A MnSOD Structural Model Complex Employing a Pyrazole-containing Ligand

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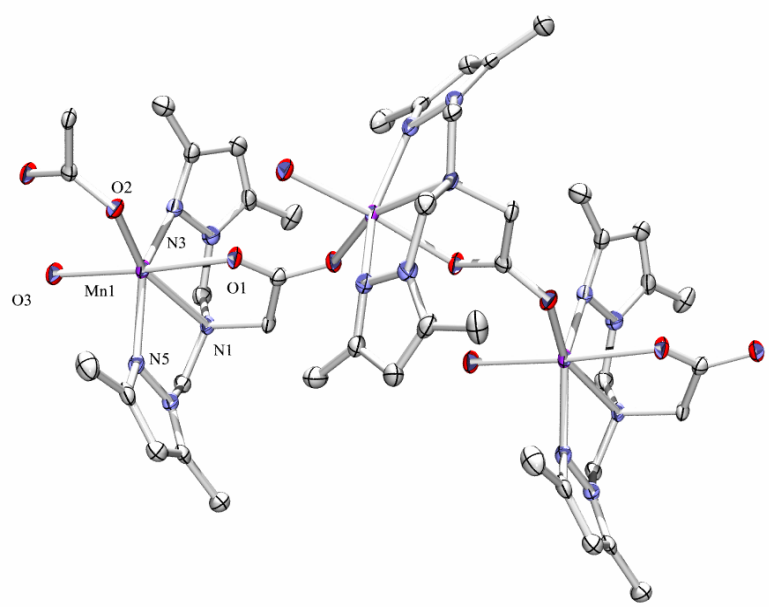
Superoxide Dismutases (SODs) are a class of metalloenzymes able to catalyse the dismutation of superoxide radicals into hydrogen peroxide using transition metals as cofactors. MnSODs have been structurally characterized and their active sites are composed by a Mn^{III} ion coordinated to three histidines, one aspartate and a hydroxo group. Attempting to model MnSODs we have designed a tripod N_3O-donor ligand containing pyrazole and carboxylate pendant arms (KBPZG: potassium *N, N*-bis(3,5-dimethylpyrazolylmethyl)glycinate), which was used to obtain a new Mn^{II} complex (**1**). Complex **1** was characterized by X-ray crystallography and EPR spectroscopy. In this complex, the Mn^{II} ion is hexacoordinated and arranged in a chain, as observed in the figure below. X-band EPR data at 4.5 K show a six line spectrum at $g \sim 2.03$ characteristic of mononuclear Mn^{II} centers. This fact indicates the chain structure is broken in solution, which was confirmed by ESI mass spectrometry. Finally, we have synthesized and characterized a new Mn^{II} complex that structurally mimics the active site of MnSODs enzymes.



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