

Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement coefficients ( $\text{\AA}^2 \times 10^4$ )

$U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U_{eq}$
Cr	2036.2 (2)	5907.1 (2)	7222.0 (2)	170 (1)
C(1)	2352 (2)	7771 (2)	7048 (2)	239 (5)
O(1)	2503 (2)	8925 (1)	6901 (1)	370 (4)
C(2)	1012 (2)	6415 (2)	8603 (2)	257 (5)
O(2)	362 (2)	6767 (2)	9408 (1)	415 (5)
C(3)	2909 (2)	5791 (2)	5684 (2)	235 (5)
O(3)	3418 (2)	5817 (1)	4758 (1)	368 (4)
C(4)	314 (2)	5922 (2)	6399 (2)	216 (4)
O(4)	-761 (1)	5900 (1)	5925 (1)	303 (4)
C(5)	4207 (2)	5040 (2)	7756 (2)	242 (5)
C(6)	3890 (2)	3548 (2)	7417 (2)	245 (5)
C(7)	3814 (2)	2909 (2)	8700 (2)	294 (5)
C(8)	2749 (2)	3976 (2)	9144 (2)	252 (5)
C(9)	3514 (2)	5307 (2)	8806 (2)	243 (5)
C(10)	1630 (2)	3854 (2)	8130 (2)	233 (5)
C(11)	2327 (2)	3594 (2)	7073 (2)	234 (5)

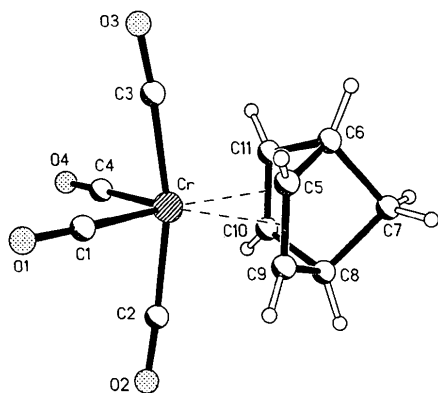


Fig. 1. The molecule of the title compound in the crystal, showing the atom-numbering scheme. Radii are arbitrary.

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

Cr—C(1)	1.861 (2)	Cr—C(2)	1.889 (2)
Cr—C(3)	1.904 (2)	Cr—C(4)	1.866 (2)
Cr—C(5)	2.310 (2)	Cr—C(9)	2.299 (2)
Cr—Cent1	2.201	Cr—C(10)	2.283 (2)
Cr—C(11)	2.290 (2)	Cr—Cent2	2.181
C(1)—O(1)	1.152 (2)	C(2)—O(2)	1.145 (2)
C(3)—O(3)	1.137 (2)	C(4)—O(4)	1.145 (2)
C(5)—C(6)	1.538 (3)	C(5)—C(9)	1.368 (3)
C(6)—C(7)	1.547 (3)	C(6)—C(11)	1.536 (2)
C(7)—C(8)	1.546 (3)	C(8)—C(9)	1.544 (3)
C(8)—C(10)	1.536 (3)	C(10)—C(11)	1.375 (3)
C(1)—Cr—C(2)	84.9 (1)	C(1)—Cr—C(3)	83.8 (1)
C(2)—Cr—C(3)	166.5 (1)	C(1)—Cr—C(4)	95.0 (1)
C(2)—Cr—C(4)	85.5 (1)	C(3)—Cr—C(4)	88.2 (1)
C(1)—Cr—C(5)	103.9 (1)	C(2)—Cr—C(5)	111.7 (1)
C(3)—Cr—C(5)	78.2 (1)	C(4)—Cr—C(5)	155.3 (1)
C(1)—Cr—C(9)	103.3 (1)	C(2)—Cr—C(9)	77.3 (1)
C(3)—Cr—C(9)	112.6 (1)	C(4)—Cr—C(9)	153.5 (1)
C(5)—Cr—C(9)	34.5 (1)	C(1)—Cr—C(10)	159.9 (1)
C(2)—Cr—C(10)	77.6 (1)	C(3)—Cr—C(10)	114.7 (1)
C(4)—Cr—C(10)	93.6 (1)	C(5)—Cr—C(10)	74.0 (1)
C(9)—Cr—C(10)	63.3 (1)	C(1)—Cr—C(11)	160.6 (1)
C(2)—Cr—C(11)	112.6 (1)	C(3)—Cr—C(11)	79.7 (1)
C(4)—Cr—C(11)	94.6 (1)	C(5)—Cr—C(11)	62.9 (1)
C(9)—Cr—C(11)	74.2 (1)	C(10)—Cr—C(11)	35.0 (1)
Cr—C(1)—O(1)	177.0 (1)	Cr—C(2)—O(2)	176.9 (2)
Cr—C(3)—O(3)	175.2 (2)	Cr—C(4)—O(4)	177.5 (1)
Cr—C(5)—C(6)	96.6 (1)	Cr—C(5)—C(9)	72.3 (1)
C(6)—C(5)—C(9)	106.8 (1)	C(5)—C(6)—C(7)	100.1 (1)
C(5)—C(6)—C(11)	102.6 (1)	C(7)—C(6)—C(11)	100.0 (1)
C(6)—C(7)—C(8)	93.3 (1)	C(7)—C(8)—C(9)	100.1 (1)
C(7)—C(8)—C(10)	99.9 (1)	C(9)—C(8)—C(10)	102.6 (1)
Cr—C(9)—C(5)	73.1 (1)	Cr—C(9)—C(8)	96.4 (1)
C(5)—C(9)—C(8)	106.4 (2)	Cr—C(10)—C(8)	97.3 (1)
Cr—C(10)—C(11)	72.8 (1)	C(8)—C(10)—C(11)	106.6 (1)
Cr—C(11)—C(6)	97.5 (1)	Cr—C(11)—C(10)	72.2 (1)
C(6)—C(11)—C(10)	106.4 (1)		

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## Structure of Poly[nickel(II)- $\mu$ -(cyano-C:N)]-{(ethylenediamine-N,N')zinc}-tri- $\mu$ -cyano(N,C)]

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**Abstract.**  $[\text{NiZn}(\text{C}_6\text{H}_8\text{N}_6)]_n$ ,  $M_r = 288.26$ , orthorhombic,  $Pbcn$ ,  $a = 8.878$  (3),  $b = 9.911$  (3),  $c = 11.106$  (5)  $\text{\AA}$ ,  $V = 977.3$  (6)  $\text{\AA}^3$ ,  $Z = 4$ ,  $D_m = 1.97$ ,  $D_x$

$= 1.96 \text{ Mg m}^{-3}$ ,  $\lambda(\text{Mo } K\alpha) = 0.71069 \text{ \AA}$ ,  $\mu = 4.37 \text{ mm}^{-1}$ ,  $F(000) = 576$ ,  $T = 295 \text{ K}$ ,  $R = 0.045$  for 812 reflections [ $F_o \geq 4\sigma(F_o)$ ]. The structure is built

Table 1. Fractional coordinates ( $\times 10^4$ ) and equivalent isotropic thermal parameters  $U_{\text{eq}}$  ( $\text{\AA}^2 \times 10^2$ ) with e.s.d.'s in parentheses

$$U_{\text{eq}} = (U_{11} + U_{22} + U_{33})/3.$$

	x	y	z	$U_{\text{eq}}$
Ni	0	0	0	2.72 (3)
Zn	5000	-732 (1)	2500	2.51 (2)
C(1)	-331 (5)	1660 (5)	773 (5)	2.9 (2)
C(2)	1708 (6)	-287 (5)	952 (5)	2.9 (2)
C(3)	5736 (7)	2132 (6)	2162 (5)	3.6 (2)
N(1)	-522 (5)	2665 (5)	1250 (4)	3.7 (2)
N(2)	2765 (5)	-509 (5)	1526 (4)	3.7 (2)
N(3)	5815 (6)	891 (5)	1406 (4)	3.6 (2)
H(1)	5702 (66)	2870 (57)	1603 (47)	5.0
H(2)	6535 (66)	2128 (57)	2795 (45)	5.0
H(3)	6840 (68)	699 (55)	1106 (52)	5.0
H(4)	5157 (67)	878 (57)	822 (50)	5.0

Table 2. Bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ )

Zn—N(1) <sup>i</sup>	2.160 (5)	N(3)—C(3)	1.491 (8)
Zn—N(2)	2.271 (5)	C(3)—C(3) <sup>ii</sup>	1.507 (9)
Zn—N(3)	2.142 (5)		
Ni—C(1)	1.879 (5)	N(3)—H(3)	0.99 (6)
Ni—C(2)	1.870 (5)	N(3)—H(4)	0.87 (6)
N(1)—C(1)	1.141 (7)	C(3)—H(1)	0.96 (6)
N(2)—C(2)	1.156 (7)	C(3)—H(2)	1.00 (5)
Ni—C(1)—N(1)	179.4 (5)	Zn—N(1) <sup>i</sup> —C(1) <sup>i</sup>	155.3 (4)
Ni—C(2)—N(2)	177.7 (5)	Zn—N(2)—C(2)	172.3 (4)
C(1)—Ni—C(2)	90.1 (2)	Zn—N(3)—C(3)	106.5 (3)
N(1) <sup>i</sup> —Zn—N(1) <sup>iii</sup>	85.3 (2)	N(2)—Zn—N(2) <sup>ii</sup>	168.8 (2)
N(1) <sup>i</sup> —Zn—N(2)	101.0 (2)	N(2)—Zn—N(3) <sup>ii</sup>	84.4 (2)
N(1) <sup>iii</sup> —Zn—N(2)	87.3 (2)	N(2)—Zn—N(3)	87.2 (2)
N(1) <sup>iii</sup> —Zn—N(3)	96.6 (2)	N(3)—Zn—N(3) <sup>ii</sup>	82.6 (2)
N(1) <sup>i</sup> —Zn—N(3)	171.7 (2)	N(3)—C(3)—C(3) <sup>ii</sup>	108.7 (5)

Symmetry codes: (i)  $0.5 + x, y - 0.5, 0.5 - z$ ; (ii)  $1 - x, y, 0.5 - z$ ; (iii)  $0.5 - x, y - 0.5, z$ .

up of an infinite three-dimensional network of Zn and Ni atoms linked together by bridging cyano groups. The Ni atom is square-planar coordinated by four bridging cyano groups. The Zn atom is coordinated in the form of an extended tetragonal bipyramid. The equatorial plane is occupied by two N atoms from a chelate bonded ethylenediamine molecule [Zn—N 2.142 (5)  $\text{\AA}$ ] and two N atoms from bridging cyano groups [Zn—N 2.160 (5)  $\text{\AA}$ ]. In the axial positions two bridging N-bonded cyano groups are placed at longer distances [Zn—N 2.271 (5)  $\text{\AA}$ ].

**Experimental.** Light-yellow crystals of  $\text{Zn(en)Ni(CN)}_4$  (en = ethylenediamine) crystallized from water solution containing a mixture of  $\text{ZnSO}_4$ , en and  $\text{K}_2[\text{Ni(CN)}_4]$ . Details of preparation and identification will be described elsewhere (Černák, Potočňák & Chomič, 1991). Preliminary Weissenberg photographs revealed space group  $Pbcn$  and indicated isostructurality with  $\text{Cd(en)Ni(CN)}_4$  (Jameson, Bachmann, Oswald & Dubler, 1981).  $D_m$  by flotation in a mixture of bromoform and chloroform. Crystal of bipyramidal shape,  $0.4 \times 0.5 \times 0.65$  mm. Data collection: Syntex  $P2_1$  diffractometer,

graphite-monochromatized Mo  $K\alpha$  radiation, unit-cell parameters from 15 reflections with  $4.11 \leq \theta \leq 10.59^\circ$ .  $\theta$ - $2\theta$  scan technique, scan angle from  $[2\theta(\text{Mo } K\alpha_1) - 1]^\circ$  to  $[2\theta(\text{Mo } K\alpha_2) + 1]^\circ$ , variable scan speed ( $4.88$ – $29.29^\circ \text{ min}^{-1}$ ), 1435 unique reflections ( $0 \leq h \leq 12, 0 \leq k \leq 13, 0 \leq l \leq 15$ ) with  $1.8 < \theta < 30^\circ$ ; of these, 812 had  $F_o \geq 4\sigma(F_o)$ . Two check reflections 133 and 224, measured after every 100 reflections, decreased by approximately 10% during data collection; the measured intensities were corrected for this decay along with Lp corrections using  $XP21$  (Pavelčík, 1986). Heavy-atom positions were determined from a Patterson map, other non-H atoms were found from a difference Fourier map. The absorption corrections were applied following Walker & Stuart (1983) after isotropic refinement using  $ABSORB$  (Ugozzoli, 1987). The absorption coefficients  $A_{p,s}$  calculated in the polar angles of the incident and diffracted beam range from 1.174 to 0.851 while the spherical absorption coefficients  $A_\theta$  range from 1.07 to 0.80. All non-H atoms refined anisotropically; H-atom positions refined, with  $U = 0.05 \text{ \AA}^2$ .  $\sum w(\Delta F)^2$  minimized, weighting scheme  $w = [\sigma^2(F_o)]^{-1}$ , changed in the last cycles to  $w = [\sigma^2(F_o) + 0.0001(F_o)^2]^{-1}$  for which the analysis of variance (Sheldrick, 1976) showed no systematic dependence on the value of  $(F_o/F_{\text{max}})^{1/2}$ . Final  $R = 0.045$ ,  $wR = 0.039$ ,  $(\Delta/\sigma)_{\text{max}} = 0.002$ ,  $-0.61 \leq \Delta\rho \leq 0.62 \text{ e \AA}^{-3}$ . Final atomic parameters are given in Table 1,\* bond distances and angles appear in Table 2. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV) (Ni and Zn atoms) and *SHELX76* (Sheldrick, 1976) (C, H and N

\* Lists of structure factors, anisotropic thermal parameters and bond angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53741 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

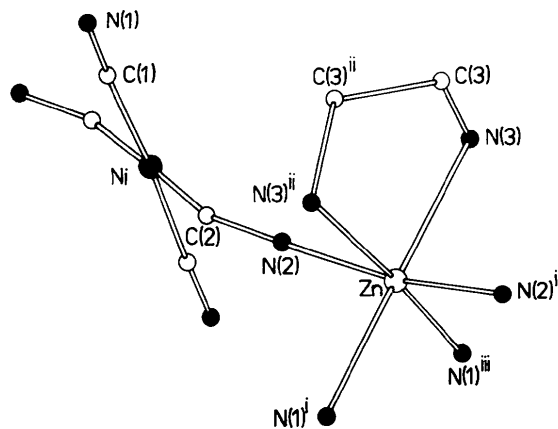


Fig. 1. The coordination of Zn and Ni atoms showing the atom-numbering scheme.

atoms) which was used for all calculations. Geometrical analysis performed using the program *PARST* (Nardelli, 1983).

**Related literature.** The formation of Zn(en)Ni(CN)<sub>4</sub> as an intermediate in the course of the thermal decomposition of Zn(en)<sub>3</sub>Ni(CN)<sub>4</sub>·H<sub>2</sub>O via Zn(en)<sub>3</sub>Ni(CN)<sub>4</sub> and Zn(en)<sub>2</sub>Ni(CN)<sub>4</sub> was not observed (Černák, Potočňák & Chomič, 1991). On the other hand, in the course of the thermal decomposition of Cd(en)<sub>3</sub>Ni(CN)<sub>4</sub>, the complexes Cd(en)<sub>2</sub>Ni(CN)<sub>4</sub> and Cd(en)Ni(CN)<sub>4</sub> are successively formed. The structure of Cd(en)Ni(CN)<sub>4</sub> consists of a three-dimensional network with CN ligands bridging Cd and Ni atoms (Jameson, Bachmann, Oswald & Dubler, 1981). Similarly, Ni(en)Ni(CN)<sub>4</sub> is formed in the course of the thermal decomposition of Ni(en)<sub>3</sub>Ni(CN)<sub>4</sub>·H<sub>2</sub>O (Černák, Chomič & Potočňák, 1989). The crystal structures of the ionic complexes Zn(en)<sub>3</sub>Ni(CN)<sub>4</sub>·H<sub>2</sub>O and Zn(en)<sub>3</sub>Ni(CN)<sub>4</sub>

were described by Černák, Chomič, Dunaj-Jurčo & Kappenstein (1984), while the chain structure of Zn(en)<sub>2</sub>Ni(CN)<sub>4</sub> was described by Černák, Potočňák, Chomič & Dunaj-Jurčo (1990).

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## Structure of (η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>W<sub>1.2</sub>Mo<sub>0.8</sub>Fe(μ<sub>3</sub>-Te)<sub>2</sub>(CO)<sub>7</sub> Containing a Te···Te Bonding Interaction

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**Abstracts.** [FeMo<sub>0.8</sub>Te<sub>2</sub>W<sub>1.2</sub>(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(CO)<sub>7</sub>], *M<sub>r</sub>* = 934.68, triclinic, *P*1̄, *a* = 13.195 (2), *b* = 15.892 (2), *c* = 21.632 (2) Å, α = 100.28 (1), β = 104.76 (1), γ = 94.07 (1)°, *V* = 4283.6 (9) Å<sup>3</sup>, *Z* = 8, *D<sub>x</sub>* = 2.899 g cm<sup>-3</sup>, λ(Mo *K*α) = 0.71073 Å, μ = 107.41 cm<sup>-1</sup>, *F*(000) = 3363.2, *T* = 295 K, *R* = 0.051 for 8302 observed reflections. The four molecules per asymmetric unit are quite similar. The title compound features Te···Te distances of 3.140–3.154 Å, which indicate strong Te···Te bonding interactions.

**Experimental.** The reaction of (η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Mo<sub>2</sub>(CO)<sub>6</sub> and (η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)W<sub>2</sub>(CO)<sub>6</sub> with Fe<sub>3</sub>Te<sub>2</sub>(CO)<sub>9</sub> in toluene yielded dark-brown crystals of the title compound. Qualitative elemental analysis showed Mo, W and Fe were present. The crystal chosen for X-ray study had approximate dimensions 0.20 × 0.20 × 0.11 mm. The intensity data were collected on an Enraf–Nonius CAD-4 diffractometer with graphite-monochroma-

tized Mo *K*α radiation. The lattice parameters were refined from the angle values of 25 reflections with 28 ≤ 2θ ≤ 30°. 15 481 reflections with 2 ≤ 2θ ≤ 50° were collected using the ω-scan mode with a variable rate of 1 to 7° min<sup>-1</sup> and a scan range of (0.40 + 0.35tan2θ)°. The index range was -15 ≤ *h* ≤ 15, -18 ≤ *k* ≤ 18, 0 ≤ *l* ≤ 25. Three standard reflections measured at exposure intervals of 2 h exhibited no significant variation. Data were corrected for Lorentz–polarization effects and empirically for absorption using the program *DIFABS* (Walker & Stuart, 1983). Max. and min. transmission factors were 1.152 and 0.820, respectively. 8302 reflections with *I* > 3σ(*I*) were used in subsequent calculations.

The structure was solved using direct methods, which located the positions of all Te, W/Mo and Fe atoms in the four independent molecules. The remaining non-H atoms were located from difference Fourier syntheses. All non-H atoms except the C atoms were refined with anisotropic temperature factors. All H atoms were located according to their

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