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PII:	S1386-1425(18)30613-9
DOI:	doi:10.1016/j.saa.2018.06.071
Reference:	SAA 16230
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	19 April 2018
Revised date:	16 June 2018
Accepted date:	18 June 2018

Please cite this article as: Xin Wang, Jingshun Zhang, Xinrui Zhu, Tiegang Ren, Li Wang , Influence of different ancillary ligand on the phosphorescent properties of platinum(II) complexes. Saa (2018), doi:10.1016/j.saa.2018.06.071

Influence of different ancillary ligand on the phosphorescent properties of platinum(II) complexes

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Abstract

In past two decades, lots of bidentate Pt(II) complexes are developed as potential organic light emitting diodes due to their simple synthetic process. The relative low quantum efficiency is one of the major blocks for their applications. Two new heteroleptic Pt(II) complexes bearing an n-hexyloxy substituted phenyllepidine-based ligand and either a picolinate (pic) (**1**) or acetylacetonate (acac) (**2**) ancillary ligand are synthesized as orange-red-emitter by Wawrzinek and coauthors. The quantum efficiency of **2** is much larger than that of **1** indicating that the variation of ancillary ligand has a great effect on the performance. Inspired by it, other two new bidentate Pt(II) complexes are theoretically designed with the same primary ligand along with pyrazolone (pzl) (**3**) or N-substituted carbazole (NCaz) (**4**) ancillary ligand. The phosphorescent properties are explored by density functional theory (DFT) and time dependent DFT (TDDFT) methods with the ultimate goal to explore the influence of

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