Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4′-Ferrocenyl-3′-(4-methoxybenzoyl)-1′-methylspiro[1*H*-indole-3(2*H*),2′-pyrrolidin]-2-one

**B. K. Satis Kumar,[a] D. Gayathri,[b] D. Velmurugan,[b]* K. Ravikumar[c] and A. R. Sureshbabu[d]**

[a]Department of Physics, Presidency College, Chennai 600 005, India, [b]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [c]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [d]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India

Correspondence e-mail: d_velu@yahoo.com

**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.039
*wR* factor = 0.113
Data-to-parameter ratio = 17.4

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

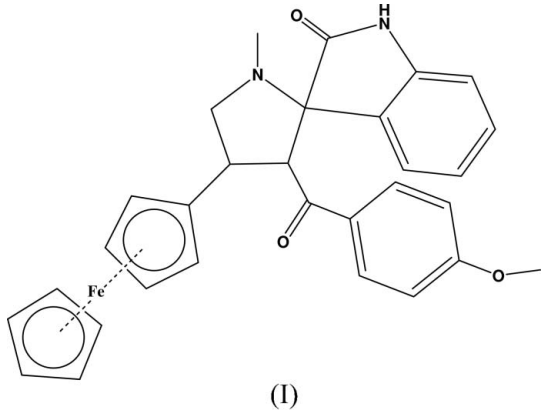


Received 27 March 2007
Accepted 2 April 2007

In the title compound, $[Fe(C_5H_5)(C_{25}H_{23}N_2O_3)]$, the pyrrolidine ring adopts a twist conformation. The oxindole ring system is planar. The crystal packing is stabilized by N—H···O and C—H···π intermolecular interactions.

## Comment

Pyrrolidine derivatives have been found to be DNA polymerase inhibitors and also exhibit characteristic inhibition of DNA metabolic enzymes (Mizushina *et al.*, 2003). Oxindole derivatives act as orally active potent growth hormone secretagogues (Tokunaga *et al.*, 2005). The literature shows that ferrocenyl compound is a multi-responsive calcium chemosensor with remarkable fluorescence properties in $CH_3CN$ (Delavaux-Nicot *et al.*, 2006). As the title compound, (I), is of great importance, we have determined its crystal structure using X-ray diffraction.




(I)

The bond lengths and bond angles of (I) are comparable with the literature values (Allen *et al.*, 1987). The sum of the bond angles around atom N1 [341.1°] indicates $sp^3$ hybridization.

The oxindole ring system of (I) is planar, with a dihedral angle of 1.0 (1) Å between the five- and six-membered rings. Atom O1 deviates by 0.072 (1) Å from the plane of the oxindole ring system. The C28—C27—O3—C30 torsion angle [1.5 (1)°] indicates that the methoxy group is coplanar with the C24–C29 benzene ring. The dihedral angle between the C24–C29 benzene ring and the benzene ring of the oxindole system in the structure is 40.1 (1)°. The dihedral angle between the two cyclopentadienyl rings is 2.8 (1) Å. The Fe—C coordination distances range from 2.031 (2) to 2.054 (2) Å.

The pyrrolidine ring (N1/C13/C12/C11/C14) adopts a twist conformation with a pseudo-twofold axis passing through atom C13 and the C11—C14 bond. The puckering parameters

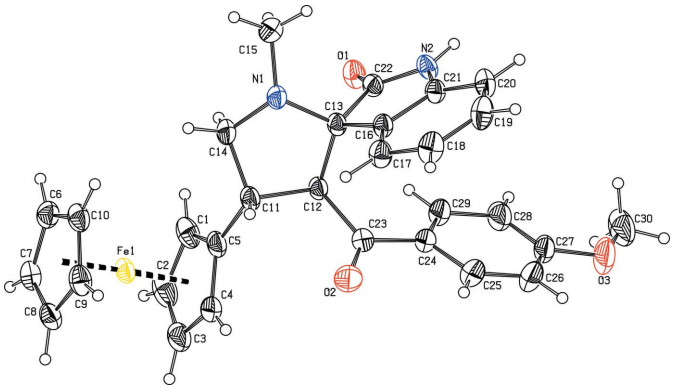



**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids.

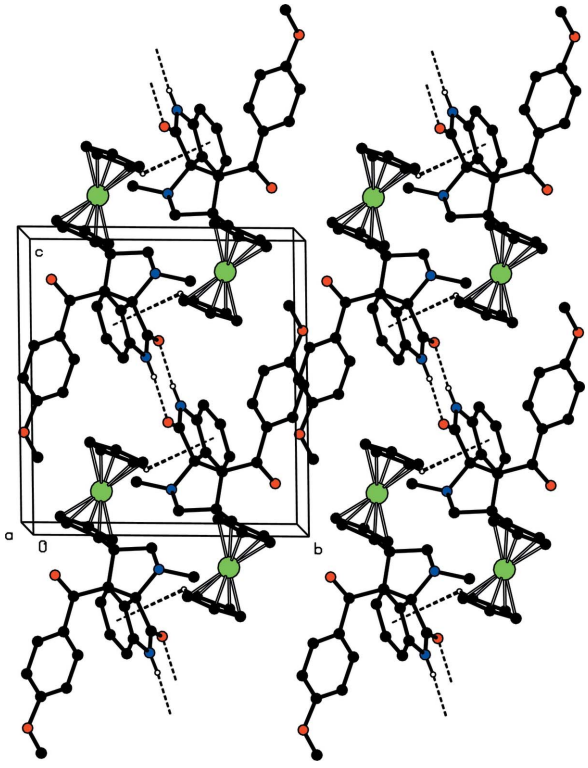



**Figure 2**
The molecular packing of (I), viewed approximately down the *a* axis. For clarity, H atoms not involved in hydrogen bonding (dashed lines) have been omitted.

(Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for the pyrrolidine ring are $q_2$ = 0.416 (2) Å, $\varphi$ = 303.9 (2)° and $\Delta_2(C_{13})$ = 1.2 (2).

The molecule of (I) is stabilized by a weak C—H···O intramolecular interaction and the crystal packing is stabilized by N—H···O and C—H···$\pi$ intermolecular interactions. The N—H···O hydrogen bond (Table 1) generates a centrosymmetric dimer with an $R_2^2(8)$ ring (Bernstein *et al.*, 1995). In the C—H···$\pi$ interaction, atom C10 acts as donor to the centroid *Cg* of the C16–C21 benzene ring at (1 − *x*, 1 − *y*, 2 − *z*), with an H···*Cg* distance of 3.022 Å.

## Experimental

A solution of (*E*)-ferrocenylidene-*p*-methoxyacetophenone (1 mmol), isatin (1 mmol) and sarcosine (1 mmol) in acetonitrile (20 ml) was refluxed until the disappearance of the starting materials. The crude product was purified by column chromatography (silica gel, 100–200 mesh) eluted with hexane:ethylacetate (8:2) and recrystallized from methanol by slow evaporation.

### *Crystal data*

$[Fe(C_5H_5)(C_{25}H_{23}N_2O_3)]$
$M_r$ = 520.39
Triclinic, $P\overline{1}$
*a* = 9.4895 (5) Å
*b* = 11.4943 (6) Å
*c* = 12.3633 (7) Å
$\alpha$ = 86.978 (1)°
$\beta$ = 71.302 (1)°
$\gamma$ = 77.822 (1)°
*V* = 1248.45 (12) Å$^3$
*Z* = 2
Mo *K*$\alpha$ radiation
$\mu$ = 0.64 mm$^{-1}$
*T* = 293 (2) K
0.26 × 0.24 × 0.23 mm

### *Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
14419 measured reflections
5703 independent reflections
5098 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
*S* = 1.02
5703 reflections
327 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1$^{i}$ | 0.86 | 2.03 | 2.859 (2) | 162 |
| C12—H12···O1$^{i}$ | 0.98 | 2.54 | 3.000 (2) | 109 |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were refined using a riding model, with N—H = 0.86 Å and C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C,N) or 1.5$U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

DG thanks the CSIR, India, for the award of a Senior Research Fellowship. DV thanks the DST, India, for a Major Research Project. The Department of Science and Technology (DST-FIST) and the University Grants Commission (UGC), Government of India, are acknowledged by DV for providing facilities to the department.

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2001). *SMART* (Version 5.625/NT/2000) and *SAINT* (Version 6.28a). Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Delavaux-Nicot, B., Maynadié, J., Lavabre, D. & Fery-Forgues, S. (2006). *Inorg. Chem.* **45**, 5691–5702.
Mizushina, Y., Xu, X., Asano, N., Kasai, N., Kato, A., Takemura, M., Asahara, H., Linn, S., Sugawara, F., Yoshida, H. & Sakaguchid, K. (2003). *Biochem. Biophys. Res. Commun.* **304**, 78–85.
Nardelli, M. (1983). *Acta Cryst.* C**39**, 1141–1142.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tokunaga, T., Hume, W. E., Nagamine, J., Kawamura, T., Taiji, M. & Nagata, R. (2005). *Bioorg. Med. Chem. Lett.* **15**, 1789–1792.