New polynuclear Re-M cyanide complexes (M = Cu, Ag)

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New class of mixed-metal square-shaped polynuclear clusters based on rhenium(I) phosphine complexes have been obtained. The heteronuclear complexes are comprising of the core that consists of Re and Cu or Ag atoms bridged by cyanide ligands resulting in the formation of cyclic structure with approximate square geometry. In studied complexes Re atoms are located in vertices of the square, while Cu or Ag atoms along with coordinated CN' ligands form their sides.

Keywords: rhenium complexes, cyanide complexes, heteronuclear clusters

Figure 1. Structure of square-shaped \(\text{[Re(μ-CN)Ag(μ-NC)(CO)P]}_4\) unit in studied complex. The aromatic rings attached to phosphorus atoms in \(\text{PPh}_3\) groups are omitted for clarity.

**MS33-P2** New polynuclear Re-M cyanide complexes (M = Cu, Ag)

**MS33-P4** Disappearing Superstructure in Crystals of Pentaphosphaferrocene-Based Supramolecules

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Since 2002, we have being systematically investigating an inorganic analogue of ferrocene, pentaphosphaferrocene, \(\text{[Cp}^\text{R})\text{Fe(η}^\text{5-P}^\text{R})_5\] \((\text{Cp}^\text{R} = \text{η}^\text{2-CH}_{\text{R}}\text{C}_{\text{R}}\text{H})\). It showed an unprecedented ability to assemble in giant supramolecules [1-7] when reacted to Cu(I) halides (X = Cl, Br, I). These supramolecules reach 2.1–4.6 nm in size and can be isolated in astonishingly high yields. Their molecular structure is usually based on inorganic hollow cage, in which the \(\text{cyclo-P}_2\) ring of the \(\text{[Cp}^\text{R})\text{Fe(η}^\text{5-P}^\text{R})_5\] ligand is coordinated to single or various aggregated CuX units. The single-layered cages often follow fullerene topology involving single \(\text{CuX}\) units [1-4]. The multi-layered cages [1-2, 6] are constructed of \(\text{CuX}^\text{n}_{\text{m}}\) polynuclear fragments.

The X-ray structural analysis of these compounds faces many difficulties as low diffraction power, disorder in \(\text{CuX}^\text{n}_{\text{m}}\) halide core, disorder of guest molecules and \(\text{Cp}^\text{R}\) ligands. The disorder can be interpreted as formation of solid solutions of co-crystallizing supramolecules with different, but similar structure. In some cases, we observed superstructural effects pointing to partial ordering. The aging of the crystals in the mother liquor unexpectedly leads the superstructure to disappear. For example, the diffraction pattern of freshly prepared \(\text{[CH} \text{Cl}_\text{1})_{\text{14}} \times \text{[(Cu}^{\text{II}}\text{FeP}^{\text{III}}\text{]}_{\text{13}}\text{(MeCN)}_{\text{56}}\) demonstrates superstructural ordering accompanied with doubling of the triclinic unit cell (see figure 1, blue). In the supercell two crystallographically unique supramolecules are related by pseudo body-centering translation. While aging, the diffraction pattern shows as superstructural reflections gradually fade. The resulting subcell (figure 1, red) contains only one unique supramolecule [1]. Other examples will also be discussed.

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Keywords: pentaphosphaferrocene, supermolecule, crystallography
Anthracene derivatives have been widely studied during the last two decades as perspective materials for luminescence [1]. Moreover, anthracene derivatives have been intensively investigated as an attractive building block and starting material in OLEDs (organic light-emitting diodes), due to their unusual photoluminescence and electroluminescence properties [1]. Coordination compounds of Cu(II) and Zn(II) have been developed in vitro as promising materials for antimicrobial properties against Staphylococcus aureus, Bacillus subtilis, Escherichia coli, Pseudomonas aeruginosa etc... [2,3]. In this work, new coordination polymers of Zn(II) and Cu(II) based on new anthracene derivatives (Figure 1) will be presented combining both luminescent and antimicrobial properties. The ligand (L1) was already investigated with Ag(I) in our group. While the shift of emission and the decrease of eximer band are observed upon coordination to silver ion in crystalline form, amorphous nanowires showed a large emission band for this system [4]. Three coordination polymers of Cu(II) and three of Zn(II) were obtained with ligands L1 and L2 by slow liquid diffusion technique. Crystalline structures of coordination compounds were obtained from X-ray single crystal measurements, and solved by SHELX-97 program. Further luminescent and antimicrobial properties will be investigated.

References