

Application of the high-resolution neutron

diffraction to the C-H bond studies

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Abstract:

This talk is mainly on the investigation of C-H bond and its related non-covalent interactions (NCI) based by using the high-resolution neutron diffraction methods (i.e.TOPAZ at ORNL, USA). Many new weak interactions involving the fluorous ponytails have been introduced into the fluorous metal complexes e.g. [trans-(3-HCF2CF2CH2OCH2-py)2PtCl2]. The new weak interactions result in several possible solid state packing of the fluorinated Pt complexes. Thus, there are several polymorphs observed for the fluorous Pt complexes with the same chemical formula. It has been also found that this type of fluorous Pt cmplexes whose special interactions can be well studied by neutron diffraction methods are good stimuli-responsive systems which are likely to have good applications in OLED or sensory industries. Additionally, the rest of C-H bond and its related NCI studies are mainly based on single crystal neutron diffraction studies. The C-H...F improper hydrogen bonding (HB) and unusual C-H bond elongation induced by tetrel bond (TB) based on single crystal neutron diffraction studies will be discussed. It has been found for the 1st time that the fluorinated Pt complexes with the terminal alkynyl H atom can intramolecularly form the blue-shifted sp C-H...F interactions such that the terminal C-H stretch appears around 3400 cm-1. The talk will also address how TB-induced C-H bond elongation can be easily offset by forming an improper HB with the H atom from this C–H bond. Very rare intramolecular TBs and significant F...pi interactions will also be discussed. Non-covalent interactions, thermodynamics and electrostatic potential analysis investigations have been used to affirm the nature of the interactions based on density functional theory (DFT), NCI and other related calculations.