

BAND GAP INVESTIGATION OF NOVEL Hf(IV)-SCHIFF BASE COMPLEXES SYNTHESISED FROM SALICYLALDEHYDE DERIVATIVES AND HEXAMETHYLENEDIAMINE

S. Lilachjini and C.V. Hettiarachchi*

Department of Chemistry, University of Peradeniya, Peradeniya, Sri Lanka.

*champikav@sci.pdn.ac.lk

Band gap energy is a fundamental concept in solid-state physics and materials chemistry, referring to the energy difference between the valence band and the conduction band in a material. This energy gap determines a material's electrical conductivity and optical properties. The importance of band gap energy lies in its ability to predict and control the behavior of materials in various applications, particularly in electronics, photovoltaics, and photocatalysis. By analysing how the structure of the ligand or the metal center influences the band gap, electronic properties of these complexes can be tailored. The purpose of studying band gap energy in Schiff base complexes of Hf(IV) was to understand their potential as functional materials. A series of novel Hf(IV)-Schiff base complexes were synthesised using salicylaldehyde derivatives (5-bromosalicylaldehyde and 5-chlorosalicylaldehyde) and hexamethylenediamine as the coordinating ligands. The Schiff base ligands were prepared via condensation reactions and subsequently complexed with Hf(IV) to yield stable coordination compounds. The resulting complexes were characterised by Fourier transform infrared spectroscopy and electronic spectra to confirm their structural integrity and coordination behavior. Special emphasis was placed on evaluating the optical properties of the complexes by employing UV-visible diffuse reflectance spectroscopy. Tauc plots were constructed to determine the optical band gap energies, which provide insight into the potential semiconducting and photocatalytic behavior of the materials. The band gap values of the Hf(IV) complexes synthesised were found to vary depending on the nature of the salicylaldehyde derivatives, indicating the possibility of tuning electronic properties through ligand modification. In conclusion, the 5-chloro-substituted complex exhibits the lowest band gap energy (2.07 eV), followed by the 5-bromo derivative (2.37 eV), while the complex derived from unsubstituted salicylaldehyde displays the highest band gap (2.40 eV) among the series. Overall, these results demonstrate that tuning the substituent on the ligand framework is an effective strategy to modulate the band gap energy of the Hf(IV)-Schiff base complexes.

Financial assistance from the AOARD US Airforce (Grant No FA2386-23-1-4036) is acknowledged.

Keywords: Bandgap, Hafnium, Photocatalysis, Salicylaldehyde, Schiff base, Tauc plot