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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.054
wR factor = 0.124
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

catena-Poly[[[acetonitrilebis[μ-bis(diphenylphosphino)-methane-κ^2P:P']dicopper(I)]-μ-(1,2-dicyanoethylene-1,2-dithiolato)-[(1,2-dicyanoethylene-1,2-dithiolato)-tungstate(IV)]-μ-(1,2-dicyanoethylene-1,2-dithiolato)] diethyl ether disolvate acetonitrile solvate]

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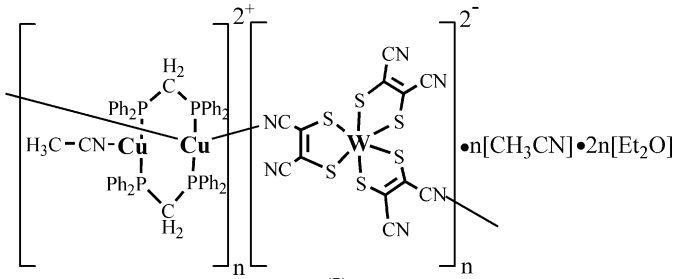
The reaction between $[Cu_2(\mu\text{-bis(diphenylphosphino)-methane})_2(MeCN)_2](ClO_4)_2$ and $(Bu_4N)_2[W(cis\text{-1,2-dicyano-ethylene-1,2-dithiolate})_3]$ gave the title compound, $\{[Cu_2W(C_4N_2S_2)_3(C_2H_3N)(C_{25}H_{22}P_2)_2]\cdot 2C_4H_{10}O\cdot C_2H_3N\}_n$. Due to the binding between a Cu atom of the binuclear copper unit $[Cu_2\{bis(diphenylphosphino)methane\}_2(MeCN)]^{2+}$ and the N atoms of the buliding block $[W(cis\text{-1,2-dicyano-ethylene-1,2-dithiolate})_3]^{2-}$, a one-dimensional zigzag chain structure is formed.

Comment

Assembly between binuclear copper(I) complexes and some ligands like chalcogenide, nitrogenide, halogenide and alkynyl have been studied extensively (Diéz *et al.*, 1987; Chen *et al.*, 2004, 2005; Liaw *et al.*, 2005). We are interested in designing heterometallic cluster complexes formed by self-assembly between metal diphosphine and metal thiolate components, where the latter shows potential bridging character.



(I)

We describe here a polymeric heterometallic complex, $[Cu_2W(\mu\text{-bis(diphenylphosphino)methane})_2(cis\text{-1,2-dicyano-ethylene-1,2-dithiolate})_3(MeCN)]_n\cdot nCH_3CN\cdot 2nEt_2O$, which resulted from the self-assembly between $[Cu_2(\mu\text{-bis(diphenylphosphino)methane})_2(MeCN)_2](ClO_4)_2$ and $(Bu_4N)_2[W(cis\text{-1,2-dicyanoethylene-1,2-dithiolate})_3]$. In the crystal structure of the title compound, the coordination geometry around the W atom is distorted octahedral, which is similar to that in $[Ph_4As]_2[W(cis\text{-1,2-dicyanoethylene-1,2-dithiolate})_3]$ (Gary & Edward, 1973). Atom Cu1 adopts an approximately triangular-planar geometry, defined by two P atoms from two bis(diphenylphosphino)methane ligands and one N atom from the MeCN solvent, while Cu2 adopts a distorted tetrahedral geometry, defined by two P atoms from two bis(diphenyl-phosphino)methane ligands and two N atoms from two dicyanoethylene-1,2-dithiolate ligands, leading to a zigzag chain structure (Fig. 2).

Experimental

All reactions were carried out under an argon atmosphere using standard Schlenk techniques and all solvents were degassed by standard methods and distilled before use. The starting compounds $(Bu_4N)_2[W(cis\text{-}1,2\text{-dicyanoethylene-1,2-dithiolate})_3]$ (Stiefel *et al.*, 1970) and $[Cu_2(\mu\text{-bis(diphenylphosphino)methane})_2(MeCN)_2](ClO_4)_2$ (Diéz *et al.*, 1987) were prepared by the literature procedures. The title compound was synthesized by the following procedure. To a solution of $[Cu_2(\mu\text{-bis(diphenylphosphino)methane})_2(MeCN)_2](ClO_4)_2$ (36 mg, 0.03 mmol) in 3 ml of MeCN was added $[Bu_4N]_2[W(cis\text{-}1,2\text{-dicyanoethylene-1,2-dithiolate})_3]$ (33 mg, 0.03 mmol). After the solution was stirred at room temperature for 12 h, the solvent was removed under vacuum, and the resulting residue was extracted by 3 ml of MeCN. Diffusing diethyl ether into the MeCN solution afforded purple crystals.

Crystal data

$[Cu_2W(C_4N_2S_2)_3(C_2H_3N)(C_{25}H_{22}P_2)_2]\cdot 2C_4H_{10}O\cdot C_2H_3N$
$M_r = 1730.55$
Monoclinic, $P2_1/n$
$a = 17.3530$ (3) Å
$b = 21.8357$ (4) Å
$c = 21.2915$ (3) Å
$\beta = 96.502$ (1)°
$V = 8015.8$ (2) Å^3
$Z = 4$
$D_x = 1.434$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.24$ mm^{-1}
$T = 293$ (2) K
Prism, purple
0.41 × 0.37 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.723$, $T_{max} = 1.000$
(expected range = 0.369–0.511)
25728 measured reflections
14033 independent reflections
9834 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.124$
$S = 1.20$
14033 reflections
875 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0261P)^2 + 28.6662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.75$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}

All H atoms were included in calculated positions with C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl and $1.2U_{eq}(C)$ for the remaining H atoms. The methyl group of the acetonitrile molecule was allowed to rotate but not to tip. One of the Et_2O (C04—C03—O01—C01—C02) solvent molecules was refined using the following distance restraints: C—C = 1.50 (1) Å, C—O = 1.42 (1) Å and non-bonded distances C01···O03 = C02···O01 = C04···O01 = 2.35 (1) Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

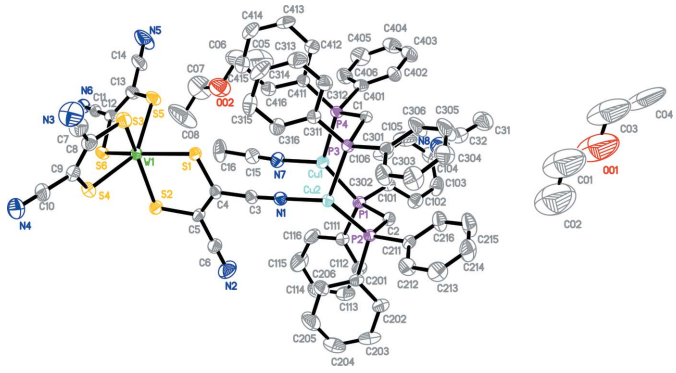


Figure 1
The asymmetric unit of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level and all H atoms have been omitted for clarity.

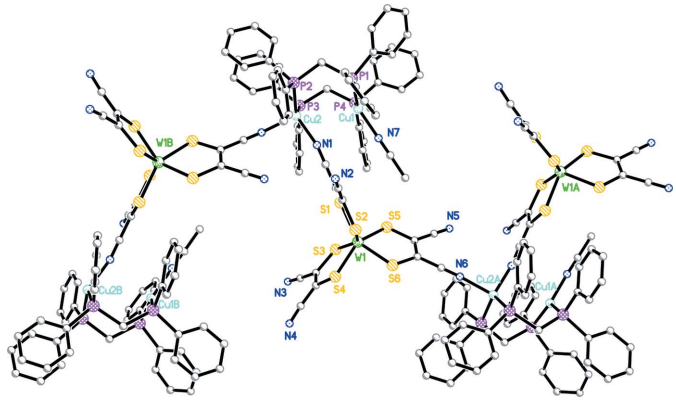


Figure 2
The zigzag structure of the title compound, viewed along the *c* axis of the unit cell; solvent molecules and H atoms were omitted. [Symmetry codes: (A) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (B) $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$.]

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