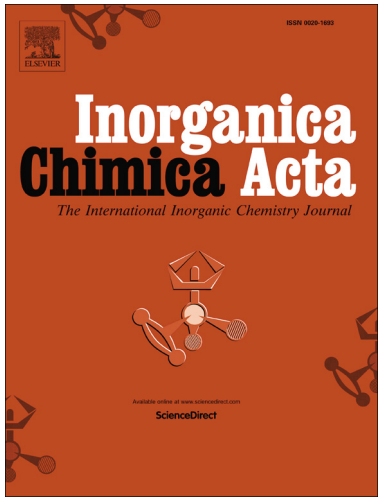

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Abstract

Schiff-base 1*H*-pyrrol-2-yl-methyleneamino-4,6-di-*tert*-butylphenol, $ONNH_2$ (**1**), and its aluminum complexes [$(ONN_2Al)AlR_2$] (R = Me (**2**), Et (**3**), and *i*Bu (**4**)) were synthesized. Complexes **2**-**4** were characterized by FT-IR, ^1H and $^{13}C\{^1H\}$ NMR, and mass spectrometry. X-ray diffraction analysis shows that **2** is a bimetallic complex with one aluminum center in an octahedral environment and the other in a tetrahedral one, **3** and **4** are also bimetallic, but with both aluminum atoms in a trigonal bipyramidal geometry. In diluted solution, **3** coexists as two isomers, namely, $\mathbf{3_{tet\text{-}oct}}$ and $\mathbf{3_{tbp\text{-}tbp}}$. The assignment of these isomers was complemented with Density Functional Theory (DFT) computations of the chemical shifts. The luminescent properties of **2** in CH_2Cl_2 were investigated using UV-Vis and photoluminescence (PL) spectroscopies, showing emission in the green region with a quantum yield of Φ = 4%. Time dependent DFT