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# Structure of Bis(2-aminothiazole)dichlorozinc(II)

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## Abstract

The structure consists of discrete $Zn(at)_2Cl_2$ (at = 2-aminothiazole) molecules. The Zn atom is tetrahedrally coordinated by two *endo*-N atoms from the heterocycle and two Cl atoms; Zn—$N_{ave}$ = 2.017, Zn—$Cl_{ave}$ = 2.247 Å. The angle Cl—Zn—Cl′ [113.47(3)°] deviates significantly from the ideal tetrahedral value. The dihedral angle between the unprimed and primed at ligands (both planar to within 0.007 Å) is 68.3(1)°. The formation of intramolecular N—H···Cl bonds causes rotation of the amino group by 15(8) for at and 32(3)° for at′ with respect to the ligand planes. The packing is stabilized by intermolecular N—H···Cl bonds and by stacking of the at′ rings along the *a* axis. The ring separation in the stack is 3.669(2) and 3.684(2) Å.

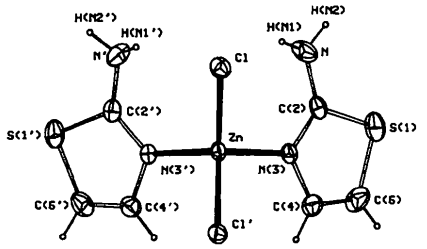



Fig. 1. The $Zn(at)_2Cl_2$ molecule with the atom-numbering scheme. Thermal ellipsoids are drawn at 20% probability; H atoms are arbitrarily reduced.

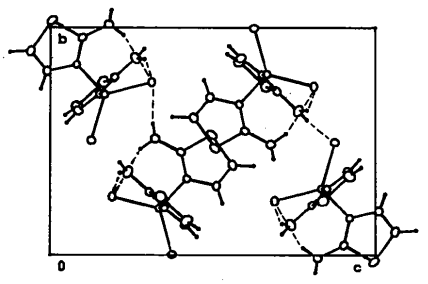
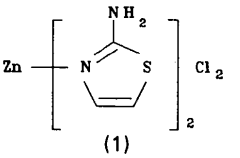



Fig. 2. Projection of the structure along the *a* axis. Dashed lines denote hydrogen bonds.

## Comment

The tetrahedral $Zn(at)_2Cl_2$ molecule (1) placed at the general position of the space group exhibits an *m* pseudosymmetry with the mirror plane defined by Zn and the two Cl atoms. In contrast, the $Co(at)_2Cl_2$ molecules in a similar complex of cobalt (Raper, Oughtred, Nowell & Marsch, 1982) are disposed on a 2 axis. A twofold molecular pseudosymmetry is also exhibited by molecules in the $Co(abt)_2Cl_2$ (abt = 2-aminobenzothiazole) complex (Macíček, Davarska & Davarski, 1987). The structure of the uncoordinated at ligand has been studied by Caranoni & Reboul (1982).




(1)

## Experimental

*Crystal data*

$[Zn(C_3H_4N_2S)_2Cl_2]$
$M_r$ = 336.56
Monoclinic
$P2_1/n$
$a$ = 8.4569 (8) Å
$b$ = 10.007 (1) Å
$c$ = 14.843 (2) Å
$\beta$ = 91.963 (9)°
$V$ = 1255.5 (4) Å$^3$
$Z$ = 4
$D_x$ = 1.780 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\lambda$ = 0.71073 Å
Cell parameters from 22 reflections
$\theta$ = 18.95–20.63°
$\mu$ = 2.72 mm$^{-1}$
$T$ = 292 K
Prismatic
0.3 × 0.3 × 0.2 mm
Transparent brownish

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Continuous scan profiles
Absorption correction: empirical
$T_{min}$ = 0.9245, $T_{max}$ = 0.9992
2806 measured reflections
2806 independent reflections
1872 observed reflections [$I>3.0\sigma(I)$]
$\theta_{max}$ = 26°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 12$
$l = -18 \rightarrow 18$
3 standard reflections
frequency: 240 min
intensity variation: 2.1%

*Refinement*

Refinement on $F$
Final $R$ = 0.024
$wR$ = 0.030
$S$ = 1.095
1839 reflections
168 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F)+(0.040F)^2]$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 0.423 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.376 e Å$^{-3}$
Atomic scattering factors from *SDP/PDP* (Enraf–Nonius, 1985)

Data collection: CAD-4 (Enraf–Nonius, 1988). Cell refinement: CAD-4. Data reduction: *SDP/PDP*. Structure solved by Patterson method. Program(s) used to refine structure: *SDP/PDP*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *KAPPA* (Macíček, 1992).

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å²)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

| | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| Zn | 0.00872 (4) | 0.20622 (3) | 0.33385 (2) | 0.03926 (7) |
| Cl | 0.0569 (1) | 0.25974 (8) | 0.18980 (5) | 0.0543 (2) |
| Cl′ | 0.09802 (9) | 0.00353 (7) | 0.37414 (5) | 0.0501 (2) |
| S(1) | −0.5236 (1) | 0.2592 (1) | 0.33853 (7) | 0.0743 (3) |
| S(1′) | 0.2658 (1) | 0.52918 (9) | 0.49490 (6) | 0.0694 (3) |
| N | −0.2988 (3) | 0.3660 (3) | 0.2384 (2) | 0.0762 (9) |
| N′ | 0.1711 (4) | 0.5127 (3) | 0.3216 (2) | 0.0686 (8) |
| N(3) | −0.2281 (3) | 0.2081 (2) | 0.3495 (1) | 0.0412 (6) |
| N(3′) | 0.1130 (3) | 0.3371 (2) | 0.4198 (1) | 0.0404 (6) |
| C(2) | −0.3325 (3) | 0.2793 (3) | 0.3036 (2) | 0.0470 (7) |
| C(2′) | 0.1754 (3) | 0.4542 (3) | 0.4019 (2) | 0.0458 (7) |
| C(4) | −0.2990 (4) | 0.1342 (3) | 0.4150 (2) | 0.0609 (9) |
| C(4′) | 0.1348 (4) | 0.3062 (3) | 0.5103 (2) | 0.0583 (9) |
| C(5) | −0.4549 (4) | 0.1503 (4) | 0.4189 (3) | 0.084 (1) |
| C(5′) | 0.2123 (5) | 0.3962 (4) | 0.5597 (2) | 0.071 (1) |

Table 2. *Interatomic distances* (Å) *and angles* (°), *and hydrogen-bond geometry* (Å, °)

| | | | |
|---|---|---|---|
| Zn—Cl | 2.2548 (8) | N—C(2) | 1.337 (4) |
| Zn—Cl′ | 2.2386 (8) | N′—C(2′) | 1.328 (4) |
| Zn—N(3) | 2.024 (2) | N(3)—C(2) | 1.307 (4) |
| Zn—N(3′) | 2.011 (2) | N(3)—C(4) | 1.376 (4) |
| S(1)—C(2) | 1.726 (3) | N(3′)—C(2′) | 1.316 (4) |
| S(1)—C(5) | 1.703 (4) | N(3′)—C(4′) | 1.384 (4) |
| S(1′)—C(2′) | 1.726 (3) | C(4)—C(5) | 1.332 (5) |
| S(1′)—C(5′) | 1.712 (4) | C(4′)—C(5′) | 1.321 (5) |
| Cl—Zn—Cl′ | 113.47 (3) | Zn—N(3′)—C(4′) | 120.7 (2) |
| Cl—Zn—N(3) | 108.54 (7) | C(2′)—N(3′)—C(4′) | 110.7 (2) |
| Cl—Zn—N(3′) | 110.94 (7) | S(1)—C(2)—N | 121.2 (2) |
| Cl′—Zn—N(3) | 107.69 (7) | S(1)—C(2)—N(3) | 113.7 (2) |
| Cl′—Zn—N(3′) | 106.50 (7) | N—C(2)—N(3) | 125.0 (3) |
| N(3)—Zn—N(3′) | 109.61 (9) | S(1′)—C(2′)—N′ | 121.6 (2) |
| C(2)—S(1)—C(5) | 89.1 (2) | S(1′)—C(2′)—N(3′) | 113.3 (2) |
| C(2′)—S(1′)—C(5′) | 89.6 (2) | N′—C(2′)—N(3′) | 125.1 (3) |
| Zn—N(3)—C(2) | 126.8 (2) | N(3)—C(4)—C(5) | 114.9 (3) |
| Zn—N(3)—C(4) | 122.2 (2) | N(3′)—C(4′)—C(5′) | 115.7 (3) |
| C(2)—N(3)—C(4) | 111.0 (2) | S(1)—C(5)—C(4) | 111.2 (3) |
| Zn—N(3′)—C(2′) | 128.5 (2) | S(1′)—C(5′)—C(4′) | 110.7 (3) |

| *D* | H | *A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|---|---|
| N | H(N1) | Cl | 0.87 (3) | 2.50 (3) | 3.294 (3) | 152 (3) |
| N′ | H(N1′) | Cl | 0.82 (3) | 2.59 (3) | 3.323 (3) | 150 (3) |
| N | H(N2) | Cl′ | 0.84 (3) | 2.46 (3) | 3.287 (3) | 174 (3) |
| N′ | H(N2′) | Cl | 0.83 (3) | 2.56 (3) | 3.385 (3) | 171 (3) |

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55683 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: NA1019]

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# Structure of 4-(9-Phenanthryl)-*N*,*N*-dimethylaniline


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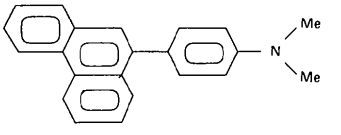
## Abstract

The molecular shape of this intramolecular donor–acceptor complex in the crystalline state is characterized by a dihedral angle of 65.0 (1)° between the phenanthrene plane and the almost planar dimethylanilino group.


## Comment

The structure determination of the title compound (I) was undertaken in order to establish the mutual orientation of the two ring systems and thereby explain its donor–acceptor properties.




(I)

The final atomic coordinates and equivalent isotropic temperature factors are listed in Table 1. A labelled view of the molecular structure is shown in Fig. 1, and bond distances and bond angles are given in Table 2.

As a result of steric overcrowding on the C(4)–C(7) side of the phenanthrene, the ring is slightly bent. The angle between the best planes through the C(1), C(2), C(3), C(4), C(5), C(14) and C(6), C(7),

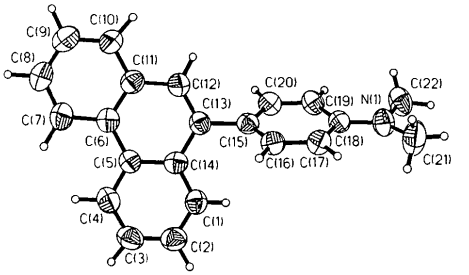



Fig. 1. *SHELXTL/PC* view of the molecule showing labelling scheme. Thermal ellipsoids are drawn at 50% probability levels with H atoms shown as small circles of arbitrary radii.