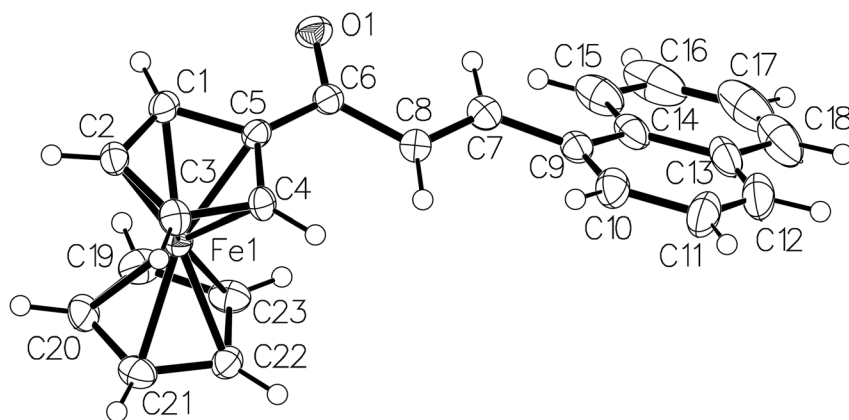


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The crystal structure of (*E*)-1-ferrocenyl-3-(naphthalen-1-yl)prop-2-en-1-one, C₂₃H₁₈FeO



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Abstract

C₂₃H₁₈FeO, orthorhombic, *Pna*2₁ (no. 33), *a* = 28.3217(11) Å, *b* = 5.7477(2) Å, *c* = 10.3071(3) Å, β = 90°, *V* = 1677.84(10) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0372, *wR*_{ref}(*F*²) = 0.0713, *T* = 150 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

At the room temperature, a mixture of 1-naphthaldehyde (10 mmol) and acetylferrocene (10 mmol) was dissolved in 25 mL ethanol solution, and then 10 mL KOH (20%) was added. After all raw material disappeared (judged by thin

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.19 × 0.14 × 0.11 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.91 mm ⁻¹
Diffractometer, scan mode:	D8 VENTURE, φ and ω
θ _{max} , completeness:	26.5°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	16,989, 3445, 0.065
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2786
<i>N</i> (<i>param</i>) _{refined} :	226
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

layer chromatography), the reaction solution was poured into 50 mL water to precipitate some solids. The solid production was gained by vacuum filtering, and then used water and 30% ethanol aqueous solution to wash it in turn. The single crystal of the title compound was achieved by recrystallization at the room temperature for seven days.

Experimental details

All H atoms were placed in geometrically idealized positions and refined riding on their parent C atoms with d(C–H) = 0.95 Å and *U*_{iso}(H) = 1.2 *U*_{eq}(C).

Comment

Ferrocene, as a classical sandwich structure, embraces the iron atom between two cyclopentadienyl rings [5],

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
C1	0.73238 (16)	0.9104 (9)	0.6859 (4)	0.0238 (11)
H1	0.726441	1.069613	0.704405	0.029*
C2	0.76457 (14)	0.7640 (7)	0.7523 (6)	0.0239 (10)
H2	0.783808	0.808656	0.823640	0.029*
C3	0.76333 (16)	0.5392 (9)	0.6946 (4)	0.0250 (11)
H3	0.781860	0.408990	0.719775	0.030*
C4	0.72957 (16)	0.5434 (9)	0.5929 (4)	0.0222 (10)
H4	0.721114	0.415953	0.539058	0.027*
C5	0.71038 (16)	0.7753 (8)	0.5858 (5)	0.0210 (10)
C6	0.67241 (15)	0.8631 (9)	0.5012 (4)	0.0217 (10)
C7	0.61331 (16)	0.7681 (9)	0.3371 (5)	0.0260 (11)
H7	0.606950	0.930326	0.336137	0.031*
C8	0.64558 (16)	0.6954 (9)	0.4223 (4)	0.0229 (11)
H8	0.651305	0.533485	0.432224	0.027*
C9	0.58666 (14)	0.6259 (9)	0.2450 (6)	0.0263 (12)
C10	0.60632 (19)	0.4278 (10)	0.1941 (5)	0.0343 (13)
H10	0.636069	0.376366	0.225519	0.041*
C11	0.5835 (2)	0.2987 (12)	0.0963 (5)	0.0478 (16)
H11	0.597319	0.159623	0.064218	0.057*
C12	0.5416 (2)	0.3741 (14)	0.0482 (6)	0.0574 (18)
H12	0.527205	0.290544	−0.020783	0.069*
C13	0.5191 (2)	0.5714 (13)	0.0976 (5)	0.0480 (16)
C14	0.54131 (18)	0.7020 (10)	0.2003 (5)	0.0345 (13)
C15	0.51718 (16)	0.8936 (10)	0.2523 (8)	0.0434 (13)
H15	0.531423	0.980643	0.320153	0.052*
C16	0.4734 (2)	0.9585 (13)	0.2073 (7)	0.066 (2)
H16	0.457546	1.087843	0.244639	0.079*
C17	0.4523 (2)	0.8327 (18)	0.1060 (8)	0.078 (2)
H17	0.422150	0.878061	0.074817	0.094*
C18	0.4741 (2)	0.6500 (17)	0.0529 (7)	0.073 (2)
H18	0.459272	0.570010	−0.016716	0.088*
C19	0.64377 (18)	0.7403 (9)	0.8801 (5)	0.0342 (13)
H19	0.634748	0.897442	0.894386	0.041*
C20	0.67762 (18)	0.6133 (10)	0.9528 (5)	0.0324 (12)
H20	0.695308	0.670881	1.024202	0.039*
C21	0.68047 (17)	0.3855 (9)	0.9004 (5)	0.0296 (11)
H21	0.700322	0.263756	0.930592	0.035*
C22	0.64869 (15)	0.3719 (9)	0.7960 (4)	0.0246 (11)
H22	0.643379	0.238783	0.743329	0.030*
C23	0.62579 (15)	0.5912 (8)	0.7822 (6)	0.0299 (12)
H23	0.602698	0.630357	0.718992	0.036*
Fe1	0.69753 (2)	0.62801 (10)	0.76204 (7)	0.02021 (15)
O1	0.66388 (11)	1.0735 (6)	0.4978 (3)	0.0286 (8)

which makes it relatively stable in aqueous and aerobic environments [6]. Factually, ferrocene derivatives hold inherent remarkable stability towards air, light, heat and show a rich photochemistry, at low cost, and low toxicity [7]. Thus they are widely applied in homogeneous catalysis [8], electrochemistry [9], polymer chemistry [10], and bioorganometallic chemistry [11]. Additionally, the

introduction of ferrocenyl into bioactive compounds is an effective way to develop more efficacious therapeutic agents [6]. Plentiful ferrocene derivatives were proved to display a wide spectrum of biological effects like anti-cancer [12], anti-HIV [13], anti-infective, anti-oxidant [14], antimalarial [15], anticonvulsant [16], and DNA-cleaving properties [17].

The title compound crystallizes with one molecule per asymmetric unit (see the figure). The C–Fe distances are in the range 2.025(5)–2.056(5) Å. The bond length of C6=O1 is 1.234(7) Å, which is close to the standard value. Two cyclopentadienyl rings of ferrocene substituent make dihedral angles of 15.06° and 14.97° respectively with the naphthyl moiety. Some weak intramolecular C–H...O interactions related to O atom of the acyl group and H atom of the adjacent compounds help to stabilize the present molecular conformation, which are similar to several previous works [18–20].

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