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(*N*-Ferrocenylmethyl)dimethylammonium nitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.067
wR factor = 0.163
Data-to-parameter ratio = 13.9

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

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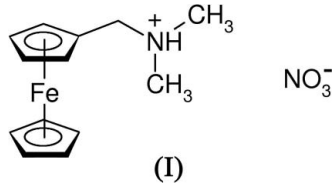
The cation of the title compound, $[Fe(C_5H_5)(C_8H_{13}N)]NO_3$, forms a bifurcated N—H···O hydrogen bond to the nitrate anion.

Comment

Ferrocene derivatives have attracted considerable attention in recent decades, owing to their biological activity and applications in areas such as electrochemistry and materials science (Hall *et al.*, 1998; Li *et al.*, 2001; Welipitiya *et al.*, 1996). (Ferrocenylmethyl)dimethylamine serves as an intermediate, playing an important role in the syntheses of many ferrocene derivatives (Rainer *et al.*, 1998). In this communication, we report a new (ferrocenylmethyl)dimethylammonium salt, (I) (Fig. 1), prepared from (ferrocenylmethyl)dimethylamine and sodium nitrate in an ethanol solution.



(I)

As is usually found for ferrocene derivatives (Shi *et al.*, 2005; Ye *et al.*, 2005; Todd *et al.*, 2006), the two cyclopentadienyl (Cp) ligands are planar, close to parallel [the dihedral angle is 2.1 (1)° between the two least-squares ring planes] and close to eclipsed. The Fe atom binds somewhat asymmetrically to the two Cp ligands. The Fe1—C distances (Table 1) range from 2.029 (5) to 2.043 (6)Å, with mean values of 2.036 and 2.025Å for the unsubstituted and substituted Cp rings, respectively. These suggest that an interaction may exist between the methyldimethylamine group and the Fe atom, drawing the less electron-rich substituted Cp ligand closer to the metal centre.

The cation forms a bifurcated hydrogen bond to atoms O2 and O3 in the nitrate anion (Fig. 1 and Table 2). Atoms O1 and O2 of the nitrate anion are also directed towards the rear of the N1—H1*N* bond in a neighbouring complex, forming an O2···N1^{i} contact of 3.637 (7)Å and an O1···N1^{ii} contact of 4.067 (7)Å [symmetry codes: (i) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $x, \frac{3}{2}-y, \frac{1}{2}+z$] (Fig. 2).

Experimental

(Ferrocenylmethyl)dimethylamine (0.1213 g, 0.5 mmol) and $NaNO_3$ (0.00425 g, 0.5 mmol) were dissolved in ethanol (15 ml). To this solution, dichloromethane (1.5 ml, 0.2 mmol) was added dropwise and the mixture was stirred for 10 h. Brown block-shaped crystals of

the title compound were obtained after several days at room temperature.

Crystal data

$[Fe(C_5H_5)(C_8H_{13}N)]NO_3$
M_r = 306.14
Monoclinic, $P2_1/c$
a = 17.4375 (14) Å
b = 7.4054 (5) Å
c = 11.0348 (9) Å
β = 104.049 (2)°
V = 1382.32 (18) Å^3
Z = 4
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 K
Block, brown
0.31 × 0.25 × 0.18 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: ψ scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.727, T_{max} = 0.821
4660 measured reflections
2445 independent reflections
1886 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.163
S = 1.07
2445 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 6.2892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—C1	2.029 (5)	Fe1—C6	2.022 (7)
Fe1—C2	2.038 (5)	Fe1—C7	2.025 (7)
Fe1—C3	2.043 (6)	Fe1—C8	2.028 (7)
Fe1—C4	2.036 (6)	Fe1—C9	2.024 (7)
Fe1—C5	2.037 (6)	Fe1—C10	2.025 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2	0.98	1.96	2.870 (8)	154
N1—H1*N*···O3	0.98	2.22	3.068 (7)	145

H atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.98, 0.97 and 0.96 Å for those on cyclopentadienyl, methylene and methyl C atoms, respectively. In the first two cases, U_{iso}(H) = 1.2U_{eq}(C), while U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups. Atom H1N was positioned geometrically and allowed to ride on N1 with N—H = 0.98 Å, with an isotropic displacement parameter refined to be 0.07 (2) Å^2.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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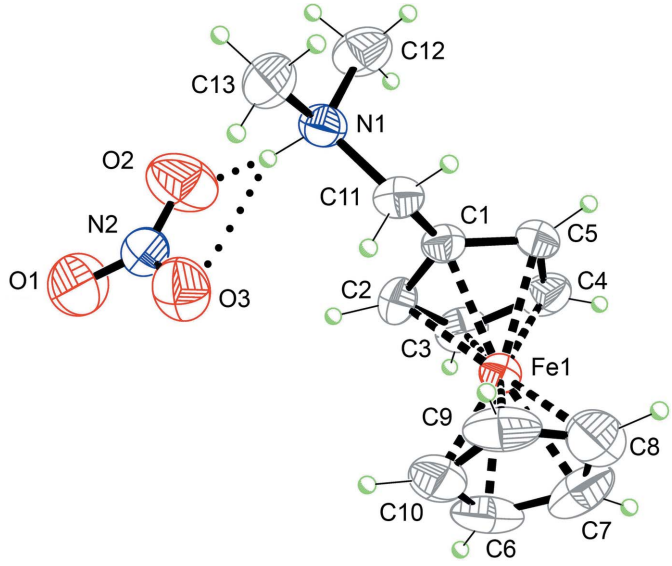

Figure 1
View of the structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms. The dotted lines indicate the bifurcated N—H···O hydrogen bond.

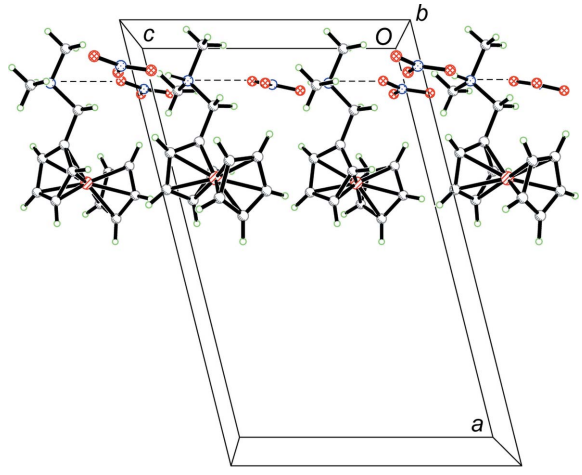

Figure 2
A partial packing diagram, viewed along the *b* direction, showing O···N contacts between molecules as dashed lines.

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