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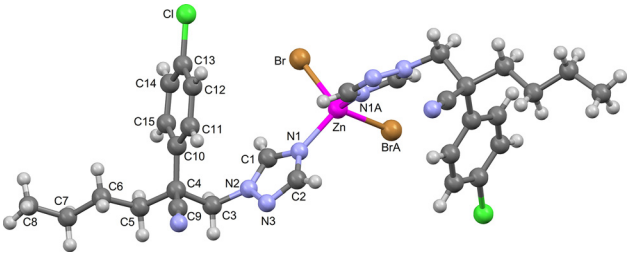
The crystal structure of dibromido-bis((*RS*)-2-(4-chlorophenyl)-2-(1,2,4-triazol-1-ylmethyl) hexanenitrile-κ^1*N*)zinc(II), $C_{30}H_{34}Br_2Cl_2N_8Zn$



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Abstract

$C_{30}H_{34}Br_2Cl_2N_8Zn$, monoclinic, *C*2/*c* (no. 15), $a = 28.500(6)$ Å, $b = 6.6384(13)$ Å, $c = 20.522(4)$ Å, $\beta = 108.376(4)°$, $V = 3684.6(13)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0485$, $wR_{ref}(F^2) = 0.1452$, $T = 296(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The (*RS*)-2-(4-chlorophenyl)-2-(1,2,4-triazol-1-ylmethyl) hexanenitrile (0.578 g, 0.200 mmol) was dissolved in ethanol absolute (10 mL). Then, $ZnBr_2$ (0.225 g, 0.100 mmol) was added. The mixture was allowed to stir at room temperature for 2 h. Colorless rod crystals of the title compound were obtained by slow evaporation from ethanol absolute.

Experimental details

All H atoms were placed geometrically and refined using a riding-model approximation, with C–H distances of 0.93 Å (aromatic), 0.97 Å (methylene), 0.96 Å (methyl), $U_{iso}(H) = 1.2U_{eq}$ (aromatic and methylene) and $1.5U_{eq}$ (methyl). The torsion angles of the methyl H atoms were allowed to refine to best fit the experimental electron density map.

Table 1: Data collection and handling.

Crystal:	Colourless rodlike
Size:	0.38 × 0.31 × 0.23 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	3.01 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9640, 3732, 0.044
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2542
$N(param)_{refined}$:	196
Programs:	Bruker [1], SHELX [2–4], Mercury [5]

Comment

As a broad spectrum systemic 1,2,4-triazole fungicide, myclobutanil (MT), (*RS*)-2-(4-chlorophenyl)-2-(1,2,4-triazol-1-ylmethyl) hexanenitrile, has been widely used to control powdery mildews and scabbing of plants [6–8] in many kinds of crops by inhibiting steroid demethylation [9]. The complexes containing transition metal Zn(II) and various 1,2,4-triazole ligands have been extensively investigated because of their structures and potential applications. The pharmacological and toxicological properties of many drugs are improved when they form Zn(II) complexes [10–12].

The title compound crystallizes in the monoclinic space group *C*2/*c* and the asymmetric unit is half of the title complex with the Zn(II) located on a twofold axis. The Zn(II) is four-coordinated by two bromido ligands and two nitrogen atoms and the Zn(II) complex has a distorted tetrahedral structure: Zn–N length (Zn–N1 = 2.031(4) Å); the Zn–Br length (Zn–Br = 2.3637(7) Å), and the N1–Zn–Br, N1–Zn–N1^i, N1–Zn–Br^i, and Br–Zn–Br^i bond angles of 104.53(9)°, 104.56(18)°, 113.67(9)°, and 115.55(4)°, respectively (symmetry code: (i) $-x$, y, $-z + 1/2$). These parameters are in agreement with closely related Zn(II) complexes reported [13, 14].

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.000000	−0.04343 (9)	0.250000	0.0419 (2)
Br	0.07393 (2)	−0.23329 (8)	0.28182 (3)	0.0720 (2)
Cl	0.22688 (7)	0.0317 (4)	0.32438 (8)	0.1308 (8)
N1	0.00635 (12)	0.1437 (5)	0.17496 (16)	0.0423 (8)
N3	0.00092 (13)	0.3953 (5)	0.09875 (17)	0.0456 (8)
N2	0.02707 (11)	0.2364 (4)	0.08599 (15)	0.0344 (7)
N4	0.07748 (16)	0.7472 (5)	0.0561 (2)	0.0624 (11)
C1	0.03060 (14)	0.0901 (6)	0.13167 (19)	0.0414 (9)
H1	0.047380	−0.030796	0.133174	0.050*
C2	−0.01073 (15)	0.3333 (6)	0.1528 (2)	0.0493 (10)
H2	−0.028871	0.410960	0.174025	0.059*
C3	0.04960 (14)	0.2450 (5)	0.03138 (18)	0.0339 (8)
H3B	0.026611	0.308109	−0.008669	0.041*
H3A	0.055547	0.108773	0.018781	0.041*
C4	0.09934 (13)	0.3640 (5)	0.05203 (18)	0.0360 (8)
C5	0.12089 (15)	0.3411 (6)	−0.0079 (2)	0.0467 (10)
H5A	0.127064	0.199297	−0.013290	0.056*
H5B	0.096204	0.385435	−0.049892	0.056*
C6	0.16842 (17)	0.4571 (8)	0.0004 (3)	0.0710 (14)
H6B	0.163253	0.597849	0.008839	0.085*
H6A	0.194185	0.405623	0.040026	0.085*
C7	0.1853 (3)	0.4407 (17)	−0.0623 (3)	0.167 (5)
H7A	0.184146	0.299662	−0.075073	0.200*
H7B	0.161445	0.511138	−0.099690	0.200*
C8	0.2342 (3)	0.5173 (17)	−0.0567 (6)	0.196 (5)
H8B	0.237385	0.652492	−0.039257	0.293*
H8C	0.238573	0.516551	−0.101182	0.293*
H8A	0.258797	0.433376	−0.025986	0.293*
C9	0.08746 (14)	0.5813 (6)	0.05617 (19)	0.0420 (9)
C10	0.13352 (14)	0.2900 (6)	0.12105 (19)	0.0391 (9)
C15	0.15861 (15)	0.1081 (6)	0.1247 (2)	0.0497 (10)
H15	0.156564	0.038805	0.084554	0.060*
C14	0.18639 (17)	0.0293 (7)	0.1871 (3)	0.0647 (13)
H14	0.202288	−0.093878	0.188820	0.078*
C13	0.19056 (18)	0.1318 (9)	0.2460 (2)	0.0721 (14)
C12	0.1674 (2)	0.3123 (10)	0.2440 (2)	0.0885 (19)
H12	0.170984	0.382603	0.284527	0.106*
C11	0.13848 (18)	0.3914 (8)	0.1817 (2)	0.0666 (13)
H11	0.122302	0.513554	0.180734	0.080*

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