Construction and Optical Properties of π-Conjugated Systems Using Bismuth Complexes with ONO Ligands

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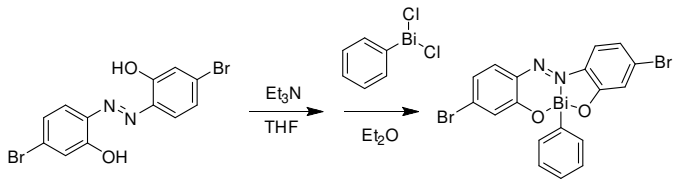
Keywords: Bismuth; π-Conjugated molecule; Azobenzene; Azomethine; Ring-fused structure

In recent years, organic molecules have been widely used in fields such as the development of OLEDs and organic thin-film solar cells. Among them, π-conjugated molecules have attracted a great deal of attention because of their high stability, electrical conductivity, and unique optical properties.

By introducing a coordination point at the center of the framework of conjugated molecules, it becomes possible to construct conjugated systems that directly reflect the characteristics of the elements. In our previous researches, we have clarified the electronic and optical properties of boron-, germanium-, and tin-complexes. We have found that complexes of highly periodic elements with ONO tridentate ligands, such as the azomethine and the azobenzene structures, in which nitrogen atoms are substituted for carbon atoms in the phenylenevinylene system, can be stably isolated. Moreover, they have the unique properties of highly periodic elements, such as control of electronic properties by hypervalent bonds.

In this study, we focused on bismuth in the sixth period, which has variable oxidation and coordination numbers. Bismuth has been used as a medicine for a long time because of its low toxicity to the human body. To investigate this element, we synthesized bismuth complexes (**BiAzBr)** using ONO ligands. (Scheme 1)



Scheme 1. Synthetic scheme of **BiAzBr**.

From the results of NMR and single crystal X-ray structure analysis, we succeeded in isolating the bismuth complex and found it to be stable under ambient condition. (Figure 1) In this presentation, the optical and electronic properties of the complexes based on highly periodic element will be discussed in detail using optical measurements and DFT calculations.

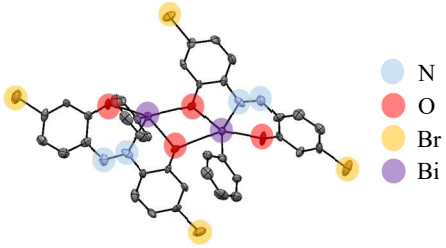


Figure 1. ORTEP illustrations of single-crystal structure of **BiAzBr**.

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