

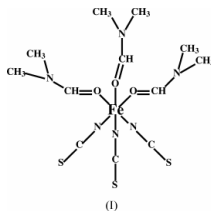
Ming-Sheng Wang,<sup>a</sup> Li-Zhen Cai,<sup>b</sup> Guo-Cong Guo<sup>b\*</sup> and Jin-Shun Huang<sup>b</sup><sup>a</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China and Graduate School of Chinese Academy of Sciences, Beijing 100039, People's Republic of China, and <sup>b</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China

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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{N}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.062  
 $wR$  factor = 0.146  
Data-to-parameter ratio = 16.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*fac*-Tris(dimethylformamide)tris(isothiocyanato)iron(III)The reaction of  $\text{FeCl}_3$ ,  $\text{NaSCN}$  and  $\text{Gd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  in 1:10 DMF/ $\text{H}_2\text{O}$  led to the formation of the title compound,  $[\text{Fe}(\text{NCS})_3(\text{C}_4\text{H}_7\text{N})_3]$ , in which the six-coordinated Fe atom is in an octahedral *fac* environment.Received 27 May 2003  
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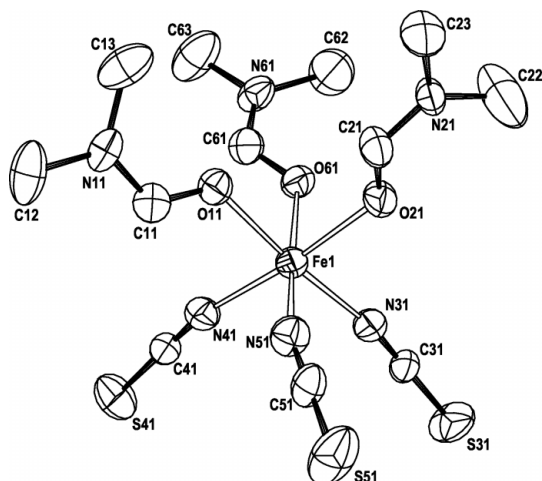
## Comment

The  $\text{SCN}^-$  ligand has been extensively investigated in recent years (Vinogradova *et al.*, 2001; Ren *et al.*, 2001; Kuang *et al.*, 2001; Sudbrake & Vahrenkamp, 2001). In most of the reported iron(III) complexes, the  $\text{SCN}^-$  ligand acts in a monodentate manner (Marchivie *et al.*, 2002; Zhu *et al.*, 2002; Marlin *et al.*, 2002). During our research on *3d-4f* metal complexes, we obtained the title compound, (I), a mononuclear iron(III) complex containing the  $\text{SCN}^-$  ligand. Here we report the structure of (I).

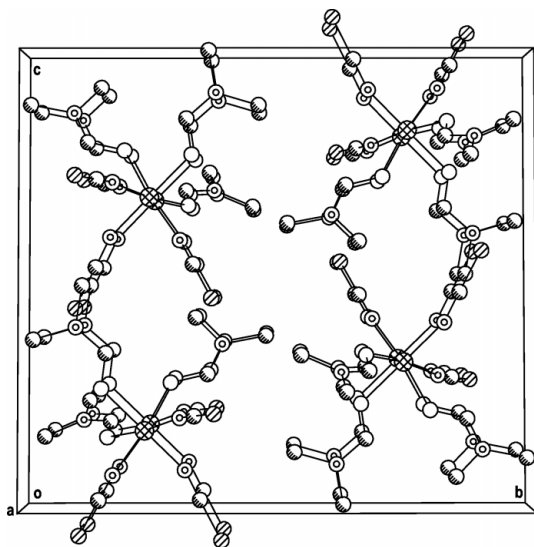
In the title complex (Fig. 1), the six-coordinated  $\text{Fe}^{\text{III}}$  atom is surrounded by three  $\text{SCN}^-$  anions and three DMF molecules with mean  $\text{Fe}-\text{N}$  and  $\text{Fe}-\text{O}$  distances of 2.009 (6) and 2.037 (8)  $\text{\AA}$ , respectively. Atoms N41, N51, O61 and O21 are coplanar, and the deviation of atom Fe1 from the above plane is 0.0554 (3)  $\text{\AA}$ . The structure of (I) is similar to that of *fac*-tris(isothiocyanato)tris(triphenylphosphineoxide)iron(III) (Olejnik *et al.*, 1995). All six *fac*-positioned ligands are monodentate. Three near-linear  $\text{SCN}^-$  ligands in (I) have an average  $\text{S}-\text{C}-\text{N}$  bond angle of 179.2 (2)°. The  $\text{S}-\text{C}$  and  $\text{C}-\text{N}$  bond distances in the  $\text{SCN}$  ligand are comparable to reported values (Olejnik *et al.*, 1995). The packing of (I) in the unit cell is shown in Fig. 2. The crystal structure is stabilized by van der Waals interactions.

## Experimental

$\text{FeCl}_3$  (1 mmol, 162 mg) was added to a 10 ml aqueous solution of  $\text{NaSCN}$  (6 mmol, 486 mg). A clear red solution was formed;  $\text{Gd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  (1 mmol, 451 mg) and DMF (1 ml) were then added successively. The final solution was filtered and allowed to stand in an ambient environment. Black-red prismatic crystals formed after several days.



**Figure 1**  
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.



**Figure 2**  
The molecular packing, viewed down the *a* axis. H atoms have been omitted for clarity.

#### Crystal data

[Fe(NCS)<sub>3</sub>(C<sub>4</sub>H<sub>7</sub>N)<sub>3</sub>]  
 $M_r = 449.38$   
 Monoclinic,  $P2_1/c$   
 $a = 8.7570$  (4) Å  
 $b = 16.8849$  (8) Å  
 $c = 15.3070$  (6) Å  
 $\beta = 97.591$  (2)°  
 $V = 2243.47$  (17) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.330$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1832 reflections  
 $\theta = 1.8$ – $25.1$ °  
 $\mu = 0.97$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, black-red  
 $0.26 \times 0.22 \times 0.18$  mm

#### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.772$ ,  $T_{\max} = 0.839$   
 7394 measured reflections

3864 independent reflections  
 1904 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.055$   
 $\theta_{\text{max}} = 25.1$ °  
 $h = -9 \rightarrow 7$   
 $k = -20 \rightarrow 14$   
 $l = -16 \rightarrow 18$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.062$   
 $wR(F^2) = 0.146$   
 $S = 1.00$   
 3864 reflections  
 232 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 1.9621P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.003$   
 $\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Fe1–N51	2.000 (2)	S31–C31	1.594 (3)
Fe1–N41	2.012 (2)	S41–C41	1.607 (3)
Fe1–N31	2.015 (2)	S51–C51	1.598 (3)
Fe1–O21	2.0261 (18)	C31–N31	1.146 (3)
Fe1–O61	2.0353 (17)	C41–N41	1.147 (3)
Fe1–O11	2.0481 (18)	C51–N51	1.164 (4)
N51–Fe1–N41	94.47 (9)	O21–Fe1–O61	83.17 (7)
N51–Fe1–N31	93.98 (9)	N51–Fe1–O11	91.21 (8)
N41–Fe1–N31	93.07 (9)	N41–Fe1–O11	89.79 (8)
N51–Fe1–O21	91.02 (9)	N31–Fe1–O11	173.86 (8)
N41–Fe1–O21	173.63 (8)	O21–Fe1–O11	86.87 (7)
N31–Fe1–O21	89.75 (8)	O61–Fe1–O11	85.40 (7)
N51–Fe1–O61	173.41 (9)	N31–C31–S31	179.5 (3)
N41–Fe1–O61	91.17 (8)	N41–C41–S41	178.9 (3)
N31–Fe1–O61	89.11 (8)	N51–C51–S51	179.2 (3)
C31–N31–Fe1	169.9 (2)	C11–O11–Fe1	127.58 (18)
C41–N41–Fe1	165.1 (2)	C21–O21–Fe1	127.97 (18)
C51–C51–Fe1	162.3 (2)	C61–O61–Fe1	129.21 (18)

H atoms were positioned geometrically and allowed to ride on their parent atoms. A rotating group model was used for the methyl groups. The low ratio (0.49) of observed to unique reflections and the relatively large  $U_{\text{eq}}$  values for the non-H atoms reflect the poor diffraction quality of the crystal.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1994); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Siemens, 1994); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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