Table 2. *Selected geometric parameters (Å, °)*

Re—Re^{i}	2.785 (3)	Te—Te^{ii}	3.486 (6)
Re—Te^{ii}	2.790 (2)	Te—Te^{iii}	3.616 (6)
Re—S^{i}	2.337 (10)		
Re^{i}—Re—Re^{iv}	60	S^{i}—Re—S^{iv}	104.6 (3)
Te^{ii}—Re—Te^{v}	77.35 (11)	Re^{ii}—Te—Re^{v}	101.36 (9)
Te^{ii}—Re—S^{iv}	87.3 (2)	Re^{i}—S—Re^{iv}	73.2 (4)
Te^{ii}—Re—S^{vi}	160.2 (2)		

Symmetry codes: (i) $-x, -y, z$; (ii) $x, \frac{1}{2} - y, \frac{1}{2} - z$; (iii) $1 - x, y, 1 - z$; (iv) $-x, y, -z$; (v) $\frac{1}{2} - x, y, \frac{1}{2} - z$; (vi) $x, -y, -z$.

Refinement of the inversed geometry gave $R = 0.048$, $wR = 0.036$ and $S = 6.82$, confirming that the absolute configuration chosen here is correct.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1991). Cell refinement: *MSC/AFC Diffractometer Control Software.* Data reduction: *EQVRFL* (Imoto, 1992). Program(s) used to solve structure: *SAPI*91 (Fan, 1991). Program(s) used to refine structure: *ANYBLK* (Imoto, Hayakawa, Morita & Saito, 1990). Software used to prepare material for publication: *ANYBLK.*

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Lists of structure factors, anisotropic displacement parameters and complete geometry, and supplementary figures, have been deposited with the IUCr (Reference: OH1089). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Copper–Zinc Oxide Catalysts. III. Structure of $[Zn(NH_3)_3][Cu(CN)_2]_2$

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Abstract

The structure of the new Cu–Zn bimetallic compound triamminezinc(II) bis[dicyanocuprate(I)] is built up from infinite —Cu—*AA*—Cu—*AA*— (where *AA* represents a disordered CN group) helical chains with 2_1 symmetry. Terminal cyano groups and —CN—$Zn(NH_3)_3$ groups are bonded alternately to the Cu atoms of the chains. Both crystallographically independent Cu^{I} atoms are trigonally coordinated by three cyano groups. The Zn^{II} atom is tetrahedrally coordinated by three ammonia molecules and one nitrogen-bonded cyano group. The intra- and interchain CN···HN hydrogen bonds contribute to the stabilization of the structure.

Comment

Copper–zinc bimetallic compounds can be used as precursors for the unconventional preparation of model catalysts for the methanolization of syngas ($CO + H_2$). The advantage of such precursors is the intimate presence of both metals at the first stage of catalyst preparation (Chinchen, Denny, Jennings, Spencer & Waugh, 1988). Our goal is to study the preparation, characterization and crystal structure of such bimetallic compounds. In previous papers we described the preparation and thermal properties of new Cu–Zn bimetallic compounds (Černák, Chomič, Kappenstein, Brahmi & Duprez, 1995) and the crystal structures of two, $Zn(NH_3)_2Cu(CN)_3$ (ZCA) and

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$[Zn(en)_3]_6[Cu_5(CN)_{17}].nH_2O$ (n = 8.4) (ZCE3), were discussed (Černák, Chomič, Kappenstein & Dunaj-Jurčo, 1994); ZCA exhibits a polymeric structure and ZCE3 is ionic. Here we report the crystal structure of $[Zn(NH_3)_3][Cu(CN)_2]_2$ (ZC2A) with a Cu:Zn atomic ratio of 2:1. This compound crystallizes from the system Zn^{2+}–NH_3–$[Cu(CN)_2]^-$ under a nitrogen atmosphere (to prevent oxidation of Cu^I) in the form of colourless irregular parallelepipeds, along with a few needle-shaped crystals of poor X-ray quality.

The centrosymmetric structure is one-dimensional with infinite left- and right-handed helical —Cu—*AA*—Cu—*AA*— chains (where *AA* represents a disordered CN group) along 2_1 axes. Terminal cyano ligands and —CN—$Zn(NH_3)_3$ groups complete the trigonal coordination of the Cu atoms such that the composition of the chains may be represented by {—Cu(CN)—*AA*—Cu[—CN—$Zn(NH_3)_3$]—*AA*—}.

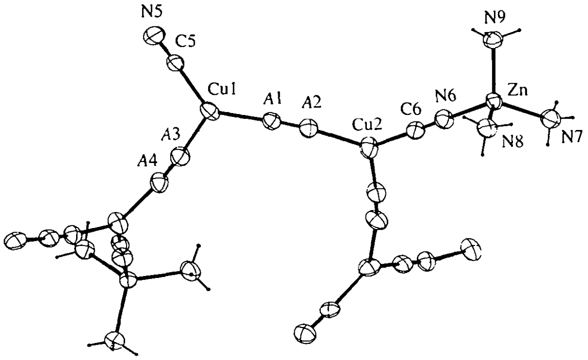

Fig. 1. *ORTEP* (Johnson, 1965) view of the title compound displaying its chain character. The displacement ellipsoids are drawn at the 50% probability level.

Cromer & Larson (1962) stated that the Cu—N bond is longer than the Cu—C bond by about 0.1 Å, thus offering the possibility of distinguishing between a C and an N atom. In our case, however, some bonds originally assigned as Cu—N and Cu—C exhibited practically the same bond lengths, thus disclosing the presence of disorder. It was possible to introduce two disordered cyano groups, *A*1–*A*2 and *A*3–*A*4, into the refinement process, leading to site-occupancy factors (defined as C/N ratio) of 0.59 (4)/0.41(4) for site *A*1 and 0.56 (4)/0.44 (4) for site *A*4. The disordered model yields a lower value of the *wR*2 agreement index (0.0927 against 0.0994 for an ordered model with *A*1 and *A*4 as C atoms). Disordered cyano groups have been found in other cyanocuprates; the C and N sites are sometimes related by symmetry elements such as mirror planes, as in $Cu(NH_3)_2Cu_4(CN)_6$ (Kappenstein & Schubert, 1980).

The same type of chain with 2_1 symmetry is present in the potassium salt $K[Cu(CN)_2]$ (Cromer, 1957), in which the K^+ ions are located between the chains. In the sodium salt, $Na[Cu(CN)_2].2H_2O$, the chains adopt glide-plane symmetry and the CuC_2N unit is planar (Kappenstein & Hugel, 1977). Such chains also exist in ZCA, but in this case they are cross-linked by [—μ-$(NC)_2$—$Zn(NH_3)_2$] groups (Černák, Chomič, Kappenstein & Dunaj-Jurčo, 1994).

The structures of the analogous compounds containing Cu^{II} instead of Zn^{II}, $Cu(NH_3)_3Cu_2(CN)_4$ (CC2A) (Williams, Cromer & Larson, 1971) and $[Cu(en)_2(H_2O)][Cu_2(CN)_4]$ (CC2E) (Williams, Larson & Cromer, 1972), are different. The structure of CC2A is built up from chains of shared pentagons formed by one pseudo-octahedrally coordinated Cu^{II} and four trigonally coordinated Cu^I atoms. It is interesting to note that three ammonia molecules statistically occupy four positions around the Cu^{II} atoms. The second compound, CC2E, contains discrete square pyramidal $[Cu(en)_2(H_2O)]^{2+}$ cations in the holes of the $[Cu_2(CN)_4]^{2-}$ polymeric framework. The formation of different structure types in the case of the Cu^{II} compounds may be a consequence of the Jahn–Teller effect and a preference for higher coordination numbers.

In ZC2A, both independent Cu atoms display planar trigonal coordination (Table 2), whereas the related ZCA compound contains tetrahedrally coordinated Cu^I atoms. The angles at Cu defined by the chain in ZC2A exhibit values lower than 120°. The Zn atom is tetrahedrally coordinated by one bridging cyano group and three ammonia molecules; this type of coordination is different from that found in ZCA, where the Zn atom is coordinated by two bridging cyano groups and two ammonia ligands. The bond distances and angles are comparable with those found in other cyanocuprate complexes (Cromer, 1957; Kappenstein & Hugel, 1977; Černák, Chomič, Kappenstein & Dunaj-Jurčo, 1994).

The N atom of the terminal cyano group and the ammonia molecules are candidates for N—H···N-type hydrogen-bond formation. There are four N···N contacts below 3.6 Å (Table 3). Two (N7—H7*A*···N5^{i} and N9—H9*C*···N5^{iii}) represent interchain hydrogen bonds, the third (N9—H9*B*···N5^{iv}) can be assigned to a weak intrachain hydrogen bond and the fourth [N8—H8*B* (or H8*A*)···N5^{ii}] exhibits a value too low for the N—H···N angle to be considered as a hydrogen bond. The hydrogen bonds contribute to the stabilization of the structure.

The distances between the metal atoms are interesting from a catalytic point of view. It is known that in some cyanocuprates relatively short distances between Cu atoms exist, *e.g.* 2.42 Å in $CuCN(NH_3)$ (Cromer, Larson & Roof, 1965) or 2.655 Å in $[Me_2PhS]Cu_2(CN)_3$ (Černák, Györyová, Sabolová & Dunaj-Jurčo, 1991). In the present compound, the shortest metal–metal distances are found between adjacent chains and are much longer: Cu2···Cu2^{v} 3.886 (1) Å, Cu1···Cu2^{v} 4.0143 (9) Å and Zn···Cu1^{v} 4.440 (2) Å [symmetry code: (v) $1-x, -y, -z$], excluding any direct metal–metal interaction.

Experimental

The addition of 1 *M* $ZnSO_4$ solution (5 mmol) to a hot 1.33 *M* $KCu(CN)_2$ solution (10 mmol) resulted in a colourless precipitate, which redissolved on bubbling NH_3 through the mixture. The solution was allowed to stand for several hours, after which colourless crystals were obtained.

Crystal data

$[Zn(NH_3)_3][Cu(CN)_2]_2$
$M_r = 347.63$
Monoclinic
$P2_1/c$
$a = 7.512$ (2) Å
$b = 11.599$ (2) Å
$c = 12.928$ (3) Å
$\beta = 102.14$ (3)°
$V = 1101.25$ (45) Å^3
$Z = 4$
$D_x = 2.0967$ Mg m^{-3}
$D_m = 2.12$ Mg m^{-3}
D_m measured by flotation in bromoform–acetone

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 36 reflections
$\theta = 7.57$–15.50°
$\mu = 6.033$ mm^{-1}
$T = 293$ (2) K
Irregular cube
0.25 × 0.20 × 0.20 mm
Colourless

Data collection

Kuma KM-4 κ-axis diffractometer
ω–2θ scans
Absorption correction: ψ scan (*ABSELI*, *KM*-4 *Software*; Kuma, 1991)
$T_{min} = 0.62$, $T_{max} = 0.97$
3441 measured reflections
3220 independent reflections
1813 observed reflections [$I > 2\sigma(I)$]

$R_{int} = 0.0419$
$\theta_{max} = 30.00°$
$h = -10 \rightarrow 0$
$k = 0 \rightarrow 16$
$l = -17 \rightarrow 18$
3 standard reflections monitored every 50 reflections intensity decay: <3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0297$
$wR(F^2) = 0.0785$
$S = 1.081$
3219 reflections
132 parameters
H atoms treated using a riding model
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = -0.156$
$\Delta\rho_{max} = 0.400$ e Å^{-3}
$\Delta\rho_{min} = -0.756$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Zn	−0.14499 (5)	−0.22579 (3)	−0.28151 (3)	0.0377 (1)
Cu1	0.60806 (7)	0.33486 (4)	0.09198 (4)	0.0507 (1)
Cu2	0.26202 (7)	−0.03504 (4)	0.02857 (4)	0.0535 (2)
N5	0.7545 (5)	0.5045 (3)	−0.0500 (3)	0.0565 (8)
C5	0.7064 (5)	0.4391 (3)	0.0037 (3)	0.0403 (7)
N6	0.0133 (4)	−0.1472 (3)	−0.1603 (2)	0.0476 (7)
C6	0.1031 (5)	−0.1041 (3)	−0.0892 (3)	0.0418 (7)
C1†	0.4562 (5)	0.2007 (3)	0.0488 (2)	0.0442 (9)
N1‡	0.4562 (5)	0.2007 (3)	0.0488 (2)	0.0442 (9)
C2‡	0.3787 (5)	0.1150 (3)	0.0319 (2)	0.0452 (9)
N2†	0.3787 (5)	0.1150 (3)	0.0319 (2)	0.0452 (9)
C4§	0.6893 (5)	0.3965 (3)	0.3308 (3)	0.0484 (9)
N4¶	0.6893 (5)	0.3965 (3)	0.3308 (3)	0.0484 (9)
C3¶	0.6601 (5)	0.3666 (3)	0.2442 (3)	0.053 (1)
N3§	0.6601 (5)	0.3666 (3)	0.2442 (3)	0.053 (1)
N7	−0.1550 (7)	−0.3935 (3)	−0.2480 (3)	0.072 (1)
N8	−0.3941 (4)	−0.1550 (3)	−0.3013 (2)	0.0469 (7)
N9	−0.0419 (4)	−0.2060 (3)	−0.4119 (2)	0.0472 (7)

† Site occupancy 0.59 (4). ‡ Site occupancy 0.41 (4). § Site occupancy 0.56 (4). ¶ Site occupancy 0.44 (4).

Table 2. *Selected geometric parameters (Å, °)*

An represents C*n* or N*n* where *n* = 1, 2, 3 or 4.

Zn—N6	1.979 (3)	Cu2—C6	1.903 (3)
Zn—N7	1.998 (3)	Cu2—*A*2	1.945 (3)
Zn—N8	2.010 (3)	Cu2—*A*4^{i}	1.947 (3)
Zn—N9	2.011 (3)	N5—C5	1.138 (5)
Cu1—C5	1.914 (3)	N6—C6	1.135 (4)
Cu1—*A*1	1.941 (3)	*A*1—*A*2	1.149 (5)
Cu1—*A*3	1.960 (4)	*A*3—*A*4	1.148 (5)
N6—Zn—N7	108.7 (2)	C6—Cu2—*A*4^{i}	122.6 (2)
N6—Zn—N8	107.5 (1)	*A*2—Cu2—*A*4^{i}	110.4 (1)
N7—Zn—N8	110.4 (2)	N5—C5—Cu1	175.7 (3)
N6—Zn—N9	109.8 (1)	C6—N6—Zn	178.4 (3)
N7—Zn—N9	109.4 (1)	N6—C6—Cu2	177.7 (4)
N8—Zn—N9	111.1 (1)	*A*2—*A*1—Cu1	172.6 (3)
C5—Cu1—*A*1	127.7 (1)	*A*1—*A*2—Cu2	170.4 (3)
C5—Cu1—*A*3	117.4 (1)	*A*3—*A*4—Cu2^{ii}	173.5 (3)
*A*1—Cu1—*A*3	114.9 (1)	*A*4—*A*3—Cu1	173.3 (3)
C6—Cu2—*A*2	126.8 (1)		

Symmetry codes: (i) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$.

Table 3. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7*A*···N5^{i}	2.194 (8)	3.024 (5)	155 (1)
N8—H8*A*···N5^{ii}	3.25 (2)	3.501 (5)	99 (1)
N8—H8*B*···N5^{ii}	3.03 (1)	3.501 (5)	115 (1)
N9—H9*C*···N5^{iii}	2.274 (9)	3.137 (5)	163 (2)
N9—H9*B*···N5^{iv}	2.65 (2)	3.363 (5)	138 (2)

Symmetry codes: (i) $x - 1, y - 1, z$; (ii) $-x, y - \frac{1}{2}, -\frac{1}{2} - z$; (iii) $x - 1, \frac{1}{2} - y, z - \frac{1}{2}$; (iv) $1 - x, y - \frac{1}{2}, -\frac{1}{2} - z$.

The scattering factor $f(A)$ of atom *A* of the disordered cyano group was considered to be formed by a sum of the scattering factors of the C and N atoms such that $f(A) = kf(\mathrm{C}) + (1 - k)f(\mathrm{N})$, where *k*, the site-occupancy factor of the C atom, was refined. The disordered model is better at the 99.5% significance level as $RFR = wR2_1/wR2_2 = 1.072 > RFR_{2,3219,0.005} = 1.002$ (*RFR* = *R*-factor ratio) (Hamilton, 1965). The ammonia H atoms were treated as idealized methyl group atoms in which the H atom was allowed to ride on the N atom, with *U* set to $1.5U_{eq}$ of the parent N atom.

Data collection: *KM*-4 *Software* (Kuma, 1991). Cell refinement: *KM*-4 *Software*. Data reduction: *KM*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *SHELXL*93. Geometrical analysis: *PARST* (Nardelli, 1983); *SHELXL*93.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BR1113). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 1070–1072

Mercury(II) Selenite Hemihydrate

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Abstract

The title compound, dimercury bis[trioxoselenate(2−)] monohydrate, $Hg_2(SeO_3)_2.H_2O$, contains two inequivalent Hg^{II} ions with coordination numbers of five and seven. The coordination polyhedra of these ions are a tetragonal pyramid and a monocapped trigonal prism, respectively. One of the two inequivalent selenite groups bridges three Hg^{II} ions and the other bridges four Hg^{II} ions, thus forming a structure extending in three dimensions.

Comment

The coordination number of divalent mercury usually varies between five and seven, and the coordination polyhedron is often a tetragonally flattened or elongated octahedron (Dubler, Beck, Linowsky & Jameson, 1981). We have described the structures of two mercury(II) selenites, $HgSeO_3$ and $Hg_3(HSeO_3)_2(SeO_3)_2$, previously (Koskenlinna & Valkonen, 1995*a*,*b*). The first compound is isostructural with the perovskite-like compounds $MSeO_3$ (M = Mg, Mn, Co, Ni, Cu, Zn and Cd; Kohn, Inoue, Horie & Akimoto, 1976; Valkonen, 1994*a*) and has a coordination polyhedron in the form of a flattened octahedron, while the latter is isostructural with the corresponding cadmium compound (Valkonen, 1994*b*) and contains coordination polyhedra of six and seven O atoms; the octahedron is tetragonally flattened and the other polyhedron has the form of a monocapped trigonal prism. In both compounds, the polyhedra of O atoms around the Hg^{II} ions are distorted compared with those of other metals in the respective isostructural series. We report here the structure of a novel mercury(II) selenite.

The title compound contains two inequivalent Hg^{II} ions, two selenite ions and a water molecule, corresponding either to the formula $Hg_2(SeO_3)_2.H_2O$ [mercury(II) selenite–water (2/1), $Z = 4$] or $HgSeO_3.0.5H_2O$ [mercury(II) selenite hemihydrate, $Z = 8$]. The structure is continuous in three dimensions, but contains a cavity. The cavity is in the middle of the unit cell and extends

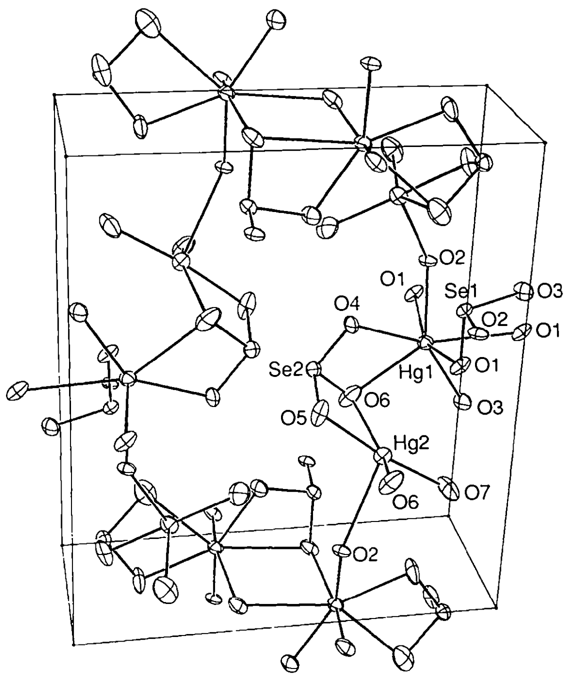

Fig. 1. An *ORTEP*II (Johnson, 1976) drawing of the unit cell with displacement ellipsoids shown at the 50% level. The *c* axis is horizontal and the *b* axis is vertical.

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