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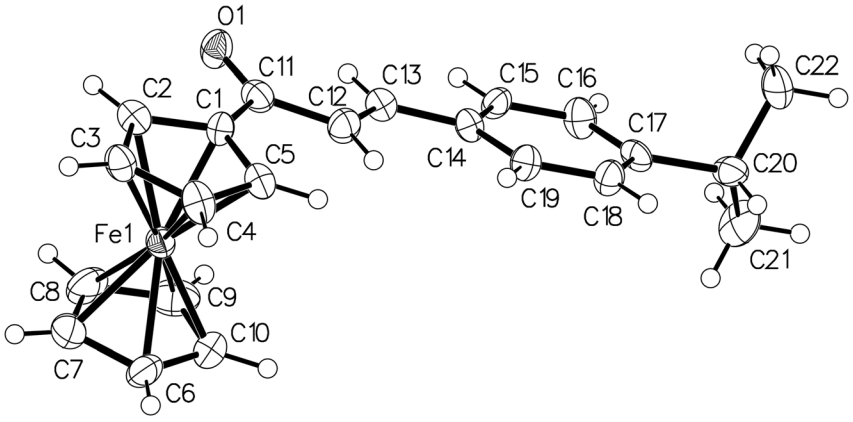
# The crystal structure of (*E*)-1-ferrocenyl-3-(4-isopropylphenyl)prop-2-en-1-one, $C_{22}H_{22}FeO$

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**Abstract**

$C_{22}H_{22}FeO$, monoclinic, $P2_1$ (no. 4), $a$ = 10.204(3) Å, $b$ = 5.7956(16) Å, $c$ = 14.591(4) Å, $\beta$ = 97.876(10)°, $V$ = 854.7(4) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0676, $wR_{ref}(F^2)$ = 0.1647, T = 170 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.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Red needle |
| Size: | 0.12 × 0.08 × 0.03 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.89 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 26.4°, 99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 4779, 3020, 0.074 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 σ($I_{obs}$), 2006 |
| $N(param)_{refined}$: | 189 |
| Programs: | Bruker [1], Olex2 [2], SHELX [3, 4] |

## Source of material

A mixture of 10 mmol acetylferrocene and 10 mmol cuminaldehyde was added to 25 mL of ethanol, and kept stirring to make mixture completely soluble at the room temperature. Then 10 mL of KOH (20%) was added to the above solution. Until all starting materials disappeared on the thin layer chromatography, the solution was added to 50 mL water, and the precipitated solids were filtered off. The solid was obtained by vacuum filtering, and washing with water and 30% ethanol respectively. Crystals were acquired by slow evaporation at the room temperature for one week.

## Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and treated as riding on their parent C atoms with d(C–H) = 0.95 Å and $U_{iso}$ (H) = 1.2 $U_{eq}$(C).

## Comment

Cuminaldehyde, i.e., 4-isopropylbenzaldehyde, is an oxidized aldehyde monoterpene compound, and is a major essential

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.8412 (7) | 0.3029 (12) | 0.4418 (3) | 0.025 (2) |
| C2 | 0.8293 (7) | 0.1697 (10) | 0.3594 (4) | 0.027 (2) |
| H2 | 0.801942 | 0.013134 | 0.353334 | 0.033* |
| C3 | 0.8654 (7) | 0.3117 (13) | 0.2876 (3) | 0.031 (3) |
| H3 | 0.866538 | 0.266769 | 0.225079 | 0.037* |
| C4 | 0.8997 (7) | 0.5326 (11) | 0.3256 (5) | 0.035 (3) |
| H4 | 0.927701 | 0.661446 | 0.293038 | 0.042* |
| C5 | 0.8847 (8) | 0.5272 (10) | 0.4209 (4) | 0.028 (3) |
| H5 | 0.900906 | 0.651735 | 0.463294 | 0.033* |
| C6 | 0.5870 (8) | 0.6932 (12) | 0.2765 (5) | 0.036 (3) |
| H6 | 0.614039 | 0.817307 | 0.240885 | 0.043* |
| C7 | 0.5483 (8) | 0.4701 (14) | 0.2428 (4) | 0.054 (3) |
| H7 | 0.544871 | 0.418723 | 0.180717 | 0.065* |
| C8 | 0.5157 (8) | 0.3373 (11) | 0.3183 (6) | 0.047 (3) |
| H8 | 0.486557 | 0.181432 | 0.315528 | 0.057* |
| C9 | 0.5342 (7) | 0.4783 (14) | 0.3986 (5) | 0.047 (3) |
| H9 | 0.519686 | 0.433362 | 0.459013 | 0.057* |
| C10 | 0.5783 (7) | 0.6983 (12) | 0.3728 (5) | 0.033 (3) |
| H10 | 0.598473 | 0.826355 | 0.412881 | 0.040* |
| C11 | 0.8016 (10) | 0.2197 (19) | 0.5311 (6) | 0.028 (2) |
| C12 | 0.8015 (10) | 0.3941 (17) | 0.6042 (6) | 0.032 (3) |
| H12 | 0.831308 | 0.546075 | 0.594138 | 0.039* |
| C13 | 0.7602 (10) | 0.3417 (17) | 0.6848 (6) | 0.027 (2) |
| H13 | 0.725369 | 0.191130 | 0.690636 | 0.033* |
| C14 | 0.7636 (6) | 0.4963 (9) | 0.7658 (3) | 0.023 (2) |
| C15 | 0.7090 (6) | 0.4192 (9) | 0.8425 (4) | 0.027 (2) |
| H15 | 0.666868 | 0.272772 | 0.841092 | 0.032* |
| C16 | 0.7159 (6) | 0.5563 (11) | 0.9211 (3) | 0.033 (3) |
| H16 | 0.678587 | 0.503617 | 0.973539 | 0.040* |
| C17 | 0.7775 (7) | 0.7705 (10) | 0.9232 (3) | 0.026 (2) |
| C18 | 0.8321 (6) | 0.8476 (8) | 0.8465 (4) | 0.029 (2) |
| H18 | 0.874224 | 0.994027 | 0.847904 | 0.035* |
| C19 | 0.8252 (6) | 0.7105 (10) | 0.7678 (3) | 0.031 (3) |
| H19 | 0.862507 | 0.763186 | 0.715456 | 0.037* |
| C20 | 0.7887 (10) | 0.924 (3) | 1.0111 (6) | 0.035 (3) |
| H20 | 0.826183 | 1.075273 | 0.994796 | 0.042* |
| C21 | 0.6571 (10) | 0.973 (3) | 1.0426 (7) | 0.048 (3) |
| H21A | 0.598545 | 1.047266 | 0.992381 | 0.072* |
| H21B | 0.669905 | 1.075368 | 1.096489 | 0.072* |
| H21C | 0.617178 | 0.827768 | 1.059448 | 0.072* |
| C22 | 0.8871 (14) | 0.818 (2) | 1.0870 (8) | 0.055 (4) |
| H22A | 0.851598 | 0.672062 | 1.107247 | 0.083* |
| H22B | 0.902200 | 0.924403 | 1.139566 | 0.083* |
| H22C | 0.970835 | 0.788607 | 1.063321 | 0.083* |
| Fe1 | 0.70803 (13) | 0.4484 (3) | 0.34352 (8) | 0.0253 (4) |
| O1 | 0.7700 (7) | 0.0189 (11) | 0.5397 (4) | 0.0334 (19) |

oil of green cumin seeds, eucalyptus, myrrh, and cassia [5, 6]. Due to its characteristic aroma, this compound has been used as a fragrance chemical in cosmetic. Additionally, cuminaldehyde has been reported to exhibit various therapeutic properties, such as anti-oxidant, anti-helminthic [7], anti-inflammatory [6], anti-nociceptive, anti-neuropathic [8], antibacterial [9], antidiabetic [10], anti-cancer [11], and antifungal effects [12, 13]. However, there is limit research on its carbonyl derivatives [14–16]. As mentioned in our previous works [17, 18], ferrocene has a stable sandwich structure. The incorporation of ferrocenyl into biological molecules offers the potential to develop better and more efficacious therapeutic drugs.

The optimized molecular structure of the title compound is displayed in the figure, and it adopts an *E* configuration about the C12–C13 double bond. There is a slight twist between the two cyclopentadienyl rings of ferrocenyl moiety forming a dihedral angle of 2.61°. The dihedral angle between the phenyl ring (C14/C15/C16/C17/C18/C19) and the cyclopentadienyl ring (C1/C2/C3/C4/C5) is 14.85°, and the dihedral angle between the phenyl ring (C14/C15/C16/C17/C18/C19) and the other cyclopentadienyl ring (C6/C7/C8/C9/C10) is 17.12°. The intramolecular hydrogen bonding interactions between the acyl O atoms and C–H atoms stabilize the crystal packing. Parameters are similar to related structures [17–19].

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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