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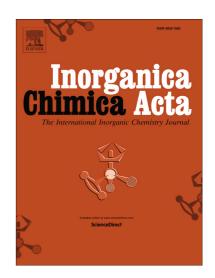
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## **ACCEPTED MANUSCRIPT**

# A Terbium Chlorobismuthate(III) Double Salt: Synthesis, Structure, and Photophysical Properties

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#### **Abstract**

We report on the structure and luminescence of a double salt trivalent rare earth ion acceptor,  $Tb^{3+}$ , with octahedral  $[BiCl_6]^{3-}$  donor clusters. The novel  $TbBiCl_6 \cdot 14H_2O$  (1) was prepared from aqueous BiOCl and  $TbCl_3 \cdot 6H_2O$ . The crystal structure of compound 1 exhibits isolated  $[BiCl_6]^{3-}$  and  $[Tb(OH_2)_8]^{3+}$  clusters. Luminescence data show energy transfer from octahedral chlorobismuthate(III) clusters to rare earth metal ions. Density Functional Theory (DFT) calculations show distinctly different emission pathways at high and low excitation energies.

### 1. Introduction

Rare earth metal ions produce sharp emission bands making them particularly useful in a variety of applications, including optoelectronics, biosensors, and photovoltaic compounds.  $^{1-7}$  The challenge in developing viable materials using these ions centers on the difficulty of excitation of the lanthanide f electrons. The f orbitals are held close to the nucleus below the f orbitals due to lanthanide contraction and f-f transitions are symmetrically forbidden. This results in weak emission intensities from these ions. Much research has focused on improving the emission intensity of solid state crystals f Energy transfer to rare earth metal centers is a

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