Supporting Information

Functionalized Bodipy with Various Sensory Units – A Versatile Colorimetric and Luminescent Probe for pH and ions

Zhendong Yin,[§,‡] Anthony Yiu-Yan Tam,[‡] Keith Man-Chung Wong,[‡] Chi-Hang Tao,[‡] Bao Li[§], Chun-Ting Poon,[‡] Lixin Wu,[§] Vivian Wing-Wah Yam*[§,‡]

[§]*State Key Laboratory of Supramolecular Structure and Materials and College of Chemistry, Jilin University, Changchun 130012, P.R. China*

[‡]*Institute of Molecular Functional Materials (Areas of Excellence Scheme, University Grants Committee (Hong Kong)) and Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong*

Email: wwyam@hku.hk

Electronic Supplementary Material (ESI) for Dalton Transactions

Tables and Figures

Table S1. Crystallographic and structural refinement data for **1**.

Table S2. Selected bond distances (Å) and bond angles (deg) for **1** with estimated standard deviations (e.s.d.s.) given in parentheses.

Figure S1. (a) Perspective drawing of **1** with atomic numbering scheme. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 50 % probability level. (b) Ball-and-stick model showing the dimeric arrangement of two molecules of **1**.

Figure S2. (a) Expanded ion cluster at *m/z* 640.5 from the positive ESI-mass spectrum of an acetonitrile solution of **1** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{1}\cdot Mg–H]^+$.

Figure S3. (a) Expanded ion cluster at *m/z* 484 from the positive ESI-mass spectrum of an acetonitrile solution of **2** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{2}\cdot 2Mg–2H]^{2+}$.

Figure S4. (a) Expanded ion cluster at *m/z* 1269 from the positive MALDI-TOF mass spectrum of an acetonitrile solution of **2** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{2}\cdot 2Mg\cdot 3ClO_4]^+$.

Figure S5. (a) Expanded ion cluster at *m/z* 972.5 from the positive ESI-mass spectrum of an acetonitrile solution of **5** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{5}\cdot Mg–H]^+$.

Table S1. Crystallographic and structural refinement data for **1**.

empirical formula	$C_{34}H_{38}BF_2N_3O_5$
formula weight	617.48
temperature	293(2) K
wavelength	0.71073 Å
crystal system,	triclinic
space group	$P\bar{1}$
a [Å]	10.291(2)
b [Å]	12.539(3)
c [Å]	12.846(3)
α [°]	70.34(3)
β [°]	88.71(3)
γ [°]	88.86(3)
volume	1560.5(5) $Å^3$
Z	2
density(Calcd)	1.314 g cm^{-3}
absorption coefficient	0.096 mm^{-1}
F(000)	652
crystal size	0.34 mm × 0.18 mm × 0.17 mm
data collection range	3.23 to 27.48°
index range	$-11 \le h \le 13$, $-16 \le k \le 16$, $-16 \le l \le 16$
no. of reflns collected	15314
no. of indep reflns	6984 [*R*(int) = 0.0490]
completeness to $\theta = 27.48°$	97.6 %
absorp corr	None
refinement method	full-matrix least-squares on F^2
no. of data/restraints/params	6984 / 0 / 408
goodness-of-fit on F^2	0.997
final *R* indices[a] [$I > 2\sigma(I)$]	$R_1 = 0.0603$, $wR_2 = 0.1234$
R indices (all data)	$R_1 = 0.1276$, $wR_2 = 0.1456$
largest diff peak and hole	0.165 and –0.202 e$Å^{-3}$

[a] $R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})|/\Sigma[F_o^2]$, $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table 2. Selected bond distances (Å) and bond angles (deg) for **1** with estimated standard deviations (e.s.d.s.) given in parentheses

B(1)–F(1)	1.378(3)	B(1)–F(2)	1.383(3)
B(1)–N(1)	1.536(3)	B(1)–N(2)	1.551(3)
C(8)–N(1)	1.398(3)	C(11)–N(1)	1.351(3)
C(13)–N(2)	1.394(3)	C(16)–N(2)	1.355(3)
C(16)–C(17)	1.437(3)	C(17)–C(18)	1.330(3)
H(1)···O(2)	1.9726(16)	N(1)–B(1)–N(2)	107.23(17)
F(1)–B(1)–F(2)	110.21(18)		

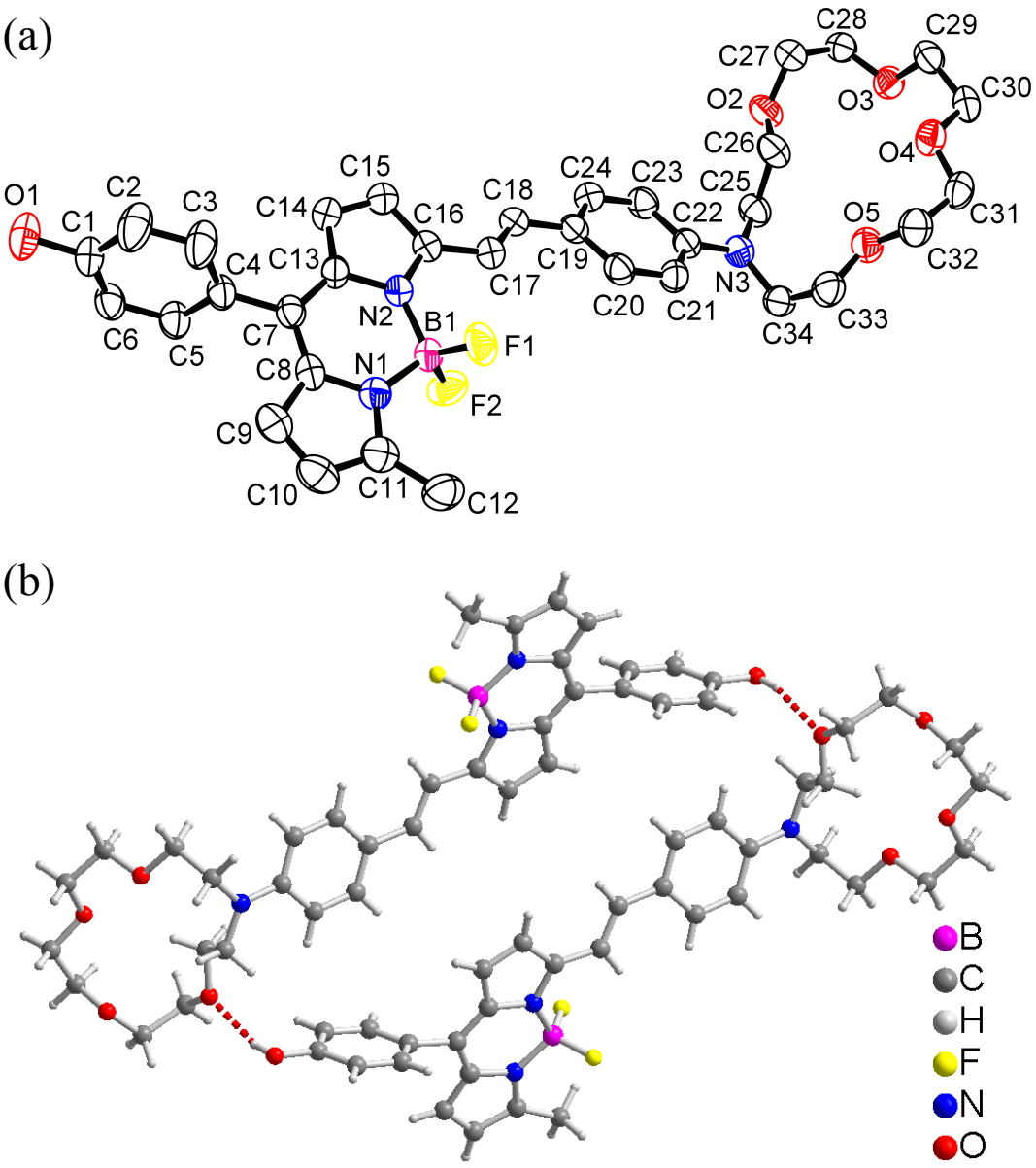

Figure S1. (a) Perspective drawing of **1** with atomic numbering scheme. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at the 50 % probability level. (b) Ball-and-stick model showing the dimeric arrangement of two molecules of **1**.

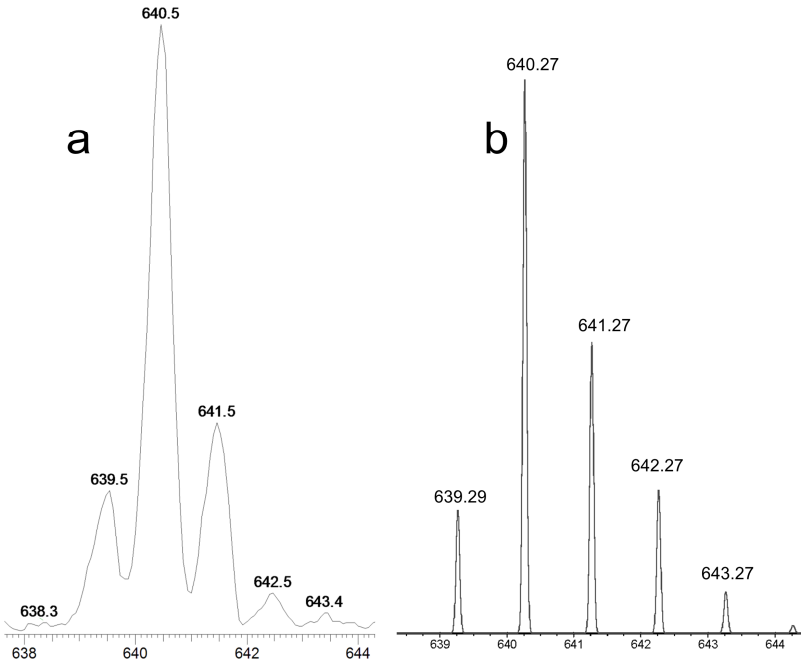

Figure S2. (a) Expanded ion cluster at *m/z* 640.5 from the positive ESI-mass spectrum of an acetonitrile solution of **1** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{1}\cdot Mg–H]^+$.

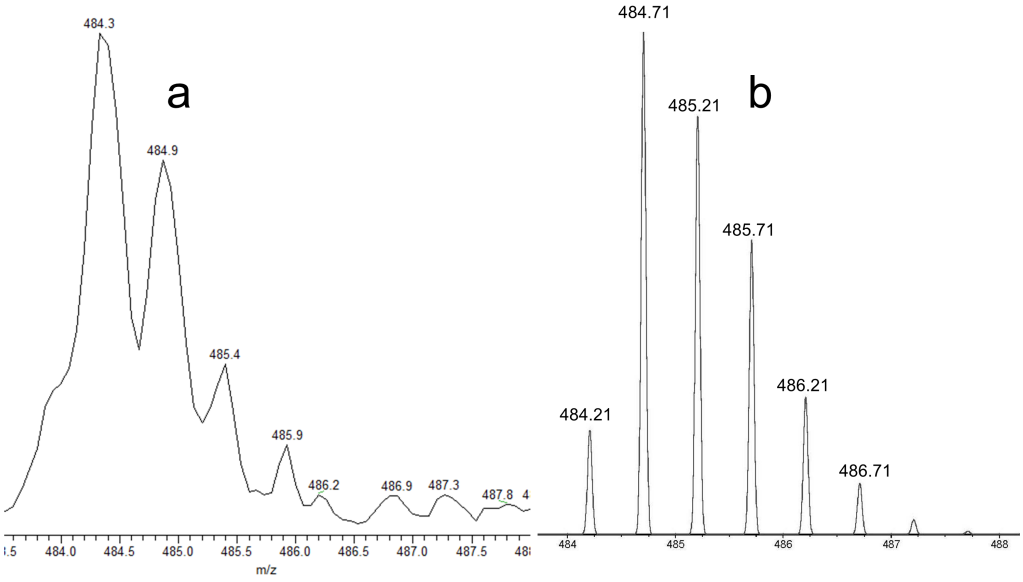

Figure S3. (a) Expanded ion cluster at *m/z* 484 from the positive ESI-mass spectrum of an acetonitrile solution of **2** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{2}\cdot 2Mg–2H]^{2+}$.

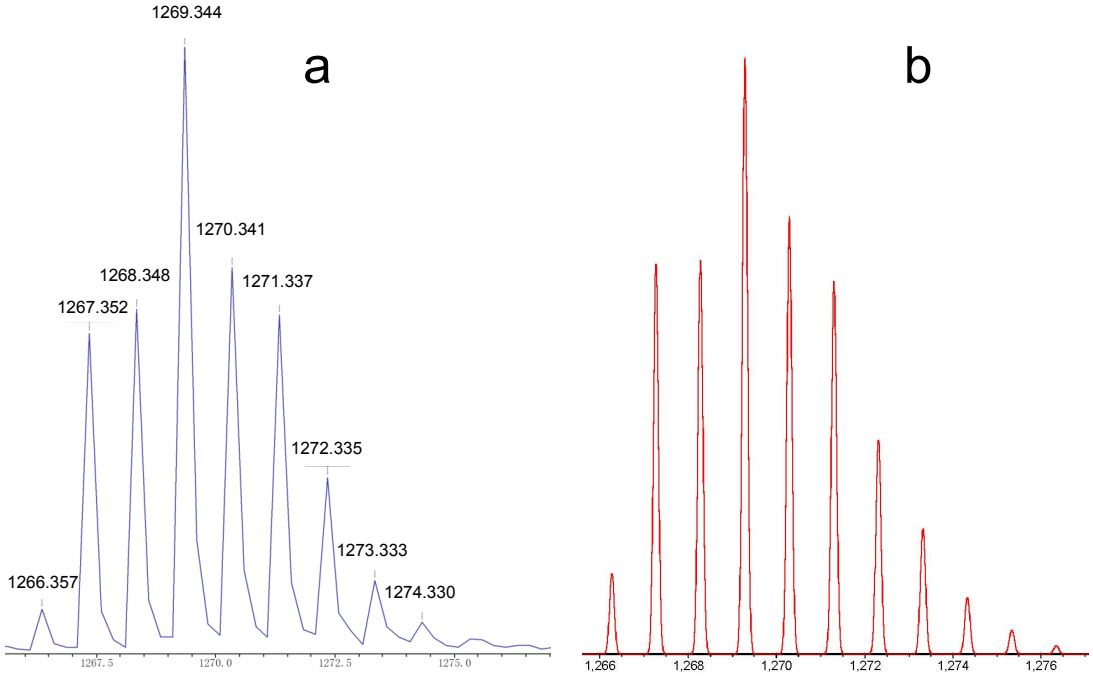

Figure S4. (a) Expanded ion cluster at *m/z* 1269 from the positive MALDI-TOF mass spectrum of an acetonitrile solution of **2** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of $[\mathbf{2}\cdot 2Mg\cdot 3ClO_4]^+$.

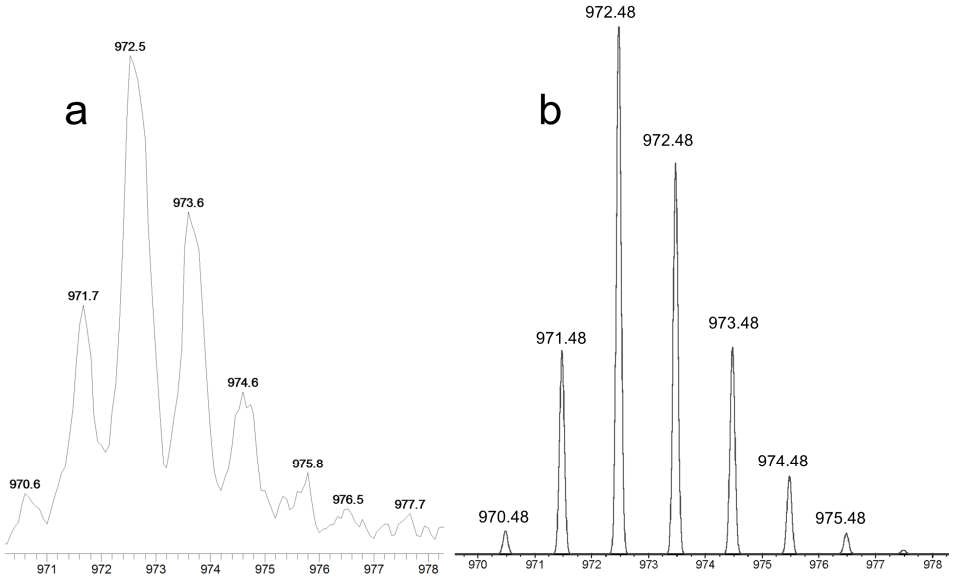

Figure S5. (a) Expanded ion cluster at *m/z* 972.5 from the positive ESI-mass spectrum of an acetonitrile solution of **5** and $Mg(ClO_4)_2$; (b) simulated isotopic pattern of

$[\mathbf{5}\cdot\mathrm{Mg–H}]^{+}$.