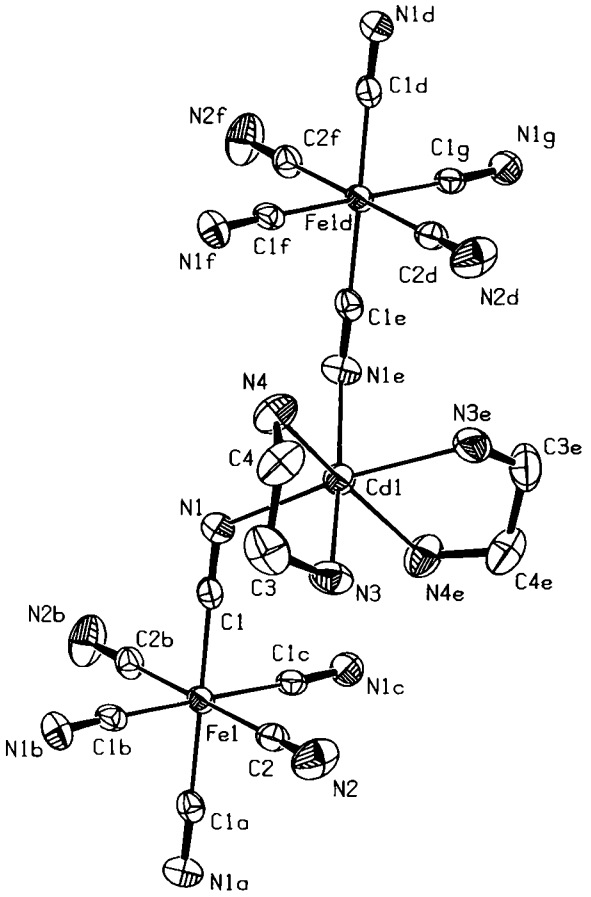
# Crystal structure of poly[{bis(cyanide-*C*)iron(II)}tetra($\mu_2$-cyanide-*C*:*N*)-bis{bis(ethylenediamine-*N*,*N'*)cadmium(II)}], $Cd_2Fe(CN)_6(C_2H_8N_2)_4$

A.-Y. Fu*,[I] and D.-Q. Wang[II]

[I] Dezhou University, Institute of New Pattern Material Chemistry, Shandong, Dezhou, 253023 P.R. China
[II] Liaocheng University, Department of Chemistry, Shandong, Liaocheng, 252059 P. R. China

Received August 3, 2005, accepted and available on-line September 12, 2005; CCDC no. 1267/1620




**Abstract**

$C_{14}H_{32}Cd_2FeN_{14}$, orthorhombic, *Fddd* (no. 70), $a = 8.686(3)$ Å, $b = 15.568(5)$ Å, $c = 36.52(1)$ Å, $V = 4938.5$ Å$^3$, $Z = 8$, $R_{gt}(F) = 0.027$, $wR_{ref}(F^2) = 0.065$, $T = 293$ K.

**Source of material**

A solution of $CdSO_4 \cdot 6H_2O$ (1.0 mmol) in 10 ml distilled water was added slowly to an aqueous mixture (20 ml) of $K_4[Fe(CN)_6]$ (0.5 mmol) and ethylenediamine (2 mmol). The mixture was stirred for 4 h and left to stand at room temperature for about three weeks. Red crystals were obtained.

Elemental analysis: found – C, 24.66 %; H, 4.52 %; N, 28.89 %; calc. for $C_{14}H_{32}Cd_2FeN_{14}$ – C, 24.83 %; H, 4.76 %; N, 28.96 %.

**Discussion**

For the development of functions such as electrical conductivities, magnetic properties, or non-linear optical properties in molecular crystals, not only the electronic properties of molecules themselves, but also the molecular arrangements in the crystals are very important. Therefore, the design of crystal structures and control of molecular arrangements has attracted much attention in recent years. Hexacyanometalate ions $[M(CN)_6]^{n-}$ act as good building blocks to provide bimetallic assemblies exhibiting spontaneous magnetization [1-4]. In this paper we show the title polymer which has layered structure.

The title compound, $[Cd_2Fe(C_2H_8N_2)_4(CN)_6]_n$, consists of $[Cd(C_2H_8N_2)_2]^{2+}$ cations and $[Fe(CN)_6]^{4-}$ anions (figure, top). Atom Fe1 is coordinated by six nitrile C atoms, of which the atoms C1, C1$^{i}$, C1$^{ii}$, C1$^{iii}$ (symmetry codes i: $-x+¾,-y+¾,z$; ii: $x,-y+¾,-z+¾$; iii: $-x+¾,y,-z+¾$) constitute the basal plane of the coordination octahedron. Within the basal plane, the Fe—C bond lengths (1.906(4) Å) are equal among each other. And on the axial positions, C2 and C2$^{iii}$ atoms have the equal Fe—C distance of 1.934(6) Å, which is longer than that in the basal plane. The complete anion is generated by inversion symmetry. The three *trans* angles for the Fe1 octahedron are 179.5(3)°, 179.5(3)°, 180°, the remaining angles are very close to 90°, indicating only slightly distorted octahedral environment. The Cd1 atom is surrounded by six N atoms from two chelated ethylenediamine ligands and two cyanide anions which belong to the octahedra of the two neighboring Cd atoms. It exhibits distorted octahedral coordination geometry. Four cyanide anions from a $FeC_6$ octahedron as bridging ligands connect four $[Cd(C_2H_8N_2)_2]^{2+}$ cations extending along the *a* and *b* axes, forming layer polymer parallel to the *a*,*b* plane. The intermolecular H-bond N3–H3A···N2$^{iv}$ (3.252(6) Å, 168.5°, symmetry code iv: $-x+1,-y+1,-z+1$) further connect the planes into 3D network.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | red block, size 0.08 × 0.10 × 0.25 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 23.17 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 47.26° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 5334, 922 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 698 |
| $N(param)_{refined}$: | 73 |
| Programs: | SHELXTL [5], SHELXTL-plus [5] |

* Correspondence author (e-mail: aiyunfu@yahoo.com.cn)

**Table 2.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(3A) | 32*h* | 0.6437 | 0.5412 | 0.4869 | 0.051 |
| H(3B) | 32*h* | 0.5938 | 0.4747 | 0.4612 | 0.051 |
| H(4A) | 32*h* | 0.9358 | 0.5934 | 0.4064 | 0.053 |
| H(4B) | 32*h* | 0.9312 | 0.6706 | 0.4290 | 0.053 |
| H(3C) | 32*h* | 0.8291 | 0.4553 | 0.4386 | 0.068 |
| H(3D) | 32*h* | 0.8470 | 0.4544 | 0.4814 | 0.068 |
| H(4C) | 32*h* | 0.9128 | 0.6013 | 0.4801 | 0.062 |
| H(4D) | 32*h* | 1.0311 | 0.5466 | 0.4575 | 0.062 |

**Table 3.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cd(1) | 16*g* | ⅝ | ⅝ | 0.41847(1) | 0.0286(3) | 0.0280(3) | 0.0283(3) | 0.0000(2) | 0 | 0 |
| Fe(1) | 8*b* | ⅜ | ⅜ | ⅜ | 0.0276(6) | 0.0181(6) | 0.0191(6) | 0 | 0 | 0 |
| N(1) | 32*h* | 0.6205(4) | 0.5161(2) | 0.3748(1) | 0.036(2) | 0.028(2) | 0.038(2) | −0.006(2) | 0.005(2) | −0.005(2) |
| N(2) | 16*g* | ⅜ | ⅜ | 0.4593(2) | 0.061(4) | 0.072(5) | 0.025(4) | −0.018(3) | 0 | 0 |
| N(3) | 32*h* | 0.6596(4) | 0.5187(2) | 0.4645(1) | 0.057(3) | 0.036(2) | 0.035(2) | −0.011(2) | −0.004(2) | 0.006(2) |
| N(4) | 32*h* | 0.8922(4) | 0.6175(3) | 0.4262(1) | 0.030(2) | 0.063(3) | 0.041(2) | −0.001(2) | −0.001(2) | 0.007(2) |
| C(1) | 32*h* | 0.5301(5) | 0.4616(3) | 0.3748(1) | 0.032(2) | 0.021(2) | 0.021(2) | 0.006(2) | 0.002(2) | −0.001(2) |
| C(2) | 16*g* | ⅜ | ⅜ | 0.4280(2) | 0.031(3) | 0.024(3) | 0.029(4) | −0.005(3) | 0 | 0 |
| C(3) | 32*h* | 0.8189(6) | 0.4898(3) | 0.4606(2) | 0.070(4) | 0.047(4) | 0.053(4) | 0.018(3) | −0.017(3) | 0.008(3) |
| C(4) | 32*h* | 0.9251(5) | 0.5663(4) | 0.4584(2) | 0.035(3) | 0.079(4) | 0.039(3) | 0.000(3) | −0.005(2) | 0.008(3) |

*Acknowledgment.* The authors thank the Education Office of Shandong Province, P. R. China, for research grant (no. J05D55).

## References

1. Clemente-León, M.; Coronado, E.; Galán-Mascarós, J. R.; Gómez-García, C. J.; Woike, Th.; Clemente-Juan, J. M.: Bimetallic Cyanide-Bridged Complexes Based on the Photochromic Nitroprusside Anion and Paramagnetic Metal Complexes. Syntheses, Structures, and Physical Characterization of the Coordination Compounds $[Ni(en)_2]_4[Fe(CN)_5NO]_2[Fe(CN)_6]\cdot 5H_2O$, $[Ni(en)_2][Fe(CN)_5NO]\cdot 3H_2O$, $[Mn(3\text{-}MeOsalen)(H_2O)]_2[Fe(CN)_5NO]$, and $[Mn(5\text{-}Brsalen)]_2[Fe(CN)_5NO]$. Inorg. Chem. **40** (2001) 87-94.
2. Ohba, M.; Fukita, N.; Okawa, H.: Magnetic characteristics of bimetallic assemblies, $[Ni(en)_2]_3[M(CN)_6]_2\cdot 2H_2O$ (en = $H_2NCH_2CH_2NH_2$; $M$ = Fe, Mn, Cr or Co), with a one-dimensional rope-ladder chain structure. J. Chem. Soc., Dalton Trans. (1997) 1733-1737.
3. Gu, Z.-Z.; Sato, O.; Einaga, Y.; Kai, M.; Iyoda, T.; Fujishima, A.; Hashimoto, K.: Crystal Structure and Photo-Reaction of a New Coordination Polymer: $[Ni(en)_2]_4[Fe(CN)_5NO]_2[Fe(CN)_6]\cdot 6H_2O$. Bull. Chem. Soc. Jpn. **74** (2001) 1617-1622.
4. Ohba, M.; Maruono, N.; Okawa, H.; Enoki, T.; Latour J.-M.: A New Bimetallic Ferromagnet, $[Ni(en)_2]_3[Fe(CN)_6]_2\cdot 2H_2O$, with a Rare Rope-Ladder Chain Structure. J. Am. Chem. Soc. **116** (1994) 11566-11567.
5. Sheldrick, G. M.: SHELXTL. Structure Determination Software Suite. Version 5.0. Siemens Industrial Automation, Analytical Instrumentation, Madison, Wisconsin, USA 1995.
6. Sheldrick, G. M.: SHELXTL-plus. Structure Determination Software Suite. Release 4.1. Siemens Analytical X-ray Instruments, Madison, Wisconsin, USA 1991.