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Title:	Microwave-assisted facile and expeditive syntheses of phosphorescent cyclometallated iridium(III) complexes
Authors:	Karanam, M. (/jspui/browse?type=author&value=Karanam%2C+M.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Cyclometallated Ir(III) complex Microwave Heteroleptic complexes Ancillary ligands
Issue Date:	2013
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Citation:	Polyhedron,53, pp. 286-294.
Abstract:	<p>The syntheses of greenish-blue light emitting [Ir(ppy)₂(dppel)] (2), [Ir(ppy)₂(dppp)] (3) and [Ir(ppy)₂(dppe)] (4) [ppy, 2-phenylpyridine; dppel, 1,2-bis(diphenylphosphino)ethylene; dppp, 1,3-bis(diphenylphosphino)propane; dppe, 1,2-bis(diphenylphosphino)ethane] complexes were carried out using [(ppy)₂Ir(μ-Cl)Ir(ppy)₂] (1) as a starting material. These complexes were characterized by elemental analyses and NMR (¹H, ¹³C and ³¹P) spectral studies. A single-crystal X-ray diffraction study confirmed a distorted octahedral geometry for 3. Complexes 2–4 were found to exhibit blue-shifted emission as compared to [Ir(ppy)₂(acac)] (acacH = acetylacetone) and [Ir(ppy)₂pic] (pic = 2-picolinic acid) because of the presence of strongly π-accepting, Ph₂P⁺PPh₂ units. The solution quantum efficiency for 2–4 was measured and 2 showed the highest quantum efficiency. Ground state geometry optimizations for 2–4 were performed using density functional theory (DFT) with the B3LYP hybrid functional and excitation energies for low lying singlet and triplet excited states were obtained via time-dependent DFT (TDDFT) calculations. Further, complexes 1–4 were synthesized by a Microwave Irradiation technique (MW) in a reasonably shorter time. This facile and expeditive synthetic route has been extended and successfully verified for other heteroleptic complexes of Ir(III) with varying different bidentate [(N⁺N) (5), (O⁺O) (6), (N⁺O) (7)] and monodentate [PPh₃ (8)] ancillary ligands.</p>
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