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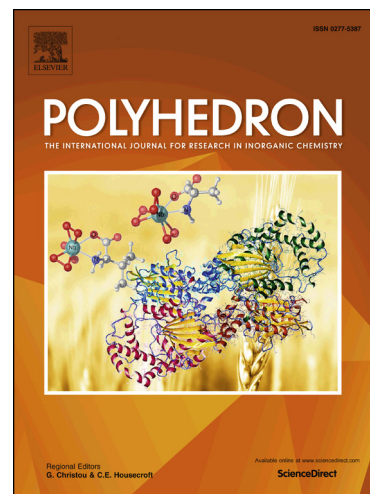
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Noncovalent Interactions and Photophysical Properties of New Ag(I) Complexes With 4-Amino-2,1,3-Benzothiadiazole

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ABSTRACT

New silver complexes $[\text{AgL}(\text{NO}_3)]_n$ (**1**), $[\text{AgL}_2(\text{NO}_3)]_n$ (**2**) and $[\text{AgL}_3(\text{NO}_3)]_2$ (**3**) (L = 4-amino-2,1,3-benzothiadiazole) were obtained as single-phase products of the reactions of AgNO_3 with L by varying their ratio. The structures of **1–3** were established by single-crystal X-ray diffraction and contain $\{\text{Ag}_2\text{L}_2\}$ units, where L acts as a bridging ligand. The other metal coordination sites are occupied by O atoms of nitrates and N atoms of L ligands. Several types of strong and weak L–L and Ag–L interactions in the complexes are discussed herein, supported by quantum chemical calculations. Differences in the structures of the complexes cause significant changes of the photoluminescence intensity: no emission for **2** and noticeable for **1** and **3**. However, similar values of luminescence maxima for **1** and **3** (630 and 620 nm, respectively) result in red emission for both compounds. Structural, topological, and spectroscopic findings are interpreted on the basis of state-of-the-art quantum mechanical calculations.

INTRODUCTION

Molecular materials containing a 2,1,3-benzothiadiazole (BTD) core attracted considerable attention over the last decade, mainly due to its electron-withdrawing properties [1-3] and high luminescence efficiency of its derivatives.[2, 4, 5] These properties have given rise to multiple studies on their potential applications as chemosensors,[6] electron-transporting layers in organic light-emitting diodes,[7, 8] fluorescent materials,[9, 10] as elements of photovoltaic cells,[11-15] fluorescent probes in biomedicine [16] *etc.* Such a high versatility encourages design and synthesis of novel BTD derivatives and in-depth investigation of their photophysical properties. At the same time, the coordination chemistry of these units is relatively scarce with a limited number of reported crystal structures, primarily containing unsubstituted BTD ligands,[17-24] though their highly pronounced tendency towards formation of intermolecular π - π interactions,[22] as well as expected secondary bonding interactions between heteroatoms of adjacent molecules [25] represent a highly obscure and therefore a very attractive field.

The introduction of additional donor substituents in the ring, e.g. hydroxyl,[26-28] amine [28-32] and thiol [33-36] can substantially improve the coordination ability, and therefore determines the binding mode. An amine-substituted derivative can be considered as one of the most promising, due to peculiar luminescent properties [37] and wide range of possibilities for further functionalization by condensation with Schiff-bases.[30, 37] Although the syntheses of several complexes with 4-amino-2,1,3-

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