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(2*Z*)-2-(Anthracen-9-ylmethylene)-5,6-dihydroimidazo[2,1-*b*]thiazol-3(2*H*)-one

Zu-Pei Liang[a]* and Jian Li[b]

[a]School of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China, and [b]Qingdao Huaren Pharmaceutical Co., Ltd, Qingdao 266001, People's Republic of China

Correspondence e-mail: zupeiliang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.074
wR factor = 0.198
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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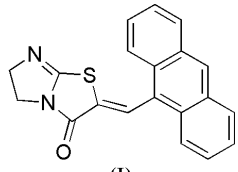
The title compound, $C_{20}H_{14}N_2OS$, was synthesized by mixing imidazolidine-2-thione, ethyl chloroacetate and anthracene-10-carbaldehyde in ethanol. The dihedral angle between the anthracene plane and the heterocyclic ring system is 61.5 (3)°. In the crystal structure, the molecules are linked *via* weak C—H···O interactions.

Comment

Dihydroimidazoles are reported to exhibit diverse biological and pharmacological properties. Examples of these include vasodepressor, sympathomimetic, antihistaminic, histamine-like and cholinomimetic activity (Gilman & Goodman, 2001; Greenhill & Lue, 1993). Dihydroimidazoles, such as midaglizole, deriglidole and efaroxan, have been found to be potent antihyperglycaemic agents (Bihan *et al.*, 1999). Thus there has been considerable interest in the chemistry of dihydroimidazole and its derivatives in recent years. In this paper, the structure of the title compound, (I), is reported.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The heterocyclic ring system is essentially planar, with a mean deviation of 0.0152 (3) Å. Selected bond lengths and angles are listed in Table 1. Taking account of the different substitution patterns, the geometry of the heterocyclic ring system compares favourably with that in the related compounds 6-(4-chlorobenzylidene)-2,3-dihydroimidazo[2,1-*b*]thiazol-5(6*H*)-one (Karolak-Wojciechowska & Kieć-Kononowicz, 1991), DL-6-phenyl-2,3,5,6-tetrahydroimidazo[2,1-*b*]thiazole and L-(−)-6-phenyl-2,3,5,6-tetrahydroimidazo[2,1-*b*]thiazole (Simon *et al.*, 1992). The anthracene ring system is planar to within 0.0306 (3) Å, and the dihedral angle between the anthracene plane and the heterocyclic ring system is 61.5 (3)°. In the crystal structure, molecules are linked *via* weak C—H···O interactions (Table 2 and Fig. 2).

Experimental

A mixture of imidazolidine-2-thione (0.02 mol), ethyl chloroacetate (0.02 mol) and pyridine (0.02 mol) was stirred under reflux in ethanol (40 ml) for 2.5 h. Anthracene-10-carbaldehyde (0.02 mol) was then added and the mixture was refluxed for 4 h. After cooling and filtration, the title compound was recrystallized from acetic acid (m.p.

481–483 K). 15 mg of (I) were dissolved in 15 ml trichloromethane, and the solution was kept at room temperature for 9 d. Natural evaporation gave straw yellow single crystals of the title compound, suitable for X-ray analysis.

Crystal data

$C_{20}H_{14}N_2OS$
M_r = 330.39
Orthorhombic, $P2_12_12_1$
a = 5.127 (2) Å
b = 13.750 (6) Å
c = 22.503 (9) Å
V = 1586.4 (11) Å^3
Z = 4
D_x = 1.383 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1622 reflections
θ = 2.3–26.1°
μ = 0.21 mm^{-1}
T = 293 (2) K
Plate, yellow
0.40 × 0.20 × 0.04 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.886, T_{max} = 0.992
7748 measured reflections
2789 independent reflections
1531 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 25.1°
$h = -4 \rightarrow 6$
$k = -16 \rightarrow 15$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.198
S = 1.12
2789 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2 + 0.2765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Absolute structure: Flack (1983), with 883 Friedel pairs
Flack parameter = −0.2 (3)

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.744 (8)	N2—C1	1.381 (9)
S1—C5	1.749 (6)	N2—C3	1.447 (8)
O1—C4	1.229 (8)	C2—C3	1.524 (10)
N1—C1	1.254 (8)	C4—C5	1.501 (9)
N1—C2	1.481 (10)	C5—C6	1.312 (8)
N2—C4	1.352 (8)	C6—C7	1.476 (8)
C1—S1—C5	91.5 (3)	N1—C2—C3	107.7 (6)
C1—N1—C2	105.3 (7)	N2—C3—C2	101.2 (6)
C4—N2—C1	117.5 (6)	O1—C4—N2	125.9 (7)
C4—N2—C3	134.1 (7)	O1—C4—C5	124.6 (6)
C1—N2—C3	108.0 (6)	N2—C4—C5	109.4 (6)
N1—C1—N2	117.7 (7)	C6—C5—C4	123.5 (6)
N1—C1—S1	131.2 (7)	C6—C5—S1	126.3 (5)
N2—C1—S1	111.1 (5)	C4—C5—S1	110.2 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···O1^{i}	0.97	2.43	3.068 (10)	123

Symmetry code: (i) $x - \frac{1}{2}, -\frac{1}{2} - y, -z$.

H atoms were positioned geometrically with C—H = 0.93–0.97 Å, and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(carrier atom).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

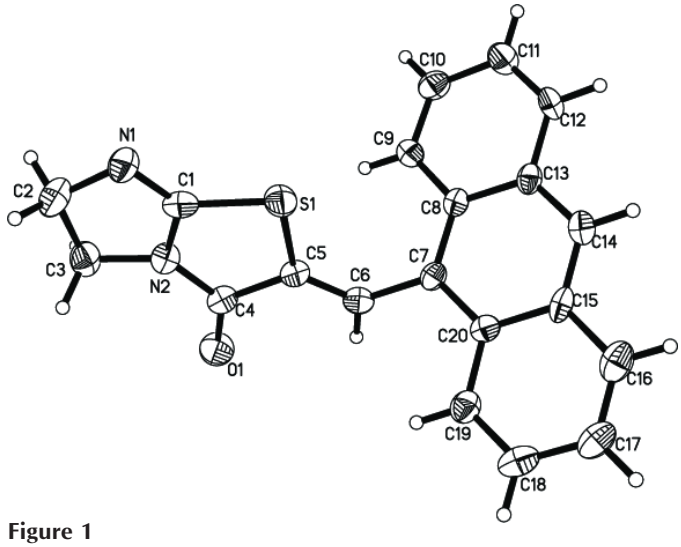


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

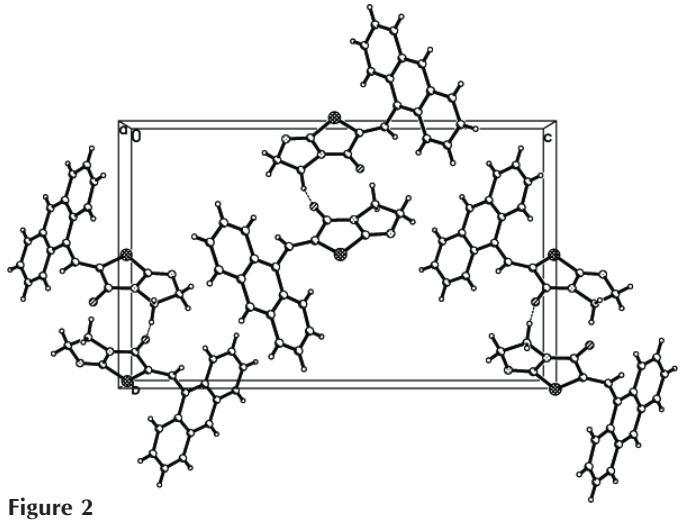


Figure 2
The crystal structure of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

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