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# Bis(*S*-benzylisothiouronium) tetrachloridozincate(II)

**D. Gayathri,[a] D. Velmurugan,[a]* P. Hemalatha,[b] V. Veeravazhuthi[c] and K. Ravikumar[d]**

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [b]Department of Physics, PSG College of Technology, Coimbatore 641 004, India, [c]Department of Physics, PSG College of Arts and Science, Coimbatore 641 101, India, and [d]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India
Correspondence e-mail: d_velu@yahoo.com

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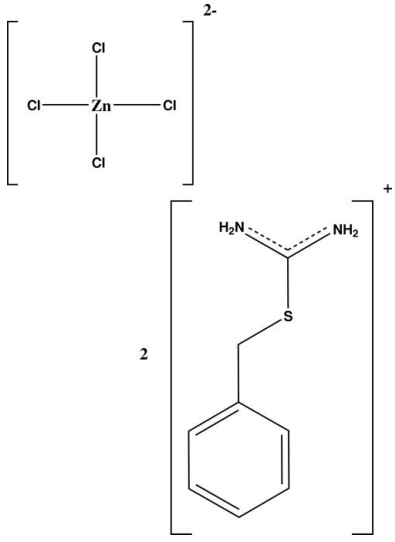
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.029; $wR$ factor = 0.074; data-to-parameter ratio = 22.5.

The asymmetric unit of the title compound, $(C_8H_{11}N_2S)_2[ZnCl_4]$, contains two *S*-benzylisothiouronium cations which differ in the C—C—S—C torsion angle [165.3 (2) and 81.9 (2)°] and a tetrahedral tetrachloridozincate anion. The crystal structure is stabilized by N—H···Cl, C—H···Cl and C—H···S interactions.

## Related literature

For related literature, see: Hemalatha *et al.* (2006); Zhang *et al.* (1994); Barker & Powell (1998).




## Experimental

### Crystal data

$(C_8H_{11}N_2S)_2[ZnCl_4]$
$M_r$ = 541.67
Monoclinic, $P2_1/c$
$a$ = 15.2135 (11) Å
$b$ = 6.4475 (5) Å
$c$ = 23.9277 (18) Å
$\beta$ = 95.368 (1)°
$V$ = 2336.8 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.70 mm$^{-1}$
$T$ = 293 (2) K
0.27 × 0.23 × 0.21 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
25129 measured reflections
5481 independent reflections
4986 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
$S$ = 1.08
5481 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cl1—Zn1 | 2.2792 (5) | Cl3—Zn1 | 2.2718 (5) |
| Cl2—Zn1 | 2.2650 (5) | Cl4—Zn1 | 2.2589 (5) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···Cl3 | 0.86 | 2.68 | 3.372 (2) | 139 |
| N1—H1$B$···Cl2$^{i}$ | 0.86 | 2.45 | 3.255 (2) | 157 |
| N2—H2$A$···Cl4 | 0.86 | 2.53 | 3.219 (2) | 138 |
| N2—H2$B$···Cl3$^{ii}$ | 0.86 | 2.62 | 3.262 (2) | 132 |
| N3—H3$A$···Cl1$^{iii}$ | 0.86 | 2.72 | 3.469 (2) | 147 |
| N3—H3$A$···Cl4$^{iii}$ | 0.86 | 2.65 | 3.244 (2) | 128 |
| N3—H3$B$···Cl1$^{iv}$ | 0.86 | 2.44 | 3.283 (2) | 166 |
| N4—H4$A$···Cl1$^{iii}$ | 0.86 | 2.49 | 3.290 (2) | 156 |
| N4—H4$B$···Cl2$^{i}$ | 0.86 | 2.62 | 3.447 (2) | 163 |
| C15—H15$A$···S1 | 0.97 | 2.87 | 3.591 (2) | 132 |
| C15—H15$A$···Cl2$^{v}$ | 0.97 | 2.77 | 3.556 (2) | 139 |
| C15—H15$B$···Cl2$^{i}$ | 0.97 | 2.65 | 3.594 (2) | 164 |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x, y+1, z$; (iii) $x-1, y, z$; (iv) $x-1, y+1, z$; (v) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2708).

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# supporting information

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## Bis(*S*-benzylisothiouronium) tetrachloridozincate(II)

**D. Gayathri, D. Velmurugan, P. Hemalatha, V. Veeravazhuthi and K. Ravikumar**

### S1. Comment

Most organic nonlinear optical (NLO) crystals have usually poor mechanical and thermal properties, and are susceptible to damage during processing. It is difficult to grow large optical quality crystals of these materials for device applications (Zhang *et al.*, 1994). For further enhancement of NLO property many efforts have been made on developing new semiorganic NLO materials. The title compound is one of the new metalorganic nonlinear optical crystals. It combines the advantages of both organic and inorganic materials.

The C—N, S—C bond lengths and C—S—C and N—C—N bond angles are comparable with the similar structure reported earlier (Barker & Powell, 1998). There is a difference in the torsion angles C6—C7—S1—C8 [165.3 (2)°] and C14—C15—S2—C16 [81.9 (2)°] in the two molecules which indicates a difference in the conformation of the two molecules in the asymmetric unit.

The crystal structure (Figs. 2 and 3) is stabilized by N—H···Cl, C—H···Cl and C—H···S interactions.

### S2. Experimental

First *S*-benzylisothiouronium chloride (SBTC) was synthesized as discussed in an earlier report (Hemalatha *et al.*, 2006). The solutions of SBTC (5 g m) and zinc chloride (1 g m) were prepared separately in minimum amount of water. Then the solutions were mixed together and stirred for 1 hr at 45°C. The resulting complex was filtered and thoroughly washed with distilled water. The product was recrystallized repeatedly from 0.2 *M* hydrochloric solution to grow transparent and good quality single crystals for NLO applications. Needle shape crystals were obtained from the saturated solution (with water) of the title compound by slow evaporation technique at room temperature.

### S3. Refinement

All H-atoms were refined using a riding model with d(C—H) = 0.93 Å or d(N—H) = 0.86 Å $U_{iso}$=1.2$U_{eq}$ (C,N) and 0.97 Å, $U_{iso}$ = 1.2$U_{eq}$ (C) for $CH_2$.

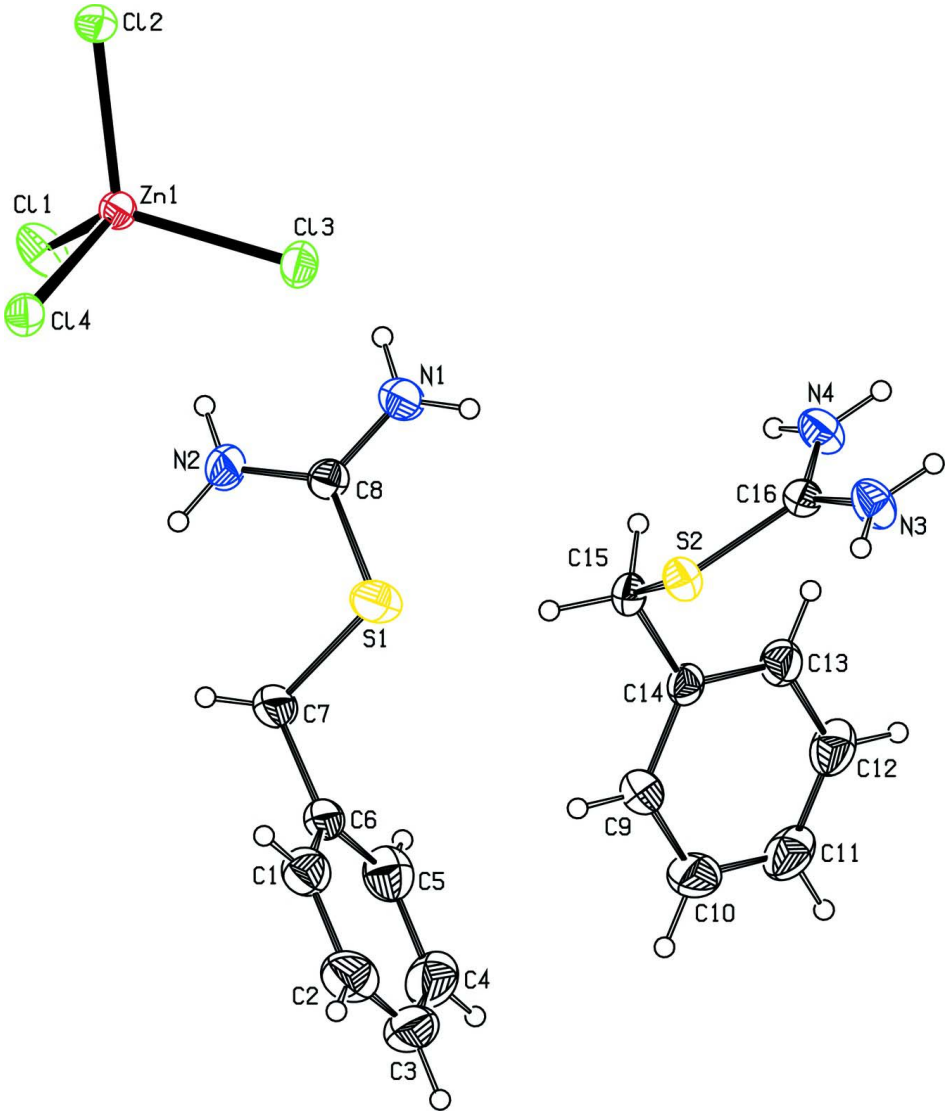


**Figure 1**

The molecular structure of title compound, showing 30% probability displacement ellipsoids.

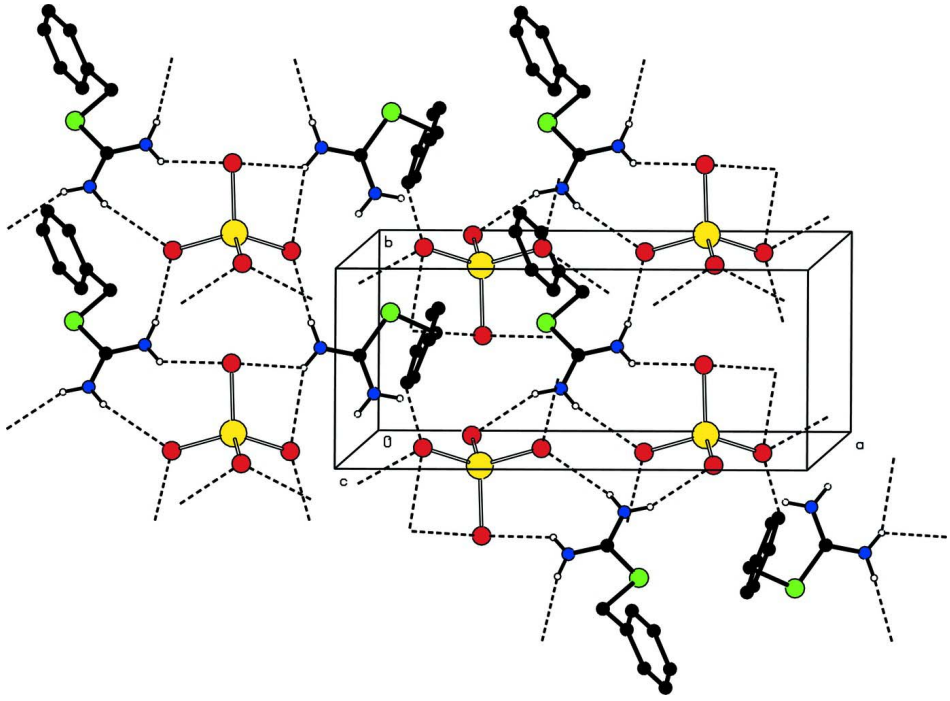


**Figure 2**

The molecular packing of the title compound showing N—H···Cl interactions viewed down *c* axis.

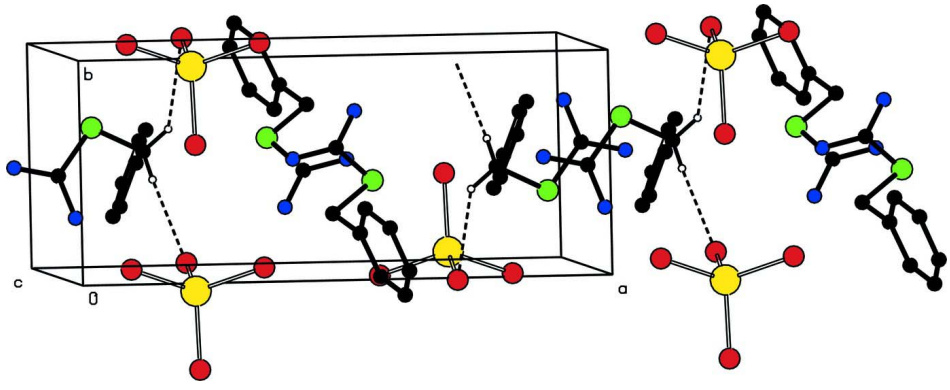


**Figure 3**

The molecular packing of the title compound showing C—H···Cl interactions viewed down *c* axis.

**Bis(*S*-benzylisothiouronium) tetrachloridozincate(II)**

*Crystal data*

$(C_8H_{11}N_2S)_2[ZnCl_4]$
$M_r = 541.67$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.2135\ (11)$ Å
$b = 6.4475\ (5)$ Å
$c = 23.9277\ (18)$ Å
$\beta = 95.368\ (1)°$
$V = 2336.8\ (3)$ Å$^3$
$Z = 4$
$F(000) = 1104$
$D_x = 1.540$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2794 reflections
$\theta = 1.3–25.0°$
$\mu = 1.70$ mm$^{-1}$
$T = 293$ K
Needle, colorless
0.27 × 0.23 × 0.21 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
25129 measured reflections
5481 independent reflections
4986 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.3°$
$h = -20 \rightarrow 20$
$k = -8 \rightarrow 8$
$l = -30 \rightarrow 31$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.073$
$S = 1.08$
5481 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 1.0433P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.32$ e Å$^{-3}$

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.38843 (3) | 0.61059 (12) | 0.36896 (3) | 0.06677 (19) |
| N1 | 0.42614 (13) | 0.2947 (3) | 0.43326 (8) | 0.0562 (5) |
| H1A | 0.4589 | 0.2133 | 0.4547 | 0.067* |
| H1B | 0.3709 | 0.2676 | 0.4258 | 0.067* |
| C1 | 0.36865 (17) | 1.0458 (4) | 0.28381 (11) | 0.0598 (6) |
| H1 | 0.3774 | 1.1179 | 0.3175 | 0.072* |
| C2 | 0.31899 (18) | 1.1338 (5) | 0.23884 (15) | 0.0783 (8) |
| H2 | 0.2949 | 1.2652 | 0.2423 | 0.094* |
| C3 | 0.3052 (2) | 1.0311 (7) | 0.19011 (14) | 0.0869 (10) |
| H3 | 0.2718 | 1.0920 | 0.1600 | 0.104* |
| C4 | 0.3395 (2) | 0.8398 (7) | 0.18442 (11) | 0.0867 (10) |
| H4 | 0.3293 | 0.7693 | 0.1505 | 0.104* |
| C5 | 0.39016 (18) | 0.7482 (4) | 0.22921 (12) | 0.0663 (7) |
| H5 | 0.4137 | 0.6165 | 0.2252 | 0.080* |
| C6 | 0.40541 (13) | 0.8523 (4) | 0.27928 (9) | 0.0475 (5) |
| C7 | 0.46069 (15) | 0.7581 (4) | 0.32779 (11) | 0.0664 (7) |
| H7A | 0.4903 | 0.8661 | 0.3506 | 0.080* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.5052 | 0.6680 | 0.3143 | 0.080* |
| C8 | 0.46009 (12) | 0.4585 (3) | 0.41203 (8) | 0.0399 (4) |
| S2 | 0.06186 (3) | 0.66804 (7) | 0.41032 (2) | 0.04038 (11) |
| N2 | 0.54328 (12) | 0.5038 (3) | 0.42243 (9) | 0.0555 (5) |
| H2A | 0.5772 | 0.4246 | 0.4438 | 0.067* |
| H2B | 0.5644 | 0.6130 | 0.4079 | 0.067* |
| C9 | 0.15114 (15) | 0.6634 (4) | 0.27656 (10) | 0.0578 (6) |
| H9 | 0.1742 | 0.7917 | 0.2880 | 0.069* |
| C10 | 0.13285 (18) | 0.6205 (6) | 0.22003 (11) | 0.0757 (8) |
| H10 | 0.1442 | 0.7203 | 0.1936 | 0.091* |
| C11 | 0.09845 (18) | 0.4338 (5) | 0.20262 (11) | 0.0743 (8) |
| H11 | 0.0859 | 0.4075 | 0.1645 | 0.089* |
| C12 | 0.08244 (17) | 0.2855 (5) | 0.24096 (10) | 0.0651 (7) |
| H12 | 0.0588 | 0.1583 | 0.2290 | 0.078* |
| C13 | 0.10135 (14) | 0.3240 (4) | 0.29755 (9) | 0.0505 (5) |
| H13 | 0.0914 | 0.2213 | 0.3235 | 0.061* |
| C14 | 0.13496 (11) | 0.5144 (3) | 0.31602 (8) | 0.0395 (4) |
| C15 | 0.15495 (11) | 0.5601 (3) | 0.37715 (8) | 0.0377 (4) |
| H15A | 0.2038 | 0.6572 | 0.3818 | 0.045* |
| H15B | 0.1737 | 0.4330 | 0.3964 | 0.045* |
| C16 | −0.00143 (12) | 0.4549 (3) | 0.42524 (8) | 0.0373 (4) |
| N3 | −0.08381 (12) | 0.4941 (3) | 0.43308 (8) | 0.0527 (4) |
| H3A | −0.1180 | 0.3953 | 0.4418 | 0.063* |
| H3B | −0.1038 | 0.6187 | 0.4295 | 0.063* |
| N4 | 0.03000 (12) | 0.2657 (3) | 0.43054 (8) | 0.0519 (4) |
| H4A | −0.0036 | 0.1658 | 0.4392 | 0.062* |
| H4B | 0.0842 | 0.2415 | 0.4253 | 0.062* |
| Cl1 | 0.85432 (4) | −0.02098 (8) | 0.44408 (3) | 0.05782 (15) |
| Cl2 | 0.76342 (3) | −0.05687 (7) | 0.57924 (2) | 0.04173 (11) |
| Cl3 | 0.60408 (3) | −0.01885 (8) | 0.44970 (3) | 0.05317 (14) |
| Cl4 | 0.73327 (3) | 0.42677 (7) | 0.49034 (2) | 0.04099 (11) |
| Zn1 | 0.738101 (13) | 0.07662 (3) | 0.491654 (9) | 0.03552 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0303 (2) | 0.0860 (4) | 0.0846 (4) | 0.0098 (3) | 0.0085 (2) | 0.0446 (4) |
| N1 | 0.0452 (10) | 0.0590 (11) | 0.0640 (12) | −0.0027 (8) | 0.0029 (8) | 0.0212 (9) |
| C1 | 0.0585 (14) | 0.0609 (14) | 0.0607 (14) | −0.0017 (11) | 0.0088 (11) | 0.0033 (11) |
| C2 | 0.0582 (15) | 0.0761 (18) | 0.101 (2) | 0.0120 (14) | 0.0101 (15) | 0.0311 (18) |
| C3 | 0.0568 (16) | 0.128 (3) | 0.073 (2) | −0.0069 (18) | −0.0079 (14) | 0.039 (2) |
| C4 | 0.079 (2) | 0.135 (3) | 0.0459 (14) | −0.027 (2) | 0.0053 (13) | −0.0046 (17) |
| C5 | 0.0617 (15) | 0.0708 (16) | 0.0684 (16) | −0.0033 (12) | 0.0167 (12) | −0.0063 (13) |
| C6 | 0.0359 (9) | 0.0567 (12) | 0.0498 (11) | −0.0044 (9) | 0.0043 (8) | 0.0124 (10) |
| C7 | 0.0423 (12) | 0.0819 (18) | 0.0735 (16) | −0.0119 (11) | −0.0031 (11) | 0.0342 (13) |
| C8 | 0.0349 (9) | 0.0424 (10) | 0.0426 (10) | 0.0044 (7) | 0.0041 (7) | 0.0031 (8) |
| S2 | 0.0369 (2) | 0.0350 (2) | 0.0500 (3) | −0.00065 (18) | 0.00816 (19) | −0.00128 (19) |
| N2 | 0.0386 (9) | 0.0523 (10) | 0.0724 (13) | −0.0025 (8) | −0.0125 (8) | 0.0143 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0515 (12) | 0.0654 (14) | 0.0565 (13) | −0.0130 (11) | 0.0048 (10) | 0.0116 (11) |
| C10 | 0.0635 (15) | 0.113 (2) | 0.0521 (14) | −0.0118 (16) | 0.0110 (12) | 0.0252 (15) |
| C11 | 0.0585 (15) | 0.123 (3) | 0.0408 (12) | −0.0074 (16) | 0.0039 (11) | −0.0090 (14) |
| C12 | 0.0599 (14) | 0.0816 (17) | 0.0530 (13) | −0.0095 (13) | 0.0019 (11) | −0.0212 (12) |
| C13 | 0.0502 (12) | 0.0544 (12) | 0.0466 (11) | −0.0072 (10) | 0.0025 (9) | −0.0054 (9) |
| C14 | 0.0277 (8) | 0.0497 (10) | 0.0409 (10) | −0.0010 (7) | 0.0021 (7) | −0.0001 (8) |
| C15 | 0.0285 (8) | 0.0400 (9) | 0.0442 (10) | −0.0021 (7) | 0.0004 (7) | −0.0029 (7) |
| C16 | 0.0372 (9) | 0.0397 (9) | 0.0351 (9) | −0.0016 (7) | 0.0040 (7) | 0.0021 (7) |
| N3 | 0.0406 (9) | 0.0461 (9) | 0.0741 (12) | −0.0004 (7) | 0.0188 (8) | 0.0060 (9) |
| N4 | 0.0483 (10) | 0.0402 (9) | 0.0687 (12) | 0.0002 (7) | 0.0130 (9) | 0.0119 (8) |
| Cl1 | 0.0586 (3) | 0.0431 (3) | 0.0774 (4) | 0.0024 (2) | 0.0365 (3) | −0.0026 (2) |
| Cl2 | 0.0459 (2) | 0.0367 (2) | 0.0417 (2) | −0.00012 (18) | −0.00090 (18) | 0.00612 (17) |
| Cl3 | 0.0417 (3) | 0.0453 (3) | 0.0688 (3) | −0.0069 (2) | −0.0143 (2) | 0.0068 (2) |
| Cl4 | 0.0366 (2) | 0.0346 (2) | 0.0508 (3) | 0.00228 (16) | −0.00096 (19) | 0.00113 (18) |
| Zn1 | 0.03067 (11) | 0.03633 (12) | 0.03951 (12) | 0.00107 (8) | 0.00309 (8) | 0.00358 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C8 | 1.732 (2) | C9—C10 | 1.383 (4) |
| S1—C7 | 1.813 (2) | C9—C14 | 1.385 (3) |
| N1—C8 | 1.300 (3) | C9—H9 | 0.9300 |
| N1—H1A | 0.8600 | C10—C11 | 1.362 (4) |
| N1—H1B | 0.8600 | C10—H10 | 0.9300 |
| C1—C6 | 1.376 (3) | C11—C12 | 1.363 (4) |
| C1—C2 | 1.378 (4) | C11—H11 | 0.9300 |
| C1—H1 | 0.9300 | C12—C13 | 1.380 (3) |
| C2—C3 | 1.340 (5) | C12—H12 | 0.9300 |
| C2—H2 | 0.9300 | C13—C14 | 1.386 (3) |
| C3—C4 | 1.351 (5) | C13—H13 | 0.9300 |
| C3—H3 | 0.9300 | C14—C15 | 1.495 (3) |
| C4—C5 | 1.391 (4) | C15—H15A | 0.9700 |
| C4—H4 | 0.9300 | C15—H15B | 0.9700 |
| C5—C6 | 1.374 (3) | C16—N3 | 1.309 (2) |
| C5—H5 | 0.9300 | C16—N4 | 1.312 (2) |
| C6—C7 | 1.497 (3) | N3—H3A | 0.8600 |
| C7—H7A | 0.9700 | N3—H3B | 0.8600 |
| C7—H7B | 0.9700 | N4—H4A | 0.8600 |
| C8—N2 | 1.300 (3) | N4—H4B | 0.8600 |
| S2—C16 | 1.734 (2) | Cl1—Zn1 | 2.2792 (5) |
| S2—C15 | 1.825 (2) | Cl2—Zn1 | 2.2650 (5) |
| N2—H2A | 0.8600 | Cl3—Zn1 | 2.2718 (5) |
| N2—H2B | 0.8600 | Cl4—Zn1 | 2.2589 (5) |
| | | | |
| C8—S1—C7 | 103.9 (1) | C14—C9—H9 | 120.1 |
| C8—N1—H1A | 120.0 | C11—C10—C9 | 120.8 (3) |
| C8—N1—H1B | 120.0 | C11—C10—H10 | 119.6 |
| H1A—N1—H1B | 120.0 | C9—C10—H10 | 119.6 |
| C6—C1—C2 | 120.6 (3) | C10—C11—C12 | 120.1 (2) |

| | | | |
|---|---|---|---|
| C6—C1—H1 | 119.7 | C10—C11—H11 | 119.9 |
| C2—C1—H1 | 119.7 | C12—C11—H11 | 119.9 |
| C3—C2—C1 | 120.4 (3) | C11—C12—C13 | 120.0 (2) |
| C3—C2—H2 | 119.8 | C11—C12—H12 | 120.0 |
| C1—C2—H2 | 119.8 | C13—C12—H12 | 120.0 |
| C2—C3—C4 | 120.6 (3) | C12—C13—C14 | 120.6 (2) |
| C2—C3—H3 | 119.7 | C12—C13—H13 | 119.7 |
| C4—C3—H3 | 119.7 | C14—C13—H13 | 119.7 |
| C3—C4—C5 | 120.1 (3) | C9—C14—C13 | 118.7 (2) |
| C3—C4—H4 | 120.0 | C9—C14—C15 | 119.82 (19) |
| C5—C4—H4 | 120.0 | C13—C14—C15 | 121.44 (18) |
| C6—C5—C4 | 120.0 (3) | C14—C15—S2 | 113.93 (12) |
| C6—C5—H5 | 120.0 | C14—C15—H15A | 108.8 |
| C4—C5—H5 | 120.0 | S2—C15—H15A | 108.8 |
| C5—C6—C1 | 118.3 (2) | C14—C15—H15B | 108.8 |
| C5—C6—C7 | 121.0 (2) | S2—C15—H15B | 108.8 |
| C1—C6—C7 | 120.6 (2) | H15A—C15—H15B | 107.7 |
| C6—C7—S1 | 108.00 (15) | N3—C16—N4 | 120.7 (2) |
| C6—C7—H7A | 110.1 | N3—C16—S2 | 115.7 (2) |
| S1—C7—H7A | 110.1 | N4—C16—S2 | 123.5 (2) |
| C6—C7—H7B | 110.1 | C16—N3—H3A | 120.0 |
| S1—C7—H7B | 110.1 | C16—N3—H3B | 120.0 |
| H7A—C7—H7B | 108.4 | H3A—N3—H3B | 120.0 |
| N1—C8—N2 | 121.5 (2) | C16—N4—H4A | 120.0 |
| N1—C8—S1 | 116.2 (2) | C16—N4—H4B | 120.0 |
| N2—C8—S1 | 122.3 (2) | H4A—N4—H4B | 120.0 |
| C16—S2—C15 | 104.82 (9) | Cl4—Zn1—Cl2 | 113.28 (2) |
| C8—N2—H2A | 120.0 | Cl4—Zn1—Cl3 | 103.76 (2) |
| C8—N2—H2B | 120.0 | Cl2—Zn1—Cl3 | 111.95 (2) |
| H2A—N2—H2B | 120.0 | Cl4—Zn1—Cl1 | 107.14 (2) |
| C10—C9—C14 | 119.7 (2) | Cl2—Zn1—Cl1 | 106.53 (2) |
| C10—C9—H9 | 120.1 | Cl3—Zn1—Cl1 | 114.24 (3) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.5 (4) | C14—C9—C10—C11 | 0.5 (4) |
| C1—C2—C3—C4 | 0.2 (5) | C9—C10—C11—C12 | −0.7 (5) |
| C2—C3—C4—C5 | −0.5 (5) | C10—C11—C12—C13 | −0.2 (4) |
| C3—C4—C5—C6 | −0.1 (4) | C11—C12—C13—C14 | 1.3 (4) |
| C4—C5—C6—C1 | 0.8 (4) | C10—C9—C14—C13 | 0.6 (3) |
| C4—C5—C6—C7 | −179.1 (2) | C10—C9—C14—C15 | 179.8 (2) |
| C2—C1—C6—C5 | −1.0 (4) | C12—C13—C14—C9 | −1.5 (3) |
| C2—C1—C6—C7 | 178.9 (2) | C12—C13—C14—C15 | 179.3 (2) |
| C5—C6—C7—S1 | −89.8 (2) | C9—C14—C15—S2 | 91.8 (2) |
| C1—C6—C7—S1 | 90.3 (2) | C13—C14—C15—S2 | −89.0 (2) |
| C8—S1—C7—C6 | 165.34 (19) | C16—S2—C15—C14 | 81.90 (15) |
| C7—S1—C8—N1 | −159.52 (19) | C15—S2—C16—N3 | −159.78 (16) |
| C7—S1—C8—N2 | 20.0 (2) | C15—S2—C16—N4 | 22.5 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···Cl3 | 0.86 | 2.68 | 3.372 (2) | 139 |
| N1—H1*B*···Cl2$^{i}$ | 0.86 | 2.45 | 3.255 (2) | 157 |
| N2—H2*A*···Cl4 | 0.86 | 2.53 | 3.219 (2) | 138 |
| N2—H2*B*···Cl3$^{ii}$ | 0.86 | 2.62 | 3.262 (2) | 132 |
| N3—H3*A*···Cl1$^{iii}$ | 0.86 | 2.72 | 3.469 (2) | 147 |
| N3—H3*A*···Cl4$^{iii}$ | 0.86 | 2.65 | 3.244 (2) | 128 |
| N3—H3*B*···Cl1$^{iv}$ | 0.86 | 2.44 | 3.283 (2) | 166 |
| N4—H4*A*···Cl1$^{iii}$ | 0.86 | 2.49 | 3.290 (2) | 156 |
| N4—H4*B*···Cl2$^{i}$ | 0.86 | 2.62 | 3.447 (2) | 163 |
| C15—H15*A*···S1 | 0.97 | 2.87 | 3.591 (2) | 132 |
| C15—H15*A*···Cl2$^{v}$ | 0.97 | 2.77 | 3.556 (2) | 139 |
| C15—H15*B*···Cl2$^{i}$ | 0.97 | 2.65 | 3.594 (2) | 164 |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*, *y*+1, *z*; (iii) *x*−1, *y*, *z*; (iv) *x*−1, *y*+1, *z*; (v) −*x*+1, −*y*+1, −*z*+1.