Supplementary Material (ESI) for Chemical Communications

Improved transparency-nonlinearity trade-off with boroxine-based octupolar molecules

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High Resolution Mass Spectra were performed by the *Centre Régional de Mesures Physiques de l'Ouest* (Rennes).
Crystal structure of compound **1** was performed by the *Centre de Diffractométrie X* at University of Rennes 1.

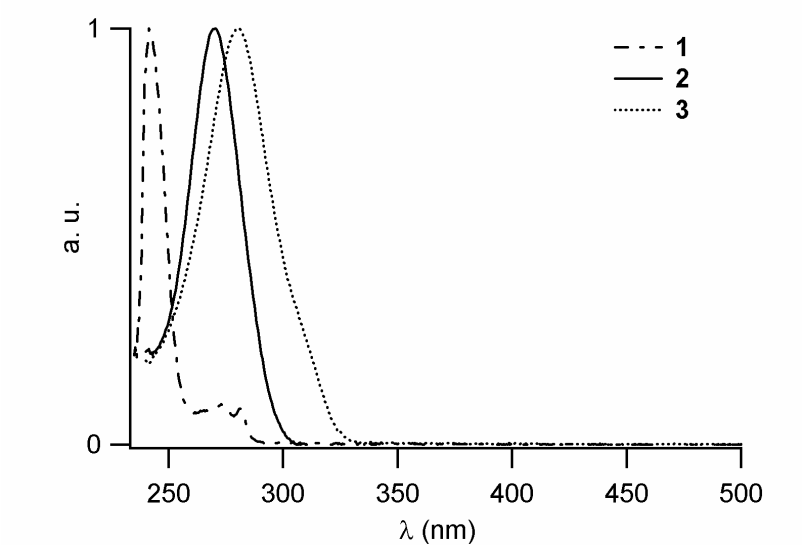
Characterization data for compounds 1-3:

1: ^{1}H (200 MHz, $CDCl_3$): δ 3.80 (s, 9H, OCH_3), 7.95 and 8.10 (d, $^{3}J_{HH}$=8.54 Hz, CH). ^{13}C (50 MHz, $CDCl_3$): δ 55.6 (s, 3C, OCH_3), 113.9 and 137.9 (s, 6C, CH), 163.6 (s, 3C, C^{IV}-OMe). ^{11}B NMR (96.3 MHz, $CDCl_3$): δ 29.3. HRMS [$M^{+\cdot}$] calcd. for $C_{21}H_{21}O_6B_3$: *m/z* 402.1617. Found 402.1649 (7 ppm). $C_{21}H_{21}O_6B_3$: C 62.77, H 5.27; found C 62.76, H 5.31.

2: ^{1}H (200 MHz, $CDCl_3$): δ 2.47 (s, 9H, SCH_3), 7.38 and 8.14 (d, $^{3}J_{HH}$=8.33 Hz, CH). ^{13}C (50 MHz, $CDCl_3$): δ 15.3 (s, SCH_3), 125.3 and 136.3 (s, 6C, CH), 145.0 (s, 3C, C^{IV}-SMe). ^{11}B NMR (96.3 MHz, $CDCl_3$): δ 33.2. HRMS [$M^{+\cdot}$] calcd. for $C_{21}H_{21}O_3S_3B_3$: *m/z* 450.0932. Found 450.0938 (1 ppm). $C_{21}H_{21}O_3S_3B_3$: C 56.05, H 4.70; found C 55.57, H 4.91

3: ^{1}H (200 MHz, $CDCl_3$): δ 3.10 (s, 18H, NMe_2), 6.83 and 8.14 (d, $^{3}J_{HH}$=8.85 Hz, CH). ^{13}C (50 MHz, $CDCl_3$): δ 40.5 (s, 6C, NMe_2), 111.5 and 137.5 (s, 6C, CH), 153.6 (s, 3C, C^{IV}- NMe_2). ^{11}B NMR (96.3 MHz, $CDCl_3$): δ 29.8. HRMS [$M^{+\cdot}$] calcd. for $C_{24}H_{30}N_3O_3B_3$: *m/z* 441.2566. Found 441.2564 (0 ppm). $C_{24}H_{30}N_3O_3B_3$: C 65.37, H 6.86, N 9.53; found C 64.67, H 6.84, N 9.25.

UV-Visible spectra for compounds 1-3:



Normalized absorption spectra of molecules **1-3** in chloroform.

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Computational details.

Calculations were conducted using the Gaussian 98 package[1] with the B3LYP[2] density functional and the 6-31G* basis set. C_{3h} symmetry has been assumed for compounds **1**-**2** and D_{3h} for compound **3**.

References:

1 Gaussian 98, Revision A.11, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, M. Head-Gordon, R. E. S. and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2001.

2 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.