☒ **Talk** ☒ **Poster**

New Schiff Base Ligands for the Remediation of Environmental Heavy Metal

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Background and Aim

Corrosion and waste products from shuttered industrial plants are contaminating food and waterways in once thriving communities. Mercury, cadmium and arsenic are major culprits. No amount of these in the body is safe. Accumulation of heavy metals damages tissues and organs. Metal accumulation is propagated through food and fish with devastating public health and economic consequences. Chelation can be used for environmental remediation. Agents such as EDTA are not easily degradable and can persist in the environment. There remains a need for better chelating agents as antidotes to metal poisoning [1].

Methods

We examined Schiff base ligand 2-benzoylpyridine-4,4-dimethyl-3-thiosemicarbazone (**Lig1**) and a new derivative 1-{[2-phenyl-1-(pyridin-2-yl)ethylidene]amino}-3-(prop-2-en-1-yl)thiourea (**Lig2**) for their efficacy in chelating cadmium using mass spectrometry, nuclear magnetic resonance, infrared spectroscopy and X-ray diffraction [2, 3].

Results

Lig1 coordinates cadmium in an efficient 1:1 ligand to metal ratio - in contrast to structure BI-HTAQ in Cambridge Structural Database that required two ligand molecules to a cadmium ion. The cadmium-bound complex of **Lig2**, 1-{[2-phenyl-1-(pyridin-2-yl)ethylidene]amino}-3-(prop-2-en-1-yl)thiourea, however, yielded two distinct monomeric cadmium-bound ligand complexes together with a dimeric cadmium-bound complex in the asymmetric unit. The cadmium centers in the dimer are connected by a dichloride bridge in a Cd_2Cl_2 metallacycle. The cadmium ions in the two monomers are independently coordinated by a chloride anion in a terminal bridge. **Lig2** shows considerable conformational freedom. Mass spectrometry analysis on the reaction product yielded species consistent with metal bound complexes of the ligand and simple higher order species. The assembly of the metal coordinated complexes of **Lig2** is maintained through two nonsymmetric hydrogen bonds between the dimeric structure and the monomers.

Conclusions

The coexistence of both monomeric and dimeric metal-bound complexes in the same unit cell is unexpected. This has implications for catalysis - and a potential for clustering that might enhance heavy metal chelation.

References

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