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N-(Ferrocenecarbonyl)-*N*′-(quinolin-8-yl)thiourea

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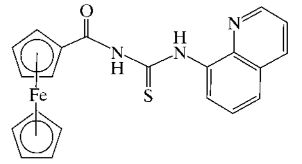
In the title compound, $[Fe(C_5H_5)(C_{16}H_{12}N_3OS)]$, the 8-aminoquinoline and acylthiourea moieties are almost planar. There are two perpendicular arrangements of the molecules in the crystal with slightly different conformations. The two cyclopentadienyl rings in each molecule are parallel and eclipsed.

Comment

Ferrocene derivatives have received much interest recently as redox-active entities, with potential applications in areas such as materials for electronics (Nguyen *et al.*, 1999; Creager & Yu, 1999; Bildstein *et al.*, 2000), electrochemical molecular recognition (Beer *et al.*, 1999), non-linear optical (NLO) materials (Long, 1995; Tian *et al.*, 1999; Roberto *et al.*, 2000), and as biologically active compounds (Li *et al.*, 1997; Kraatz *et al.*, 1997). A variety of ferrocene derivatives have been investigated in this respect. Ligand design is a key factor for developing an efficient system for molecular recognition and catalysis. We report herein the crystal structure of a novel ferrocene derivative containing an *N*-heterocyclic and acylthiourea coordination site.

The title compound, (I), is an amino-substituted ferrocenecarbonyl thiourea. There are two perpendicular arrangements of the molecules in the crystal with slightly different conformations (Fig. 1). Bond lengths and angles in the two molecules (*A* and *B*) are similar and the C═S bond distances are similar to those reported in the literature [1.671 (3) and 1.664 (3) Å (Fun *et al.*, 1995) and 1.680 (3) Å (Tian *et al.*, 1996)]. Each molecule can be described as consisting of ferrocenyl, *N*-heterocyclic and acylthiourea fragments. For molecule *A*, the Fe—C$_{ring}$ distances are as expected for a ferrocene derivative, ranging from 2.031 (3) to 2.053 (3) Å, with an average of 2.045 (3) Å, which agree with the values found in acetylferrocene (2.046 Å; Palenik, 1970) and ferrocene (2.058 Å; Haaland & Silson, 1968). The dimensions of the cyclopentadienyl (Cp) rings [C—C distance 1.400 (4)–1.435 (3) Å, average 1.414 (3) Å, and C—C—C angles 107.3 (3)–108.9 (3)°, average 108.0°] are also normal. The conformation of the Cp ring is close to eclipsed, which is common for ferrocene derivatives. The two Cp rings are planar and nearly parallel, the tilt between the two rings being 1.2 (2)°. Molecule *B* is similar.



(I)

The *N*-heterocyclic and acylthiourea fragments for each molecule almost lie in one plane. For molecule *A*, the *N*-heterocyclic fragment is planar with a maximum deviation of 0.023 (3) Å for C13*A*, and the acylthiourea fragment is planar with a maximum deviation of 0.103 (1) Å for O1*A*. The mean planes through the *N*-heterocyclic and acylthiourea fragments form a dihedral angle of 14.2 (2)°. However, for molecule *B*, the *N*-heterocyclic fragment is planar with a maximum deviation of 0.040 (3) Å for C20*B*, and the acylthiourea fragment is planar with a maximum deviation of 0.045 (1) Å for O1*B*. The mean planes through the two fragments of molecule *B* form a dihedral angle of 1.9 (2)°, indicating that the two fragments in molecule *B* are more planar than those in molecule *A*.

There are intramolecular and intermolecular hydrogen bonds (Table 2), weak N2*A*—H2*AB*···N3*A* [2.638 (3) Å], N2*B*—H2*BB*···N3*B* [2.632 (3) Å], C14*A*—H14*A*···S1*A* [3.204 (3) Å] and C14*B*—H14*B*···S1*B* [3.225 (3) Å] intramolecular interactions and a weak C6*A*—H6*AA*···O1*B*($-\frac{1}{2}+x$, $\frac{1}{2}-y$, $\frac{1}{2}+z$) [3.214 (3) Å] intermolecular interaction.

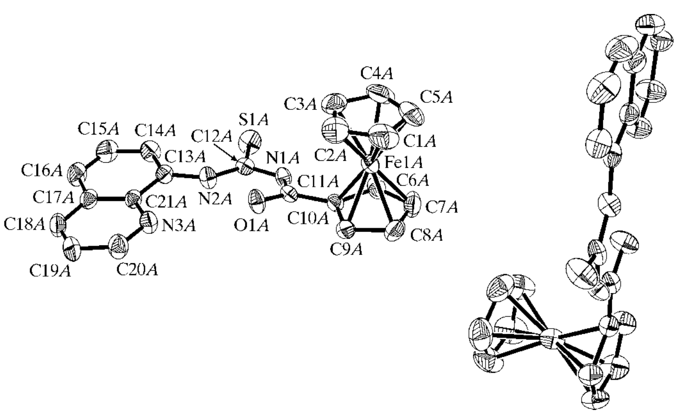


Figure 1
The title complex drawn with 50% probability displacement ellipsoids. H atoms are not shown.

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Table 1
Selected interatomic distances (Å).

S1*A*—C12*A*	1.662 (3)	S1*B*—C12*B*	1.661 (3)
O1*A*—C11*A*	1.229 (3)	O1*B*—C11*B*	1.229 (3)
C11*A*—N1*A*	1.367 (3)	C11*B*—N1*B*	1.376 (3)
N1*A*—C12*A*	1.393 (3)	N1*B*—C12*B*	1.408 (3)
N2*A*—C12*A*	1.343 (3)	N2*B*—C12*B*	1.328 (3)
N2*A*—C13*A*	1.404 (3)	N2*B*—C13*B*	1.415 (3)
N3*A*—C20*A*	1.318 (3)	N3*B*—C20*B*	1.320 (3)
N3*A*—C21*A*	1.358 (3)	N3*B*—C21*B*	1.365 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*AB*···O1*B*$^{\rm i}$	0.86	2.2068	3.009 (3)	155
N2*A*—H2*AB*···O1*A*	0.86	1.8997	2.621 (3)	141
N1*B*—H1*BB*···O1*A*$^{\rm ii}$	0.86	2.1807	3.026 (3)	167
N2*B*—H2*BB*···O1*B*	0.86	1.8871	2.625 (3)	143
C15*B*—H15*B*···S1*A*$^{\rm iii}$	0.93	2.8269	3.715 (3)	160
C9*B*—H9*BA*···O1*A*$^{\rm ii}$	0.98	2.2371	3.140 (3)	153

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $-x, -y, 1 - z$; (iii) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$.

Experimental

The title compound was prepared by treating the product from the reaction of chlorocarbonylferrocene and potassium isothiocyanate with 8-aminoquinoline (Yuan *et al.*, 1997; Wang *et al.*, 1994, 1996). Single crystals were grown by slow evaporation from a dichloromethane/2-propanol solution.

Crystal data

$[Fe(C_5H_5)(C_{16}H_{12}N_3OS)]$
M_r = 415.29
Monoclinic, $P2_1/n$
a = 12.9519 (1) Å
b = 18.1406 (1) Å
c = 15.6117 (2) Å
β = 95.230 (1)°
V = 3652.78 (6) Å^3
Z = 8

D_x = 1.510 Mg m^{-3}
Cell parameters from 6038 reflections
θ = 1.7–28.4°
μ = 0.96 mm^{-1}
T = 293 (2) K
Slab, dark brown
0.36 × 0.34 × 0.28 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.725, $T_{\rm max}$ = 0.776
25 618 measured reflections

8936 independent reflections
5352 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.083
$\theta_{\rm max}$ = 28.3°
$h = -15 \rightarrow 16$
$k = -18 \rightarrow 24$
$l = -20 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.105
S = 0.97
8936 reflections
487 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0150P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 0.46 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.71 e Å^{-3}

After checking their presence in a difference map, all H atoms were fixed geometrically and allowed to ride on their attached atoms, with $U_{\rm iso} = 1.2U_{\rm eq}$ for the attached atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DA1205). Services for accessing these data are described at the back of the journal.

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