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# (*R*)-*N*-(Ferrocenylmethyl)-1-hydroxy-3-phenylpropan-2-aminium (*E*)-but-2-enoate

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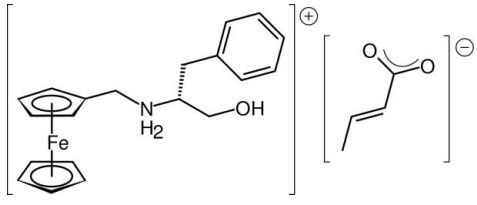
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.030; $wR$ factor = 0.067; data-to-parameter ratio = 18.4.

The crystal structure of the title salt, $[Fe(C_5H_5)(C_{15}H_{19}NO)](C_4H_5O_2)$, consists of discrete ammonium and carboxylate ions, which associate into infinite chains parallel to [100] by means of N—H···O and O—H···O interactions. These chains are further cross-linked into a three-dimensional network by additional C—H···O contacts and by offset $\pi$–$\pi$ stacking interactions of inversion-related aromatic rings [centroid–centroid distance = 3.7040 (14) Å]. The molecular parameters of the ionic components are in no way unexpected, the geometry of the ammonium cation being similar to that found in other structurally characterized salts obtained from *N*-ferrocenylmethyl $\beta$-aminoalcohols. The (*E*)-but-2-enoate anion consists of two approximately planar subunits, *viz* the delocalized carboxylate unit and the butenyl group (the latter being planar within *ca.* 0.002 Å), which are mutually rotated by 30.3 (4)°.

## Related literature

For crystal structures of *N*-ferrocenylmethyl $\beta$-aminoalcohols and their salts, see: Štěpnička *et al.* (2004, 2008*a*,*b*). For the preparation of a simple *N*-ferrocenylmethyl $\beta$-aminoalcohol, $FcCH_2NHCH_2CH_2OH$ (Fc = ferrocenyl), see: Hess *et al.* (1999). For an overview of organometallic crystal engineering, see: Braga *et al.* (2008) and references cited therein.




## Experimental

### Crystal data

$[Fe(C_5H_5)(C_{15}H_{19}NO)](C_4H_5O_2)$
$M_r$ = 435.33
Monoclinic, $P2_1$
$a$ = 5.9730 (2) Å
$b$ = 15.3905 (3) Å
$c$ = 11.7713 (4) Å
$\beta$ = 100.4986 (13)°
$V$ = 1063.99 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.73 mm$^{-1}$
$T$ = 150 K
0.33 × 0.12 × 0.10 mm

### Data collection

Nonius KappaCCD diffractometer
15916 measured reflections
4864 independent reflections
4511 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.067
$S$ = 1.05
4864 reflections
265 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$
Absolute structure: Flack (1983), 2329 Friedel pairs
Flack parameter: −0.016 (12)

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H91···O2$^{i}$ | 0.95 | 1.74 | 2.685 (2) | 173 |
| N1—H92···O3 | 0.82 | 1.94 | 2.747 (2) | 170 |
| O1—H93···O3$^{i}$ | 0.87 | 1.85 | 2.712 (2) | 172 |
| C16—H16···O1$^{ii}$ | 0.93 | 2.56 | 3.447 (3) | 159 |
| C18—H18···O2$^{iii}$ | 0.93 | 2.58 | 3.435 (3) | 154 |

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+1, y-\frac{1}{2}, -z+1$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2388).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m1619-m1620 [ **doi:10.1107/S1600536811044096** ]

# (*R*)-*N*-(Ferrocenylmethyl)-1-hydroxy-3-phenylpropan-2-aminium (*E*)-but-2-enoate

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## Comment

With our recent work (Štěpnička *et al.*, 2004 and 2008*a,b*), we demonstrated that *N*-ferrocenylmethyl *β*-aminoalcohols with general formula $FcCH_2NHCR^1R^2CR^3R^4OH$ (Fc = ferrocenyl) are potentially useful building blocks for organometallic crystal engineering (Braga *et al.*, 2008 and references therein). These compounds possess a balanced number of conventional H-bond donors and acceptors (OH and NH) in their native form. When reacted with protonic acids, they are readily converted to the corresponding ammonium salts, the crystal assembly of which receives additional support from charge interactions. This contribution reports the crystal structure of a salt obtained from a chiral aminoalcohol, namely (*R*)-2-[(ferrocenylmethyl)azonia]-3-phenylpropan-1-ol (*E*)-but-2-enoate.

Several crystals of the title compound were isolated unexpectedly during attempted crystallization of (*R*)-2-[(ferrocenylmethyl)amino]-3-phenylpropan-1-ol from ethyl acetate/hexane, apparently resulting from the reaction of the free amine with (*E*)-but-2-enoic acid present as a trace impurity in reagent grade ethyl acetate. A view of the molecular structure is presented in Fig. 1.

The geometry of the cation is rather unexceptional, and compares well with those reported earlier for salts obtained from $FcCH_2CMe_2CH_2OH$ and similar *N*-ferrocenylmethyl *β*-aminoalcohols (Štěpnička *et al.*, 2004 and 2008*a,b*). The ferrocenylmethyl and benzyl group attached to the 'central' N1—C12 bond assume an *anticlinal* eclipsed conformation (*cf.* torsion angle C11—N1—C12—C14) while their aromatic rings, C(1–5) and C(15–20), are nearly parallel [dihedral angle 7.75 (12)°] but mutually offset. The $CH_2OH$ pendant group is appended in a *gauche* position (*cf.* torsion angle C11—N1—C12—C13). Atom C13 is directed towards the ferrocenyl group and the C13—O1 bond extends away from the N1—C12 bond (*cf.* torsion angle N1—C12—C13—O1).

The ferrocenyl group shows negligible tilting [dihedral angle of the least-squares cyclopentadienyl planes is 1.63 (13)°] and similar Fe1—ring centroid distances [1.6461 (10) Å and 1.6565 (10) Å for the rings C(1–5) and C(6–10), respectively]. Although the Fe—C distances between Fe1 and individual carbon atoms in the substituted cyclopentadienyl ring C(1–5) differ by less than 0.03 Å [2.0271 (16)–2.054 (2) Å], there is a clear trend with the Fe—C distance gradually increasing from the $C_{ipso}$ to the opposite edge of the five-membered ring (*ipso* < *α* < *β*). The Fe—C distances observed for the unsubstituted cyclopentadienyl ring vary significantly less [2.040 (2)–2.058 (2) Å].

The C═C double bond within the (*E*)-but-2-enoate anion has an almost ideal *trans* configuration with the torsion angle C21—C22—C23—C24 of -179.6 (3)°, which renders the whole $CH_3$—CH═CH—C group nearly perfectly planar (within *ca*. 0.002 Å). The terminal carboxyl group (C21, O2, O3) is symmetrically rotated from the plane of the $CH_3$—CH═CH—C moiety by as much as 30.3 (4)° and shows a delocalized character. The individual C—O distances differ by only *ca*. 0.02 Å and even this relatively small difference may come mainly from crystal packing effects as the longer C—O distance is associated with O3 acting as a double H-bond acceptor, while the shorter one involves O2 atom for which only one strong H-bond was detected.

The ions constituting the crystal of the title compound assemble by means of H-bonds between OH and NH groups and carboxylate oxygen atoms to form infinite chains in the [1 0 0] direction (Fig. 2). Distances between the H-bond donors and acceptors are close to 2.7 Å while the H-bond angles fall into the range 170–173° (Table 2). In addition, these conventional H-bonds are supported by the softer C—H···O interactions formed by CH groups at the terminal phenyl ring and proximal oxygen atoms O1 and O2 and further by π···π stacking interactions between the unsubstituted cyclopentadienyl ring C(6–10) and phenyl ring in a molecule related by unit-cell translation along the *c*-axis (Fig. 3). Least-squares planes of the interacting aromatic rings make a dihedral angle of 6.22 (12)°, and the distance of their respective centroids is 3.7040 (14) Å.

### Experimental

(*R*)-2-[(Ferrocenylmethyl)amino]-3-phenylpropan-1-ol was prepared by an established two-step procedure (Hess *et al.*, 1999; Štěpnička *et al.* 2004 and 2008*b*) consisting of condensation of ferrocene carboxaldehyde with (*R*)-phenylalaninol and subsequent reduction of the intermediate Schiff base as follows.

Ferrocene carboxaldehyde (428 mg, 2.00 mmol) and (*R*)-2-amino-3-phenylpropan-1-ol (318 mg, 2.1 mmol) were dissolved in dry chloroform (20 ml). The resulting solution was refluxed under argon for 90 min and then evaporated under vacuum. The residue was immediately re-dissolved in dry methanol (20 ml) and the solution was cooled in ice. An amount of $NaBH_4$ (380 mg, 10 mmol) was added over 30 min causing the colour of the reaction mixture to change from initial orange red to orange yellow. After the addition, the reaction mixture was stirred at 0 °C for 1 h and at room temperature for 90 min before being quenched by addition of 10% aqueous NaOH and extracted with dichloromethane (2×20 ml). The combined organic extracts were washed with brine (2×20 ml) and dried over $MgSO_4$ overnight.

The drying agent was filtered off and the filtrate was evaporated under vacuum leaving a residue which was purified by column chromatography over silica gel. Elution with dichloromethane–methanol (10:1 *v*/*v*) led to the development of two yellow bands. The first one containing ferrocenylmethanol was discarded. The second one was collected and evaporated under vacuum to afford (*R*)-2-[(ferrocenylmethyl)amino]-3-phenylpropan-1-ol (371 mg, 53%) as an orange amorphous solid.

Characterization. $^1$H NMR ($CDCl_3$): δ 2.31 (br s, 2 H, NH and OH), 2.78 (dd, $^2J_{HH}$ = 13.7, $^3J_{HH}$ = 6.7 Hz, 1 H, $CH_2Ph$), 2.83 (dd, $^2J_{HH}$ = 13.7, $^3J_{HH}$ = 7.6 Hz, 1 H, $CH_2Ph$), 3.01 (m, 1 H, CHN), 3.38 (dd, $^2J_{HH}$ = 10.8, $^3J_{HH}$ = 4.7 Hz, 1 H, $CH_2O$), 3.42 and 3.53 (2×d, $^2J_{HH}$ = 12.9 Hz, 1 H, *AB* spin system of $FcCH_2$), 3.67 (dd, $^2J_{HH}$ = 10.8, $^3J_{HH}$ = 3.8 Hz, 1 H, $CH_2O$), 3.99 (s, 5 H, $C_5H_5$), 4.06 (m, 1 H, $C_5H_4$), 4.08 (virtual t, 2 H, $C_5H_4$), 4.14 (m, 1 H, $C_5H_4$), 7.18–7.34 (m, 5 H, Ph).

$^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 38.15 ($CH_2Ph$), 46.01 ($FcCH_2$), 59.65 (CHN), 62.29 ($CH_2O$), 67.66 (2 C), 67.77 and 67.89 (CH of $C_5H_4$); 68.34 ($C_5H_5$), 86.61 ($C_{ipso}$ of $C_5H_4$), 126.61 (1 C), 128.70 (2 C) and 129.18 (2 C) (3×CH of Ph); 138.44 ($C_{ipso}$ of Ph).

IR (neat): ν/cm$^{-1}$ 3296 br s, 3086 s, 3026 m, 2924 s, 2856 m, 1653 br m, 1603 w, 1495 s, 1454 very strong, 1412 m, 1352 m, 1329 m, 1232 m, 1105 very strong, 1041 very strong br, 1001 s, 818 br very strong, 746 very strong, 700 very strong, 484 very strong.

MS: *m*/*z* (relative abundance) 350 (9), 349 (38, $M^{+\cdot}$), 347 (3), 331 (3, $[M - H_2O]^{+\cdot}$), 266 (2), 200 (16), 199 (100, $[FcCH_2]^+$), 197 (6), 186 (2, $FcH^{+\cdot}$), 148 (3), 147 (3), 138 (2), 121 (28, $[C_5H_5Fe]^+$), 91 (11), 78 (4), 77 (3), 65 (4), 56 (11, $Fe^+$).

Few crystals of the title compound have been obtained upon attempted recrystallization of (*R*)-2-[(ferrocenylmethyl)amino]-3-phenylpropan-1-ol from ethyl acetate/hexane, resulting by a reaction of this compound with tiny amounts of (*E*)-but-2-enoic acid present in the commercial solvent (Lach-Ner).

## Refinement

N– and O-bonded H atoms were identified on the difference electron maps and isotropically refined as riding atoms. The remaining H-atoms were included in their calculated positions and refined as riding atoms with $U_{iso}$(H) assigned to a multiple of $U_{eq}$(C) of their bonding carbon atoms.

## Figures

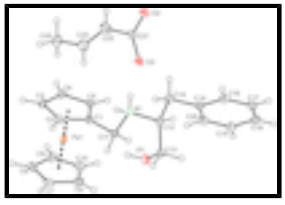

Fig. 1. View of the structure of the title compound showing displacement ellipsoids for non-H atoms at the 30% probability level.

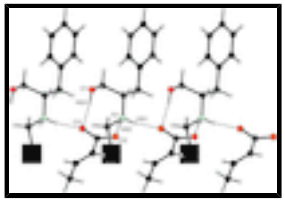

Fig. 2. Section of the infinite H-bonded chains in the crystal structure of the title compound. The bulky ferrocenyl moieties were replaced with filled squares for clarity.

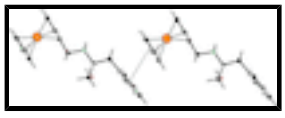

Fig. 3. π···π Stacking interactions of the aromatic rings in the structure of the title compound (indicated by a dotted line). The molecules depicted relate by unit-cell translation in the direction of the *c*-axis.

## (*R*)-*N*-(Ferrocenylmethyl)-1-hydroxy-3-phenylpropan-2-aminium (*E*)-but-2-enoate

*Crystal data*

| | |
|---|---|
| $[Fe(C_5H_5)(C_{15}H_{19}NO)](C_4H_5O_2)$ | $F(000) = 460$ |
| $M_r = 435.33$ | $D_x = 1.359$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 5.9730$ (2) Å | Cell parameters from 2535 reflections |
| $b = 15.3905$ (3) Å | $\theta = 1.0$–$27.5°$ |
| $c = 11.7713$ (4) Å | $\mu = 0.73$ mm$^{-1}$ |
| $\beta = 100.4986$ (13)° | $T = 150$ K |
| $V = 1063.99$ (6) Å$^3$ | Block, yellow |
| $Z = 2$ | 0.33 × 0.12 × 0.10 mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD diffractometer | 4511 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.043$ |
| horizontally mounted graphite crystal | $\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$ |
| Detector resolution: 9.091 pixels mm$^{-1}$ | $h = -7 \rightarrow 7$ |
| ω and φ scans to fill the Ewald sphere | $k = -19 \rightarrow 20$ |
| 15916 measured reflections | $l = -15 \rightarrow 15$ |
| 4864 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | H-atom parameters constrained |
| $wR(F^2) = 0.067$ | $w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 0.4582P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 4864 reflections | $\Delta\rho_{max} = 0.36$ e Å$^{-3}$ |
| 265 parameters | $\Delta\rho_{min} = -0.27$ e Å$^{-3}$ |
| 1 restraint | Absolute structure: Flack (1983), 2329 Friedel pairs |
| 0 constraints | Flack parameter: −0.016 (12) |
| Primary atom site location: structure-invariant direct methods | |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe1 | 0.34726 (4) | 0.852498 (19) | 1.26047 (2) | 0.01975 (7) |
| N1 | 0.2364 (3) | 0.79109 (11) | 0.88685 (13) | 0.0188 (3) |
| H91 | 0.1215 | 0.8326 | 0.8611 | 0.025 (6)* |
| H92 | 0.3616 | 0.8129 | 0.8869 | 0.045 (8)* |
| O1 | −0.2057 (3) | 0.69386 (11) | 0.78892 (14) | 0.0335 (4) |
| H93 | −0.2303 | 0.7427 | 0.8211 | 0.034 (7)* |
| O2 | 0.9374 (3) | 0.91779 (11) | 0.81113 (14) | 0.0316 (4) |
| O3 | 0.6734 (2) | 0.84425 (12) | 0.88161 (12) | 0.0279 (3) |
| C1 | 0.3185 (3) | 0.84770 (18) | 1.08632 (14) | 0.0202 (3) |
| C2 | 0.1952 (4) | 0.92054 (14) | 1.11836 (18) | 0.0235 (4) |
| H2 | 0.0400 | 0.9306 | 1.0956 | 0.028* |
| C3 | 0.3518 (4) | 0.97480 (13) | 1.19111 (18) | 0.0260 (5) |
| H3 | 0.3165 | 1.0267 | 1.2243 | 0.031* |
| C4 | 0.5715 (4) | 0.93652 (14) | 1.20475 (18) | 0.0243 (4) |
| H4 | 0.7044 | 0.9587 | 1.2487 | 0.029* |
| C5 | 0.5524 (3) | 0.85864 (18) | 1.13951 (15) | 0.0209 (4) |
| H5 | 0.6712 | 0.8211 | 1.1324 | 0.025* |
| C6 | 0.2180 (4) | 0.73848 (15) | 1.30972 (19) | 0.0322 (5) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.1563 | 0.6940 | 1.2603 | 0.039* |
| C7 | 0.0964 (4) | 0.80938 (16) | 1.3456 (2) | 0.0319 (5) |
| H7 | −0.0592 | 0.8194 | 1.3245 | 0.038* |
| C8 | 0.2551 (4) | 0.86256 (18) | 1.41971 (17) | 0.0302 (5) |
| H8 | 0.2219 | 0.9138 | 1.4551 | 0.036* |
| C9 | 0.4725 (4) | 0.82358 (14) | 1.42989 (18) | 0.0297 (5) |
| H9 | 0.6072 | 0.8445 | 1.4736 | 0.036* |
| C10 | 0.4491 (4) | 0.74712 (15) | 1.36194 (19) | 0.0301 (5) |
| H10 | 0.5659 | 0.7091 | 1.3532 | 0.036* |
| C11 | 0.2253 (4) | 0.77346 (13) | 1.01152 (17) | 0.0220 (4) |
| H11A | 0.0684 | 0.7634 | 1.0190 | 0.026* |
| H11B | 0.3118 | 0.7214 | 1.0368 | 0.026* |
| C12 | 0.2090 (4) | 0.71216 (13) | 0.80983 (17) | 0.0211 (4) |
| H12 | 0.3477 | 0.6771 | 0.8297 | 0.025* |
| C13 | 0.0092 (4) | 0.65595 (13) | 0.82677 (19) | 0.0242 (4) |
| H13A | 0.0162 | 0.6017 | 0.7857 | 0.029* |
| H13B | 0.0245 | 0.6423 | 0.9083 | 0.029* |
| C14 | 0.1931 (4) | 0.74385 (14) | 0.68492 (18) | 0.0255 (4) |
| H14A | 0.0653 | 0.7834 | 0.6659 | 0.031* |
| H14B | 0.3305 | 0.7756 | 0.6785 | 0.031* |
| C15 | 0.1632 (4) | 0.66929 (13) | 0.59961 (17) | 0.0220 (4) |
| C16 | 0.3474 (4) | 0.61840 (14) | 0.58549 (18) | 0.0261 (5) |
| H16 | 0.4909 | 0.6307 | 0.6280 | 0.031* |
| C17 | 0.3201 (4) | 0.54932 (15) | 0.5087 (2) | 0.0307 (5) |
| H17 | 0.4447 | 0.5151 | 0.5009 | 0.037* |
| C18 | 0.1077 (5) | 0.53108 (15) | 0.4434 (2) | 0.0304 (5) |
| H18 | 0.0896 | 0.4851 | 0.3912 | 0.037* |
| C19 | −0.0769 (4) | 0.58170 (15) | 0.45646 (19) | 0.0294 (5) |
| H19 | −0.2199 | 0.5700 | 0.4129 | 0.035* |
| C20 | −0.0487 (4) | 0.65025 (15) | 0.53490 (19) | 0.0258 (5) |
| H20 | −0.1739 | 0.6837 | 0.5440 | 0.031* |
| C21 | 0.7467 (4) | 0.91227 (15) | 0.83988 (18) | 0.0259 (4) |
| C22 | 0.6023 (5) | 0.99310 (18) | 0.8262 (2) | 0.0466 (7) |
| H22 | 0.6189 | 1.0309 | 0.7667 | 0.056* |
| C23 | 0.4576 (5) | 1.01401 (17) | 0.8904 (2) | 0.0474 (7) |
| H23 | 0.4445 | 0.9754 | 0.9496 | 0.057* |
| C24 | 0.3080 (5) | 1.09256 (16) | 0.8816 (3) | 0.0422 (6) |
| H24A | 0.3545 | 1.1333 | 0.8287 | 0.063* |
| H24B | 0.3207 | 1.1190 | 0.9563 | 0.063* |
| H24C | 0.1528 | 1.0757 | 0.8541 | 0.063* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.02130 (13) | 0.02038 (12) | 0.01725 (12) | 0.00067 (14) | 0.00270 (9) | 0.00026 (14) |
| N1 | 0.0175 (9) | 0.0220 (8) | 0.0167 (8) | −0.0016 (7) | 0.0030 (6) | −0.0008 (6) |
| O1 | 0.0226 (8) | 0.0361 (9) | 0.0408 (9) | −0.0039 (7) | 0.0033 (7) | −0.0117 (7) |
| O2 | 0.0224 (8) | 0.0355 (9) | 0.0386 (9) | 0.0020 (7) | 0.0104 (7) | 0.0121 (7) |

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|---|---|---|---|---|---|---|
| O3 | 0.0221 (7) | 0.0293 (8) | 0.0337 (7) | 0.0016 (8) | 0.0089 (5) | 0.0043 (8) |
| C1 | 0.0221 (8) | 0.0229 (9) | 0.0153 (7) | 0.0016 (11) | 0.0027 (6) | 0.0010 (10) |
| C2 | 0.0229 (11) | 0.0263 (10) | 0.0206 (10) | 0.0053 (8) | 0.0020 (8) | 0.0042 (8) |
| C3 | 0.0335 (12) | 0.0196 (10) | 0.0245 (11) | 0.0028 (9) | 0.0042 (9) | 0.0014 (8) |
| C4 | 0.0244 (11) | 0.0250 (11) | 0.0235 (10) | −0.0048 (8) | 0.0041 (8) | −0.0013 (8) |
| C5 | 0.0202 (9) | 0.0226 (9) | 0.0204 (8) | 0.0010 (10) | 0.0046 (7) | 0.0029 (10) |
| C6 | 0.0433 (14) | 0.0284 (11) | 0.0238 (11) | −0.0115 (10) | 0.0031 (10) | 0.0039 (9) |
| C7 | 0.0259 (12) | 0.0436 (13) | 0.0277 (12) | −0.0029 (10) | 0.0086 (9) | 0.0068 (10) |
| C8 | 0.0413 (12) | 0.0327 (13) | 0.0195 (9) | 0.0010 (11) | 0.0131 (8) | 0.0008 (10) |
| C9 | 0.0325 (12) | 0.0380 (13) | 0.0171 (10) | −0.0031 (9) | 0.0005 (9) | 0.0027 (8) |
| C10 | 0.0389 (13) | 0.0278 (11) | 0.0228 (11) | 0.0075 (10) | 0.0038 (9) | 0.0069 (9) |
| C11 | 0.0266 (11) | 0.0232 (10) | 0.0162 (9) | −0.0033 (8) | 0.0039 (8) | 0.0018 (8) |
| C12 | 0.0226 (10) | 0.0219 (10) | 0.0187 (10) | −0.0024 (8) | 0.0037 (8) | −0.0022 (8) |
| C13 | 0.0233 (11) | 0.0255 (11) | 0.0241 (10) | −0.0038 (8) | 0.0051 (8) | −0.0030 (8) |
| C14 | 0.0299 (12) | 0.0243 (10) | 0.0217 (10) | −0.0019 (9) | 0.0033 (9) | 0.0004 (8) |
| C15 | 0.0273 (11) | 0.0240 (10) | 0.0147 (9) | −0.0031 (9) | 0.0034 (8) | 0.0020 (8) |
| C16 | 0.0236 (11) | 0.0298 (11) | 0.0242 (11) | 0.0000 (9) | 0.0023 (9) | 0.0044 (9) |
| C17 | 0.0309 (13) | 0.0296 (12) | 0.0337 (12) | 0.0046 (9) | 0.0114 (10) | 0.0034 (10) |
| C18 | 0.0430 (16) | 0.0248 (12) | 0.0244 (11) | −0.0063 (10) | 0.0085 (10) | −0.0012 (9) |
| C19 | 0.0292 (13) | 0.0349 (12) | 0.0228 (11) | −0.0055 (10) | 0.0013 (9) | 0.0005 (9) |
| C20 | 0.0246 (12) | 0.0304 (12) | 0.0216 (11) | 0.0020 (10) | 0.0026 (9) | 0.0014 (9) |
| C21 | 0.0241 (11) | 0.0303 (11) | 0.0234 (10) | 0.0041 (9) | 0.0043 (9) | 0.0058 (9) |
| C22 | 0.0508 (17) | 0.0441 (15) | 0.0521 (16) | 0.0222 (13) | 0.0286 (13) | 0.0257 (13) |
| C23 | 0.064 (2) | 0.0370 (14) | 0.0464 (16) | 0.0139 (13) | 0.0238 (14) | 0.0131 (12) |
| C24 | 0.0431 (16) | 0.0321 (13) | 0.0530 (16) | 0.0061 (11) | 0.0133 (13) | 0.0033 (12) |

*Geometric parameters (Å, °)*

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| Fe1—C1 | 2.0271 (17) | C9—H9 | 0.9300 |
| Fe1—C10 | 2.040 (2) | C10—H10 | 0.9300 |
| Fe1—C2 | 2.041 (2) | C11—H11A | 0.9700 |
| Fe1—C5 | 2.0430 (18) | C11—H11B | 0.9700 |
| Fe1—C6 | 2.043 (2) | C12—C13 | 1.516 (3) |
| Fe1—C9 | 2.047 (2) | C12—C14 | 1.536 (3) |
| Fe1—C8 | 2.0533 (19) | C12—H12 | 0.9800 |
| Fe1—C4 | 2.053 (2) | C13—H13A | 0.9700 |
| Fe1—C3 | 2.054 (2) | C13—H13B | 0.9700 |
| Fe1—C7 | 2.059 (2) | C14—C15 | 1.514 (3) |
| N1—C11 | 1.506 (2) | C14—H14A | 0.9700 |
| N1—C12 | 1.507 (2) | C14—H14B | 0.9700 |
| N1—H91 | 0.9454 | C15—C16 | 1.385 (3) |
| N1—H92 | 0.8195 | C15—C20 | 1.385 (3) |
| O1—C13 | 1.407 (3) | C16—C17 | 1.386 (3) |
| O1—H93 | 0.8666 | C16—H16 | 0.9300 |
| C1—C2 | 1.429 (3) | C17—C18 | 1.387 (4) |
| C1—C5 | 1.433 (3) | C17—H17 | 0.9300 |
| C1—C11 | 1.487 (3) | C18—C19 | 1.381 (3) |
| C2—C3 | 1.419 (3) | C18—H18 | 0.9300 |
| C2—H2 | 0.9300 | C19—C20 | 1.392 (3) |

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|---|---|---|---|
| C3—C4 | 1.420 (3) | C19—H19 | 0.9300 |
| C3—H3 | 0.9300 | C20—H20 | 0.9300 |
| C4—C5 | 1.417 (3) | O2—C21 | 1.249 (3) |
| C4—H4 | 0.9300 | O3—C21 | 1.268 (3) |
| C5—H5 | 0.9300 | C21—C22 | 1.505 (3) |
| C6—C10 | 1.411 (3) | C22—C23 | 1.288 (4) |
| C6—C7 | 1.417 (3) | C22—H22 | 0.9300 |
| C6—H6 | 0.9300 | C23—C24 | 1.496 (3) |
| C7—C8 | 1.424 (3) | C23—H23 | 0.9300 |
| C7—H7 | 0.9300 | C24—H24A | 0.9600 |
| C8—C9 | 1.415 (3) | C24—H24B | 0.9600 |
| C8—H8 | 0.9300 | C24—H24C | 0.9600 |
| C9—C10 | 1.415 (3) | | |
| C1—Fe1—C10 | 121.63 (10) | C10—C6—H6 | 125.9 |
| C1—Fe1—C2 | 41.13 (9) | C7—C6—H6 | 125.9 |
| C10—Fe1—C2 | 158.18 (9) | Fe1—C6—H6 | 125.6 |
| C1—Fe1—C5 | 41.24 (7) | C6—C7—C8 | 107.7 (2) |
| C10—Fe1—C5 | 106.98 (10) | C6—C7—Fe1 | 69.19 (13) |
| C2—Fe1—C5 | 68.83 (8) | C8—C7—Fe1 | 69.54 (12) |
| C1—Fe1—C6 | 106.79 (10) | C6—C7—H7 | 126.1 |
| C10—Fe1—C6 | 40.44 (10) | C8—C7—H7 | 126.1 |
| C2—Fe1—C6 | 122.59 (9) | Fe1—C7—H7 | 126.7 |
| C5—Fe1—C6 | 122.90 (10) | C9—C8—C7 | 107.8 (2) |
| C1—Fe1—C9 | 157.79 (9) | C9—C8—Fe1 | 69.58 (12) |
| C10—Fe1—C9 | 40.52 (9) | C7—C8—Fe1 | 69.93 (12) |
| C2—Fe1—C9 | 159.87 (9) | C9—C8—H8 | 126.1 |
| C5—Fe1—C9 | 121.99 (9) | C7—C8—H8 | 126.1 |
| C6—Fe1—C9 | 68.08 (9) | Fe1—C8—H8 | 126.0 |
| C1—Fe1—C8 | 159.80 (8) | C8—C9—C10 | 108.1 (2) |
| C10—Fe1—C8 | 68.07 (10) | C8—C9—Fe1 | 70.04 (12) |
| C2—Fe1—C8 | 123.80 (9) | C10—C9—Fe1 | 69.47 (12) |
| C5—Fe1—C8 | 158.01 (9) | C8—C9—H9 | 126.0 |
| C6—Fe1—C8 | 68.15 (10) | C10—C9—H9 | 126.0 |
| C9—Fe1—C8 | 40.38 (9) | Fe1—C9—H9 | 126.1 |
| C1—Fe1—C4 | 68.90 (9) | C6—C10—C9 | 108.2 (2) |
| C10—Fe1—C4 | 123.05 (10) | C6—C10—Fe1 | 69.89 (12) |
| C2—Fe1—C4 | 68.52 (9) | C9—C10—Fe1 | 70.01 (12) |
| C5—Fe1—C4 | 40.47 (10) | C6—C10—H10 | 125.9 |
| C6—Fe1—C4 | 159.02 (9) | C9—C10—H10 | 125.9 |
| C9—Fe1—C4 | 107.71 (9) | Fe1—C10—H10 | 125.8 |
| C8—Fe1—C4 | 122.89 (10) | C1—C11—N1 | 111.13 (16) |
| C1—Fe1—C3 | 68.67 (10) | C1—C11—H11A | 109.4 |
| C10—Fe1—C3 | 159.57 (9) | N1—C11—H11A | 109.4 |
| C2—Fe1—C3 | 40.55 (9) | C1—C11—H11B | 109.4 |
| C5—Fe1—C3 | 68.13 (10) | N1—C11—H11B | 109.4 |
| C6—Fe1—C3 | 158.90 (9) | H11A—C11—H11B | 108.0 |
| C9—Fe1—C3 | 123.88 (9) | N1—C12—C13 | 112.49 (16) |
| C8—Fe1—C3 | 108.60 (10) | N1—C12—C14 | 107.53 (15) |
| C4—Fe1—C3 | 40.47 (9) | C13—C12—C14 | 113.21 (17) |

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| C1—Fe1—C7 | 123.06 (9) | N1—C12—H12 | 107.8 |
| C10—Fe1—C7 | 67.96 (10) | C13—C12—H12 | 107.8 |
| C2—Fe1—C7 | 108.04 (10) | C14—C12—H12 | 107.8 |
| C5—Fe1—C7 | 159.48 (9) | O1—C13—C12 | 114.61 (17) |
| C6—Fe1—C7 | 40.43 (10) | O1—C13—H13A | 108.6 |
| C9—Fe1—C7 | 67.97 (9) | C12—C13—H13A | 108.6 |
| C8—Fe1—C7 | 40.53 (10) | O1—C13—H13B | 108.6 |
| C4—Fe1—C7 | 158.99 (9) | C12—C13—H13B | 108.6 |
| C3—Fe1—C7 | 123.54 (10) | H13A—C13—H13B | 107.6 |
| C11—N1—C12 | 114.96 (15) | C12—C14—C15 | 111.95 (17) |
| C11—N1—H91 | 106.0 | C15—C14—H14A | 109.2 |
| C12—N1—H91 | 111.0 | C12—C14—H14A | 109.2 |
| C11—N1—H92 | 105.9 | C15—C14—H14B | 109.2 |
| C12—N1—H92 | 109.2 | C12—C14—H14B | 109.2 |
| H91—N1—H92 | 109.5 | H14A—C14—H14B | 107.9 |
| C13—O1—H93 | 116.1 | C16—C15—C20 | 118.7 (2) |
| C2—C1—C5 | 107.5 (2) | C16—C15—C14 | 120.54 (19) |
| C2—C1—C11 | 127.15 (18) | C20—C15—C14 | 120.7 (2) |
| C5—C1—C11 | 125.4 (2) | C15—C16—C17 | 120.7 (2) |
| C2—C1—Fe1 | 69.96 (11) | C15—C16—H16 | 119.6 |
| C5—C1—Fe1 | 69.98 (9) | C17—C16—H16 | 119.6 |
| C11—C1—Fe1 | 125.48 (16) | C16—C17—C18 | 120.2 (2) |
| C3—C2—C1 | 107.84 (18) | C16—C17—H17 | 119.9 |
| C3—C2—Fe1 | 70.21 (12) | C18—C17—H17 | 119.9 |
| C1—C2—Fe1 | 68.91 (11) | C19—C18—C17 | 119.5 (2) |
| C3—C2—H2 | 126.1 | C19—C18—H18 | 120.3 |
| C1—C2—H2 | 126.1 | C17—C18—H18 | 120.3 |
| Fe1—C2—H2 | 126.4 | C18—C19—C20 | 119.9 (2) |
| C2—C3—C4 | 108.53 (18) | C18—C19—H19 | 120.0 |
| C2—C3—Fe1 | 69.24 (12) | C20—C19—H19 | 120.0 |
| C4—C3—Fe1 | 69.75 (12) | C15—C20—C19 | 120.9 (2) |
| C2—C3—H3 | 125.7 | C15—C20—H20 | 119.6 |
| C4—C3—H3 | 125.7 | C19—C20—H20 | 119.6 |
| Fe1—C3—H3 | 126.9 | O2—C21—O3 | 123.9 (2) |
| C5—C4—C3 | 107.96 (19) | O2—C21—C22 | 116.6 (2) |
| C5—C4—Fe1 | 69.37 (12) | O3—C21—C22 | 119.5 (2) |
| C3—C4—Fe1 | 69.79 (12) | C23—C22—C21 | 125.2 (2) |
| C5—C4—H4 | 126.0 | C23—C22—H22 | 117.4 |
| C3—C4—H4 | 126.0 | C21—C22—H22 | 117.4 |
| Fe1—C4—H4 | 126.4 | C22—C23—C24 | 128.1 (3) |
| C4—C5—C1 | 108.2 (2) | C22—C23—H23 | 115.9 |
| C4—C5—Fe1 | 70.16 (11) | C24—C23—H23 | 115.9 |
| C1—C5—Fe1 | 68.79 (10) | C23—C24—H24A | 109.5 |
| C4—C5—H5 | 125.9 | C23—C24—H24B | 109.5 |
| C1—C5—H5 | 125.9 | H24A—C24—H24B | 109.5 |
| Fe1—C5—H5 | 126.7 | C23—C24—H24C | 109.5 |
| C10—C6—C7 | 108.2 (2) | H24A—C24—H24C | 109.5 |
| C10—C6—Fe1 | 69.67 (13) | H24B—C24—H24C | 109.5 |
| C7—C6—Fe1 | 70.37 (13) | | |

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| C10—Fe1—C1—C2 | 162.25 (13) | C4—Fe1—C6—C10 | 44.6 (3) |
| C5—Fe1—C1—C2 | −118.3 (2) | C3—Fe1—C6—C10 | −166.5 (2) |
| C6—Fe1—C1—C2 | 120.65 (14) | C7—Fe1—C6—C10 | −119.01 (19) |
| C9—Fe1—C1—C2 | −166.4 (2) | C1—Fe1—C6—C7 | −121.63 (14) |
| C8—Fe1—C1—C2 | 48.5 (4) | C10—Fe1—C6—C7 | 119.01 (19) |
| C4—Fe1—C1—C2 | −81.09 (14) | C2—Fe1—C6—C7 | −79.43 (15) |
| C3—Fe1—C1—C2 | −37.53 (13) | C5—Fe1—C6—C7 | −163.87 (13) |
| C7—Fe1—C1—C2 | 79.43 (17) | C9—Fe1—C6—C7 | 81.30 (15) |
| C10—Fe1—C1—C5 | −79.49 (18) | C8—Fe1—C6—C7 | 37.63 (13) |
| C2—Fe1—C1—C5 | 118.3 (2) | C4—Fe1—C6—C7 | 163.6 (2) |
| C6—Fe1—C1—C5 | −121.09 (16) | C3—Fe1—C6—C7 | −47.5 (3) |
| C9—Fe1—C1—C5 | −48.1 (3) | C10—C6—C7—C8 | 0.6 (2) |
| C8—Fe1—C1—C5 | 166.7 (3) | Fe1—C6—C7—C8 | −59.06 (16) |
| C4—Fe1—C1—C5 | 37.17 (15) | C10—C6—C7—Fe1 | 59.66 (15) |
| C3—Fe1—C1—C5 | 80.73 (16) | C1—Fe1—C7—C6 | 76.56 (17) |
| C7—Fe1—C1—C5 | −162.31 (14) | C10—Fe1—C7—C6 | −37.74 (14) |
| C10—Fe1—C1—C11 | 40.3 (2) | C2—Fe1—C7—C6 | 119.41 (14) |
| C2—Fe1—C1—C11 | −122.0 (2) | C5—Fe1—C7—C6 | 41.7 (3) |
| C5—Fe1—C1—C11 | 119.8 (3) | C9—Fe1—C7—C6 | −81.61 (14) |
| C6—Fe1—C1—C11 | −1.3 (2) | C8—Fe1—C7—C6 | −119.3 (2) |
| C9—Fe1—C1—C11 | 71.7 (3) | C4—Fe1—C7—C6 | −163.7 (2) |
| C8—Fe1—C1—C11 | −73.5 (4) | C3—Fe1—C7—C6 | 161.43 (13) |
| C4—Fe1—C1—C11 | 156.9 (2) | C1—Fe1—C7—C8 | −164.13 (15) |
| C3—Fe1—C1—C11 | −159.50 (19) | C10—Fe1—C7—C8 | 81.57 (16) |
| C7—Fe1—C1—C11 | −42.5 (2) | C2—Fe1—C7—C8 | −121.28 (15) |
| C5—C1—C2—C3 | −0.5 (2) | C5—Fe1—C7—C8 | 161.0 (2) |
| C11—C1—C2—C3 | 179.57 (19) | C6—Fe1—C7—C8 | 119.3 (2) |
| Fe1—C1—C2—C3 | 59.65 (15) | C9—Fe1—C7—C8 | 37.70 (14) |
| C5—C1—C2—Fe1 | −60.19 (13) | C4—Fe1—C7—C8 | −44.4 (3) |
| C11—C1—C2—Fe1 | 119.9 (2) | C3—Fe1—C7—C8 | −79.26 (17) |
| C1—Fe1—C2—C3 | −119.19 (18) | C6—C7—C8—C9 | −0.6 (2) |
| C10—Fe1—C2—C3 | −163.5 (2) | Fe1—C7—C8—C9 | −59.48 (14) |
| C5—Fe1—C2—C3 | −80.69 (14) | C6—C7—C8—Fe1 | 58.85 (15) |
| C6—Fe1—C2—C3 | 162.97 (13) | C1—Fe1—C8—C9 | 160.5 (3) |
| C9—Fe1—C2—C3 | 45.8 (3) | C10—Fe1—C8—C9 | 37.68 (14) |
| C8—Fe1—C2—C3 | 78.92 (16) | C2—Fe1—C8—C9 | −163.12 (13) |
| C4—Fe1—C2—C3 | −37.10 (13) | C5—Fe1—C8—C9 | −43.3 (4) |
| C7—Fe1—C2—C3 | 120.86 (14) | C6—Fe1—C8—C9 | 81.42 (15) |
| C10—Fe1—C2—C1 | −44.3 (3) | C4—Fe1—C8—C9 | −78.40 (17) |
| C5—Fe1—C2—C1 | 38.51 (13) | C3—Fe1—C8—C9 | −120.82 (14) |
| C6—Fe1—C2—C1 | −77.83 (15) | C7—Fe1—C8—C9 | 119.0 (2) |
| C9—Fe1—C2—C1 | 165.0 (2) | C1—Fe1—C8—C7 | 41.6 (4) |
| C8—Fe1—C2—C1 | −161.88 (13) | C10—Fe1—C8—C7 | −81.28 (16) |
| C4—Fe1—C2—C1 | 82.10 (13) | C2—Fe1—C8—C7 | 77.92 (18) |
| C3—Fe1—C2—C1 | 119.19 (18) | C5—Fe1—C8—C7 | −162.3 (3) |
| C7—Fe1—C2—C1 | −119.94 (13) | C6—Fe1—C8—C7 | −37.54 (15) |
| C1—C2—C3—C4 | 0.0 (2) | C9—Fe1—C8—C7 | −119.0 (2) |
| Fe1—C2—C3—C4 | 58.83 (15) | C4—Fe1—C8—C7 | 162.64 (14) |
| C1—C2—C3—Fe1 | −58.83 (14) | C3—Fe1—C8—C7 | 120.22 (15) |

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| C1—Fe1—C3—C2 | 38.06 (12) | C7—C8—C9—C10 | 0.4 (2) |
| C10—Fe1—C3—C2 | 162.4 (2) | Fe1—C8—C9—C10 | −59.28 (15) |
| C5—Fe1—C3—C2 | 82.56 (13) | C7—C8—C9—Fe1 | 59.70 (15) |
| C6—Fe1—C3—C2 | −43.3 (3) | C1—Fe1—C9—C8 | −162.3 (2) |
| C9—Fe1—C3—C2 | −162.72 (13) | C10—Fe1—C9—C8 | −119.2 (2) |
| C8—Fe1—C3—C2 | −120.63 (13) | C2—Fe1—C9—C8 | 44.5 (3) |
| C4—Fe1—C3—C2 | 120.14 (18) | C5—Fe1—C9—C8 | 162.37 (16) |
| C7—Fe1—C3—C2 | −78.28 (15) | C6—Fe1—C9—C8 | −81.59 (16) |
| C1—Fe1—C3—C4 | −82.08 (13) | C4—Fe1—C9—C8 | 120.28 (15) |
| C10—Fe1—C3—C4 | 42.3 (3) | C3—Fe1—C9—C8 | 78.66 (17) |
| C2—Fe1—C3—C4 | −120.14 (18) | C7—Fe1—C9—C8 | −37.84 (15) |
| C5—Fe1—C3—C4 | −37.58 (12) | C1—Fe1—C9—C10 | −43.1 (3) |
| C6—Fe1—C3—C4 | −163.4 (2) | C2—Fe1—C9—C10 | 163.7 (2) |
| C9—Fe1—C3—C4 | 77.14 (15) | C5—Fe1—C9—C10 | −78.40 (16) |
| C8—Fe1—C3—C4 | 119.22 (13) | C6—Fe1—C9—C10 | 37.63 (14) |
| C7—Fe1—C3—C4 | 161.58 (13) | C8—Fe1—C9—C10 | 119.2 (2) |
| C2—C3—C4—C5 | 0.5 (2) | C4—Fe1—C9—C10 | −120.49 (14) |
| Fe1—C3—C4—C5 | 59.07 (15) | C3—Fe1—C9—C10 | −162.11 (14) |
| C2—C3—C4—Fe1 | −58.52 (15) | C7—Fe1—C9—C10 | 81.39 (15) |
| C1—Fe1—C4—C5 | −37.85 (13) | C7—C6—C10—C9 | −0.3 (2) |
| C10—Fe1—C4—C5 | 76.95 (15) | Fe1—C6—C10—C9 | 59.76 (15) |
| C2—Fe1—C4—C5 | −82.15 (13) | C7—C6—C10—Fe1 | −60.10 (15) |
| C6—Fe1—C4—C5 | 44.0 (3) | C8—C9—C10—C6 | −0.1 (2) |
| C9—Fe1—C4—C5 | 118.85 (13) | Fe1—C9—C10—C6 | −59.68 (15) |
| C8—Fe1—C4—C5 | 160.63 (13) | C8—C9—C10—Fe1 | 59.63 (15) |
| C3—Fe1—C4—C5 | −119.32 (18) | C1—Fe1—C10—C6 | −78.49 (15) |
| C7—Fe1—C4—C5 | −166.6 (2) | C2—Fe1—C10—C6 | −45.8 (3) |
| C1—Fe1—C4—C3 | 81.46 (14) | C5—Fe1—C10—C6 | −121.15 (14) |
| C10—Fe1—C4—C3 | −163.74 (12) | C9—Fe1—C10—C6 | 119.15 (19) |
| C2—Fe1—C4—C3 | 37.17 (12) | C8—Fe1—C10—C6 | 81.60 (15) |
| C5—Fe1—C4—C3 | 119.32 (18) | C4—Fe1—C10—C6 | −162.53 (13) |
| C6—Fe1—C4—C3 | 163.3 (2) | C3—Fe1—C10—C6 | 166.1 (2) |
| C9—Fe1—C4—C3 | −121.83 (13) | C7—Fe1—C10—C6 | 37.73 (14) |
| C8—Fe1—C4—C3 | −80.05 (15) | C1—Fe1—C10—C9 | 162.36 (13) |
| C7—Fe1—C4—C3 | −47.3 (3) | C2—Fe1—C10—C9 | −165.0 (2) |
| C3—C4—C5—C1 | −0.9 (2) | C5—Fe1—C10—C9 | 119.70 (14) |
| Fe1—C4—C5—C1 | 58.45 (14) | C6—Fe1—C10—C9 | −119.15 (19) |
| C3—C4—C5—Fe1 | −59.33 (15) | C8—Fe1—C10—C9 | −37.56 (14) |
| C2—C1—C5—C4 | 0.9 (2) | C4—Fe1—C10—C9 | 78.31 (16) |
| C11—C1—C5—C4 | −179.22 (19) | C3—Fe1—C10—C9 | 46.9 (3) |
| Fe1—C1—C5—C4 | −59.30 (14) | C7—Fe1—C10—C9 | −81.43 (15) |
| C2—C1—C5—Fe1 | 60.18 (13) | C2—C1—C11—N1 | 91.1 (2) |
| C11—C1—C5—Fe1 | −119.9 (2) | C5—C1—C11—N1 | −88.8 (2) |
| C1—Fe1—C5—C4 | 119.7 (2) | Fe1—C1—C11—N1 | −178.21 (13) |
| C10—Fe1—C5—C4 | −121.38 (14) | C12—N1—C11—C1 | 163.62 (17) |
| C2—Fe1—C5—C4 | 81.30 (14) | C11—N1—C12—C13 | 47.3 (2) |
| C6—Fe1—C5—C4 | −162.76 (13) | C11—N1—C12—C14 | 172.66 (17) |
| C9—Fe1—C5—C4 | −79.66 (16) | N1—C12—C13—O1 | 68.3 (2) |
| C8—Fe1—C5—C4 | −48.1 (3) | C14—C12—C13—O1 | −53.8 (2) |

| | | | |
|---|---|---|---|
| C3—Fe1—C5—C4 | 37.57 (13) | N1—C12—C14—C15 | −179.54 (17) |
| C7—Fe1—C5—C4 | 166.3 (2) | C13—C12—C14—C15 | −54.7 (2) |
| C10—Fe1—C5—C1 | 118.91 (16) | C12—C14—C15—C16 | −78.0 (2) |
| C2—Fe1—C5—C1 | −38.41 (15) | C12—C14—C15—C20 | 101.5 (2) |
| C6—Fe1—C5—C1 | 77.52 (17) | C20—C15—C16—C17 | −0.4 (3) |
| C9—Fe1—C5—C1 | 160.63 (15) | C14—C15—C16—C17 | 179.08 (19) |
| C8—Fe1—C5—C1 | −167.8 (3) | C15—C16—C17—C18 | 1.0 (3) |
| C4—Fe1—C5—C1 | −119.7 (2) | C16—C17—C18—C19 | −0.7 (3) |
| C3—Fe1—C5—C1 | −82.14 (16) | C17—C18—C19—C20 | −0.1 (4) |
| C7—Fe1—C5—C1 | 46.6 (3) | C16—C15—C20—C19 | −0.4 (3) |
| C1—Fe1—C6—C10 | 119.37 (13) | C14—C15—C20—C19 | −179.93 (19) |
| C2—Fe1—C6—C10 | 161.56 (13) | C18—C19—C20—C15 | 0.7 (4) |
| C5—Fe1—C6—C10 | 77.12 (15) | O2—C21—C22—C23 | −149.0 (3) |
| C9—Fe1—C6—C10 | −37.71 (13) | O3—C21—C22—C23 | 29.3 (4) |
| C8—Fe1—C6—C10 | −81.38 (14) | C21—C22—C23—C24 | −179.6 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H91···O2$^{i}$ | 0.95 | 1.74 | 2.685 (2) | 173 |
| N1—H92···O3 | 0.82 | 1.94 | 2.747 (2) | 170 |
| O1—H93···O3$^{i}$ | 0.87 | 1.85 | 2.712 (2) | 172 |
| C16—H16···O1$^{ii}$ | 0.93 | 2.56 | 3.447 (3) | 159 |
| C18—H18···O2$^{iii}$ | 0.93 | 2.58 | 3.435 (3) | 154 |

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) −*x*+1, *y*−1/2, −*z*+1.

**Fig. 1**

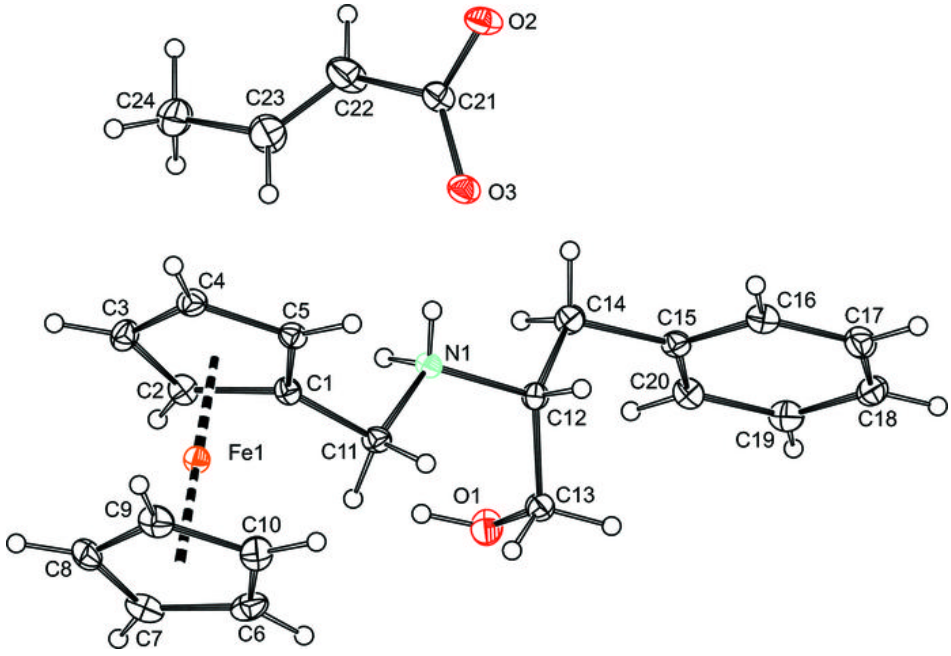
O2
C24
C23
C22
C21
O3
C4
C3
C5
N1
C14
C15
C16
C17
C2
C1
C12
C20
C18
C19
Fe1
C11
O1
C13
C9
C10
C8
C7
C6

**Fig. 2**

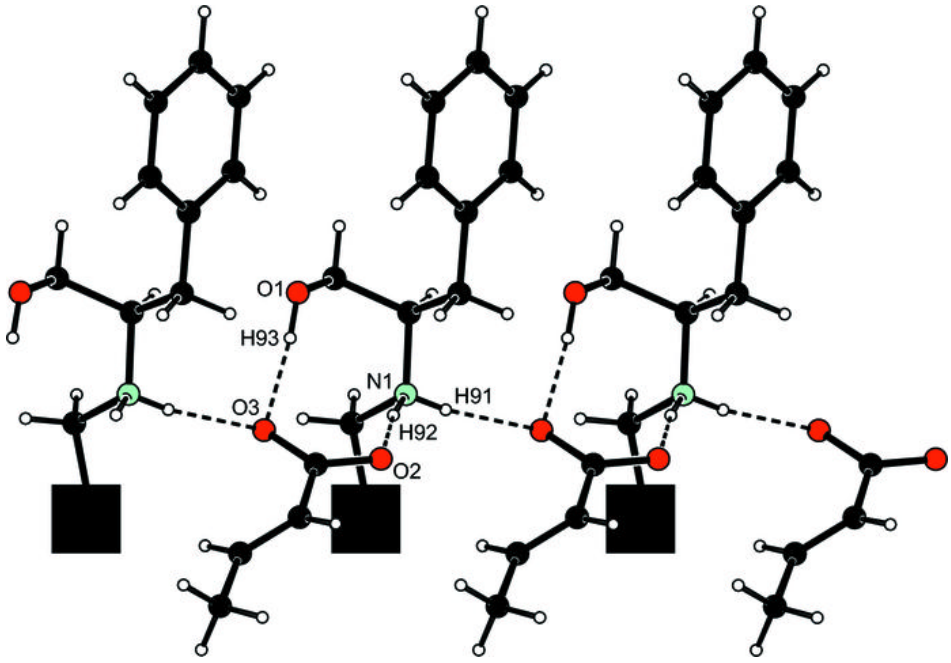

**Fig. 3**