



Library Indian Institute of Science Education and Research Mohali



DSpace@IISERMohali (/jspui/)
/ Publications of IISER Mohali (/jspui/handle/123456789/4)
/ Research Articles (/jspui/handle/123456789/9)

Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/3112>


Title:	Aggregation-Induced Emission Activity in Iridium(III) Diimine Complexes: Investigations of Their Vapochromic Properties
Authors:	Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Luminescence Iridium Nitrogen heterocycles Density functional calculations
Issue Date:	2014
Publisher:	Wiley-VCH Verlag
Citation:	European Journal of Inorganic Chemistry, 2014(23), pp.3710-3719.
Abstract:	Two iridium(III) diimine complexes [mono(1,10-phenanthroline) bis(triphenylphosphine) (dihydrido)iridium(III) hexafluorophosphate (1) and mono(1,10-phenanthroline)bis(triphenylphosphine)(hydrido)(chloro)iridium(III) hexafluorophosphate (2)] have been synthesized from a single two-step reaction. The structures of 1 and 2 both adopt distorted octahedral geometries, as established by single-crystal X-ray diffraction. The complexes, upon irradiation with UV light at 365 nm, emit faint light in solution and bright light in the solid state. The ground- and excited-state properties of these complexes were investigated through density functional theory (DFT) and time-dependent DFT calculations. The calculated energies for the transitions from the ground state to the singlet and triplet excited states were close to those determined from the experimental absorption and emission. Their molecular orbitals were also exploited to compute the ground-state dipole moments and redox potentials. Several experiments were performed to demonstrate the "aggregation-induced emission" (AIE) activity of these complexes. AIE was triggered by the restricted intramolecular rotation of the rotating units (phenyls in triphenylphosphines) in these molecules in the solid state. The solid thin films of 1 and 2 exhibit solvent-polarity-dependent vapour-responsive emission properties (vapoluminescent). The rationale for the different emission behavior in the solid state has been thoroughly investigated. The packing diagrams of 1 and 2 show that there is enough space available to accommodate small organic solvent molecules inside the crystal lattices.
Description:	Only IISERM authors are available in the record.
URI:	https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/ejic.201402222 (https://chemistry-europe.onlinelibrary.wiley.com/doi/abs/10.1002/ejic.201402222) http://hdl.handle.net/123456789/3112 (http://hdl.handle.net/123456789/3112)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format
Need to add pdf.odt (/jspui/bitstream/123456789/3112/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text

[View/Open \(/jspui/bitstream/123456789/3112/1/Need%20to%20add%20pdf.odt\)](#)

Show full item record (</jspui/handle/123456789/3112?mode=full>)

 (</jspui/handle/123456789/3112/statistics>)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.