Bis(1-alkylimidazol-2-yl)propionates: Biomimetic N,N,O ligands

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The 2-His-1-carboxylate facial triad has recently emerged as a common structural motif for the activation of dioxygen by non-heme iron (II) enzymes. [1a] Two histidine residues and a carboxylate from either glutamate or aspartate occupy one face of the iron coordination octahedron, leaving the other three sites available for the binding of exogeneous ligands such as dioxygen and the substrate. This flexibility at the active site is reflected in the wide range of oxidative transformations catalyzed by these enzymes. The same facial capping by two histidines and one carboxylate is found in several zinc containing enzymes, e.g. carboxypeptidase and thermolysin, enforcing tetrahedral coordination geometries. [1b]

This facial triad is an interesting target for structural and functional modeling. Suitable structural mimics of this triad should preferably be tridentate, tripodad, and monoanionic ligand systems with a potentially facially coordinating N,N,O donor set. Recently, we developed a relatively straightforward, high yielding, two-step route for the synthesis of a class of new N,N,O ligands, incorporating biologically relevant imidazole-groups as the N donors. [2] Here we report on our recent studies on the coordination chemistry of these N,N,O ligands and on the reactivity of their metal complexes.


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