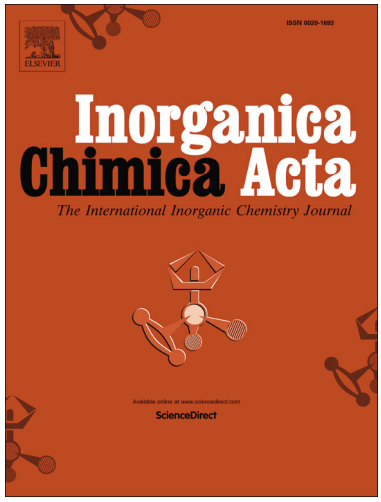

Research paper

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PII: S0020-1693(18)30207-X
DOI: https://doi.org/10.1016/j.ica.2018.03.040
Reference: ICA 18185

To appear in: *Inorganica Chimica Acta*

Received Date: 6 February 2018
Accepted Date: 27 March 2018

Please cite this article as: J.C. Ahern, A.D. Nicholas, A.W. Kelly, B. Chan, R.D. Pike, H.H. Patterson, A Terbium Chlorobismuthate(III) Double Salt: Synthesis, Structure, and Photophysical Properties, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.03.040

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

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Keywords: luminescence; crystallography; rare-earths; iodobismuthate; energy transfer

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 $TbBiCl_6 \bullet 14H_2O$ (**1**) was prepared from aqueous BiOCl and $TbCl_3 \bullet 6H_2O$. 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 *d* orbitals due to lanthanide contraction and *f-f* transitions are symmetrically forbidden.[8] This results in weak emission intensities from these ions. Much research has focused on improving the emission intensity of solid state crystals [9–11] Energy transfer to rare earth metal centers is a