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(4-Pyridylaminocarbonyl)ferrocene

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Key indicators

Single-crystal X-ray study
T = 85 K
Mean σ(C–C) = 0.002 Å
R factor = 0.019
wR factor = 0.047
Data-to-parameter ratio = 14.3

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

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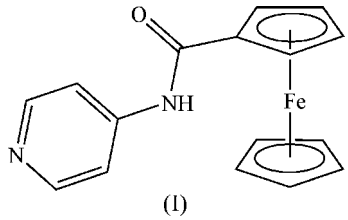
Molecules of the title compound, $[Fe(C_5H_5)(C_{11}H_9N_2O)]$, form (101) alternating sheets of the pyridylamide and ferrocene groups *via* amide to pyridine N—H···N hydrogen-bonding interactions and cyclopentadienyl to pyridine C—H···π interactions.

Comment

The title molecule, (I), was first reported in photophysical studies of its coordination complex with fluorinated zinc porphyrins (Kashiwagi *et al.*, 2003) and in studies of third-order nonlinear optical properties of structurally characterized zinc and mercury complexes (Li *et al.*, 2003). More recently, the structure of a zinc porphyrin coordination complex has been reported (Boyd & Hosseini, 2006).



(I)

The molecular structure of (I) is shown in Fig. 1. A ferrocene cyclopentadienyl ring and the pyridine amide groups are nearly coplanar [r.m.s. deviation = 0.098 (3) Å], with a small tilting of the C1–C5 cyclopentadienyl plane [r.m.s. deviation = 0.002 (1) Å] with respect to the pyridine amide unit [r.m.s. deviation = 0.051 (1) Å] of 7.8 (1)°. The cyclopentadienyl rings have a near eclipsed arrangement within the ferrocene group, with values of the C—$Cg1$—$Cg2$—C pseudo-torsion angles varying from 5.14 to 5.59° ($Cg1$ and $Cg2$ are the centroids of the C1–C5 and C6–C10 rings, respectively). The Fe···$Cg1$ and Fe···$Cg2$ distances are 1.6508 (9) and 1.6551 (9) Å, respectively, with a $Cg1$·Fe···$Cg2$ angle of 177.66 (4)°. The bond lengths in (I) (Table 1) are similar to those found in zinc and mercury complexes (Li *et al.*, 2003) and a zinc porphyrin complex (Boyd & Hosseini, 2006).

The molecules assemble as chains in the crystal structure, along the *a* axis, formed by hydrogen-bonding interactions between the amide N2—H group and the pyridine N1 atom (N—H···N = 2.266 Å; symmetry code: $-\frac{1}{2}+x, -y, -z$). These chains stack along the *ac* plane and are held together by two C—H···π interactions from neighbouring ferrocene groups at ($\frac{1}{2}+x, -y, z$) and ($\frac{3}{2}-x, y, \frac{1}{2}+z$) to opposite faces of a pyridine ring (C9—H···$Cg3$ = 2.91 Å and C8—H···$Cg3$ = 2.70 Å; $Cg3$ is the centroid of the N1/C12–C16 ring). This leads to the formation of alternating regions of pyridine amide and ferrocene groups in the crystal structure (Fig. 2).

Experimental

Compound (I) was prepared by reaction of ferrocene carbonyl chloride with 4-aminopyridine in dichloromethane (Li *et al.*, 2003; Kashiwagi *et al.*, 2003). Crystals of (I) suitable for X-ray diffraction were grown from a slowly evaporating chloroform/hexane (1:1) solution of 4-ferrocenamidopyridine.

Crystal data

$[Fe(C_5H_5)(C_{11}H_9N_2O)]$
M_r = 306.14
Orthorhombic, $Pca2_1$
a = 10.5859 (1) Å
b = 12.6355 (1) Å
c = 9.6041 (1) Å
V = 1284.63 (2) Å^3
Z = 4
D_x = 1.583 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 85 (2) K
Block, orange
0.28 × 0.22 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.775, T_{max} = 0.827
(expected range = 0.815–0.869)
11891 measured reflections
2581 independent reflections
2471 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.047
S = 1.07
2581 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 0.372P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1188 Friedel pairs
Flack parameter: 0.023 (12)

Table 1
Selected bond lengths (Å).

Fe1—C1	2.0504 (18)	C6—C7	1.428 (3)
Fe1—C2	2.0490 (18)	C8—C7	1.425 (3)
Fe1—C3	2.0515 (18)	C9—C8	1.425 (3)
Fe1—C4	2.0520 (14)	C9—C10	1.426 (2)
Fe1—C5	2.0498 (17)	C10—C6	1.432 (3)
Fe1—C6	2.0531 (18)	C5—C11	1.484 (2)
Fe1—C7	2.0579 (18)	O1—C11	1.227 (2)
Fe1—C8	2.0556 (18)	N2—C11	1.381 (2)
Fe1—C9	2.0477 (15)	N2—C12	1.396 (2)
Fe1—C10	2.0492 (17)	C13—C12	1.404 (2)
C2—C1	1.427 (2)	C14—C13	1.387 (2)
C2—C3	1.423 (3)	C14—N1	1.350 (2)
C4—C3	1.430 (2)	N1—C15	1.342 (2)
C4—C5	1.436 (3)	C15—C16	1.392 (3)
C5—C1	1.435 (3)	C12—C16	1.400 (2)

H atoms were placed in calculated positions and refined using a riding model [C—H = 0.93 Å and N—H = 0.86 Å), with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Version 1.4.1; Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

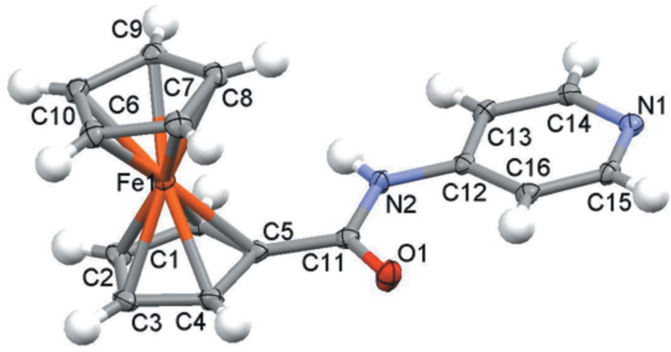


Figure 1
Structure of (I) showing 50% probability displacement ellipsoids for non-H atoms and H atoms as arbitrary spheres.

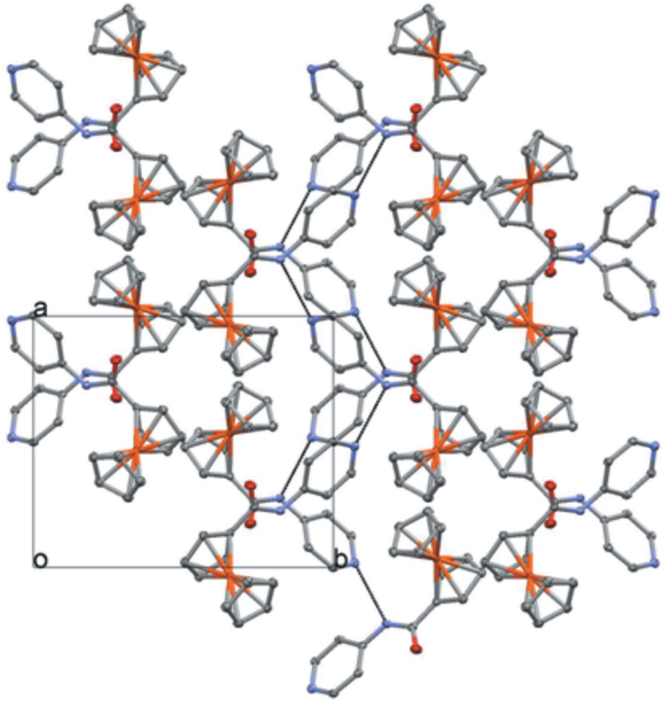


Figure 2
View of the crystal structure of (I) along [001], showing the formation of (101) alternating sheets of pyridylamide and ferrocene groups assembled from amide N2—H to pyridine N1 hydrogen-bonding interactions and cyclopentadienyl C8—H and C9—H to pyridine C—H$\cdots\pi$ interactions. H atoms have been omitted.

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