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# [2-(4-Nitrophenoxyl)-2-(1*H*-1,2,4-triazol-1-yl)-acetyl]ferrocene

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.036
*wR* factor = 0.088
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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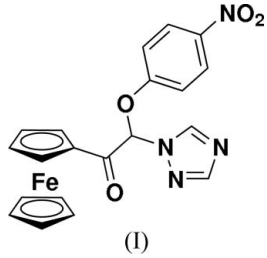
The title compound $[Fe(C_5H_5)(C_{15}H_{11}N_4O_4)]$, has been synthesized as a potent fungicidal agent and its crystal structure was determined. In the crystal structure, there are weak intermolecular C—H···N interactions. The dihedral angles between the plane of the unsubstituted ferrocenyl cyclopentadienyl and thiazole rings, and between the substituted phenyl and thiazole rings are 89.3 (3) and 92.3 (2)°, respectively.

## Comment

Triazole antifungals are known as potent inhibitors of cytochrome P450 monooxygenase in the process of fungal biosynthesis of ergosterol, which is an important constituent of fungal cell membrane (Hiroshi *et al.*, 1995; Fang *et al.*, 2003*a*,*b*). They are widely applied in the fields of medication and plant protection. In addition, ferrocenyl is ideal for use in drug design because of its low toxicity, its stability and lipophilicity (Biot *et al.*, 2000). Ferrocenyl groups have already been shown to advantageously replace phenyl moieties in biologically active compounds (Huang & Wang, 2001).




(I)

The incorporation of ferrocenyl moieties in a bioactive compound would induce great changes in its molecular properties, such as solubility and hydrophobicity. Therefore, in a search for novel potent fungicides, we have synthesized compounds which consist of ferrocenyl and 1*H*-1,2,4-triazole units. We report here the crystal structure of [2-(4-nitrophenoxyl)-2-(1*H*-1,2,4-triazol-1-yl)acetyl]ferrocene, (I).

Fig. 1 shows the molecular structure of (I) which contains the following four planar subunits: the substituted cyclopentadienyl ring C1–C5 (*p*1), the cyclopentadienyl ring C6–C10 (*p*2), the triazole ring (*p*3) and the substituted phenyl ring (p4). The dihedral angles between *p*1 and p3, and between *p*3 and *p*4 are 89.3 and 92.3°, respectively. Plane *p*1 is oriented nearly perpendicular to planes *p*3 and *p*4.

The Fe1—C bond lengths for the substituted cyclopentadienyl ring range between 2.027 (2) (Fe1–C2) and 2.052 (3) Å (Fe1—C3), similar to those in the other cyclopentadienyl ring [between Fe—C = 2.038 (3) Å (Fe1—C7) and 2.045 (2) Å (Fe1—C9)]. The Fe atom is slightly shifted in the direction of the substituted cyclopentadienyl ring. The distances between

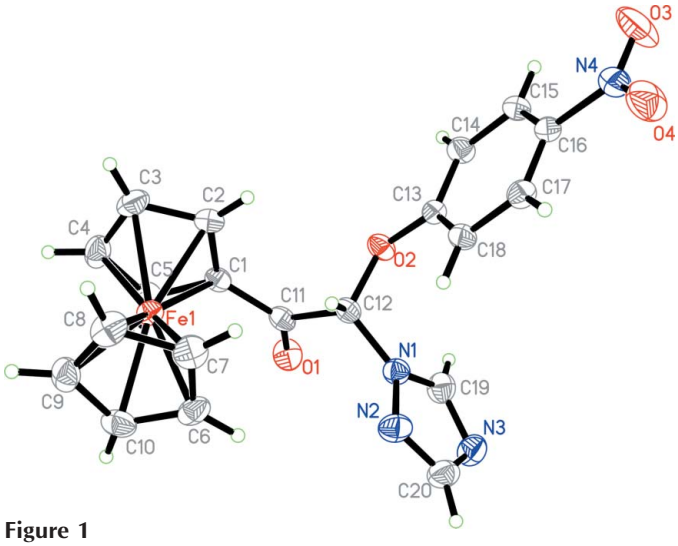



**Figure 1**
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids at the 30% probability level.

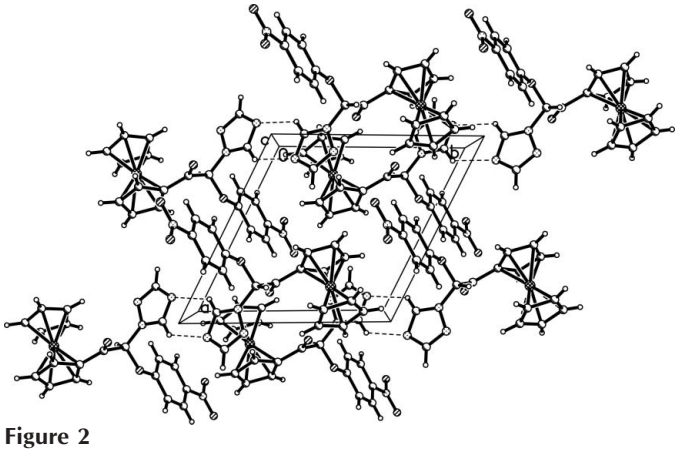


**Figure 2**
Packing of the title compound, viewed down the *c* axis. Dashed lines indicate C—H···N hydrogen-bond interactions.

the Fe atom and the centroids of the cyclopentadienyl rings *Cg*1 (C1–C5) and *Cg*2 (C6–C10) are 1.648 (2) and 1.654 (3) Å. The cyclopentadienyl rings are in an almost eclipsed conformation, as evidenced by the C1···*Cg*1···*Cg*2···C6 and C3···*Cg*1···*Cg*2···C8 pseudo-torsion angles of −4.4 (4) and −4.4 (3)°.

In the crystal structure, weak intermolecular C—H···N interactions are found [C19—H19···N2: C—H = 0.93 Å, H···N = 2.52 Å, C···N = 3.245 (1) Å and C19—H19···N = 101°; symmetry code: (i) $-x, 2-y, 1-z$] (Fig. 2).

## Experimental

The title compound was prepared by reacting (2-bromo-2–1*H*-1,2,4-triazol-1-ylacetyl)ferrocene (2.7 mmol), 4-nitrophenol (2.8 mmol) and $K_2CO_3$ (2.8 mmol) in acetonitrile (10 ml) at 343 K for 2 h under nitrogen. After cooling to room temperature, water (50 ml) was added and an amber-coloured precipitate formed. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate (*v*/*v*) = 3:1) (yield 75%). Analysis calculated for $C_{20}H_{16}FeN_4O_4$: C 55.58, H 3.73, N 12.96%; found: C 55.50, H 3.70, N 13.05%.

*Crystal data*

| | |
|---|---|
| $[Fe(C_5H_5)(C_{15}H_{11}N_4O_4)]$ | $Z = 2$ |
| $M_r = 432.22$ | $D_x = 1.528$ Mg m$^{-3}$ |
| Triclinic, $P\overline{1}$ | Mo $K\alpha$ radiation |
| $a = 9.863$ (2) Å | Cell parameters from 774 reflections |
| $b = 10.081$ (2) Å | $\theta = 2.3$–$24.5°$ |
| $c = 10.731$ (3) Å | $\mu = 0.84$ mm$^{-1}$ |
| $\alpha = 98.839$ (6)° | $T = 293$ (2) K |
| $\beta = 95.787$ (5)° | Parallelepiped, red |
| $\gamma = 114.928$ (7)° | 0.26 × 0.22 × 0.18 mm |
| $V = 939.6$ (4) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3791 independent reflections |
| $\varphi$ and $\omega$ scans | 3026 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $R_{int} = 0.017$ |
| $T_{min} = 0.800$, $T_{max} = 0.860$ | $\theta_{max} = 26.4°$ |
| 5443 measured reflections | $h = -9 \rightarrow 12$ |
| | $k = -12 \rightarrow 12$ |
| | $l = -13 \rightarrow 13$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.1868P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.088$ | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| $S = 1.03$ | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| 3791 reflections | |
| 262 parameters | |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Fe1—C2 | 2.027 (2) | Fe1—C3 | 2.052 (3) |
| Fe1—C1 | 2.028 (2) | N1—C19 | 1.333 (3) |
| Fe1—C7 | 2.038 (3) | N1—N2 | 1.356 (3) |
| Fe1—C8 | 2.040 (2) | N1—C12 | 1.441 (3) |
| Fe1—C6 | 2.042 (2) | N4—O4 | 1.213 (3) |
| Fe1—C5 | 2.043 (2) | N4—C16 | 1.468 (3) |
| Fe1—C10 | 2.044 (3) | O1—C11 | 1.211 (3) |
| Fe1—C9 | 2.045 (2) | O2—C13 | 1.383 (3) |
| Fe1—C4 | 2.050 (3) | O2—C12 | 1.413 (3) |
| | | | |
| C19—N1—N2 | 109.6 (2) | C1—C11—C12 | 115.93 (19) |
| C19—N1—C12 | 130.9 (2) | O2—C12—N1 | 110.72 (17) |
| C20—N2—N1 | 101.7 (2) | O2—C12—C11 | 104.24 (17) |
| C19—N3—C20 | 102.4 (2) | C18—C13—O2 | 124.5 (2) |
| O4—N4—O3 | 123.4 (2) | C14—C13—O2 | 114.4 (2) |
| O4—N4—C16 | 118.4 (2) | C17—C16—N4 | 118.3 (2) |
| C13—O2—C12 | 118.13 (17) | N3—C19—H19 | 124.8 |
| C5—C1—C11 | 124.7 (2) | N2—C20—N3 | 115.8 (2) |
| O1—C11—C1 | 124.4 (2) | | |
| | | | |
| C12—N1—N2—C20 | 176.7 (2) | N2—N1—C12—C11 | −98.6 (2) |
| C5—C1—C11—C12 | −158.4 (2) | O1—C11—C12—O2 | 94.4 (2) |
| C2—C1—C11—C12 | 12.9 (3) | C1—C11—C12—O2 | −85.0 (2) |
| C13—O2—C12—N1 | −75.4 (2) | O1—C11—C12—N1 | −25.4 (3) |
| C13—O2—C12—C11 | 163.84 (17) | C1—C11—C12—N1 | 155.21 (19) |
| C19—N1—C12—O2 | −39.7 (3) | C12—O2—C13—C18 | 3.5 (3) |
| N2—N1—C12—O2 | 145.4 (2) | C12—O2—C13—C14 | −177.45 (19) |
| C19—N1—C12—C11 | 76.3 (3) | O4—N4—C16—C17 | −1.1 (3) |

All H atoms were placed in calculated positions and were refined isotropically, with $U_{iso}(H) = 1.2U_{eq}(C)$ using a riding model with C—H = 0.93 Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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