H-bonding in complexes of chelating ligands with ureayl and guanidinyl functional groups

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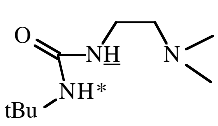
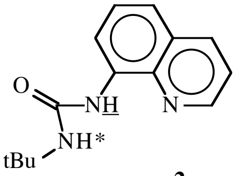
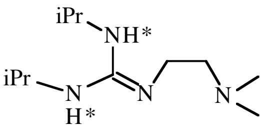
We report the syntheses of, and investigations of metal binding by, several new chelating ligands containing *N'*-alkyl-*N*-ureayl or *N',N"*-dialkyl-*N*-guanidinyl functional groups. These groups are potentially useful for catalyzing reactions of O_2 because they provide steric bulk and second-coordination sphere H-bonding opportunities (for instance, see MacBeth, et al., *Science* **2000**, *289*, 938-941). Three such ligands are shown below.



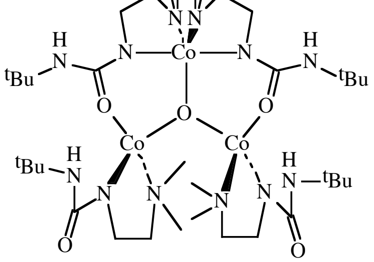
H_2L^1



H_2L^2



H_2L^3



$Co_3(O)(HL^1)_4$

We report the coordination properties of these ligands with cobalt(II) and nickel(II). UV:vis spectroscopic studies (Job's plots) in dimethylacetamide of the reaction between $Co(OAc)_2$ and KHL^1 reveal the formation of complexes with several different cobalt:HL^1 stoichiometries including 1:3 and 3:4. The structure of the 3:4 cluster has been determined and is shown above; the three cobalt(II) ions each bind to a central oxo ligand that presumably arises from adventitious water in the solvent.

RCS is grateful for support from the Andrew W. Mellon Foundation (New Directions program) for a sabbatical year spent in part at the University of Kansas.