Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

The 2,7-Bis(diphenylamino)-9,9'-spirobifluorene Functionalized Ir(III) Complex; A Conceptual Design En Route to A Three-in-one System Possessing Emitting Core and Electron and Hole Transport Peripherals

Hsiao-Fan Chen, Ken-Tsung Wong*, Yi-Hung Liu, Yu Wang, Yi-Ming Cheng,

Min-Wen Chung and Pi-Tai Chou* and Hai-Ching Su

H.-F. Chen, Prof. K.-T. Wong,

Department of Chemistry,

National Taiwan University, Taipei 10617 (Taiwan)

Fax (+886) 2-3366-1667; Tel: (+886)2-3366-1665; E-mail: kenwong@ntu.edu.tw

Y.-H. Liu, Y. Wang, Y.-M. Cheng, M.-W. Chung, Prof. P.-T. Chou,

Department of Chemistry,

National Taiwan University, Taipei 10617 (Taiwan)

Fax: (+886)2-2369-5208; E-mail: chop@ntu.edu.tw

H.-C. Su
Institute of Lighting and Energy Photonics,
National Chiao Tung University, Tainan 71150 (Taiwan)

Table S1. Calculated energy levels, oscillator strength (*f*), orbital transition analyses and %MLCT for complex **3**. Note: The TDDFT calculation is combined with an integral equation formalism-polarizable continuum model (IEF-PCM) in acetonitrile to consider the solvation effect.

States	λ_{cal}	*f*	Assignments	MLCT (%)
T_1	682.2	0	HOMO→LUMO (100%)	0
S_1	681.5	0.0002	HOMO→LUMO (100%)	0
T_2	544	0	HOMO-1→LUMO (99%)	0
S_2	539.5	0.0001	HOMO-1→LUMO(99%)	0
T_3	526	0	HOMO-2→LUMO (100%)	32.6
S_3	525.8	0.0001	HOMO-2→LUMO (100%)	32.6

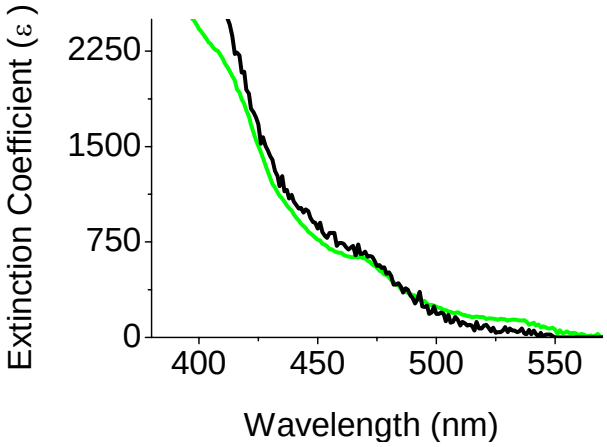


Figure S1 Expanded UV-Vis absorption spectra of complexes **2** (green) and **3** (black) between 400 ~ 560 nm in acetonitrile.

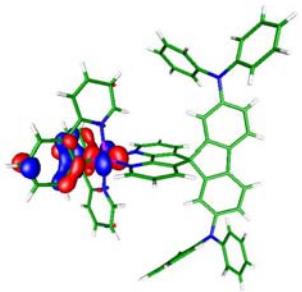
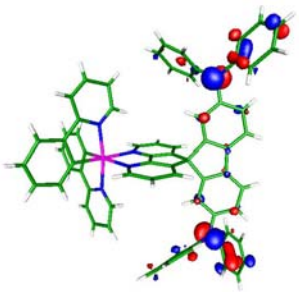
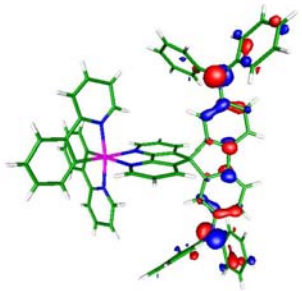
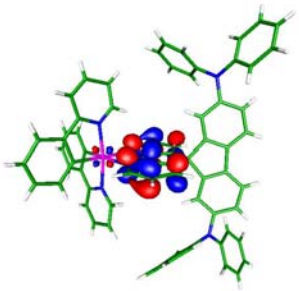
HOMO-2	HOMO-1
	
HOMO	LUMO
	

Figure S2. Frontier orbitals involved in the lower-lying electronic transitions for **3**.

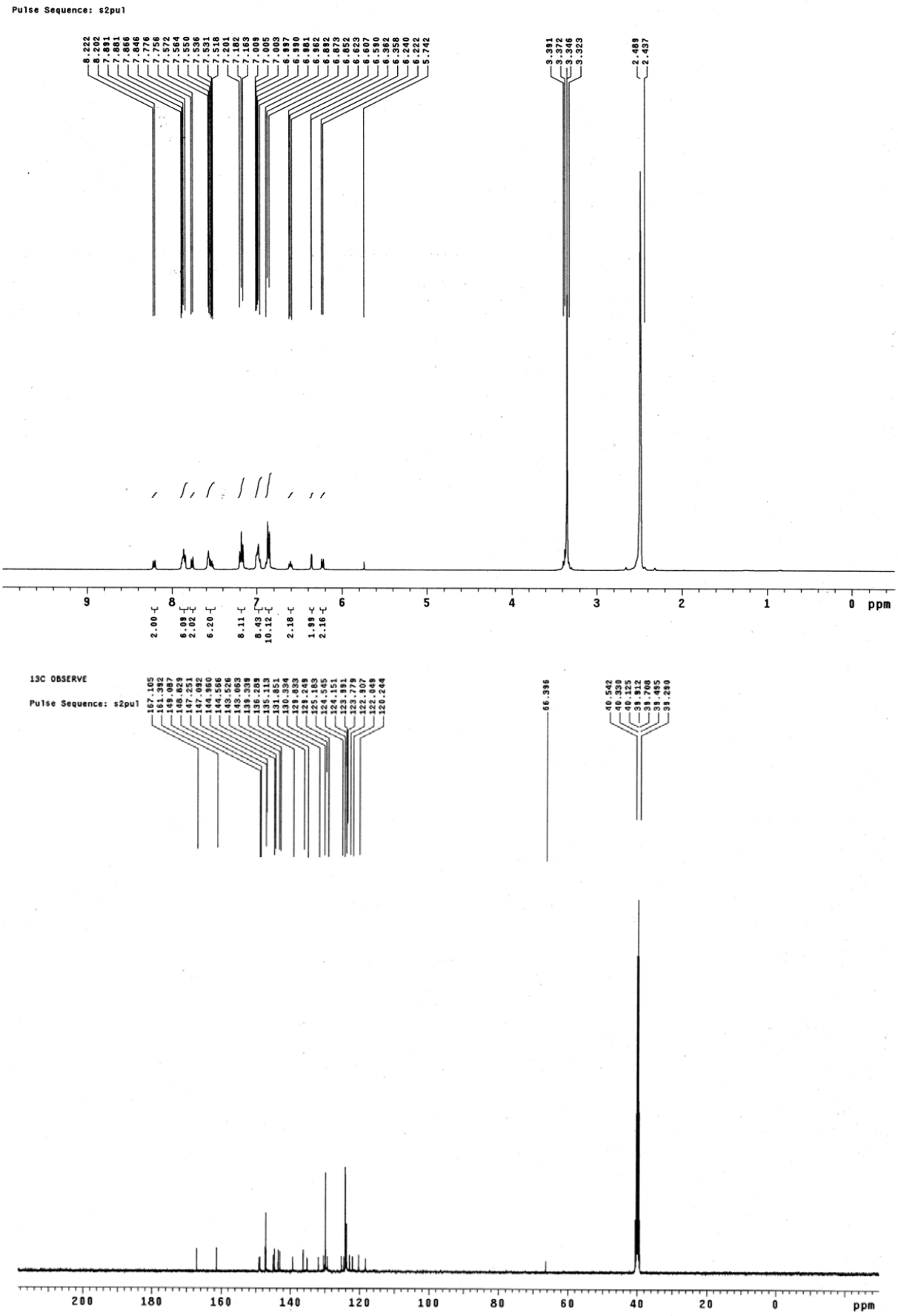


Figure S3. ^{1}H and ^{13}C NMR spectra for complex **3**.