

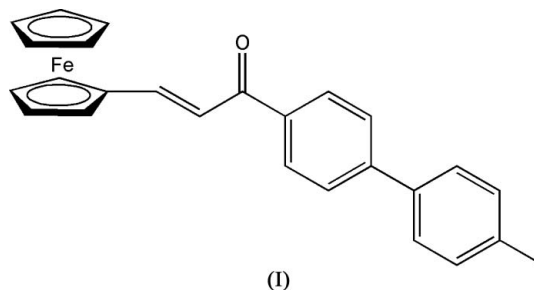
Ming-Yu Teng,<sup>a</sup> Xin-Biao Mao,<sup>a</sup>  
Qing-Bao Song<sup>a\*</sup> and  
Edward R. T. Tiekink<sup>b\*</sup><sup>a</sup>The State Key Laboratory Breeding Base of Green Chemistry–Synthesis Technology, College of Chemical Engineering and Materials Science, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China, and <sup>b</sup>Department of Chemistry, The University of Texas at San Antonio, 6900 North Loop 1604 West, San Antonio, Texas 78249-0698, USA

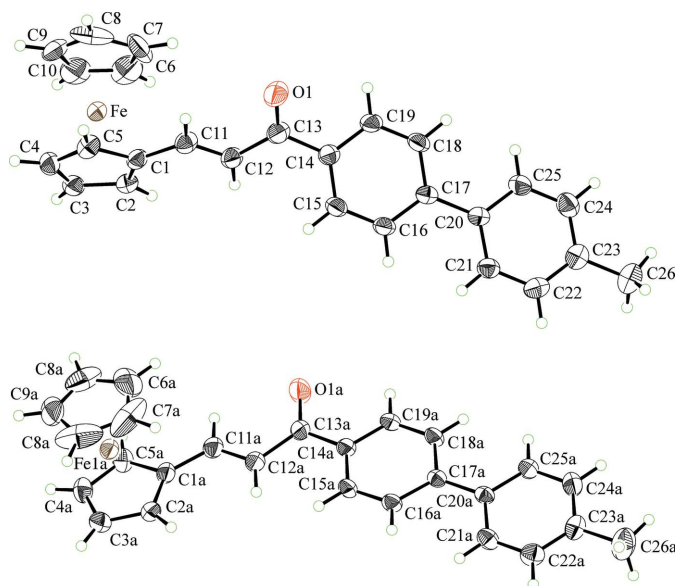
Correspondence e-mail: qbsong6@163.com, edward.tiekink@utsa.edu

## Key indicators

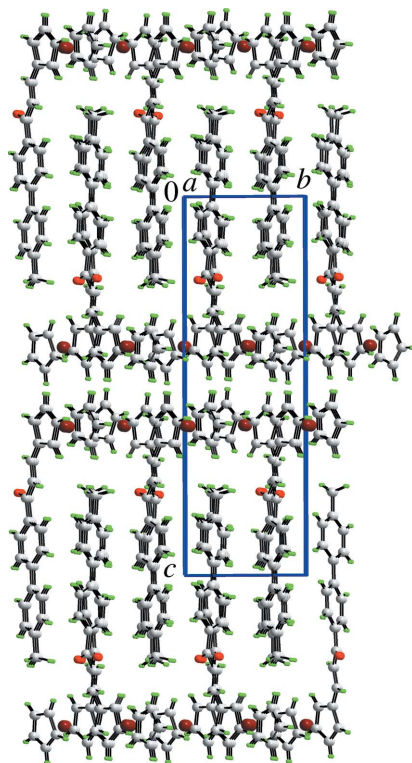
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.041  
 $wR$  factor = 0.101  
Data-to-parameter ratio = 17.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(E)-3-Ferrocenyl-1-(4-tolylphenyl)prop-2-en-1-one**In the title compound,  $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{21}\text{H}_{17}\text{O})]$ , significant conformational differences in the ferrocenyl- $\text{C}(\text{H})=\text{C}(\text{H})-\text{C}(=\text{O})R$  groups distinguish the two independent molecules comprising the asymmetric unit.  $\text{C}-\text{H}\cdots\pi$  interactions appear to influence the crystal packing.

## Comment

Interest in ferrocenyl chalcones related to the title compound, (I) (Song *et al.*, 2004, 2005), arises in part owing to their antiplasmodial activity (Wu *et al.*, 2006). There are three crystal structures available in the literature containing the ferrocenyl- $\text{C}(\text{H})=\text{C}(\text{H})\text{C}(=\text{O})R$  group as found in (I), namely  $R = \text{phenyl}$  and 4-(*n*-butoxy)phenyl (Wu *et al.*, 2006), and  $R = \text{anthracenyl}$  (Hursthouse *et al.*, 2003).Two independent molecules comprise the asymmetric unit of (I) (Fig. 1). While the configuration about the  $\text{C}11=\text{C}12$  bond in each case is *E*, as found in the aforementioned derivatives, there are non-trivial differences between the independent molecules in (I). In particular, there are twists about the  $\text{C}1-\text{C}11$ ,  $\text{C}14-\text{C}14$  and  $\text{C}17-\text{C}20$  bonds as seen in the  $\text{C}2-\text{C}1-\text{C}11-\text{C}12$ ,  $\text{O}1-\text{C}13-\text{C}14-\text{C}15$  and  $\text{C}16-\text{C}17-\text{C}20-\text{C}21$  torsion angles of  $-18.6$  (6),  $148.1$  (4) and  $-11.4$  (5)°, respectively, for the first independent molecule compared with  $15.1$  (6),  $171.5$  (4) and  $-1.1$  (4)°, respectively, for the second molecule. These features preclude the adoption of a higher-symmetry space group, even though a *PLATON* (Spek, 2003) analysis of (I) indicated significant pseudo-symmetry. By contrast, there are no significant differences in terms of bond distances and angles, which are as expected (Wu *et al.*, 2006; Hursthouse *et al.*, 2003).The conformations of the ferrocenyl groups in (I) are effectively eclipsed; it was not possible to resolve the disorder apparent in the cyclopentadienyl rings into well defined orientations. An eclipsed conformation was also found in the  $R = \text{phenyl}$  derivative mentioned above, in contrast to the almost perfectly staggered conformation found in the other two structures.Received 27 March 2006  
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**Figure 1**  
The atom-labelling scheme used for the two independent molecules in (I), showing 35% probability displacement ellipsoids (arbitrary spheres for the H atoms).



**Figure 2**  
The crystal packing in (I), viewed down the *a* axis. Colour code: Fe brown, O red, C grey and H green.

A view of the crystal packing in (I) is shown in Fig. 2. The structure may be described as a layered arrangement stacked along the *c* axis. Thus, layers of ferrocenyl entities, comprising both independent molecules, face similar layers. These double layers are separated by layers comprising the organic residues.

There is no evidence of significant  $\pi$ - $\pi$  interaction but there are C—H... $\pi$  contacts between ferrocenyl residues as well as between the non-ferrocenyl residues. The closest C—H... $\pi$  contact of 2.82 Å occurs between C19a/H19a and the ring centroid of C20<sup>i</sup>—C25<sup>i</sup> so that the C19...centroid distance is 3.517 (3) Å and the angle at H is 133° [symmetry code: (i) *x*, *y*, 1 + *z*]. The closest interaction between ferrocenyl groups occurs between C3a—H3a and the ring centroid of C6<sup>ii</sup>—C10<sup>ii</sup> so that the respective parameters are 2.98 Å, 3.851 (5) Å and 156° [symmetry code: (ii) 1 - *x*,  $\frac{3}{2}$  + *y*, 1 - *z*].

## Experimental

The title compound was prepared in accord with the literature procedure (Song *et al.*, 2004, 2005). Brown crystals of (I) suitable for the X-ray study were grown by the slow evaporation of an acetone solution of the compound; m.p. 494–495 K.

### Crystal data

[Fe(C<sub>5</sub>H<sub>5</sub>)(C<sub>21</sub>H<sub>17</sub>O)]  
*M<sub>r</sub>* = 406.29  
 Monoclinic, *P*2<sub>1</sub>  
*a* = 11.140 (3) Å  
*b* = 7.518 (2) Å  
*c* = 24.123 (6) Å  
 $\beta$  = 102.207 (9)°  
*V* = 1974.6 (9) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.367 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.78 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, brown  
 0.31 × 0.20 × 0.10 mm

### Data collection

Rigaku R-AXIS RAPID  
 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.773, *T<sub>max</sub>* = 0.925

19618 measured reflections  
 8973 independent reflections  
 7893 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.026  
 $\theta_{\max}$  = 27.5°

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.041  
*wR* (*F*<sup>2</sup>) = 0.101  
*S* = 1.09  
 8973 reflections  
 508 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 1.3096P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 ( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{\max}$  = 0.47 e Å<sup>-3</sup>  
 $\Delta\rho_{\min}$  = -0.33 e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 4106 Friedel pairs  
 Flack parameter: 0.212 (18)

**Table 1**

Selected bond angles (°).

C2—C1—C11	127.6 (3)	C2a—C1a—C11a	127.6 (3)
C1—C11—C12	126.5 (4)	C1a—C11a—C12a	127.0 (3)
C11—C12—C13	120.4 (3)	C11a—C12a—C13a	121.2 (3)
O1—C13—C12	121.3 (3)	O1a—C13a—C12a	120.6 (3)
O1—C13—C14	119.8 (3)	O1a—C13a—C14a	120.4 (3)
C12—C13—C14	118.9 (3)	C12a—C13a—C14a	118.9 (3)

The H atoms were included in the riding-model approximation with C—H distances of 0.93 Å (aromatic H atoms) and 0.96 Å (methyl), and with *U*<sub>iso</sub>(H) values of 1.2 or 1.5 times *U*<sub>eq</sub>(C) for aromatic and methyl H atoms, respectively. The structure was refined as a racemic twin with twin fractions 0.212 (18):0.788 (18).

Data collection: *CrystalStructure* (Rigaku/MS, 2004); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*;

program(s) used to solve structure: *PATY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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