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Ru(II) organometallic complexes containing aroylthiourea ligands: Synthesis, characterization, and antibacterial activity

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Thiourea-based compounds have several medicinal uses[1] and ruthenium organometallic complexes with this ligand have potential as cytotoxic agents due to ruthenium's unique properties, such as ligand exchange rates, oxidation states, and its ability to mimic iron in binding with certain biomolecules[2]. In this sense, the present work reports the synthesis and characterization of Ru(II) organometallic complexes containing aroylthiourea ligands, leading to three new series of complexes with the general formula: [Ru(HL-κ*S*)(Cl)$_2$] **(1a-1d)**, [Ru(HL-κ*S*)$_2$(Cl)]BF$_4$ **(2a-2c)** , [Ru(HL-κ*O*,*S*)Cl] and [Ru(η^6-*p*-cym)(HL-κ*O*,*S*)$_2$] **(3a;3d)**, where **L**= *N*-benzoyl (*N',N'*-diethylthiourea) **(a)**, *N*-benzoyl(*N',N'*-diisobutylthiourea) **(b)**, *N*-benzoyl(*N',N'*,-morpholylthiourea) **(c)** and *N*-benzoyl(*N',N'*-dibenzylthiourea) **(d)**. In series 1, the ligand acts as a monodentate (κ-*S*) donor, while in series 2, two ligands act as a monodentate (κ-*S*) donor, forming cationic species after the addition of the BF_4 or PF_6 counterion. Series 3 consists in complexes where the ligand is coordinated in a bidentate (κ-*O,S*) fashion. The complexes of this class are formed from the crystallization of series 1 complexes in a DCM/MeOH solvent mixture. For this series, only the complexes containing the ligand (a and d) were isolated. Furthermore, an antibacterial evaluation of the precursor, ligands, and complexes was conducted against *Gram-positive* bacteria (*S. aureus* and *S. epidermidis*) and *Gram-negative* bacteria (*E. coli*). It was observed that the complexes exhibit significantly higher antibacterial activity when compared to the precursor, free ligands or tested antibiotic reference. Complexes 1a and 2a presented the lowest MIC values demonstrated more efficient antibacterial activity. In contrast, when irradiated with blue light, there was no difference in the antibacterial test results, despite the electronic spectroscopy study showing the formation of another species. This newly formed species likely has no antibacterial activity. Figure 1 depicts the molecular structure of **1a**, **2a** and **3a** respectively

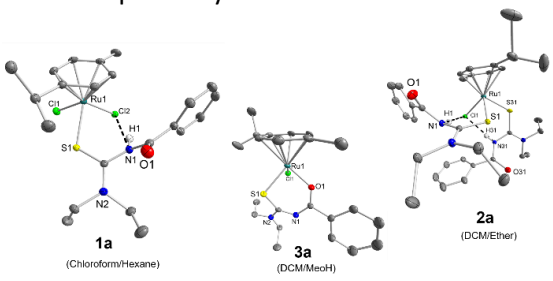

Figure 1. Molecular structures of complexes **1a**, **2a** and **3a**. Hydrogen atoms are omitted in both projections except for *N-H* bond. In (2a) contraíon is omitted.

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