**PS07.02.14  CRISTAL STRUCTURE AND EPR DATA OF A**
**DINUCLEAR Cu(II) COMPLEX [Cu(N)_{2}(NCO)(C_{6}H_{5}N)]**

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The [Cu(N)_{2}(NCO)(C_{6}H_{5}N)] molecules are arranged as
centrosymmetric dimers in which two azide ligands bridge neighboring
ammonium ions in an asymmetric head-to-head fashion. The Cu(II) ion is
coordinated to five nitrogen atoms which form a distorted tetragononal
pyramid. At the pyramid base are the two N atoms of a dimethene molecule
[d(๊Cu-N)=2.08(1), 2.12(1) Å], an azide end atom [d(๊Cu-N)=1.99(1) Å] and
a NCO group [d(๊Cu-N)=1.95(1) Å]. At the pyramid apex is the
other ion, inversion related to the first one, azide N atom in the dimer
[d(๊Cu-N)=2.38(1) Å]. This Cu-N contact links the monomers within a dimer
providing a electronic path to transmit the superexchange coupling
between the Cu(II) neighbors. Unpaired electrons in neighboring
dimers are coupled y weak N-H-O contacts. Single crystal EPR data at X-band show that the
pair of nitrogen axes expected for neighboring, magnetically nonequivalent dimers, collapse into a single line, a signature of inter-
dimers superexchange-coupling. The observed crystal gyromagnetic tensor is used to disclose the
electronic and magnetic structure around Cu(II) ions. Metal Clusters

**PS07.03.01  CRISTAL STRUCTURE OF 6,9-BIS(4-
STILBAZOLE)-NIDO-DECABORANE(12), 6,9-(4-
PhC_{6}H_{4}C=)-
P_{2}B_{12}H_{12}{\text{H}}_{12}V. Alekseev, T.M. Polyanskaya, S.T. Dumene, E.A. Incik,
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A single-crystal X-ray study has been performed for the title
decaborane(14) derivative. The sample used was prepared by the
well known type of displacement reaction of (SM_{2})_2B_{12}H_{12} with
4-stilbazole and was recrystallized from hot dimethylformamide.

The most interesting feature of the compound is that four
crystallographically independent asymmetrical molecules exist in the
unit cell due to different arrangements of both the two cycle aromatic pyridine and phenol fragments and those in respect to the
three-dimensional aromatic B_{12}H_{12} nido-cluster.

The nitrogen atoms of pyridine are linked to the 6,9-boron
atoms on the open face of the B_{12} basket at the mean distance of
1.60 Å. The following mean bond lengths are B-B 1.80, C-N 1.33,
C-C 1.40 and 1.38 Å for Py and Ph, respectively.

Crystal data: dark red color, triclinic P1, a=11.285(1), b=13.061(2),
c=21.176(2) Å, α=85.37(1), β=102.26(1), γ=115.58(1)°, V=2750(7) Å^3, Z=4, D=1.165 g cm^{-1}, CAD-4, λ=MoKα.

As a solid, this compound exhibits a photoluminescence
(λ_{ex}=653 nm) with the quantum yield approximating that of
rhodamine 6G.

**PS07.03.02  INCOMPLETE CUBANES M_{2}X_{2}^{+}, Alan Hazell,*
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The structural formulae of the type M_{2}X_{2}^{+} and M_{3}X_{M}^{+}+(M=Mo,W;
X=O,S,M=Cu,Ni,Fe) are being studied as catalysts for homogeneous
hydrogenolysis of e.g.

\[ \text{CuH}_{2}S + 2H_{2} \rightarrow \text{CuH}_{10} + H_{2}S \]

The structures of two such compounds have been studied:

1. \( \text{NH}_{2}S_{2}K_{3}[\text{Mo}_{2}O_{4}](\text{CHOOH})_{3}\text{H}_{2}O \) (x = 0.80) and
2. \( 2 \text{K}_{2}[\text{W}_{2}S_{2}](\text{CHOOH})_{3}\text{H}_{2}O \) (x = 0.94).

1 is triclinic, space group P-1 with a = 11.011(2), b = 13.310(2), c = 9.993(1) Å, \( \alpha = 105.81(7)°, \beta = 91.65(7)°, \gamma = 88.340(1)^\circ \), Z = 2, R(F) = 0.026 for N = 3972 and N = 451. 2 is monoclinic, space group C2/m with a = 19.606(6), b = 14.348(7), c = 13.627(5) Å and \( \beta = 118.94(2)^\circ \), Z = 4, R(F) = 0.049 for N = 2656 and N = 226.

1 contains isolated \( \text{Mo}^{2+} \text{O}_{4} \text{CHOOH})_{3} \) ions with one of the for-
mate ions bridging two molybdenum atoms whereas in 2 all nine monodentate formate ions are bound to a W(IV)S_{2} cluster. In both com-
pounds there is a free formate ion. In 1 two of the cation sites are disor-
dered and are occupied by either potassium or ammonium ions. 2 is
either disordered or has a lower symmetry than C2/m, but refinement
in lower symmetry space groups did not give a lower R-value.

**PS07.03.03  SYNTHESIS AND STRUCTURE OF DI-
ACETATOBIS [DICARBONYLPYRAZOLORUTHENIUM(II)]
(Ru-Ru) By C. H. Huang1, T. H. Liu1, W. M. Lee2 and K. B. Shi1

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Nucleophilic substitution of \( \text{[Ru}_{2}(\text{CO})_{6} \text{(O}_{2} \text{CMe)}_{2} \text{(NMe}_{2})] \) with
excess pyrazole (HPz) gave almost quantitatively the title compound
\( \text{[Ru}_{2}(\text{CO})_{6} \text{(O}_{2} \text{CMe)}_{2} \text{(HPz)}_{2}] \)

X-ray structure of the compound was determined after crystal
dimensions of 0.30 x 0.35 x 0.45 mm had been selected. The cell dimen-
sions are a=8.332(1), b=9.5236(7), c=15.339(2) Å, \( \beta = 90.02(8), \gamma = 100.33(2), \) \( \mu_{\text{abs}} = 11.34 \text{mm}^{-1} \) with
centrosymmetric space group of P1 bar. The unit cell is
9820(2) Å^3 containing two molecules. Calculated density is
1.922 Mg m^{-3}. The linear absorption coefficient of the crystal is
1.55 mm^{-1}. Absorption corrections were made. The final R/Re factors
were 0.0260/0.042 for 3886 reflections with I>2\sigma(I) collected on a Nonius diffractometer, using the theta/2
theta scan mode. Weights based on
counting-statistics were used. The maximum shift/sigma ratio was
approximately 0.001. In the last difference Fourier
diagram, the deepest hole was -54 eÅ^3
and the highest peak 0.88 eÅ^3. The secondary extinction coefficient is
0.13(2). The Ru-Ru distance is
2.6746(6) Å. Both rutheniums have six bonds. The distances of Ru-O range from 2.110(2) to 2.136(2) Å, those of Ru-C span from 1.822(3) to
1.829(3) Å and those of Ru-N from 2.203(2) to 2.205(3) Å. The intramol-
ecular hydrogen bonds of N2-H...O4 and N4-H...O6 are 2.790(3) and
2.774(3) Å respectively, and help stabilize the crystal structure. The con-
formations and interactions of five member rings will be presented.