

## NOTES

一个新型氢氧根桥联的双核铬(III)配合物 $[\text{Cr}(\text{saltn})\text{OH}]_2 \cdot 4\text{H}_2\text{O}$ 的合成、结构与磁性

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摘要 合成了一个新型氢氧根桥联的反铁磁耦合双核铬(III)配合物 $[\text{Cr}(\text{saltn})\text{OH}]_2 \cdot 4\text{H}_2\text{O}$

$[\text{H}_2\text{saltn} = N,N'\text{-bis}(\text{salicylidene})\text{trimethylenediamine}]$ , 并对其晶体结构和磁性进行了研究。该配合物为三斜晶系,  $P-1$ 空间群, 晶胞参数为 $a=0.95828(19)$  nm,  $b=0.95926(19)$  nm,  $c=1.0437(2)$

nm,  $\alpha=86.77(3)^\circ$ ,  $\beta=82.48(3)^\circ$ ,  $\gamma=64.93(3)^\circ$ 。每个铬(III)离子处于畸变八面体配位环境。由于晶体对称性的需要, 桥联的 $\text{Cr}_2\text{O}_2$ 单元在一个平面内。桥联的Cr-O-Cr'键角是 $99.94(16)^\circ$ , Cr...Cr'间的距离是0.3019

nm。测定了配合物在2-300 K的变温磁化率, 并应用自旋-自旋耦合模型对 $S_1=S_2=3/2$ 双核体系进行了拟合,

得到最佳拟合参数 $g=2.01(1)$ ,  $J=-0.85(2)$   $\text{cm}^{-1}$ 和 $zJ'=0.18(3)$   $\text{cm}^{-1}$ , 结果表明该双核铬配合物金属离子间存在弱的反铁磁自旋交换作用。

关键词 [铬\(III\)](#), [双核配合物](#), [合成](#), [晶体结构](#), [磁性](#)

分类号

## A New Hydroxo-bridged Chromium(III) Dimer $[\text{Cr}(\text{saltn})\text{OH}]_2 \cdot 4\text{H}_2\text{O}$ : Synthesis, Crystal Structure and Magnetic Properties

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**Abstract** A new hydroxo-bridged dimeric Cr(III) complex  $[\text{Cr}(\text{saltn})\text{OH}]_2 \cdot 4\text{H}_2\text{O}$  [ $\text{H}_2\text{saltn} = N,N'\text{-bis}(\text{salicylidene})\text{tri-methylenediamine}$ ] has been synthesized and its structural and magnetic properties have been investigated. The complex crystallizes in the triclinic space group  $P-1$  with one dimeric formula unit in a cell of dimensions  $a=0.95828(19)$  nm,  $b=0.95926(19)$  nm,  $c=1.0437(2)$  nm,  $\alpha=86.77(3)^\circ$ ,  $\beta=82.48(3)^\circ$ , and  $\gamma=64.93(3)^\circ$ . The geometry around each chromium (III) center is six-coordinate, distorted-octahedral. The bridging  $\text{Cr}_2\text{O}_2$  unit is strictly planar, as required by the crystallographic symmetry. The Cr-O-Cr' bridging angle is  $99.94(16)^\circ$ , and the distance between Cr...Cr' is 0.3019 nm. The magnetic susceptibility of the complex has been examined in the range of 2—300 K. By using the spin-spin coupled model for an  $S_1=S_2=3/2$  dimeric system ( $\hat{H}=-2\hat{S}_1\hat{S}_2$ ), the magnetic data were fitted to give the parameters of  $g=2.01(1)$ ,  $J=-0.85(2)$   $\text{cm}^{-1}$ , and  $zJ'=0.18(3)$   $\text{cm}^{-1}$ , indicating the presence of a weak anti-ferromagnetic spin-exchange interaction between the Cr(III) ions in the binuclear complex.

**Key words** [chromium](#) [dimer](#) [synthesis](#) [crystal structure](#) [magnetic property](#)

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