

# 1-(2,4-Dinitrophenyl)-5-ferrocenyl-3-methyl-1H-pyrazole

V. Stalin Elanchezian,<sup>a</sup> M. Kandaswamy<sup>a</sup> and  
M. N. Ponnuswamy<sup>b\*</sup>

<sup>a</sup>Department of Inorganic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and <sup>b</sup>Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India  
Correspondence e-mail: mnpsy2004@yahoo.com

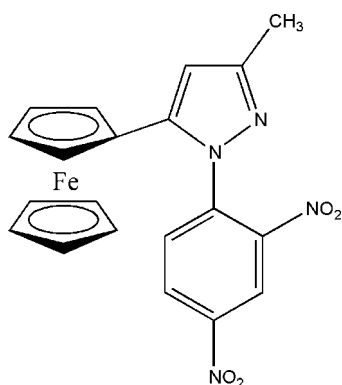
Received 17 November 2007; accepted 17 December 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.107; data-to-parameter ratio = 23.2.

In the title compound,  $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{15}\text{H}_{11}\text{N}_4\text{O}_4)]$ , the dinitrophenyl and cyclopentadienyl rings make dihedral angles of 53.61 (6) and 23.11 (9)°, respectively, with the pyrazole unit. The two cyclopentadienyl rings are in an eclipsed conformation. The crystal structure is stabilized by intermolecular C—H...O interactions, which link molecules into chains parallel to the  $b$  axis.

## Related literature

For related literature, see: Beer *et al.* (1998); Erasmus *et al.* (1996); Fabbrizzi & Poggi (1995); Gilchrist (1997); Basurto *et al.* (2007); Shi *et al.* (2005).



## Experimental

### Crystal data

$[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{15}\text{H}_{11}\text{N}_4\text{O}_4)]$   
 $M_r = 432.22$   
Triclinic,  $P\bar{1}$   
 $a = 7.1073$  (2) Å  
 $b = 11.5339$  (3) Å  
 $c = 11.7575$  (3) Å  
 $\alpha = 103.822$  (1)°  
 $\beta = 93.061$  (1)°  
 $\gamma = 98.822$  (2)°  
 $V = 920.76$  (4) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.85$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.25 \times 0.15 \times 0.15$  mm

### Data collection

Bruker Kappa APEXII diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.815$ ,  $T_{\max} = 0.882$   
24588 measured reflections  
6096 independent reflections  
4741 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.107$   
 $S = 1.01$   
6096 reflections  
263 parameters  
10 restraints  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8}\cdots\text{O4}^i$	0.93	2.46	3.380 (3)	170

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: SAINT (Bruker, 2004); 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).

We thank the CSIR, India, for financial support.

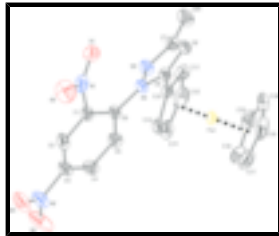
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2122).

## References

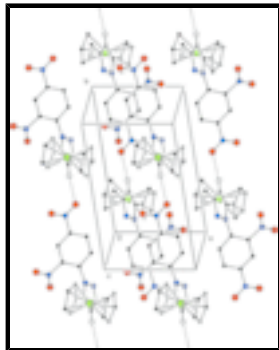
- Basurto, S., Riant, O., Moreno, D., Rojo, J. & Torroba, T. (2007). *J. Org. Chem.* **72**, 4673–4688.  
Beer, D. P., Gale, A. P. & Chen, Z. (1998). *Adv. Phys. Org. Chem.* **31**, 1–89.  
Bruker (2004). SAINT (Version 6.0a) and APEX2 (Version 1.22). Bruker AXS Inc., Madison, Wisconsin, USA.  
Erasmus, J. J. C., Lamprecht, G. J., Swarts, J. C., Roodt, A. & Oskarsson, Å. (1996). *Acta Cryst.* **C52**, 3000–3002.  
Fabbrizzi, L. & Poggi, A. (1995). *Chem. Soc. Rev.* **24**, 197–202.  
Gilchrist, T. L. (1997). *Heterocyclic Chemistry*, 3rd ed. London: Addison Wesley Longman Limited.  
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.  
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
Shi, Y.-C., Sui, C.-X. & Cheng, H.-J. (2005). *Acta Cryst.* **E61**, m1563–m1565.  
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.







& ( ! " " " " + " ! " ! + "



& \* % " ! . " " " ! # + + "

! " # \$

& 8 \* 8((E6: 6 @ 64 @ 666  
 ( / @ ( ) F<sup>4</sup>  
 8 % \$ < G ( F H " I @ -( -4 B \* ! " 4- "  
 @ - ( -4 B J @ > K L @ A  
 @ (( 44) 4 B H @ ( 4 ( K @ )4 ?  
 @ (( - - 4 B M @ )4 ( ( K G \$ .  
 H @ ( 4 ( K N @ ) K O ( O (  
 @ ) - 4 6 B

! !"  
 , . PG QRR ? !! ) ! " "  
 S " < " 6-6( " # T+U#  
 F " < ! " "@ -  
 @ )4 ? J / @ 4( K  
 V W J @ K  
 P\$ !" " < " \$ @ X(  
 3P;P,32 3 . ( )



















