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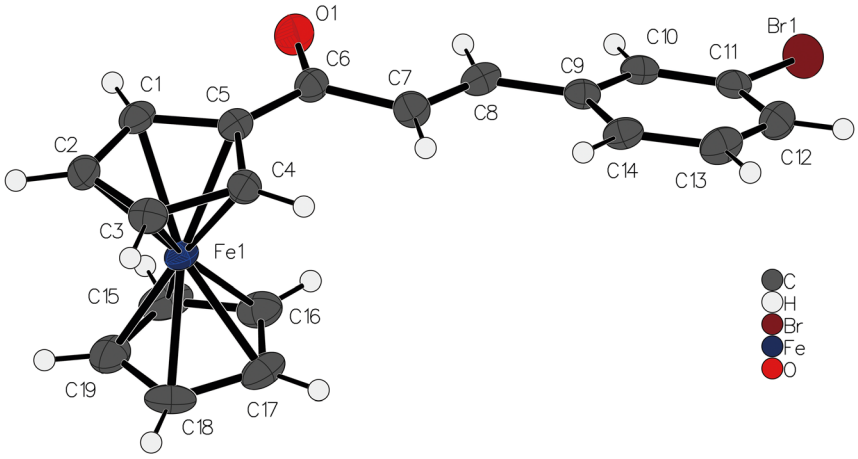
Crystal structure of (E)-(3-(3-bromophenyl) acryloyl)ferrocene, $C_{19}H_{15}BrFeO$



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Abstract

$C_{19}H_{15}BrFeO$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.7615(2) Å, b = 10.5534(4) Å, c = 25.7793(10) Å, V = 1567.47(10) Å^3, Z = 4, $R_{gt}(F)$ = 0.0399 w$R_{ref}(F^2)$ = 0.0861, T = 170 K.

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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.

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.12 × 0.06 × 0.05 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	3.51 mm^{-1}
Diffractometer, scan mode:	Bruker Apex-II, φ and ω scans
θ_{max}, completeness:	28.5°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12190, 3935, 0.072
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3,006
$N(param)_{refined}$:	199
Programs:	Bruker,[1] Shelx,[2,3] Olex2[4]

1 Source of materials

The 3-bromobenzaldehyde (3.68 g, 20.0 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 solved via Direct Methods employing SHELXT,[2] followed by anisotropic refinement of non-hydrogen atoms using full-matrix least-squares calculations (SHELXL,[3]) within the Olex2 platform.[4]

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3 Comment

The elucidation of crystal structures in ferrocene derivatives is pivotal for understanding their supramolecular organization, which governs bulk physicochemical properties such as charge transport, thermal stability, and solubility.[5–7] Precise crystallographic analysis reveals intermolecular interactions that dictate packing motifs, while also confirming regioselectivity and stereochemical fidelity in synthetic designs.[8–10]

The molecular architecture of (*E*)-(3-(3-bromophenyl) acryloyl)ferrocene features a central ferrocene core comprising an iron atom (Fe1) coordinated symmetrically between two cyclopentadienyl (Cp) rings. The left Cp ring remains unsubstituted, preserving its planar aromatic character,[11–15] while the right Cp ring is functionalized with an acryloyl moiety extending into a propenoyl chain. This chain terminates at the C8 position of the acryloyl unit with a 3-bromophenyl substituent, introducing steric and electronic asymmetry. The acryloyl bridge adopts an *E* configuration at the C7=C8 double bond, as confirmed by the antiperiplanar arrangement of the carbonyl oxygen (O1) and the brominated phenyl group.

The stereochemical rigidity of the *E*-configured acryloyl group enforces a planar geometry across the conjugated system, facilitating electronic communication between the electron-withdrawing bromophenyl group and the electron-rich ferrocene core. The 3-bromophenyl substituent, positioned orthogonally to the Cp rings, introduces significant steric bulk, likely influencing π-π stacking interactions and solubility properties.[16–18] This structural duality (planar aromatic cores vs. flexible substituents) suggests tailored applications in catalysis or materials science, where tunable electronic and steric profiles are critical.

All geometric parameters are in the expected ranges for such complexes containing a halogenophenyl moiety.[11,14,19]

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