Electric Supplementary Information

π-Conjugation modification of photochromic and redox-active dimethyldihydropyrene by phenyl- and ethynyl-terpyridines and Ru(bis-terpyridine) complexes

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Table S1. Crystal Data and Refinement Parameters for **2**·4$CHCl_3$

	2·4$CHCl_3$
Empirical formula	$C_{72}H_{62}N_6Cl_{12}$
Fw	1436.68
Crystal dimension /mm	0.2 × 0.1 × 0.1
Crystal system	Triclinic
a /Å	9.509(2)
b /Å	13.741(2)
c /Å	15.412(2)
α /°	62.573(4)
β /°	73.988(6)
γ /°	87.296(7)
V /Å^3	1710.6(4)
Space group	P–1 (#2)
Z value	1
T /K	113
μ (Mo Kα) /cm^{-1}	5.33
D(calc) /g cm^{-3}	1.395
R_1[a]	0.0515
wR_2[b]	0.1393
GOF[c]	1.058

[a] $R_1 = \Sigma||F_O|-|F_C||/\Sigma|F_O|$ ($I > 2\sigma(I)$).

[b] $wR_2 = [\Sigma(w(F_O^2-F_C^2)^2)/\Sigma(w(F_O^2)^2)]^{1/2}$ ($I > 2\sigma(I)$).

[c] GOF = $[\Sigma(w(F_O^2-F_C^2)^2)/\Sigma(N_0-N_v)^2)]^{1/2}$.

Table S2. Selected Bond Lengths for **2**

Bonds	Bond length /Å
C22–C23	1.400(2)
C23–C24	1.394(3)
C24–C25	1.393(2)
C25–C26	1.399(3)
C26–C27	1.409(3)
C27–C28	1.389(2)
C28–C22	1.413(3)
C24–C29	1.516(3)
C28–C29	1.530(3)
C29–C29’	1.527(4)

Table S3. UV/vis Absorption Spectral Data of **1**, **2**, and **3** in Dichloromethane, and **4**, **5**, and $Ru(tpy)_2 \cdot 2PF_6$ in Acetonitrile (All concentrations are 1.0×10^{-5} M.)

	1	**2**	**3**	**4**	**5**	$Ru(tpy)_2 \cdot 2PF_6$
Band	λ_{max} /nm (ε_{max} /10^4 M^{-1} cm^{-1})					
^1L_b	643 (0.1)	658 (0.2)	689 (1.0)	659 (0.3)	698 (1.3)	–
^1L_a	478 (1.1)	492 (1.2)	528 (3.5)	Not observed	562 (5.9)	–
^{1}MLCT	–	–	–	486 (6.8)	483 (4.5)	475 (1.6)
^1B_b	380 (3.7)	404 (7.4)	418 (13)	399 (5.3)	419 (4.9)	–
^1B_a	342 (9.5)	358 (5.3)	373 (5.9)	350 (6.8)	361 (3.8)	–
^{1}LC(tpy)	–	279 (7.0)	277 (7.4)	309 (15)	308 (11)	307 (6.7)
^{1}LC(tpy)	–	253 (6.3)	250 (9.5)	273 (11)	273 (8.8)	270 (4.1)

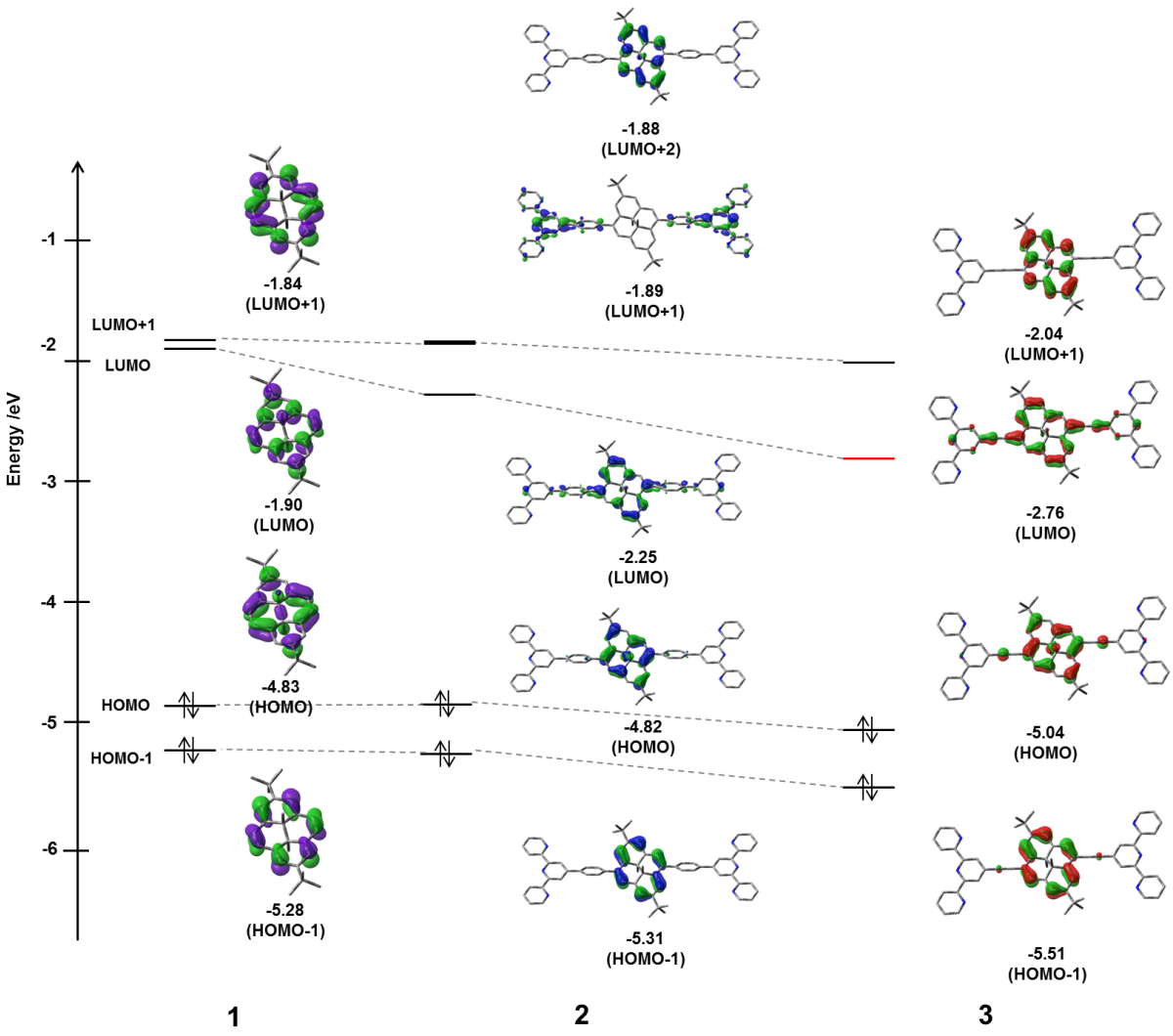

Fig. S1. Valence orbital energy diagrams and selected valence orbitals of **1**, **2**, and **3** from DFT (B3LYP) calculations.

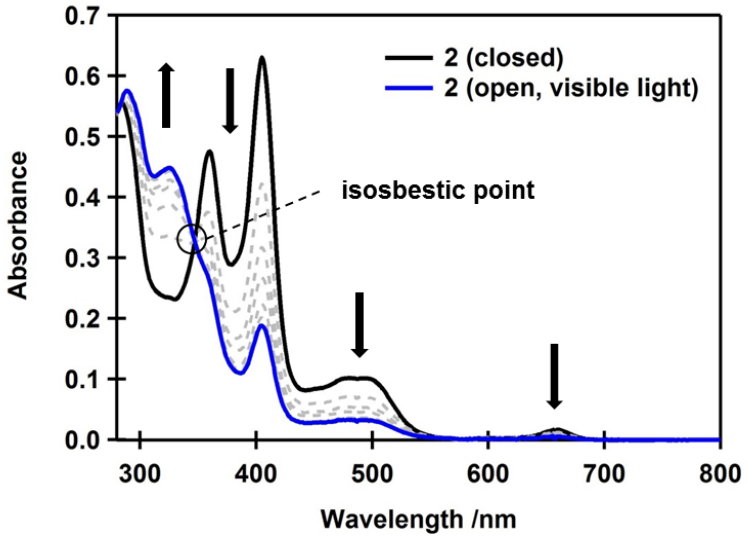

Fig. S2. UV/vis spectral change of **2** (in benzene) upon irradiation of visible light (400-700 nm). (Concentration is 1.0×10^{-5} M.)

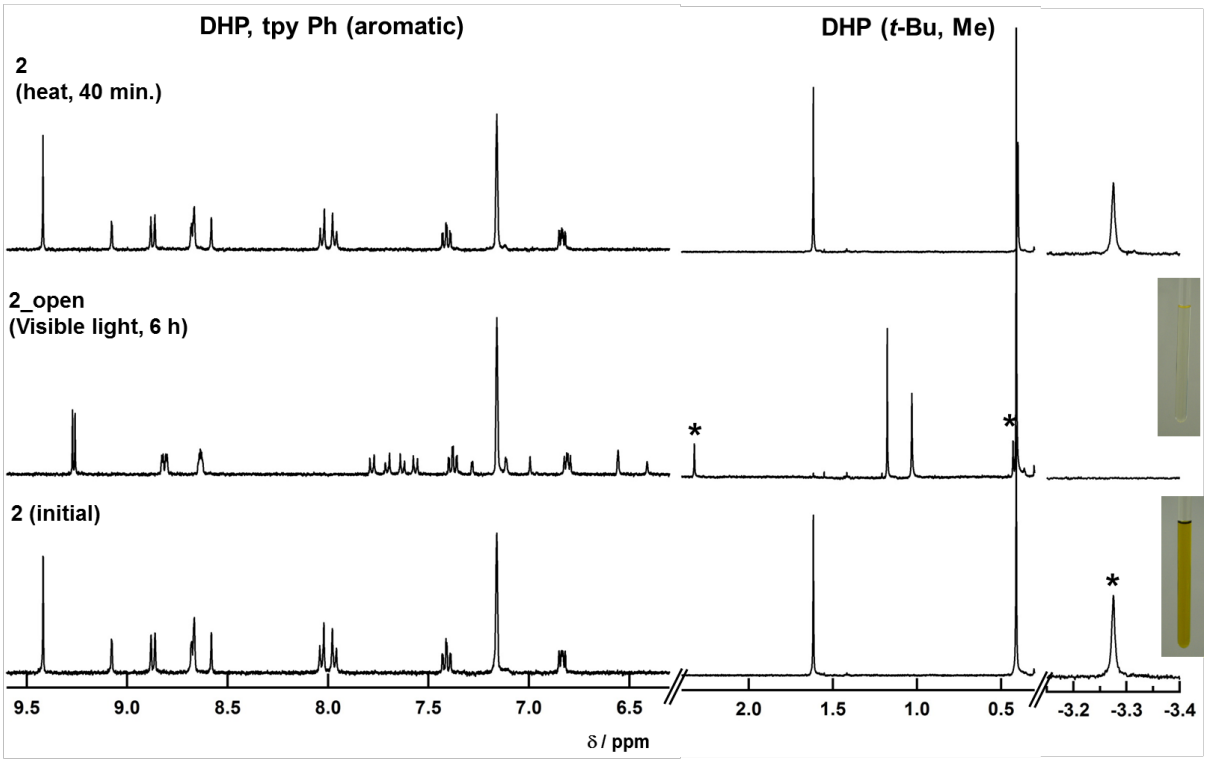

Fig. S3. ^{1}H NMR spectral change of **2** (in benzene-d^{6}) upon irradiation of visible light (400-700 nm) and heating. *: peak of *t*-Bu. (Concentration is 1.0×10^{-3} M.)

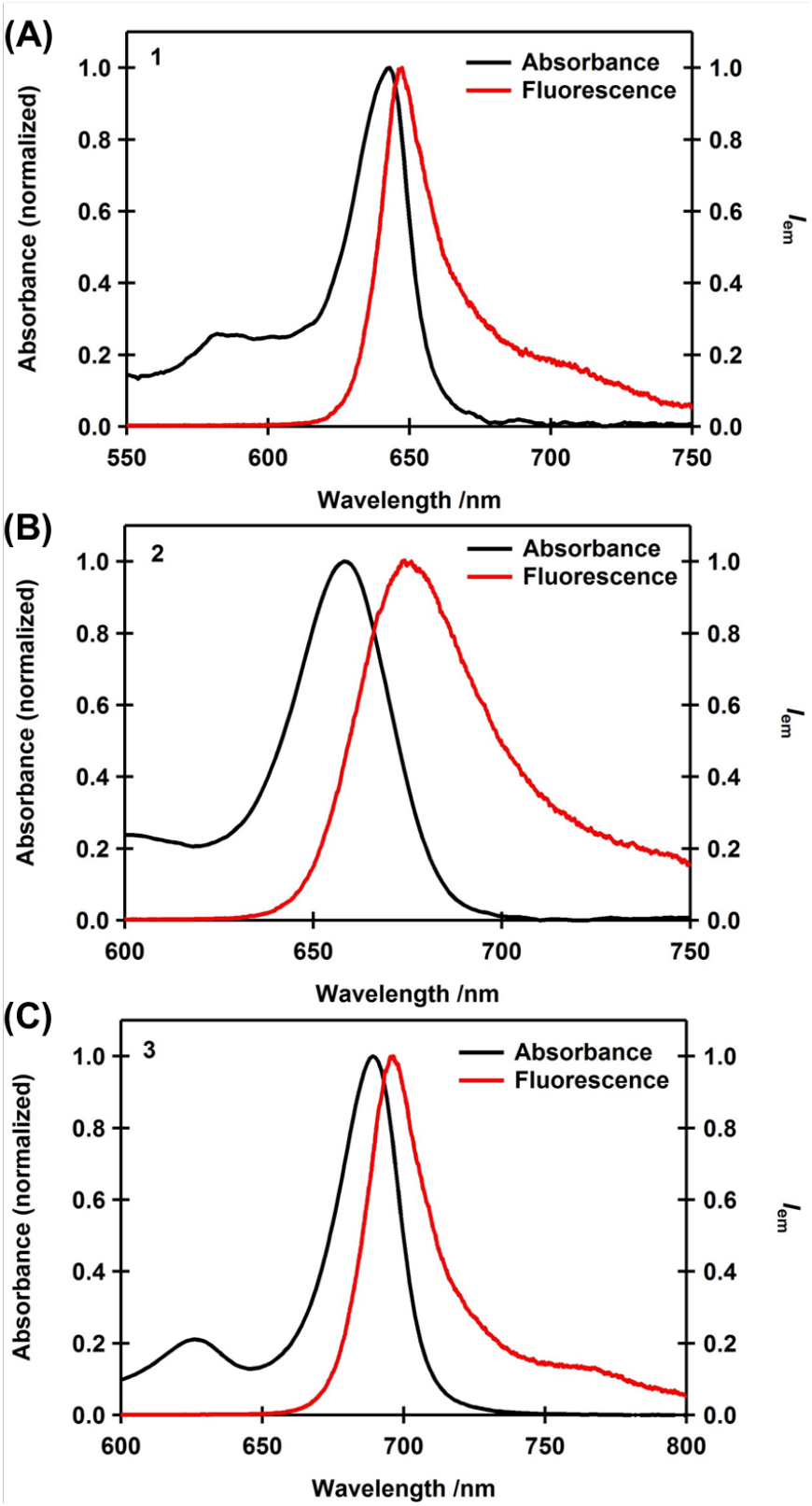

Fig. S4. A normalized UV/vis absorption spectrum and a normalized fluorescence spectrum of (A) **1**, (B) **2**, and (C) **3** in dichloromethane at 293 K (excitation: 355 nm). (All concentrations are = 1.0×10^{-5} M.)

Reference 69.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford CT, **2010**.