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Data Article

Experimental data on synthesis and characterization of chiral dinuclear manganese (II-II) compounds as biomimetic models of the active center of catalase

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ABSTRACT

Dinuclear manganese (II– III) compounds, which are potential models of the active center of catalase, were synthetized. This type of metalloenzymes presents biological importance due to three factors: they are redox catalyst centres, they are able to carry out hydrolytic reactions and they participate in activated processes via Lewis acids. Structurally, their active centre is composed by dinuclear manganese compounds, linked to nitrogen and oxygen donor atoms. An octahedral geometry around the metal ions were found, with acetate, hydroxy and aquo ligands; which can work as molecule bridges between them. The acid medium favours the electronic transfer between Mn^{3+} - Mn^{2+} as redox centre at 1.559 V and the consequent oxidation of hydrogen peroxide or organic molecules. The work also reports the data of two chiral novel compounds, $[Mn_2(S,S(+)Hcpse)_4(NaClO_4)_2(NaOH)(CH_4O)]_n\cdot[(C_2H_6O)_2]_n\cdot[(CH_4O)_2]_n$ and its respective enantioisomer, in which μ-oxo being as bridge metal centre. The X-ray structural was obtained as well as the optical and magnetic properties using Circular Dichroism,

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Electronic Paramagnetic Resonance, Magnetic Susceptibility and X-ray photoelectron spectroscopy.

Specifications Table

Subject	Inorganic Chemistry
Specific subject area	Bioinorganic chemistry, Science Materials
Type of data	Tables and Figures
How data were acquired	X-ray crystallographic study (DRX) Valence metal centres (XPS) Chiral activity (Circular dichroism) Electrochemical study (Voltammetry cyclic) Magnetic properties (Susceptibility magnetic at variable temperature)
Data format	Raw
Parameters for data collection	The data shown in this article are obtained from the methanol synthesis of the tridentate ligand - N acetyl pseudoephedrine with manganese (II), as structural biomimetic models of catalase and peroxidases. Likewise, its structural (X- ray crystal), optical (CD spectra), electronic (electrochemical analyses) and magnetic (EPR and susceptibility magnetic) characterization was carried out.
Description of data collection	The data collection was obtained of the synthesis and crystal structures of two manganese (II) complexes containing chiral aminoalcohols (*R,R* (−)H_2cpse) and (*S,S* (+) H_2cpse). The 1:1 reaction between $Mn(CH_3COOH)\cdot 4H_2O$ and ligands, followed by the addition of NaOH and $NaClO_4$ in methanol afforded the polymeric compounds. In solution, a change of the oxidation state of the manganese ion was observed using voltammetry cyclic and circular dichroism in comparison with XPS, which will serve to understand the electronic exchange in dissolution when using these models as catalase or peroxidases.
Data source location	Institution: Universidad Santiago de Cali City/Town/Region: Santiago de Cali Country: Colombia
Data accessibility	The data are found only in this article.

Value of the Data

- The new chiral ligands with manganese (II) reported are new interesting biomimetic models of metalloenzymes such as catalases. The characterization of these synthetic models emulating biological processes allows the design of new structures and to test experimentally the models reported here.
- Data can be used to compare the stability of the biomimetic compounds in solid state and in solution.
- Data are useful in the study of the mechanism of chiral compounds action in oxidases, which oxidize organic molecules and substrates such as hydrogen peroxide with several potential applications in water treatment and decorating dyes among others.
- These data show molecules that are related to enantioselective synthesis, where the metallic centre and the chiral ligand provide important optical properties that can affect intermolecular interactions in processes associated with metalloenzymes, such as: manganese peroxidases and catalase manganese.

1. Data

The data files of $[Mn_2(S,S(+)Hcpse)_4(NaClO_4)_2(NaOH)(CH_4O)]_n\cdot[(C_2H_6O)_2]_n\cdot[(CH_4O)_2]_n$ and its respective isomer showed that in solid state the asymmetric unit is composed by a dinuclear manganese (II) entity, Tables 1–3; likewise Hydrogen Bonds (°) and distances (Å) in Table 4 and Figs. 1–3. These structures showed similar coordination to metal center, as in metalloenzimes catalases. This was confirmed by X-ray crystal analysis, Fig. 4; spectra XPS, Fig. 5 and Fig. 6; and their antiferromagnetic properties, Fig. 7. Furthemore, in solution the electrochemical characterization indicated that the