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Title:	Exploring the Origin of "Aggregation Induced Emission" Activity and "Crystallization Induced Emission" in Organometallic Iridium(III) Cationic Complexes: Influence of Counterions
Authors:	Kaur, Gurpreet (/jspui/browse?type=author&value=Kaur%2C+Gurpreet) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Aggregation induced emission (AIE) Interestingly Cationic iridium(III) Complex exhibiting
Issue Date:	2016
Publisher:	American Chemical Society
Citation:	Crystal Growth and Design, 16(10), pp.5738–5752.
Abstract:	A new cationic iridium(III) complex exhibiting "aggregation induced emission (AIE)" activity, [Ir(PPH ₃) ₂ (bipy)(H) ₂]A (bipy = 2,2'-bipyridine; A = counterions), has been synthesized in a straightforward synthetic route. Interestingly, the emission color of solid state samples of this complex varied with different counteranions [A = Cl ⁻ , BF ₄ ⁻ , PF ₆ ⁻ , N(CN) ₂ ⁻] and crystallization induced emission was observed. The emission properties for the compounds with A= Cl ⁻ , PF ₆ ⁻ are discussed by analyzing the crystal packing, the frontier molecular orbitals, and the calculation of the relevant low-lying excited states using time-dependent density functional theory. The restriction of internal rotation of the phenyl rings in the phosphine ligands due to intermolecular interactions is suggested as the most plausible origin of the observed AIE effect in these crystals.
Description:	Only IISERM authors are available in the record.
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