

Supporting Information

Intrinsic quantum efficiency enhancement in famous
Ir(III) complexes by virtue of the simple and
controllable deuteration way.

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1 Spin orbit coupling

The spin orbital coupling matrix elements play an indispensable role in both radiative and non-radiative decay processes. Accordingly, the calculation of SOC integrals is crucial in determination of photophysical property for a phosphor. The one-electron SOC Hamiltonian for heavy transition metals can be expressed as:

$$\hat{H}_{SOC} = \sum_i \hat{l}_i \cdot \hat{s}_i \xi_c \quad (S1)$$

where \hat{l}_i and \hat{s}_i are denoted as orbital and spin angular momentum operator for the i -th electron, respectively. ξ_c is the one-electron spin-orbital coupling constant. In this study, only iridium d electrons are considered to be contributing to the SOC strength, since ξ_c for d electrons in Ir atom is significantly larger than the other main group atoms. Further simplified one-center one-electron direct SOC integrals are reducing to products of the normalized configuration interaction coefficients (1a_i and 3a_j) of S_n and T_m excitation states, the atomic orbital coefficients (1c_k and 3c_k) of iridium 1d_k and 3d_k involved in correlative excitation states, as well as its SOC constant, which can be expressed as:[1, 2]

$$\langle S_n | H_{SOC} | T_m \rangle = \sum_k {}^1a_i {}^3a_j {}^1c_k {}^3c_k \xi_c \langle {}^1d_k {}^1\pi^* | \hat{l} \cdot \hat{s} | {}^3d_k {}^3\pi^* \rangle \quad (S2)$$

Table. S1 Calculated and experimental key parameters for complex **1** - **4** at optimized S_0 states and T_1 states.

	1 - S_0 (theo/exp ^a)	1 - T_1 (theo)
<i>Ir</i> - <i>N1</i>	2.155 (2.130)	2.128
<i>Ir</i> - <i>N2</i>	2.155 (2.130)	2.167
<i>Ir</i> - <i>N3</i>	2.155 (2.130)	2.178
<i>Ir</i> - <i>C1</i>	2.018 (2.016)	1.974
<i>Ir</i> - <i>C2</i>	2.018 (2.016)	2.030
<i>Ir</i> - <i>C3</i>	2.017 (2.016)	2.017
	2 - S_0 (theo)	2 - T_1 (theo)
<i>Ir</i> - <i>N1</i>	2.146	2.108
<i>Ir</i> - <i>N2</i>	2.147	2.157
<i>Ir</i> - <i>N3</i>	2.147	2.157
<i>Ir</i> - <i>C1</i>	2.016	1.993
<i>Ir</i> - <i>C2</i>	2.016	2.013
<i>Ir</i> - <i>C3</i>	2.016	2.028
	3 - S_0 (theo)	3 - T_1 (theo)
<i>Ir</i> - <i>N1</i>	2.048	2.035
<i>Ir</i> - <i>N2</i>	2.048	2.067
<i>Ir</i> - <i>C1</i>	1.992	1.956
<i>Ir</i> - <i>C2</i>	1.992	1.991
<i>Ir</i> - <i>O1</i>	2.181	2.186
<i>Ir</i> - <i>O2</i>	2.181	2.180
	4 - S_0 (theo/exp ^b)	4 - T_1 (theo)
<i>Ir</i> - <i>N1</i>	2.062 (2.059)	2.053
<i>Ir</i> - <i>N2</i>	2.049 (2.040)	2.073
<i>Ir</i> - <i>C1</i>	1.997 (2.011)	2.019
<i>Ir</i> - <i>C2</i>	1.990 (1.992)	2.009
<i>Ir</i> - <i>O</i>	2.152 (2.131)	2.035
<i>Ir</i> - <i>N3</i>	2.170 (2.115)	2.139

^aFrom ref.3

^bFrom ref.4

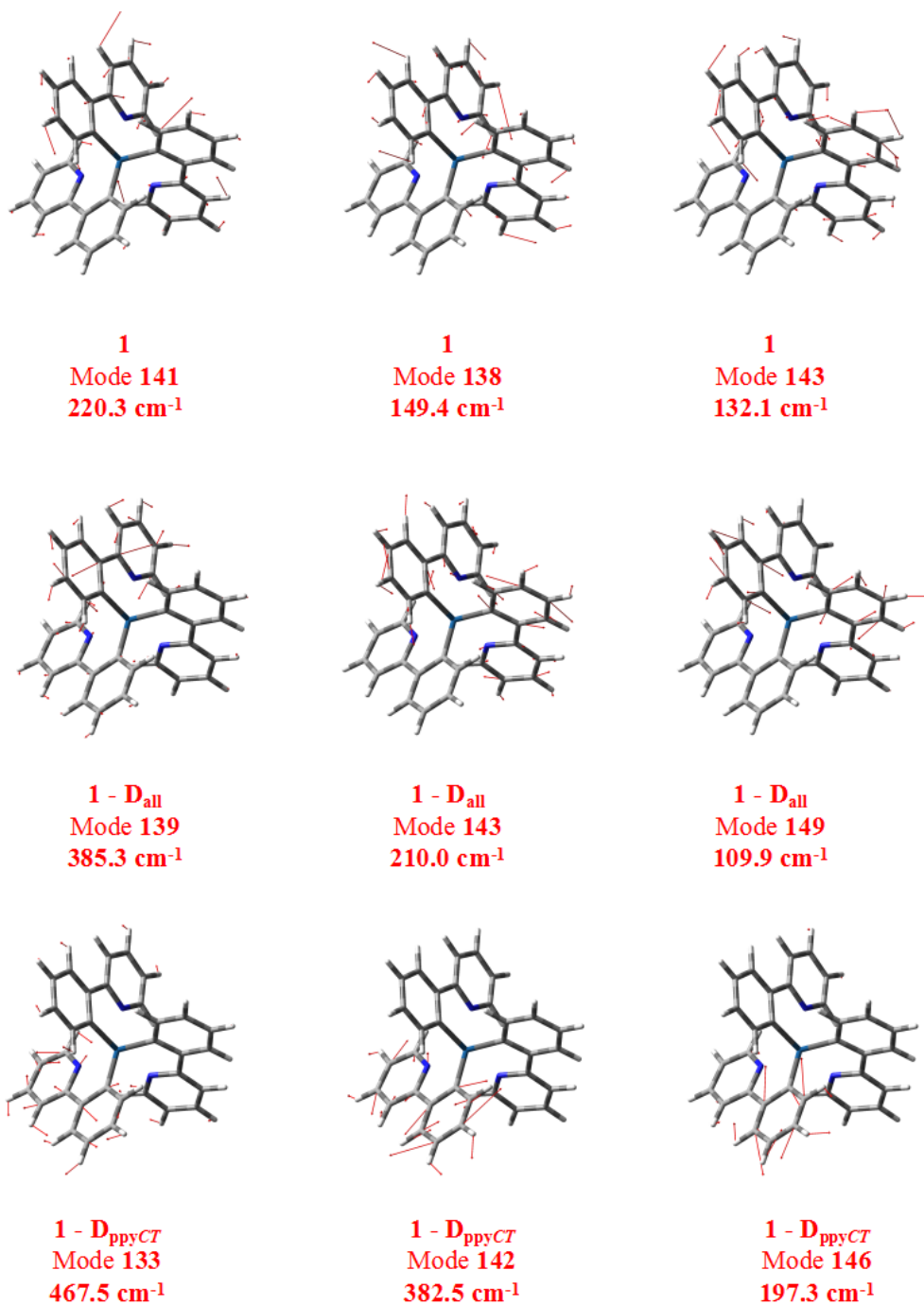


Fig. S1 Normal mode displacement vectors for the first several largest reorganization energy of complexes **1**, together with its corresponding complete and partial deuterated ones.

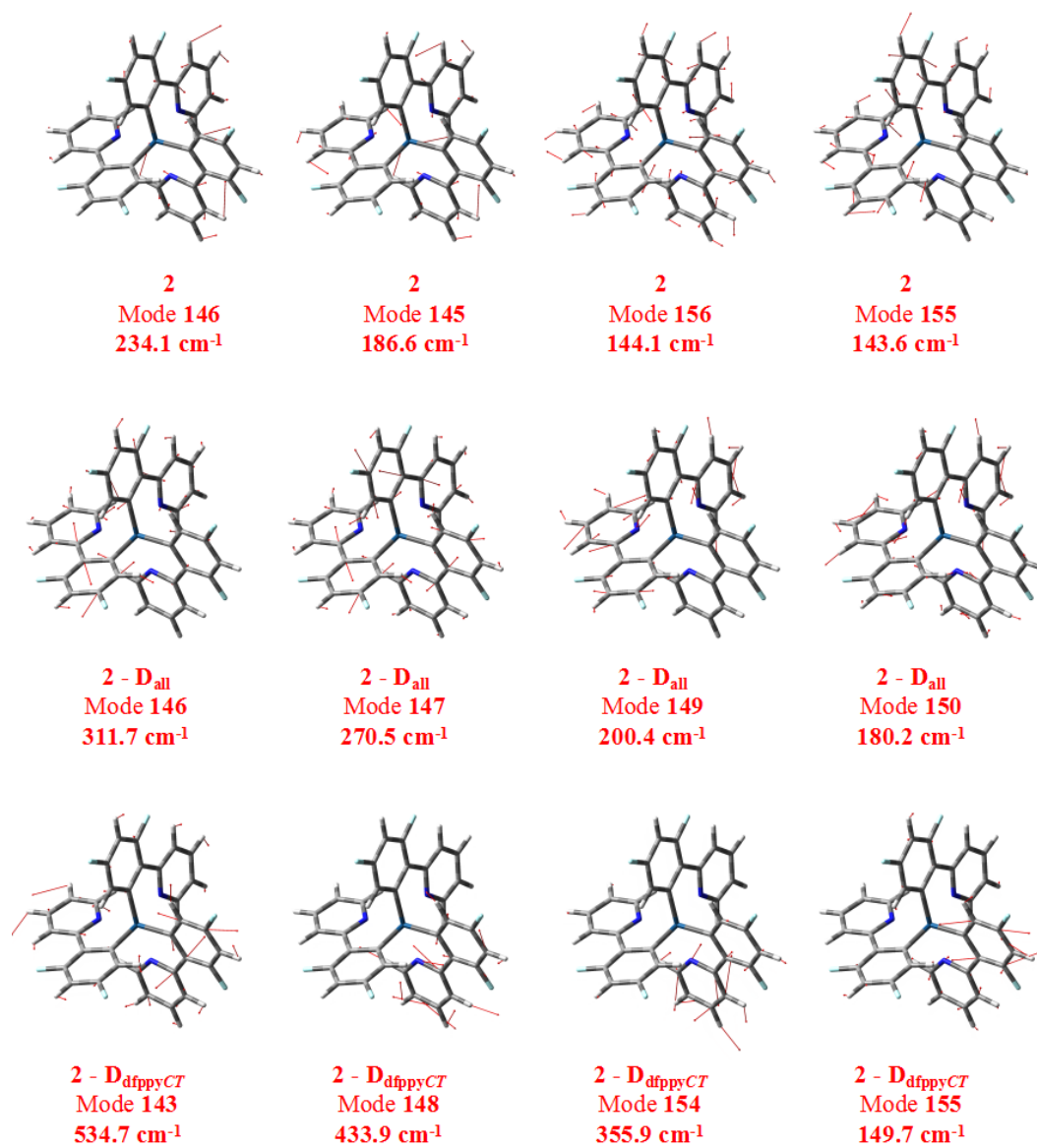


Fig. S2 Normal mode displacement vectors for the first several largest reorganization energy of complexes **2**, together with its corresponding complete and partial deuterated ones.

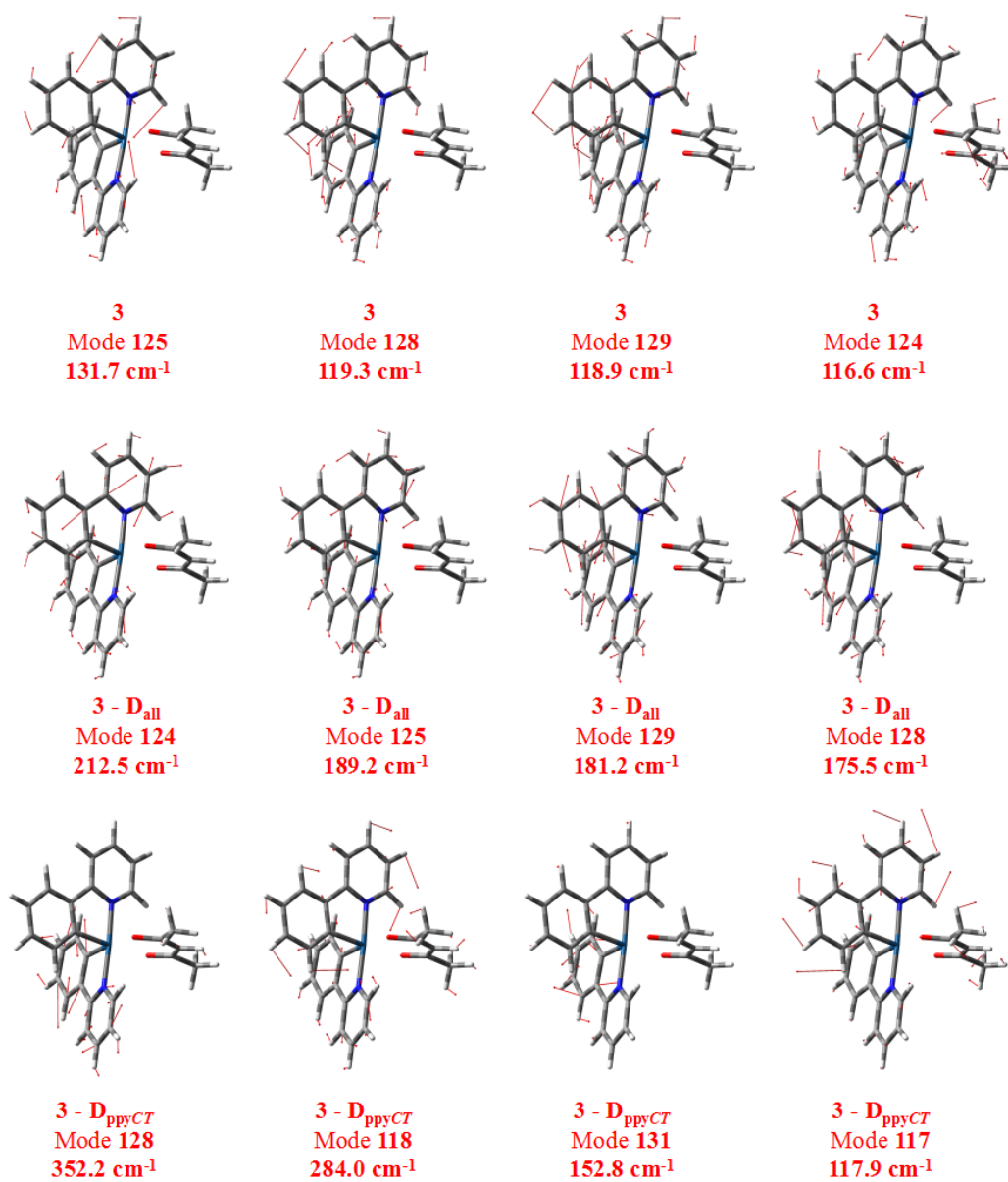


Fig. S3 Normal mode displacement vectors for the first several largest reorganization energy of complexes **3**, together with its corresponding complete and partial deuterated ones.

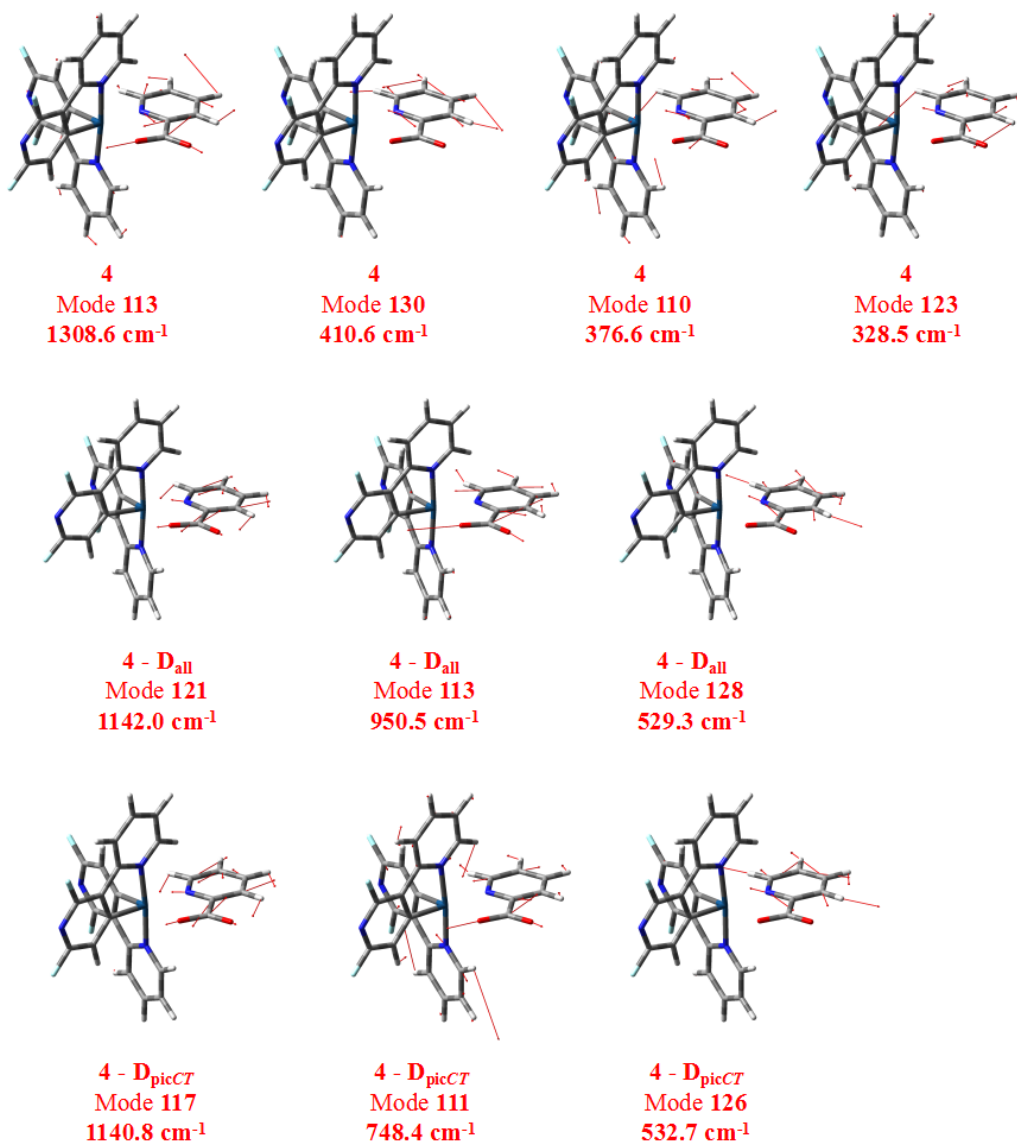


Fig. S4 Normal mode displacement vectors for the first several largest reorganization energy of complexes **4**, together with its corresponding complete and partial deuterated ones.

References

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