XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Structural and magnetic characterization of a new oxalate complex of ruthenium(III)

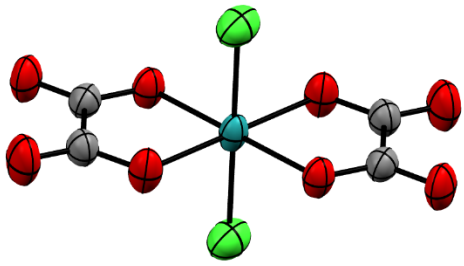
Federico Mesa[1], Carolina Pacheco[1], Lorena Matinez[1], Nicolás Veiga[1], Javier Gonzalez-Plata[2], Carlos Cruz[3], Verónica Paredes-García[3] and Raúl Chiozzone[1]

[1]Area Química Inorgánica, DEC, Facultad de Química, Universidad de la República, Montevideo, Uruguay
[2] Departamento de Física Fundamental II, Universidad de la Laguna, Tenerife, Spain
[3] Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andrés Bello, Santiago, Chile
fmesa@fq.edu.uy

Thematic Area: Materials Chemistry

Keywords: Molecular magnetism, ruthenium, coordination complex

Ruthenium(III) coordination compounds have been of great interest in several fields, including molecular magnetism due to the fact that 4*d*-based building blocks can be used for constructing intriguing polynuclear magnetic molecules [1,2]. In this work, *trans*-$[PPh_4]_2[RuCl_2(ox)(Hox)]\cdot 5H_2O$ (ox = oxalate) has been obtained in a one-pot microwave-assisted hydrothermal synthesis, directly from $RuCl_3\cdot xH_2O$, oxalic acid and potassium oxalate. In DMF solution, a quasi-reversible redox couple is observed with E^o = 340 mV vs Ag/AgCl. Single-crystal XRD shows that the compound crystallizes in a triclinic P-1 space group, where the $[Ru(ox)(Hox)]^{2-}$ anions are located in the four vertices and the centre of the unit cell. These anions and the water molecules of crystallization are arranged in parallel planes, layered by the PPh_4^+ cations, the entire structure being stabilized mainly by hydrogen bonds. The minimum distance between metallic centres is 9.77 Å. Static magnetic measurements show that $\chi_M T$ at room temperature is equal to 0.73 cm^3 K mol^{-1}, and upon cooling this value remains practically constant until 8 K. This is in good agreement with the expected behavior for an isolated ruthenium(III) mononuclear complex. Dynamic magnetic measurements reveal field-induced slow relaxation of magnetization below 8.5 K under a dc field of 1 kOe. The relaxation turns out to be a combination of Raman and direct processes.



ORTEP-type drawing of $[RuCl_2(Hox)(ox)]^{2-}$ with thermal ellipsoids plotted at 50% probability level

Acknowledgments: Comisión Sectorial de Investigación Científica (CSIC-Udelar) and Prof. Lucía Otero for her contribution in the discussion of cyclic votammetry results.

References

(1) D. Zhang, L. Zhang, Y. Chen, H. Wang, Z. Ni, W. Wernsdorfer and J. Jiang, Chem. Commun., 2010, 46, 3550.
(2) S. Langley, D. Wielechowski, V. Vieru, N. Chilton, B. Moubaraki, L. Chibotaru and K. Murray, Chem. Commun., 2015, 51, 2044.