Electronic Supplementary Information

Heteroleptic ruthenium antenna-dye for high-voltage dye-sensitized solar cells

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Supplementary Figure & Table:

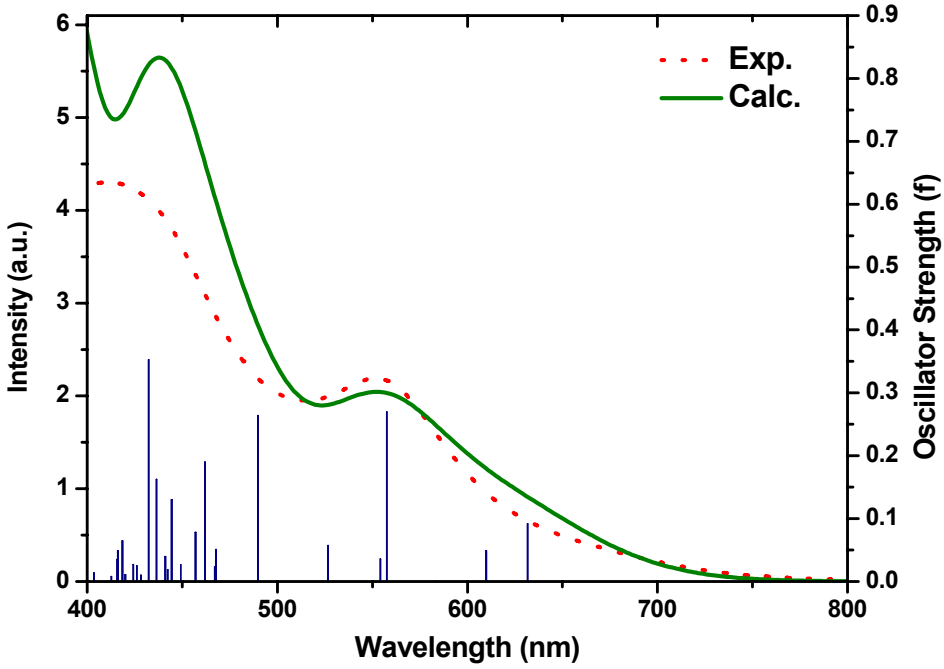

Fig. S1. Comparsion between calculated (solid green line) and experimental (dot red line) absorption spectra of **CYC-B7** in DMF. The calculated line spectra (excitation energy and oscillator strengths) are shown in the blue vertical lines. The calculated spectrum was obtained by Gaussian convolution with σ = 0.15 eV.

Table S1. Properties of ground-state vertical excitation with the energy lower 3.1 eV and oscillator strengths (*f*) larger than 0.01.

Transition Energy/nm	**Oscillator Strength (*f*)**	**Transition Assignment (H=HOMO; L=LUMO)**
631.7	0.0921	H→L (63.5 %), H→L+1 (21.0 %), H-2→L+1 (13.1 %),
609.84	0.0491	H→L+1 (58.4 %), H-2→L+1 (19.5 %), H-1→L+1 (12.1 %)
557.58	0.2701	H-1→L (38.1 %), H-2→L+1 (36.8 %), H-2→L (19.8 %)
554.27	0.0360	H-2→L (64.2 %)
526.64	0.0578	H-2→L+1 (47.7 %)
489.8	0.2645	H→L+2 (65.2 %), H-2→L+1 (12.0 %)
467.74	0.0511	H-3→L (45.9 %), H-4→L (34.7 %), H-4→L+2 (13.0 %)
467.15	0.0239	H-4→L (50.1 %), H-3→L+1 (19.0 %), H-4→L+2 (14.5 %)
461.89	0.1900	H-1→L+2 (61.9 %), H→L+3 (21.2 %), H-3→L (14.6 %)
456.97	0.0784	H→L+3 (62.1 %)
449.16	0.0270	H-2→L+2 (68.2 %)
444.39	0.1306	H-5→L (59.2 %), H-3→L+1 (19.1 %), H-2→L+2 (10.8 %)
442.32	0.0189	H-3→L+1 (53.0 %), H-3→L (36.1 %), H-5→L+1 (14.2 %)
441.05	0.0399	H→L+4 (49.0 %), H-6→L (29.3 %), H-9→L (28.6%)
436.49	0.1625	H→L+4 (41.3 %)
432.28	0.3525	H-6→L (41.8 %)
428.28	0.0101	H-1→L+3 (64.4 %)
426.06	0.0253	H-9→L+1 (42.2 %), H-6→L+1 (28.5 %), H-6→L (23.9 %)
424.23	0.0271	H-5→L+1 (55.4 %), H-5→L (25.5 %), H-9→L (21.2 %)
420	0.0113	H-2→L+3 (52.8 %), H-6→L+1 (24.4 %)
418.5	0.0645	H-6→L+1 (44.2 %), H-2→L+4 (13.0 %)

416.11	0.0489	H-3→L+2 (55.7 %), H-6→L+1 (16.6 %)
415.77	0.0356	H-4→L+2 (59.5 %), H-3→L+2 (21.8 %), H-4→L+1 (16.3 %)
403.53	0.0137	H-2→L+4 (61.2 %), H-2→L+3 (30.7 %)

Complete Reference 6:

Gaussian 09, Revision A.02, 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, 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, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.