Electronic Supplementary Information

Unveiling the mechanisms of organic room temperature phosphorescence in various surrounding environments: a computational study

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Content

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Computational details for NTO

To begin with, the central molecule is relaxed while the molecules of low level region are frozen during the QM/MM geometry optimizations with the ωB97XD functional and 6-31G** basis. Then, the molecules of low level region are replaced by background charges in NTO calculation with iop(9/40=4).

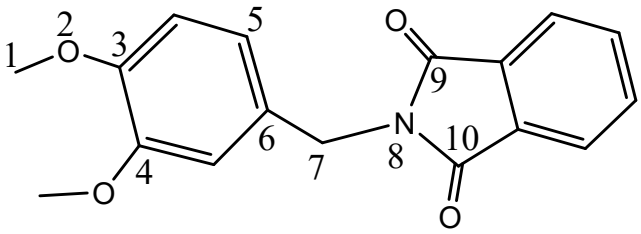

Fig. S1 Molecular structures with the labeled atom index of complex b.

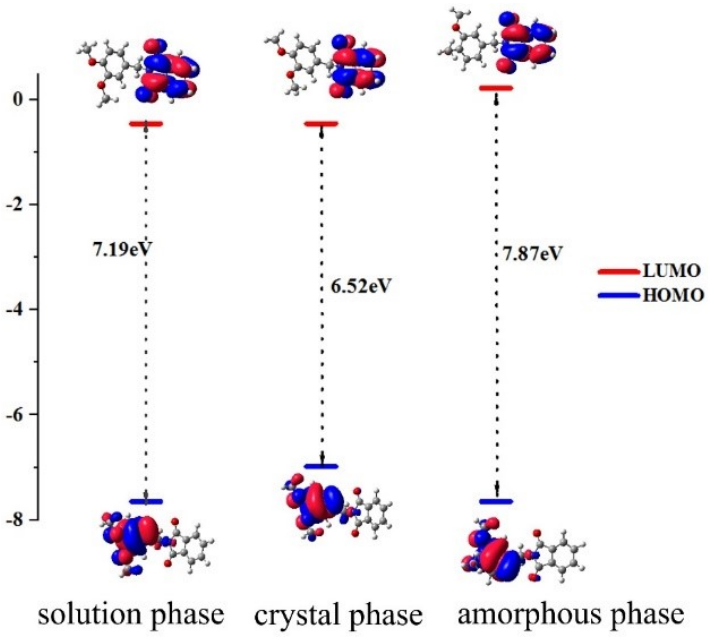

Fig. S2 Calculated orbital energy levels, energy gaps and electron density contours of HOMOs and LUMOs for complex at S_0 equilibrium geometries in three cases.

Table. S1 Representative dihedral angles and bond angles are detailed in the table.

	solution	crystal phase	amorphous phase
θ_1	C5-C6-C7-N8	C5-C6-C7-N8	C5-C6-C7-N8
θ_2	C1-O2-C3-C4	C1-O2-C3-C4	C1-O2-C3-C4
θ_3	C6-C7-N8-C10	C6-C7-N8-C10	C6-C7-N8-C10
α_1	C5-C6-C7	C5-C6-C7	C5-C6-C7
α_2	C6-C7-C8	C6-C7-C8	C6-C7-C8
α_3	C7-N8-C10	C7-N8-C10	C7-N8-C10

Table. S2 Selected dihedral angles and bond angles (in deg, marked in Fig. S_1) of S_0, S_1, and T_1 states in solution, crystal and amorphous phase, respectively.

	solution phase			crystal phase			amorphous phase		
	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
θ_1	101.1	73.1	66.7	106.9	109.1	107.3	95.7	94.0	95.6
θ_2	179.8	179.5	179.8	174.3	177.5	177.8	173.6	176.0	174.1
θ_3	90.1	73.6	84.1	103.3	103.3	107.5	79.9	81.0	79.4
α_1	121.1	118.1	117.8	120.6	120.6	120.7	119.7	119.0	119.6
α_2	112.4	101.0	109.4	113.0	109.1	108.1	115.2	112.3	115.2
α_3	124.1	122.2	122.8	124.4	123.4	123.9	123.6	122.8	122.4

Table. S3 Packing structure of complex b and excitonic coupling in crystal phase.

Dimer	J	Dimer	J
V1	-0.215	V5	0.006
V2	-0.206	V6	0.016
V3	0.084	V7	-0.023
V4	-0.006	V8	0.083

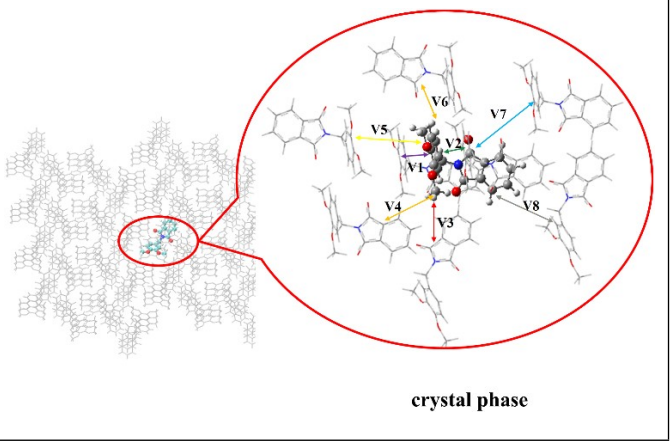

Table. S4 Packing structure of complex b and excitonic coupling in amorphous phase.

Dimer	J	Dimer	J	Dimer	J
V1	-0.196	V6	0.031	V11	-0.056
V2	-0.006	V7	-0.010	V12	0.092
V3	0.443	V8	-0.001	V13	0.011
V4	0.035	V9	0.026	V14	-0.033
V5	0.003	V10	-0.051