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Spectroscopic Study on Luminescent Mechanochromic Transition Metal Complexes

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Abstract

Luminescent mechanochromic materials that are capable of undergoing reversible mechanical-induced transformations between two forms with different luminescent behaviors have received great attention. To date, a number of different types of luminescent mechanochromic compounds including simple organic compounds, polymers and transition metal complexes have been reported [1-2]. The luminescent mechanochromism of many of these solids is derived from reversible switching between the crystalline states and the amorphous state through which the intermolecular interactions, such as π - π , H-bonding, dipole-dipole, metal-metal and metal-ligand interactions, and thus the energy of the electronic states and the luminescence are varied [1-2].

Fig. 1: Luminescent Mechanochromic Properties of Cyclometallated Ir(III) Acyclic Carbene Complexes.

As the luminescent mechanochromism of many of the reported systems mainly involves alternation of the intermolecular interactions, which are less predictable and difficult to control from the molecular frameworks or substituents. The lack of thorough understanding on the mechanochemical changes and their correlation with the macroscopic properties also contribute to the difficulty in designing compounds with tailored luminescent mechanochromism. Inspired by the strong sensitivity of the emission characteristics of the luminescent acyclic carbene complexes to the structural and conformational changes of the acyclic carbene ligands [3], herein, we report the design, syntheses and study of a new class of luminescent mechanochromic cyclometalated Ir(III) complexes with pyridyl acyclic carbene ligands, which exhibit mechanochromic behavior derived from intramolecular mechanochemical changes. On the basis of XRD, X-ray crystallography, Raman spectroscopy, time-resolved emission spectroscopy and DFT calculation, the mechanically-induced variations of the molecular packing and the structural conformation have been elucidated. With the understanding of their mechanochemical changes, it enables the design of luminescent mechanochromic compounds with tailored mechanochromic properties, including the emission color and the mechanochromic shift, through judicious structural modifications of the ligands [4].

Keywords: luminescent mechanochromism, Raman spectroscopy, time-resolved and steady-state emission spectroscopy, computational study, transition metal acyclic carbene complexes

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