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## Key indicators

Single-crystal X-ray study  
 $T = 113$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.061  
 $wR$  factor = 0.152  
Data-to-parameter ratio = 14.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

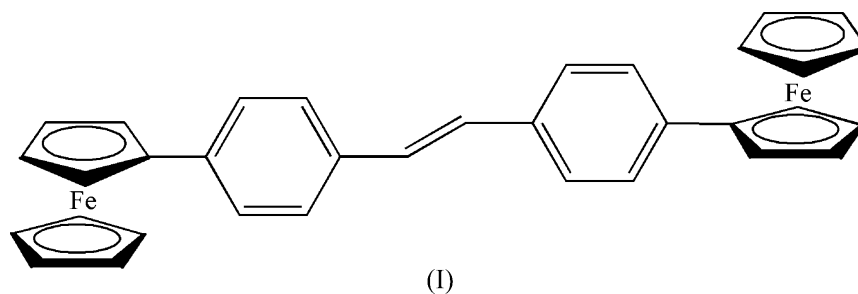
## 1,2-Bis(4-ferrocenylphenyl)ethene

The molecular structure of the centrosymmetric title compound,  $[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{24}\text{H}_{18})]$ , represents a new application of cross-metathesis for the preparation of functionalized olefins containing two organometallic groups. The two benzene and attached cyclopentadienyl (Cp) rings and the double bond are almost coplanar.

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## Comment

Dinuclear complexes featuring unsaturated bridging ligands between the metal centres have been extensively investigated over the past decade (Bunel *et al.*, 1988; Tarraga *et al.*, 2001). As a result of their unique structures and properties, dinuclear complexes find applications in many areas, such as catalysis, non-linear optics (Jayaprakash *et al.*, 1999) and as combustion reagents (Neuse *et al.*, 1988). Here we describe the synthesis and crystal structure of the title compound, (I).



The molecular structure of the title compound, (I), is shown in Fig. 1. The molecule is disposed about a crystallographic centre of symmetry. The two benzene and attached cyclopentadienyl (Cp) rings and the double bond are almost coplanar. The two Cp rings in the each ferrocene unit are almost parallel, making a dihedral angle of  $11.5(3)^\circ$ .

## Experimental

The title compound, (I), was prepared according to the literature procedure of Seshadri & Lovely (2000). A  $\text{CH}_2\text{Cl}_2$  (45 ml) solution containing 4-ferrocenylphenylethane (0.578 g, 2 mmol) and the Grubbs catalyst  $\text{RuCl}_2(\text{=CHPh})(\text{PCy}_3)_2$  (0.822 g, 1 mmol) (Schwab *et al.*, 1996) was heated at reflux until the starting materials were consumed (TLC analysis, 17–24 h). The solvent was removed, and the residue was purified by flash column chromatography ( $\text{CH}_2\text{Cl}_2$ /hexane 1:1), providing the product, which was dried and recrystallized from  $\text{CH}_2\text{Cl}_2$  as orange crystals suitable for X-ray diffraction analysis.

## Crystal data

[Fe<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(C<sub>24</sub>H<sub>18</sub>)] $M_r = 548.26$ Monoclinic,  $P2_1/c$  $a = 12.452 (2) \text{ \AA}$  $b = 8.1688 (14) \text{ \AA}$  $c = 12.5419 (18) \text{ \AA}$  $\beta = 104.880 (9)^\circ$  $V = 1233.0 (3) \text{ \AA}^3$  $Z = 2$  $D_x = 1.477 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation $\mu = 1.20 \text{ mm}^{-1}$  $T = 113 (2) \text{ K}$ 

Platelet, orange

 $0.20 \times 0.16 \times 0.02 \text{ mm}$ 

## Data collection

Rigaku Saturn diffractometer

 $\omega$  scans

Absorption correction: multi-scan

(Jacobson, 1998)

 $T_{\min} = 0.796$ ,  $T_{\max} = 0.976$ 

12668 measured reflections

2424 independent reflections

2113 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.066$  $\theta_{\text{max}} = 26.0^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.152$  $S = 1.13$ 

2424 reflections

165 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0721P)^2$  $+ 1.1009P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.92 \text{ e \AA}^{-3}$  $\Delta\rho_{\text{min}} = -0.90 \text{ e \AA}^{-3}$ 

All the H atoms were positioned geometrically and refined as riding atoms, with C—H distances =  $0.95 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *CrystalStructure* (Rigaku/MS, 2004); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1995); software used to prepare material for publication: *CrystalStructure*.

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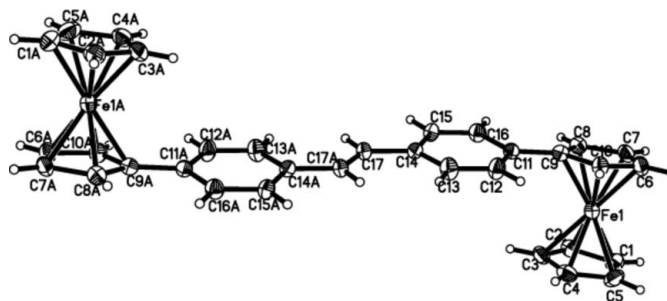


Figure 1

The molecular structure of compound (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (A)  $-x, -y, 1 - z$ .]

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