Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Tris(1,10-phenanthroline-*N*,*N*′)iron(II) dithiocyanate trihydrate

Gakuse Hoshina,[a] Shigeru Ohba,[a]* Naoko Tsuchiya,[b] Tetsuhiko Isobe[b] and Mamoru Senna[b]

[a]Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan, and [b]Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan
Correspondence e-mail: ohba@chem.keio.ac.jp

Received 31 March 2000
Accepted 11 April 2000

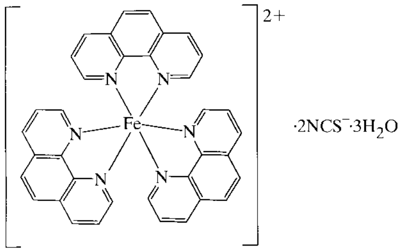
Data validation number: IUC0000103

The title mononuclear iron(II) complex, $[Fe(C_{12}H_8N_2)_3](NCS)_2{\cdot}3H_2O$, has a slightly distorted octahedral coordination. One of the thiocyanate ions and one of the water molecules of crystallization show positional disorder.

Comment

The October 1999 release of the Cambridge Structural Database (Allen & Kennard, 1993) contains 12 crystal structures which involve the title complex cation, *i.e.* $[Fe(phen)_3]^{2+}$. Among them, those of the simple inorganic counter-ions are $[Fe(phen)_3]I_2{\cdot}H_2O{\cdot}C_6H_5NO_2$ (Fujiwara *et al.*, 1984), $[Fe(phen)_3]I_2{\cdot}2H_2O$ (Johansson *et al.*, 1978) and $[Fe(phen)_3](ClO_4)_2{\cdot}0.5H_2O$ (Koh *et al.*, 1994).

Mechanochemical effects on the molecular structures, chemical states and magnetic properties have been investigated for the title compound, (I), by Tsuchiya *et al.* (1996).



(I)

Experimental

Crystals of the title compound, $[Fe(phen)_3](NCS)_2{\cdot}3H_2O$, were grown from an aqueous solution.

Crystal data

$[Fe(C_{12}H_8N_2)_3](NCS)_2{\cdot}3H_2O$
$M_r = 766.67$
Triclinic, $P\overline{1}$
$a = 12.083$ (3) Å
$b = 14.234$ (4) Å
$c = 12.050$ (2) Å
$\alpha = 93.19$ (2)°
$\beta = 109.53$ (1)°
$\gamma = 111.55$ (2)°
$V = 1778.7$ (8) Å^3
$Z = 2$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 14.9$–15.0°
$\mu = 0.591$ mm^{-1}
$T = 295$ (1) K
Prismatic, violet
0.6 × 0.5 × 0.5 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.658$, $T_{max} = 0.744$
10 804 measured reflections
10 354 independent reflections
8387 reflections with $I > 2\sigma(I)$
$R_{int} = 0.007$
$\theta_{max} = 30.0°$
$h = 0 \rightarrow 16$
$k = -20 \rightarrow 20$
$l = -16 \rightarrow 16$
3 standard reflections every 150 reflections intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.062$
$wR(F^2) = 0.201$
$S = 1.030$
8387 reflections
461 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1141P)^2 + 1.4911P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.27$ e Å^{-3}
$\Delta\rho_{min} = -1.55$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N1	1.974 (3)	Fe1—N4	1.969 (3)
Fe1—N2	1.976 (2)	Fe1—N5	1.982 (2)
Fe1—N3	1.978 (2)	Fe1—N6	1.973 (2)
N1—Fe1—N2	82.8 (1)	N2—Fe1—N6	94.35 (10)
N1—Fe1—N3	93.6 (1)	N3—Fe1—N4	82.8 (1)
N1—Fe1—N4	174.05 (7)	N3—Fe1—N5	92.27 (10)
N1—Fe1—N5	95.9 (1)	N3—Fe1—N6	174.25 (10)
N1—Fe1—N6	89.7 (1)	N4—Fe1—N5	89.03 (10)
N2—Fe1—N3	90.74 (9)	N4—Fe1—N6	94.3 (1)
N2—Fe1—N4	92.46 (10)	N5—Fe1—N6	82.69 (10)
N2—Fe1—N5	176.8 (1)		

There is a positional disorder of one of the NCS^- ions (N8—C38—S2) and one water molecule of crystallization (O5). It was assumed that occupancy factors of two possible combinations (N8—C38—S2 and O5, and N8*—C38*—S2 and O5*) were 50% each, and their positional parameters were refined isotropically. H-atom positional parameters of $[Fe(phen)_3]^{2+}$ were calculated geometrically and fixed with $U_{iso}(H) = 1.2U_{eq}$(parent atom). H atoms of the water molecules of crystallization were not introduced. The maximum residual density of 1.27 e Å^{-3} was located 0.09 Å from the S2 atom.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

References

Allen, F. H. & Kennard, O. (1993). *Chem. Des. Autom. News*, **8**, 31–37.

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.

Fujiwara, T., Iwamoto, E. & Yamamoto, Y. (1984). *Inorg. Chem.* **23**, 115–117.

Johansson, L., Molund, M. & Oskarrson, A. (1978). *Inorg. Chim. Acta*, **31**, 117–123.

Koh, L. L., Xu, Y. & Hsieh, K. (1994). *Acta Cryst.* C**50**, 884–886.

Molecular Structure Corporation (1993). *MSC/AFC Diffractmeter Control Software*. MSC, Research Forest Drive, The Woodlands, TX 77381, USA.

Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, Research Forest Drive, The Woodlands, TX 77381, USA.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

Tsuchiya, N., Isobe, T., Senna, M., Yoshioka, N. & Inoue, H. (1996). *Solid State Commun.* **99**, 525–529.

e192 Gakuse Hoshina *et al.* • $[Fe(C_{12}H_8N_2)_3](NCS)_2 \cdot 3H_2O$ *Acta Cryst.* (2000). C**56**, e191–e192