

(II) has a distorted square-pyramidal coordination, involving two bridging O and two N atoms from a bisN,N'-(salicylidene)-1,3-propanediaminato (SALPD) ligand as basal plane. One O atom from a dimethylformamide group for (I) and one O atom from a dioxane molecule for (II) complete the coordination number to five. The inner Cu ions have also irregular square-pyramidal environment, consisting of two bridging O atoms from a SALPD ligand, two bridging N atoms from two azido groups and one N atom from the third azido group. The Cu-N-Cu angles in the central azido bridges are 102.5(2)° for (I) and 102.1(3)° for (II). In (I) and (II), Cu-O-Cu angles in the O bridges have values 104.8(2)° and 105.6(2)°, respectively. The Cu-Cu distance in the azido bridge is 3.1462(7) Å for (I) and 3.1156(15) Å for (II). The Cu-Cu distances in the O bridges are 3.1501(7) Å and 3.1582(15) Å in (I) and (II), respectively. Crystal data is given below: (I) [Cu(N₃)₂Cu(C₁₇H₁₆N₂O₂)(C₃H₇NO)], Triclinic *P*-1, 9.211(1), 10.394(2), 12.941(1) Å, 77.831(1), 92.293(2), 71.104(1)°, $I_{obs} > 2\sigma(I) = 3194$, $R = 0.037$; (II) [Cu(N₃)₂Cu(C₁₇H₁₆N₂O₂)(C₄H₈O₂)], Monoclinic *P*2₁/*n*, 11.292(1), 15.413(1), 13.610(1) Å, $\beta = 97.402(5)^\circ$, $I_{obs} > 2\sigma(I) = 2575$, $R = 0.07$. Enraf-Nonius CAD-4, $\omega/2\theta$ scans, MoK α 0.71073 Å

Keywords: copper complexes, copper coordination compounds, structures of tetranuclear copper complexes

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Crystal structure of platinum 2-methyl- and palladium 2,4-dimethyl-8-hydroselenoquinolate

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In the course of study of complexing activity of 8-hydroselenoquinoline and comparative investigation of structure of analogous internal complexes platinum 2-methyl-8-hydroselenoquinolate Pt[C₉H₅(CH₃)SeN]₂ (I) and palladium 2,4-dimethyl-8-hydroselenoquinolate Pd[C₉H₄(CH₃)₂SeN]₂ (II) have been synthesized. The crystal structure of complex I and II is formed by neutral asymmetric molecules in which central atom is connected bidentatically (Se,N) with two 8-hydroselenoquinoline ligands. The presence of methyl groups in the position 2 causes the steric hindrance to the formation of planar complexes and gives use both to the changes in the structure of coordination polyhedrons: *trans*-square (2Se+2N) (I) and *cis*-square (2Se+2N) (II). The squares (2Se+2N) occur to be somewhat tetrahedrally distorted: the diagonal angles SePtSe 160.05(5)°, NPtN 178.06(38)° for (I), SePdN 163.08(14)°, 163.14(14)° for (II). Dihedral angles between the SeMN/SeMN coordination planes are 19.67(1)° (I) and 159.82(5)° (II), between quinoline planes - 94° (I) and 102° (II). The bonds M-Se are covalent. The transition of *trans*- to *cis*-coordination causes the weakening of the M-N bond only. The bond strength in the analogous complexes M(C₉H₆NSe)₂, M[C₉H₅(CH₃)SN]₂ (M=Pt, Pd) have been compared. Crystal data: I-Monoclinic, space group *P*2₁/*c*, *a*=12.5661(7), *b*=7.8072(5), *c*=18.6684(12) Å, β =97.328(2)°, *V*=1816.5(2) Å³, *Z*=4, $R=0.0629$, $wR2=0.1438$ for 4086 reflections; II-Monoclinic, space group *P*2₁/*n*, *a*=9.0092(4), *b*=16.3290(7), *c*=14.1073(6) Å, β =106.710(2)°, *V*=1987.7(2) Å³, $R=0.0499$, $wR2=0.1242$ for 4495 reflections (diffractometer Bruker-Nonius KappaCCD, λ MoK α).

[1] J. Ashaks, Yu. Bankovsky, D. Zaruma, I. Shestakova, I. Domracheva, A. Nesterova, E. Lukevics. *Chem. of Heteroc. Comp.*, 2004, 6, 905.

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Indenocorannulene: Molecular geometry, solid state packing, and metal binding

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Nonplanar polyaromatic hydrocarbons are unique molecules in which inside and outside surfaces exhibit different chemical and physical properties. Those include a novel class of bowl-shaped carbon-rich polyarenes that map onto the surfaces of fullerenes and therefore referred to as fullerene fragments or buckybowl. Systematic investigation of their properties is a new area of research that should stimulate the use of curved-surface carbon molecules in materials synthesis. Herein as part of our broad investigation of the structures and reactivity of bowl-shaped polyaromatic hydrocarbons we report the molecular geometry, solid state packing and ligating properties of indenocorannulene, C₂₆H₁₂. The structure of this polyarene will be compared with the parent corannulene and other buckybowl to evaluate effects of bowl size and curvature on the solid state packing. Then the reactivity of the curved unsaturated pi-carbon surface of indenocorannulene toward di- and trinuclear electrophilic metal complexes will be discussed. The structural effects of coordination on the geometry of bowl and metal complexes will be revealed.

Keywords: metal coordination compounds, arenes, intermolecular interactions and packing

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Quaternions, molecular motion and diffuse scattering

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For molecules which may be considered as independent rigid bodies oscillating with large angular amplitudes, the algebra of quaternions offers a neat method for calculating diffuse X-ray scattering [1]. This is because rotations may be combined in a relatively simple way. For an ensemble of independent angular simple harmonic oscillators with a Boltzmann distribution of energies, the probability distribution of angular displacements is Gaussian [2]. The latter distribution may be used to smear the molecular form factor to calculate the influence of librations on the X-ray scattering. The effect of translational vibrations may also be included by applying the well-known Debye-Waller factor, $[1 - \exp(-2M)]$, where *M* is proportional to the mean square displacement. Three globular molecular crystals of increasing molecular size have been chosen as examples to illustrate the method: sulphur hexafluoride (SF₆), adamantane (C₁₀H₁₆) and fullerene (C₆₀). In maps of diffuse X-ray scattering, librations tend to flatten peaks and to raise minima. This quaternion technique can be developed further for anisotropic librations and for larger molecular systems, such as proteins, in which whole assemblies of atoms may be moving through appreciable angles. We thank Dr Sandra Lonie and Dr Lucy MacNay for calculations of thermal motion.

[1] J S Reid, M Moore & L MacNay, *Acta Cryst.* A63 (2007)