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“Structural and Magnetic Susceptibility Study of an Octanuclear Mn^{III}-Oxo-Pyrazolido Complex”

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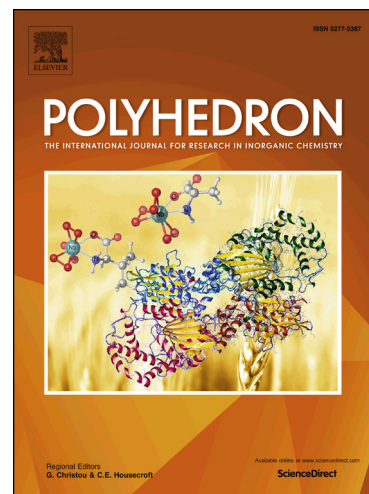
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“Structural and Magnetic Susceptibility Study of an Octanuclear Mn^{III}-Oxo-Pyrazolido Complex”

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Dedication:

Dedicated to Professor Spyros Perlepes with our best wishes for a happy 65th birthday.

Abstract

A novel octanuclear Mn^{III} bimodal motif, {3².4}{3⁴.4⁶}, has been recognized in the crystal structure of [Mn^{III}₈(μ₃-O)₄(μ-pz)₈(μ-OMe)₄(OMe)₄] (**2**). Its magnetic analysis, by fitting magnetic susceptibility data, guided by DFT calculations, has revealed both strong ferromagnetic (+7.6 cm⁻¹) and antiferromagnetic exchange (-9.3 cm⁻¹) between Mn^{III} centers of the inner Mn₄O₄-cubane core and antiferromagnetic exchange (-8.4 cm⁻¹ and -0.08 cm⁻¹) between the four cubane and four outer Mn centers, resulting in a diamagnetic ground state.

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