Joint meeting

VII Latin American Crystallographic Association

and

XXVII Brazilian Crystallographic Association

BOOK OF ABSTRACTS

October 14 to 17, 2025

Fortaleza, Brazil

Effects of halogen substitution on a new Ru(II)-arene complex stabilized by N-H···Cl interactions

C. B. Pinto[1,2], P. H. O. Santiago[1], J. Ellena[1]

[1]São Carlos Institute of Physics, University of São Paulo, São Carlos, SP, Brazil, [2]Institute of Chemistry, São Paulo State University, Araraquara, SP, Brazil
camila.batista@unesp.br

Hydrazides are a class of compounds known for their antimicrobial, anti-inflammatory and anticancer activities, among others [1]. The coordination of these compounds with Ru might enhance its properties, given that biological studies with Ru complexes have shown to increase the biological activity of a variety of ligands (*e.g.* [2]). In addition, halogen atoms are important in molecular recognition processes and in the binding of small molecules to receptors [3]. In this context, here we describe the synthesis and characterization of a new Ru-arene complex (*C1*), presenting 2-fluorobenzhydrazide (*L1*) as ligand. The interactions involving halogen atoms (F and Cl) are explored and compared with those in an analogue compound presenting a -OH group in the *para*- position of the ligand [4].

The reaction synthesis consisted of mixing a solution of dichloro(*p*-cymene)ruthenium(II) dimer to a solution of *L1* in dichloromethane under stirring. The reaction mixture was then filtered and left to evaporate under ambient conditions. Yellow single-crystals were formed and used for the X-ray diffraction experiment, which was performed on a XtaLAB Synergy-S diffractometer, using Cu Kα radiation at 200 K. Infrared spectra was also acquired for both *C1* and *L1*.

Compound *C1* is comprised of a Ru(II) center, coordinated with one Cl, one *p*-cymene and one *L1* ligand, crystallizing in the triclinic space group $P\bar{1}$. The coordination of *L1* to the Ru center happens in a bidentate mode through the oxygen and the nitrogen from the terminal -NH_2 group. The structure is also corroborated by the IR spectra, which indicates all expected shifts associated with the coordination. The structure is mainly stabilized by non-classic H-bonds, of N-H···Cl type, between *L1* and the Cl counter-ion, C-H···Cl and C-H···F contacts. However, through Hirshfeld Surfaces (HS) it is possible to see other interactions involving halogens, such as, π···F (on the fluorobenzene ring) and a very small amount of Cl···F contact. While in the analogue structure from literature, the HS indicates the presence of a π···Cl contact involving the *p*-cymene group and the counter-ion, along with N-H···Cl, C-H···Cl and O-H···Cl contacts.

In conclusion, the use of HS allowed identification of halogen interactions, which could be one of the directional forces shaping the solid-state conformation and packing of the compounds. The Hirshfeld Atom Refinement is being undertaken in order to explore these interactions.

[1] Popiołek, Ł. (2016). Med Chem Res., 26(2), 287–301.
[2] Teixeira, T. *et al*. (2025). Inorg. Chem., 64(8),3707-3718.
[3] Thomas, S. P. *et al*. (2022). Molecules, 27, 3690.
[4] Lapasam, A. *et al.* (2021). J. Coord. Chem., 74(14), 2365-2379.

Keywords: Hydrazide; Intermolecular Interaction; Hirshfeld Surface

The authors are grateful to Brazilian Funding Agency FAPESP (grant # 2023/10889-7, 2021/10066-5 and 2017/15850-0).