

Jing Zhou,<sup>a</sup> Lin Yan,<sup>b</sup> Dong-Qin Bi<sup>a</sup> and Ming-Xue Li<sup>a\*</sup><sup>a</sup>Institute of Molecular and Crystal Engineering, School of Chemistry and Chemical Engineering, Henan University, Kaifeng, Henan 475001, People's Republic of China, and <sup>b</sup>College of Pharmacy, Henan University, Kaifeng, Henan 475001, People's Republic of ChinaCorrespondence e-mail:  
limingxue@henu.edu.cn

## Key indicators

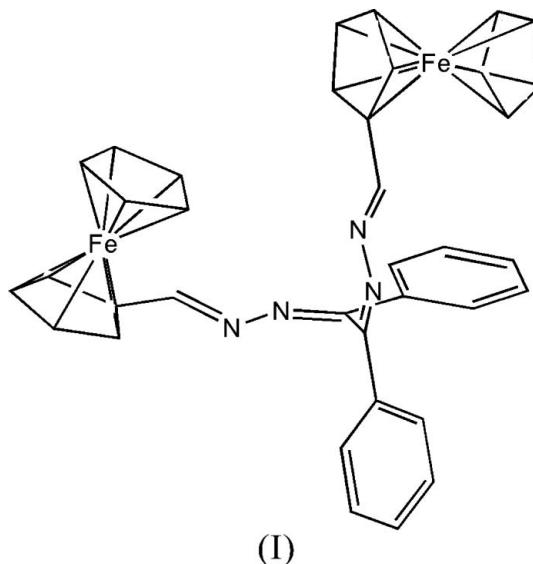
Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
*R* factor = 0.044  
*wR* factor = 0.109  
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Bis(ferrocenecarbaldehyde) (1,2-diphenyl-ethane-1,2-diylidene)dihydrazone

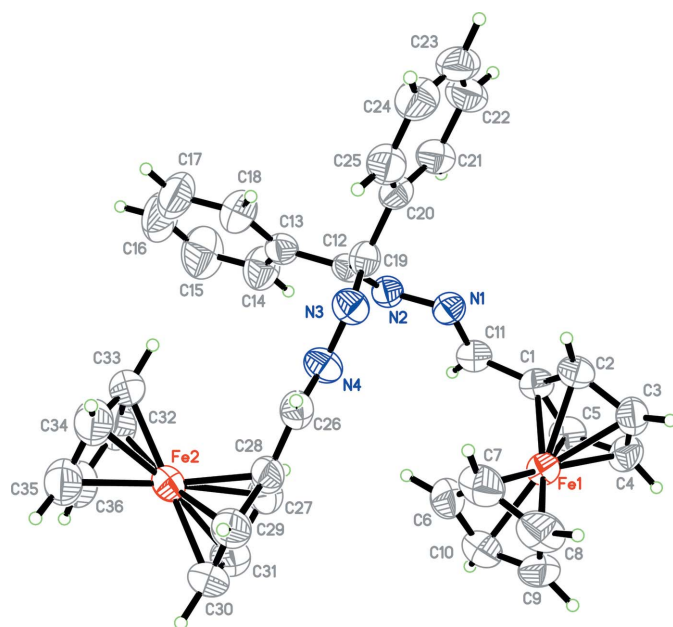
In the title compound,  $[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{26}\text{H}_{20}\text{N}_4)]$ , two ferrocene units are bridged by a Schiff base linker with an intramolecular Fe...Fe separation of 7.42 (2) Å.Received 19 October 2006  
Accepted 1 November 2006

## Comment

Numerous examples of complexes with ferrocenyl fragments are being investigated for their potential applications in many and diverse areas of chemistry (Togni *et al.*, 1995). As a model of an intramolecular electron-transfer reaction, the process of intervalence charge transfer in mixed-valence (MV) dinuclear complexes with various bridging ligands (BL) has been widely studied since the preparation of the Creutz–Taube ion (Creutz & Taube, 1969, 1973). In continuation of our research work in the assembly and properties of ferrocene-containing Schiff base compounds (Li *et al.*, 2006), we report here the crystal structure analysis of biferrocene Schiff base complex (I).



In (I), the two ferrocene groups are bridged by the Schiff base linker (Fig. 1), with an intramolecular Fe...Fe separation of about 7.42 (2) Å; the N2–C12–C19–N3 torsion angle is  $-91.80(2)^\circ$ . In addition, the two ferrocene groups position themselves perpendicular to each other with a dihedral angle of  $83.80(4)^\circ$  between the substituted Cp rings. The Fe–C distances are within normal ranges (Seiler & Dunitz, 1979; Mammano *et al.*, 1977). The dihedral angle between the two phenyl rings in the bridging group is  $74.50(3)^\circ$ . The C=N bond distances are within the normal range of C=N double bonds, but the N1–N2 and N3–N4 bond distances suggest that they are single bonds. Moreover, the C12–C19 bond



**Figure 1**  
The molecular structure of (I), showing atomic displacement ellipsoids drawn at the 50% probability level.

distance is within the normal range for a C–C single bond, so the C11=N1–N2=C12–C19=N3–N4=C26 sequence contains alternating single and double bonds (Table 1).

### Experimental

All reagents were commercially available and of analytical grade. A mixture of ferrocenecarboxaldehyde (0.107 g, 0.5 mmol) and dihydrazonotobenzyl (0.119 g, 0.5 mmol) containing five drops of acetic acid was stirred in ethanol (40 ml) for 24 h at room temperature and in the absence of light; a red precipitate was formed. Ferrocenecarboxaldehyde (0.107 g, 0.5 mmol) was then added and the mixture refluxed for 7 h in the absence of light under N<sub>2</sub>. Subsequently the solid formed was filtered off, washed with ethanol and dried *in vacuo* (yield, 62%). Red rod-shaped crystals suitable for X-ray structure analysis were obtained by slowly diffusing hexane into a dichloromethane solution containing complex (I) in a test tube. Analysis calculated for C<sub>36</sub>H<sub>30</sub>Fe<sub>2</sub>N<sub>4</sub>: C 68.60, H 4.80, N 8.89%; found: C 68.44, H 4.82, N 8.91%.

### Crystal data

[Fe<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(C<sub>26</sub>H<sub>20</sub>N<sub>4</sub>)]  
M<sub>r</sub> = 630.34  
Monoclinic, P2<sub>1</sub>/c  
a = 12.066 (3) Å  
b = 11.187 (3) Å  
c = 22.402 (6) Å  
β = 96.284 (5)°  
V = 3005.6 (13) Å<sup>3</sup>

Z = 4  
D<sub>x</sub> = 1.393 Mg m<sup>-3</sup>  
Mo Kα radiation  
μ = 1.00 mm<sup>-1</sup>  
T = 293 (2) K  
Rod, red  
0.26 × 0.18 × 0.16 mm

### Data collection

Bruker SMART APEX CCD diffractometer  
ω scans  
Absorption correction: none  
14449 measured reflections

5285 independent reflections  
3782 reflections with I > 2σ(I)  
R<sub>int</sub> = 0.070  
θ<sub>max</sub> = 25.0°

### Refinement

Refinement on F<sup>2</sup>  
R[F<sup>2</sup> > 2σ(F<sup>2</sup>)] = 0.044  
wR(F<sup>2</sup>) = 0.110  
S = 1.00  
5285 reflections  
379 parameters

H-atom parameters constrained  
w = 1/[σ<sup>2</sup>(F<sub>o</sub><sup>2</sup>) + (0.0524P)<sup>2</sup>]  
where P = (F<sub>o</sub><sup>2</sup> + 2F<sub>c</sub><sup>2</sup>)/3  
(Δ/σ)<sub>max</sub> = 0.001  
Δρ<sub>max</sub> = 0.57 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = -0.34 e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Fe1–C1	2.022 (3)	Fe2–C31	2.043 (3)
Fe1–C2	2.028 (3)	Fe2–C32	2.042 (4)
Fe1–C3	2.040 (3)	Fe2–C33	2.033 (4)
Fe1–C4	2.044 (3)	Fe2–C34	2.044 (4)
Fe1–C5	2.031 (3)	Fe2–C35	2.034 (4)
Fe1–C6	2.028 (3)	Fe2–C36	2.029 (4)
Fe1–C7	2.023 (3)	C11–N1	1.282 (3)
Fe1–C8	2.026 (3)	C19–N3	1.287 (3)
Fe1–C9	2.043 (3)	N1–N2	1.411 (3)
Fe1–C10	2.036 (3)	C12–C19	1.514 (4)
Fe2–C27	2.028 (3)	C12–N2	1.277 (3)
Fe2–C28	2.028 (3)	C26–N4	1.275 (3)
Fe2–C29	2.051 (4)	N3–N4	1.404 (3)
Fe2–C30	2.052 (4)		

All H atoms were positioned geometrically and refined as riding with C–H = 0.93–0.98 Å and with U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

This work was supported by the Natural Science Foundation of Henan Province (No. 0611011900).

### References

- Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.  
Creutz, C. & Taube, H. (1969). *J. Am. Chem. Soc.* **91**, 3988–3989.  
Creutz, C. & Taube, H. (1973). *J. Am. Chem. Soc.* **95**, 1086–1094.  
Li, M.-X., Yan, L., Wang, J.-P. & Zhou, J. (2006). *Acta Cryst.* **E62**, m2517–m2518.  
Mammano, N. J., Zalkin, A., Landers, A. & Rheingold, A. L. (1977). *Inorg. Chem.* **16**, 297–300.  
Seiler, P. & Dunitz, J. D. (1979). *Acta Cryst.* **B35**, 1068–1074.  
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
Togni, A. & Hayashi, T. (1995). Editors. *General Overview in Ferrocenes*. Weinheim: VCH.