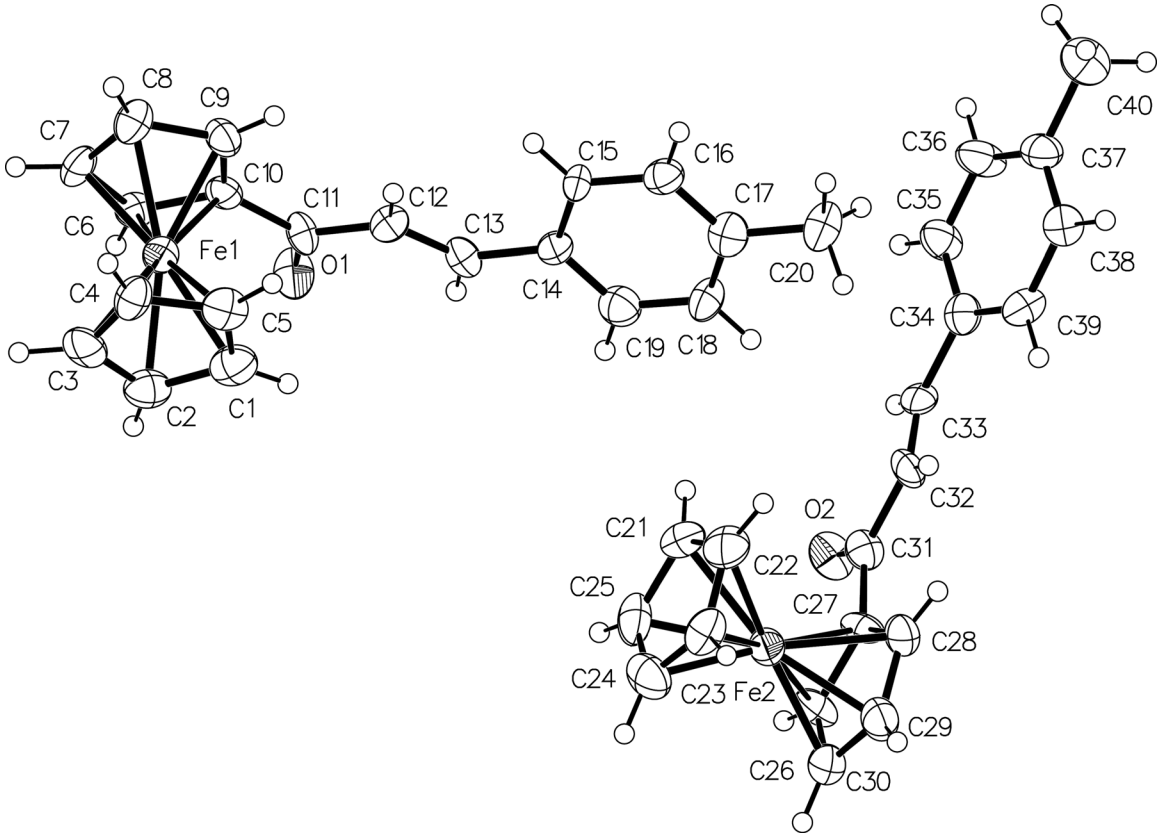
Dandan Cui, Chanchan Liu, Mengjia Yang, Jingyin Yu and Bin Liu*

Crystal structure of (*E*)-(3-(*p*-tolyl)acryloyl) ferrocene, $C_{20}H_{18}FeO$



https://doi.org/10.1515/ncrs-2025-0254
Received June 1, 2025; accepted July 2, 2025;
published online July 10, 2025

Abstract

$C_{20}H_{18}FeO$, monoclinic, *Cc* (no. 9), a = 25.941(4) Å, b = 5.8017(7) Å, c = 20.350(3) Å, β = 90.188(4)°, V = 3062.7(7) Å^3, Z = 8, $R_{gt}(F)$ = 0.0621, $wR_{ref}(F^2)$ = 0.1446, T = 170 K.

CCDC no.: 2445568

***Corresponding author: Bin Liu**, Xianyang Key Laboratory of Molecular Imaging and Drug Synthesis, School of Pharmacy, Shaanxi Institute of International Trade & Commerce, Xianyang, Shaanxi, China, E-mail: lb125lb@163.com. https://orcid.org/0000-0003-2852-7739
Dandan Cui, Chanchan Liu, Mengjia Yang and Jingyin Yu, Xianyang Key Laboratory of Molecular Imaging and Drug Synthesis, School of Pharmacy, Shaanxi Institute of International Trade & Commerce, Xianyang, Shaanxi, China

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.12 × 0.06 × 0.05 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.98 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	26.4°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3468, 3142, 0.062
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2621
$N(param)_{refined}$:	340
Programs:	Bruker,[1] SHELX,[2,3] Olex2[4]

The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

The 4-methylbenzaldehyde (2.64 g, 22.0 mmol), acetylferrocene (2.28 g, 10.0 mmol) and KOH (0.67 g, 12.0 mmol) were added to the mortar. After stirring well, the reaction mixture was ground for 20 min, until the TLC indicated the reaction was completed, then diluted with water and filtered. The solid was collected and washed with water, and dried overnight under vacuum. The crude product was further purified by flash silica chromatography to afford a single crystal of high quality. For crystal growth, the crude product was dissolved in a minimal amount of hot ethanol and slowly cooled to room temperature.

2 Experimental details

The crystal structure was determined by Direct Methods using SHELXT[2] and subsequently refined anisotropically for all non-hydrogen atoms by full-matrix least-squares in SHELXL,[3] utilizing the Olex2 platform.[4]

3 Comment

Crystallographic analysis of ferrocene derivatives is essential for elucidating supramolecular organization, which governs bulk properties like charge transport and thermal stability.[5–7] This study presents the structure of (*E*)-(3-(*p*-tolyl)acryloyl)ferrocene (Figure), confirming its regioselectivity and stereochemical integrity while revealing intermolecular interactions critical for material design.[8,9]

There are two crystallographically independent molecules in the asymmetric unit. Each molecule features a central ferrocene core with an iron atom symmetrically coordinated between two cyclopentadienyl (Cp) rings. The unsubstituted left Cp ring (C1–C5) maintains planar aromaticity,[10–13] while the right Cp ring (C6–C10) is functionalized *via* an acryloyl group extending into a propenoyl chain. This chain terminates at the C13 position with a *p*-tolyl substituent (C14–C20), introducing steric asymmetry.

The acryloyl bridge adopts an *E*-configuration at the C12=C13 double bond, evidenced by the antiperiplanar arrangement of the carbonyl oxygen (O1) and the *p*-tolyl group. The rigid *E*-geometry enforces coplanarity across the conjugated system, dihedral angle Cp–C12–C13–C14 about 180°, facilitating electronic communication between the electron-donating *p*-tolyl group and the electron-rich ferrocene core.

This duality-planar conjugation combined with steric differentiation-suggests utility in tunable optoelectronic materials where controlled solid-state organization and electronic delocalization are paramount.

Research funding: This work was financially supported by the Natural Science Foundation of Shaanxi Province (2025JC–YBMS-888) Scientific research plan project of Shaanxi Provincial Department of Education (24JK0331, 24JK0334) The 2024 Key Scientific Research Program Projects of the Shaanxi Provincial Department of Education (Key Laboratory Projects, 24JS004) Key Laboratory of Molecular Imaging and Drug Synthesis of Xianyang city (2021QXNL–PT-0008) School-level Scientific and Technological Innovation Team for Design, Synthesis and Structural Modification of Drug Molecules (2024KCTD04).

References

1. Bruker. Saint, Apex2 and Sadabs; Bruker AXS Inc.: Madison, WI, USA, 2012.
2. Sheldrick, G. M. Shelxt – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. Sheldrick, G. M. Crystal Structure Refinement with Shelxl. *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A.; Puschmann, H. Olex2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
5. Novoa, N.; Roisnel, T.; Dorcet, V.; Hamon, J. –R.; Carrillo, D.; Manzur, C.; Robin–Le Guen, F.; Cabon, N. Anisyl and Ferrocenyl Adducts of Methylenepyran-Containing *β*-Diketone: Synthesis, Spectral, Structural, and Redox Properties. *J. Organomet. Chem.* **2014**, *762*, 19–28.
6. Allison, M.; Caramés–Méndez, P.; Pask, C. M.; Phillips, R. M.; Lord, R. M.; McGowan, P. C. Bis(Bipyridine)Ruthenium(II) Ferrocenyl *β*–Diketonate Complexes: Exhibiting Nanomolar Potency Against Human Cancer Cell Lines. *Chem. – Eur J.* **2021**, *27*, 3737–3744.
7. Artigas, V.; González, D.; Fuentealba, M. Syntheses, Characterisation and Crystal Structures of Ferrocenyl *β*-Diketones and Their Schiff Base NNO Ligand Derivatives with 2-Picolylamine. *J. Mol. Struct.* **2017**, *1129*, 325–332.
8. Anizaim, A. H.; Zainuri, D. A.; Zaini, M. F.; Razak, I. A.; Bakhtiar, H.; Arshad, S. Comparative Analyses of New Donor-*π*-Acceptor Ferrocenyl-Chalcones Containing Fluoro and Methoxy-Fluoro Acceptor Units as Synthesized Dyes for Organic Solar Cell Material. *PLoS One* **2020**, *15*, e0241113.
9. Allison, M.; Caramés–Méndez, P.; Hofmann, B. J.; Pask, C. M.; Phillips, R. M.; Lord, R. M.; McGowan, P. C. Cytotoxicity of Ruthenium(II) Arene Complexes Containing Functionalized Ferrocenyl *β*–Diketonate Ligands. *Organometallics* **2023**, *42*, 1869–1881.
10. Zhang, J.; Hu, X.; Liu, X.; He, Y. The Crystal Structure of (*E*)-1-Ferrocenyl-3-(4-isopropylphenyl)prop-2-en-1-One, $C_{22}H_{22}FeO$. *Z. Kristallogr. – N. Cryst. Struct.* **2022**, *237*, 437–439.
11. Tian, H.; Chen, G.; Ma, J.; Liu, B. Crystal Structure of (4-(4-Isopropylphenyl)-1*H*-pyrrol-3-yl)(ferrocenyl)methanone. *Z. Kristallogr. - N. Cryst. Struct.* **2025**, *240*, 483–485.
12. Muškinja, J.; Burmudžija, A.; Ratković, Z.; Ranković, B.; Kosanić, M.; Bogdanović, G. A.; Novaković, S. B. Ferrocenyl Chalcones with O-Alkylated Vanillins: Synthesis, Spectral Characterization, Microbiological Evaluation, and Single-Crystal X-ray Analysis. *Med. Chem. Res.* **2016**, *25*, 1744–1753.
13. Gao, Y.; Xu, X.; Zhu, Z.; Tang, W. Crystal Structure of (E)-(3-(3,4-Dimethylphenyl)acryloyl)ferrocene. *Z. Kristallogr. – N. Cryst. Struct.* **2025**, *240*, 345.