7
S106—C107—H1072	107.6	C210—C211—C212	119.3 (3)
C108—C107—H1072	110.7	C210—C211—H2111	120.4
H1071—C107—H1072	110.1	C212—C211—H2111	120.2
C107—C108—C109	121.4 (2)	C211—C212—C213	120.4 (3)
C107—C108—C113	120.2 (2)	C211—C212—H2121	120.2
C109—C108—C113	118.4 (2)	C213—C212—H2121	119.3
C108—C109—C110	121.0 (2)	C208—C213—C212	121.1 (2)
C108—C109—H1091	119.2	C208—C213—H2131	118.3
C110—C109—H1091	119.8	C212—C213—H2131	120.6
C109—C110—C111	120.0 (2)	C201—C214—N215	115.68 (18)
C109—C110—H1101	121.3	C201—C214—C219	122.15 (19)
C111—C110—H1101	118.7	N215—C214—C219	122.17 (19)
C110—C111—C112	119.8 (2)	Zn1—N215—C214	111.17 (13)
C110—C111—H1111	120.4	Zn1—N215—C216	128.93 (14)
C112—C111—H1111	119.9	C214—N215—C216	117.82 (18)
C111—C112—C113	120.0 (2)	N215—C216—C217	123.1 (2)
C111—C112—H1121	120.3	N215—C216—H2161	118.6
C113—C112—H1121	119.7	C217—C216—H2161	118.3
C108—C113—C112	120.7 (2)	C216—C217—C218	118.6 (2)
C108—C113—H1131	119.3	C216—C217—H2171	119.8
C112—C113—H1131	120.0	C218—C217—H2171	121.5
C101—C114—N115	115.93 (18)	C217—C218—C219	118.9 (2)
C101—C114—C119	122.40 (19)	C217—C218—H2181	120.8
N115—C114—C119	121.67 (19)	C219—C218—H2181	120.3
Zn1—N115—C114	114.19 (13)	C214—C219—C218	119.2 (2)
Zn1—N115—C116	126.82 (14)	C214—C219—H2191	118.7
C114—N115—C116	118.53 (18)	C218—C219—H2191	122.1
N115—C116—C117	122.9 (2)	C201—C220—C221	118.48 (18)
N115—C116—H1161	116.8	C201—C220—C225	122.21 (19)
C117—C116—H1161	120.3	C221—C220—C225	119.30 (19)
C116—C117—C118	118.6 (2)	C220—C221—C222	120.3 (2)
C116—C117—H1171	119.5	C220—C221—H2211	119.8
C118—C117—H1171	121.8	C222—C221—H2211	119.9
C117—C118—C119	119.2 (2)	C221—C222—C223	119.9 (2)
C117—C118—H1181	120.2	C221—C222—H2221	119.6
C119—C118—H1181	120.6	C223—C222—H2221	120.5
C114—C119—C118	119.1 (2)	C222—C223—C224	120.1 (2)
C114—C119—H1191	120.1	C222—C223—H2231	120.3

C118—C119—H1191	120.9	C224—C223—H2231	119.6
C101—C120—C121	120.65 (19)	C223—C224—C225	120.3 (2)
C101—C120—C125	120.0 (2)	C223—C224—H2241	119.4
C121—C120—C125	119.3 (2)	C225—C224—H2241	120.3
C120—C121—C122	120.0 (2)	C220—C225—C224	120.1 (2)
C120—C121—H1211	119.9	C220—C225—H2251	120.1
C122—C121—H1211	120.0	C224—C225—H2251	119.8
C121—C122—C123	120.3 (2)	C302—C301—H3012	109.6
C121—C122—H1221	119.5	C302—C301—H3011	107.4
C123—C122—H1221	120.2	H3012—C301—H3011	111.6
C122—C123—C124	119.9 (2)	C302—C301—H3013	108.6
C122—C123—H1231	119.5	H3012—C301—H3013	110.3
C124—C123—H1231	120.6	H3011—C301—H3013	109.2
C123—C124—C125	120.0 (2)	C301—C302—N303	178.5 (3)
C123—C124—H1241	121.2	C301—C302—N303	178.5 (3)
C125—C124—H1241	118.8	C301—C302—N303	178.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C216—H2161···N103	0.95	2.62	3.285 (3)	127