

Poster Presentation

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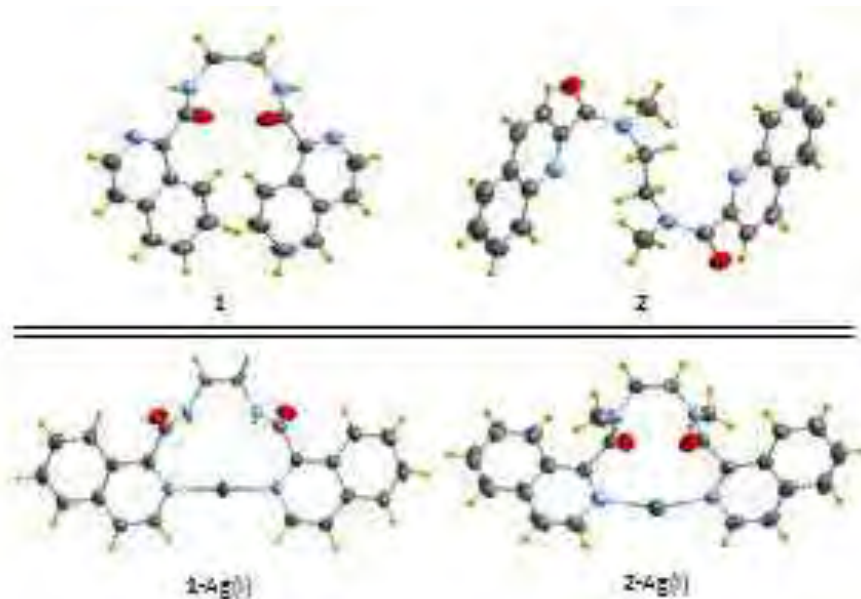
New Ag(I) Coordination Complexes Based on Bis(1-isoquinolinecarboxamide)ethane.

N. Parra¹, J. Belmar¹, C. Jiménez¹, J. Pasán², C. Ruiz-Pérez²

¹Universidad de Concepción, Departamento de Química Orgánica, Concepción, Chile, ²Universidad de la Laguna, Departamento de Física Fundamental II, Santa Cruz de Tenerife, España

Crystal Engineering is an interdisciplinary research area that involves chemists, physicists, biologists and materials scientists.¹ It is an important field inside Supramolecular Chemistry which has been considered as a new form of synthesis, named Supramolecular Synthesis.² It is known that important properties in molecular solids are closely related with the way that molecules are aggregated in the condensed phase. Consequently, the ability to control the molecular association in the crystal packing could offer control over specific properties and potential applications. Because of that, the main goal of Crystal Engineering is the rational design and synthesis of functional materials using the nature of the intermolecular forces as a toolkit. Our strategy is the systematic study of non-covalent forces in homologous series.³ In this work our interest is focused on the study of crystal packing of two homologous ligands N,N'-bis(1-isoquinolinecarboxamide)-1,2-ethane (1) and N,N'-dimethyl-N,N'-bis(1-isoquinolinecarboxamide)-1,2-ethane (2) and their Ag(I) coordination complexes. The compound 1 consists of two isoquinoline rings and one ethylene bridge linked by amide functional groups. Compound 2 is the result of the N-methylation of 1. The main difference in the molecular structures is that while 1 present a gauche conformation in the 1,2-ethanediamine bridge (60°) 2 present a staggered conformation (180°). Curiously, in spite of this fact, the Ag(I) complexes in both cases present a small torsion angle of 45° 1-Ag(I) and 65° 2-Ag(I). These orientations allow the torsion of the isoquinoline moiety and the formation of homonuclear OD coordination complexes, over the 1D coordination polymer expected. The main intermolecular interaction in 1 is the amide-to-amide hydrogen bond that is replaced by a weak CH...O interaction in 2. On the other hand, both Ag(I) complexes use the nitrate counteranion to build a chain using NH...O(nitrate) in 1 and CH(quinoline)...O(nitrate) in 2. Acknowledgment: Grant DIUC 212.023.049-1.0

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