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Structure and properties of \( \text{o-carboranylalcohols} \) pyridines metal complexes
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The recently reported series of \( \text{o-carboranylalcohols} \) bearing pyridine substituents [1] opens a new door to the synthesis of very attractive carborane based transition metal complexes (Figure). The two different functionalities (OH and N) together with the chance to vary the nitrogen position along the aromatic ring, the metal, as well as the hydrophobic icosahedral heteroborane cluster, give place to compounds which exhibit different structural architectures and properties.

When an ethanolic or acetone solution of \( \text{o-carboranylalcohols} \) pyridine or quinoloyne derivatives is mixed with a solution containing the desired metallic ion, the corresponding complexes are obtained (Figure). The electronic transfer can be evidenced by the change in the metal-ligand bond length [4] or in some cases only in the bond lengths within the organic ligand. Typical examples of such systems are coordination compounds of Co and ligands like quinolones [4].

Few works investigating the electronic transfer in compounds formed by naphthoquinones and transition metal ion have been reported so far. The reasons concerning electron transfer in this compounds are discordant [5,6].

In this work we present synthesis and characterization of \([\text{Co(Law)}(\text{Im})_2]_2\) \(\text{C}_7\text{H}_6\text{C}_8\text{H}_4\) \([\text{Co(Law)}(\text{Phen})_2](\text{C}_7\text{H}_5\text{O})_2, \) \([\text{Co(Law)}(2,2\text{-Dipy})]_2\) and \([\text{Co(Law)}(2,2\text{-Dipy})]\) \(\text{C}_7\text{H}_5\text{C}_8\text{H}_4\), where Law stands for 2-hydroxy 1,4 naphthoquinone or Lawsone. The compounds were isolated after evaporation or slow cooling of solvents and later characterized with elementary analysis, atomic absorption and IR spectroscopy. Single crystal X-ray diffraction experiments performed in the temperature range between 120 K and 150 K allowed the structural determination of compounds. The average bond lengths for \(\text{Co-N} \) (2.10(2) Å) and \(\text{Co-O} \) (2.10(6) Å) found in all investigated structures are typical of \(\text{Co}^\text{II} \) L. The typical bond lengths for \(\text{Co}^\text{II} \) L in the systems that present electron transfer should be 0.1-0.15 Å shorter than \(\text{Co}^\text{II} \) bond length [4]. Furthermore the \(\text{Co-O} \) length value (1.22(1) Å) suggests a double bond in naphthoquinone [7]. Thus, in the investigated temperature range, the X-ray diffraction results did not show any evidence of charge transfer between Co-naphthoquinone complexes.

The compound \([\text{Co(Law)}(2,2\text{-Dipy})]\) formed both a unsolvated and a solvated structure with toluene. The solvated structure crystallizes in triclinic symmetry while the unsolvated crystal structure is orthorhombic. A number of weak intermolecular interactions like \(\text{C}_7\text{H}_5\text{H}^-\text{O} \) can explain the difference in the crystal packing.

Additional X-ray diffraction as well as spectroscopy studies at temperatures down to 10 K will be performed to investigate the presence of electron transfer in Co-naphthoquinone complexes.

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Keywords: crystal engineering, magnetic properties, heteroborane clusters

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Poster Sessions

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Crystallographic study of labile systems: Cobalt and lawsons complexes
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The two different functionalities (OH and N) together with the chance to vary the nitrogen position along the aromatic ring, the metal, as well as the hydrophobic icosahedral heteroborane cluster, give place to compounds which exhibit different structural architectures and properties.

When an ethanolic or acetone solution of \(\text{o-carboranylalcohols} \) pyridine or quinoloyne derivatives is mixed with a solution containing the desired metallic ion, the corresponding complexes are obtained (Figure). The average bond lengths for \(\text{Co-N} \) (2.10(2) Å) and \(\text{Co-O} \) (2.10(6) Å) found in all investigated structures are typical of \(\text{Co}^\text{II} \) L. The typical bond lengths for \(\text{Co}^\text{II} \) L in the systems that present electron transfer should be 0.1-0.15 Å shorter than \(\text{Co}^\text{II} \) bond length [4]. Furthermore the \(\text{Co-O} \) length value (1.22(1) Å) suggests a double bond in naphthoquinone [7]. Thus, in the investigated temperature range, the X-ray diffraction results did not show any evidence of charge transfer between Co-naphthoquinone complexes.

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Additional X-ray diffraction as well as spectroscopy studies at temperatures down to 10 K will be performed to investigate the presence of electron transfer in Co-naphthoquinone complexes.

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Keywords: valence tautomerism, naphthoquinones, cobalt complexes

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