Crystal structure of 11-chloro-2-methyl-7,8,9,10-tetrahydro[1,3]thiazolo-[5,4-*a*]acridine, $C_{15}H_{13}ClN_2S$

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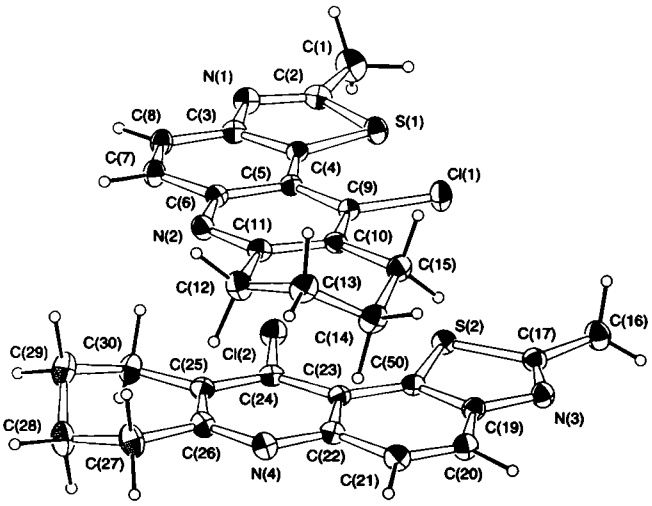

Abstract

$C_{15}H_{13}ClN_2S$, triclinic, $P\bar{1}$ (No. 2), $a = 10.225(1)$ Å, $b = 11.4840(9)$ Å, $c = 12.019(1)$ Å, $\alpha = 96.732(5)°$, $\beta = 99.616(4)°$, $\gamma = 102.884(4)°$, $V = 1338.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.048$, $wR_{ref}(F^2) = 0.056$, $T = 298$ K.

Source of material

The compound was synthesized as described by us in [1]. The recrystallization was done from methylene chloride.

Discussion

Tetrahydroaminoacridine (THA, Cognex) [2] has been the first approval drug for the treatment of Alzheimer's Disease AD. Since this period, Acetylcholine Esterase Inhibitors (AcHEI) derived from tetrahydroacridine, like Tacrine-Huperzine A (Huprines) [3], have been under consideration. In an attempt to obtain potent AchEI, we modified the saturated ring by introducing a thiazolo supplementary ring [1]. In the crystal structure of the title compound, the molecules 11-chloro-2-methyl-7,8,9,10-tetrahydro[1,3]thiazolo[5,4-a]acridine are stacked and rotated on the angle of 74.22°. The distance between the two planar part of the tetracycle is 3.642 Å.

Table 1. Data collection and handling.

Crystal:	colourless cube, size 0.3 × 0.3 × 0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.8 cm^{-1}
Diffractometer, scan mode:	KappaCCD, 90 frames, $\Delta\varphi$ =2°, $\Delta\omega$ = 2°
$2\theta_{max}$:	52.68°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4945, 4945
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\,\sigma(I_{obs})$, 3437
$N(param)_{refined}$:	343
Programs:	maXus [4], SHELXS-97 [5], SIR92 [6], ORTEPIII [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(7)	2*i*	–0.1195	0.5894	0.2960	0.069
H(8)	2*i*	0.1048	0.6876	0.2520	0.068
H(1A)	2*i*	0.6137	0.5090	0.3301	0.090
H(1B)	2*i*	0.5874	0.5603	0.2427	0.090
H(1C)	2*i*	0.6139	0.6545	0.3496	0.090
H(20)	2*i*	–0.1325	–0.2080	0.2209	0.071
H(21)	2*i*	–0.3296	–0.1194	0.1771	0.069
H(12A)	2*i*	–0.3814	0.3177	0.4547	0.077
H(12B)	2*i*	–0.4156	0.2119	0.3306	0.077
H(13A)	2*i*	–0.4639	0.1132	0.5008	0.079
H(13B)	2*i*	–0.3300	0.1984	0.5832	0.079
H(14A)	2*i*	–0.2903	–0.0023	0.5261	0.081
H(14B)	2*i*	–0.3299	0.0147	0.3626	0.081
H(15A)	2*i*	–0.0875	0.1423	0.5674	0.072
H(15B)	2*i*	–0.0921	0.0471	0.4373	0.072
H(16A)	2*i*	0.4262	–0.0195	0.1562	0.081
H(16B)	2*i*	0.3708	–0.1290	0.2140	0.081
H(16C)	2*i*	0.4194	–0.0028	0.2911	0.081
H(27A)	2*i*	–0.4556	0.2779	0.1581	0.090
H(27B)	2*i*	–0.5283	0.1627	0.0284	0.090
H(28A)	2*i*	–0.4362	0.2848	–0.0988	0.095
H(28B)	2*i*	–0.5340	0.3660	–0.0079	0.095
H(29A)	2*i*	–0.3063	0.4885	0.1164	0.095
H(29B)	2*i*	–0.3131	0.4929	–0.0293	0.095
H(30A)	2*i*	–0.0954	0.4471	0.0731	0.078
H(30B)	2*i*	–0.1604	0.3834	–0.0704	0.078

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	2*i*	0.15767(2)	0.20795(2)	0.45276(2)	0.0487(1)	0.0541(1)	0.0782(2)	0.01840(9)	0.0116(1)	0.0282(1)
Cl(2)	2*i*	0.07572(2)	0.30199(2)	0.05724(2)	0.0493(1)	0.0457(1)	0.0659(1)	0.00428(8)	0.01871(9)	0.0181(1)
S(1)	2*i*	0.34559(2)	0.41292(2)	0.36640(2)	0.0423(1)	0.0556(1)	0.0554(1)	0.01527(9)	0.01276(9)	0.0166(1)
S(2)	2*i*	0.20219(2)	0.10205(2)	0.14426(2)	0.0392(1)	0.0446(1)	0.0492(1)	0.00413(8)	0.01175(8)	0.01152(9)
N(1)	2*i*	0.33243(6)	0.60913(5)	0.28454(5)	0.0469(3)	0.0526(4)	0.0495(4)	0.0099(3)	0.0193(3)	0.0147(3)
N(2)	2*i*	−0.17821(5)	0.39721(5)	0.36352(5)	0.0396(3)	0.0470(4)	0.0499(4)	0.0102(3)	0.0072(3)	0.0136(3)
N(3)	2*i*	0.12574(6)	−0.10293(5)	0.21295(5)	0.0456(3)	0.0463(3)	0.0525(4)	0.0101(3)	0.0100(3)	0.0153(3)
N(4)	2*i*	−0.32404(5)	0.08970(5)	0.12198(5)	0.0454(4)	0.0569(4)	0.0496(4)	0.0135(3)	0.0166(3)	0.0174(3)
C(1)	2*i*	0.56224(7)	0.57155(7)	0.30379(7)	0.0484(5)	0.0866(6)	0.0745(6)	0.0153(4)	0.0299(4)	0.0239(5)
C(2)	2*i*	0.41548(7)	0.54235(7)	0.31294(6)	0.0460(4)	0.0571(5)	0.0442(5)	0.0066(4)	0.0153(3)	0.0064(4)
C(3)	2*i*	0.20328(7)	0.55829(6)	0.30470(6)	0.0436(4)	0.0457(4)	0.0382(4)	0.0091(3)	0.0124(3)	0.0059(4)
C(4)	2*i*	0.18807(6)	0.45099(6)	0.34928(6)	0.0411(4)	0.0367(4)	0.0350(4)	0.0120(3)	0.0075(3)	0.0034(3)
C(5)	2*i*	0.06092(6)	0.39058(6)	0.37136(6)	0.0379(4)	0.0368(4)	0.0341(4)	0.0073(3)	0.0083(3)	0.0050(3)
C(6)	2*i*	−0.05041(6)	0.44611(6)	0.34697(6)	0.0392(4)	0.0401(4)	0.0389(4)	0.0097(3)	0.0084(3)	0.0075(3)
C(7)	2*i*	−0.03038(7)	0.55717(7)	0.30426(7)	0.0458(4)	0.0477(4)	0.0539(5)	0.0142(3)	0.0138(3)	0.0170(4)
C(8)	2*i*	0.09245(7)	0.61297(6)	0.28223(6)	0.0499(4)	0.0418(4)	0.0520(5)	0.0126(3)	0.0154(3)	0.0185(4)
C(9)	2*i*	0.02800(6)	0.28076(6)	0.41454(6)	0.0411(4)	0.0380(4)	0.0399(4)	0.0124(3)	0.0041(3)	0.0060(3)
C(10)	2*i*	−0.10060(7)	0.22916(6)	0.43015(6)	0.0420(4)	0.0409(4)	0.0343(4)	0.0054(3)	0.0052(3)	0.0072(3)
C(11)	2*i*	−0.20282(7)	0.29351(6)	0.40255(6)	0.0432(4)	0.0433(4)	0.0408(4)	0.0067(3)	0.0097(3)	0.0080(4)
C(12)	2*i*	−0.34784(7)	0.24456(7)	0.41660(7)	0.0417(4)	0.0621(5)	0.0671(6)	0.0098(4)	0.0142(4)	0.0225(4)
C(13)	2*i*	−0.36093(7)	0.14960(6)	0.49550(7)	0.0528(5)	0.0495(4)	0.0742(6)	0.0034(4)	0.0280(4)	0.0184(4)
C(14)	2*i*	−0.28610(7)	0.05544(7)	0.46158(7)	0.0549(5)	0.0499(5)	0.0772(6)	0.0021(4)	0.0207(4)	0.0156(4)
C(15)	2*i*	−0.13329(7)	0.11074(6)	0.47778(6)	0.0535(5)	0.0412(4)	0.0617(5)	0.0046(3)	0.0128(4)	0.0180(4)
C(16)	2*i*	0.37248(7)	−0.04942(7)	0.21077(7)	0.0448(4)	0.0664(5)	0.0708(6)	0.0151(4)	0.0119(4)	0.0192(5)
C(17)	2*i*	0.23208(7)	−0.02793(6)	0.19326(6)	0.0482(4)	0.0496(4)	0.0406(4)	0.0129(3)	0.0082(3)	0.0072(4)
C(19)	2*i*	0.01097(7)	−0.05715(6)	0.18951(6)	0.0454(4)	0.0401(4)	0.0446(4)	0.0083(3)	0.0091(3)	0.0094(3)
C(20)	2*i*	−0.12083(7)	−0.11988(6)	0.20371(6)	0.0446(4)	0.0453(4)	0.0619(5)	0.0040(3)	0.0142(4)	0.0167(4)
C(21)	2*i*	−0.22668(7)	−0.06872(6)	0.18046(6)	0.0427(4)	0.0502(4)	0.0552(5)	0.0006(3)	0.0143(4)	0.0174(4)
C(22)	2*i*	−0.21032(6)	0.04549(6)	0.14231(6)	0.0399(4)	0.0473(4)	0.0382(4)	0.0054(3)	0.0115(3)	0.0077(4)
C(23)	2*i*	−0.08006(6)	0.10937(6)	0.12577(5)	0.0414(4)	0.0360(4)	0.0323(4)	0.0074(3)	0.0086(3)	0.0066(3)
C(24)	2*i*	−0.07721(6)	0.21968(6)	0.08468(6)	0.0415(4)	0.0421(4)	0.0340(4)	0.0018(3)	0.0127(3)	0.0031(3)
C(25)	2*i*	−0.19134(7)	0.26561(6)	0.06386(6)	0.0496(4)	0.0465(4)	0.0319(4)	0.0132(3)	0.0104(3)	0.0052(3)
C(26)	2*i*	−0.31453(7)	0.19423(7)	0.08569(6)	0.0461(4)	0.0574(5)	0.0412(4)	0.0155(3)	0.0133(3)	0.0128(4)
C(27)	2*i*	−0.44477(7)	0.23704(8)	0.06803(7)	0.0521(5)	0.0871(6)	0.0707(6)	0.0316(4)	0.0197(4)	0.0313(5)
C(28)	2*i*	−0.44213(8)	0.33387(8)	−0.00960(8)	0.0594(5)	0.0793(6)	0.0868(7)	0.0349(5)	0.0206(5)	0.0308(5)
C(29)	2*i*	−0.31079(9)	0.43231(7)	0.02911(8)	0.0767(6)	0.0654(5)	0.0842(7)	0.0386(5)	0.0294(5)	0.0227(5)
C(30)	2*i*	−0.18710(7)	0.38235(6)	0.01645(7)	0.0643(5)	0.0501(4)	0.0608(5)	0.0220(4)	0.0225(4)	0.0205(4)

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