Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ammonium bis{3-anilinocarbonyl-1-[(5-chloro-2-oxidophenyl)diazenyl]-2-naphtholato}ferrate(III) acetone solvate

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Received 25 February 2007
Accepted 3 April 2007

Key indicators

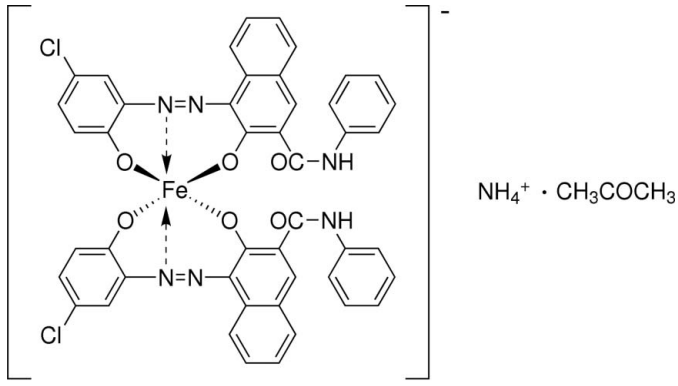
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.008 Å
R factor = 0.089
wR factor = 0.257
Data-to-parameter ratio = 13.8

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

The title compound, $(NH_4)[Fe(C_{23}H_{24}ClN_3O_3)_2]\cdot C_3H_6O$, is a charge-control agent used in electrophotography. The central Fe^{III} atom is coordinated by four O atoms and two N atoms of two symmetry-independent ligands. The metallic complex has no crystallographic symmetry.

Comment

This paper reports a structural study of the title compound, (I). For the background to this study see the preceding paper (Mizuguchi *et al.*, 2007), which describes the structure of the methanol-solvated complex.



(I)

Fig. 1 shows the molecular structure of (I). The network of hydrogen bonds that links the metallic complexes is different from that reported in the preceding paper. In (I) the ammonium ion shares its H atoms with the O atoms of three different complexes (Table 1) and the solvent molecule, while in the methanol-solvated structure, the ammonium ion shares its H atoms with two metal complexes and the solvent molecule. Interestingly the ions are again assembled in chains that run along the *a* axis.

Experimental

Compound (I) was prepared as described by Mizuguchi *et al.* (2007) and recrystallized from an acetone solution.

Crystal data

$(NH_4N)[Fe(C_{23}H_{24}ClN_3O_3)_2]\cdot C_3H_6O$
M_r = 963.61
Monoclinic, $P2_1/n$
a = 11.3199 (14) Å
b = 13.7962 (17) Å
c = 27.757 (4) Å
β = 93.747 (3)°
V = 4325.6 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 100 K
0.10 × 0.10 × 0.04 mm

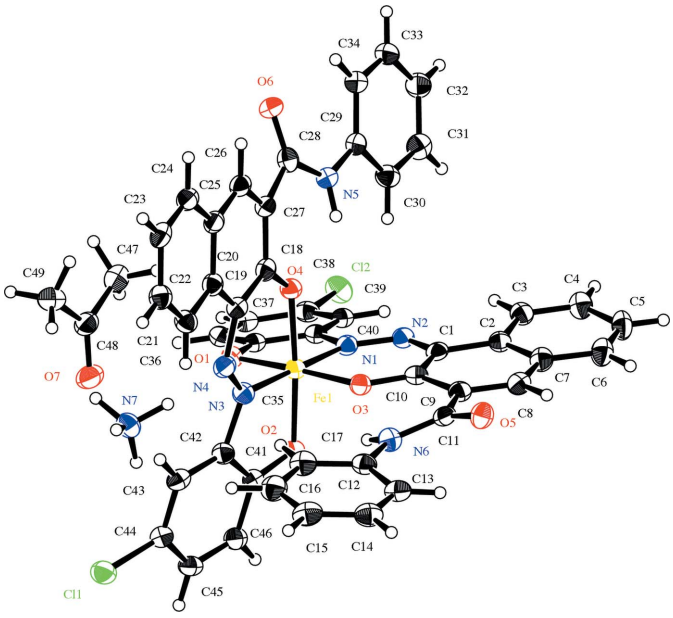


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids.

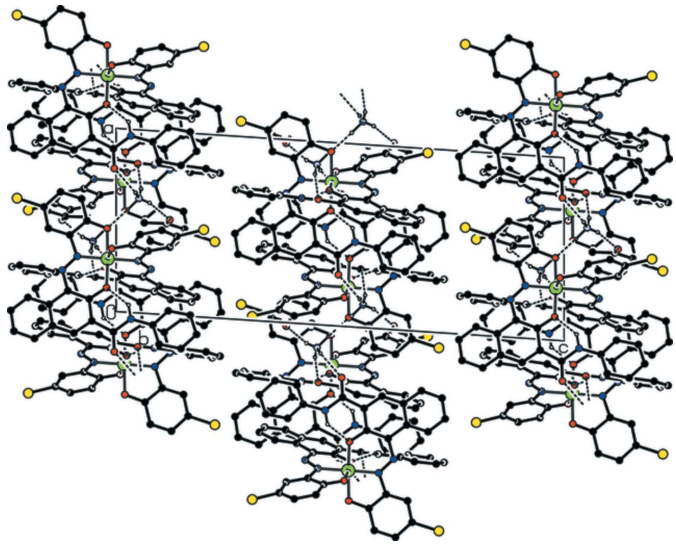


Figure 2
The packing of (I) showing the chain formation through hydrogen bonding. H atoms not involved in hydrogen bonding have been omitted for clarity.

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.950, T_{max} = 0.979
53581 measured reflections
8466 independent reflections
4761 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.196

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.089
$wR(F^2)$ = 0.257
S = 1.00
8466 reflections
612 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···O4	0.88	1.99	2.675 (5)	134
N6—H6*N*···O3	0.88	1.98	2.661 (6)	133
N7—H1*A*···O7	0.70 (7)	2.28 (6)	2.860 (8)	140 (6)
N7—H1*B*···O5^{i}	1.00 (7)	2.06 (7)	2.791 (7)	128 (5)
N7—H1*C*···O6^{ii}	0.98 (8)	1.87 (8)	2.797 (7)	156 (7)
N7—H1*D*···O1	1.01 (6)	1.80 (6)	2.800 (7)	172 (5)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z+1$.

The four H atoms of the ammonium cation were found in difference maps and their parameters were refined. All remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.95 and 0.98 Å, N—H = 0.88 Å, and U_{iso}(H) = 1.2U_{eq}(parent atom). Although the data collection was performed at 100 K, R_{int} was found to be rather poor (0.196).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

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