Electronic Supplementary Material (ESI) for Chemical Communications

Boolean operations mediated by an ion-pair receptor of a multi-readout molecular logic gate†

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Electronic Supplementary information

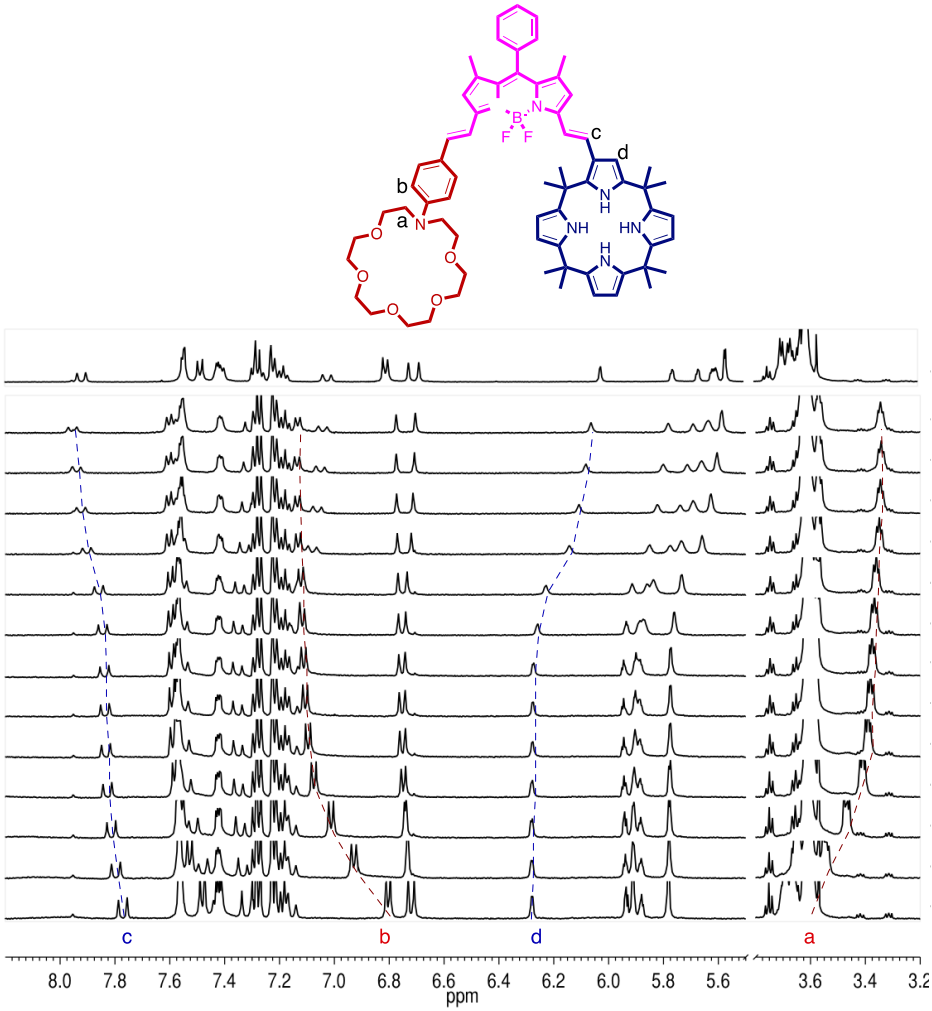


Figure S1- ^{1}H-NMR titration of compound **1** (5 mM in CD_3CN) with different amounts of $KClO_4$ and then TBAF. ^{1}H-NMR of **1** (5 mM in CD_3CN) with 3 eq. of TBAF is included on top for comparison purposes.

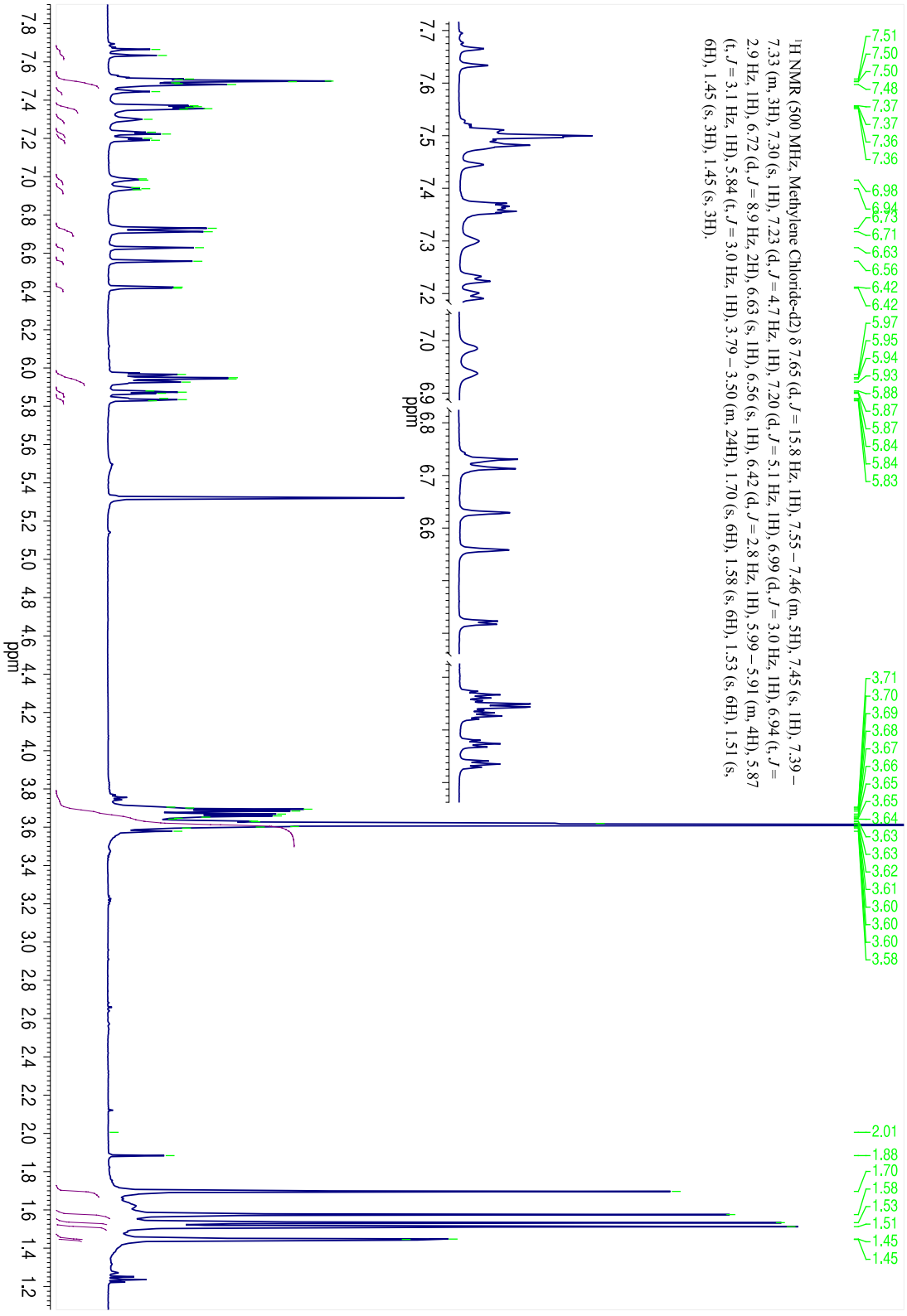
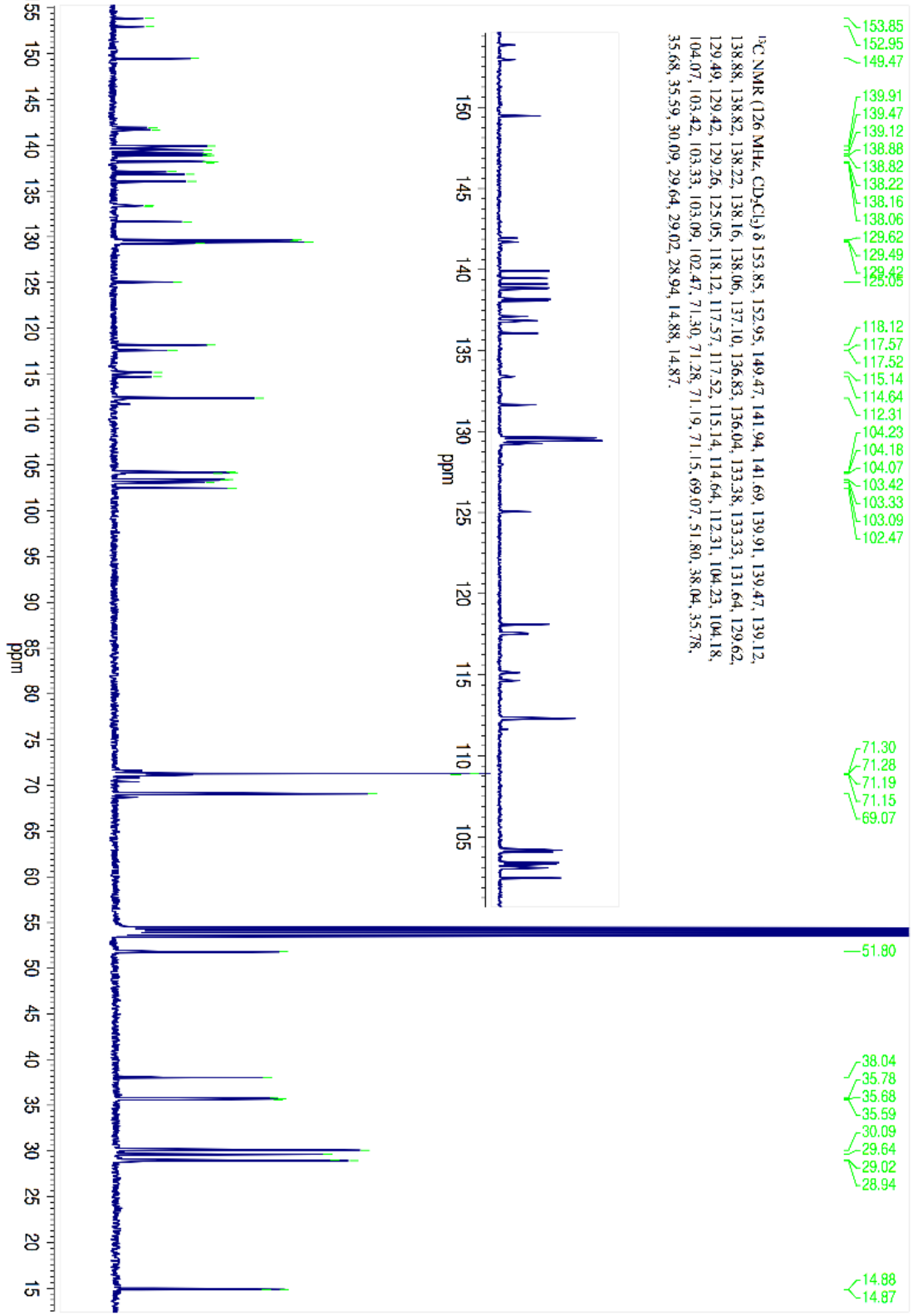
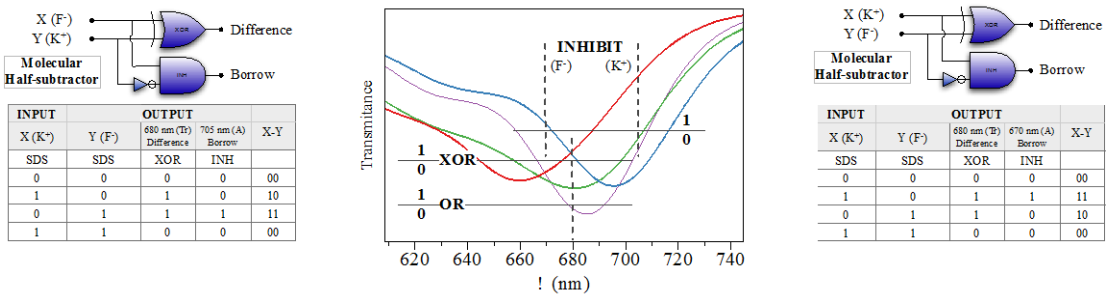


Figure S2- ^{1}H-NMR spectrum of **1** in CD_2Cl_2



^{13}C NMR (126 MHz, CD_2Cl_2) δ 153.85, 152.95, 149.47, 141.94, 141.69, 139.91, 139.47, 139.12, 138.88, 138.82, 138.22, 138.16, 138.06, 137.10, 136.83, 136.04, 133.38, 133.33, 131.64, 129.62, 129.49, 129.42, 129.26, 125.05, 118.12, 117.57, 117.52, 115.14, 114.64, 112.31, 104.23, 104.18, 104.07, 103.42, 103.33, 103.09, 102.47, 71.30, 71.28, 71.19, 71.15, 69.07, 51.80, 38.04, 35.78, 35.68, 35.59, 30.09, 29.64, 29.02, 28.94, 14.88, 14.87.

Figure S3- ^{13}C-NMR spectrum of **1** in CD_2Cl_2



INPUT		OUTPUT		
X (K⁺)	Y (F⁻)	680 nm (Tr) Difference	705 nm (A) Borrow	X-Y
SDS	SDS	XOR	INH	
0	0	0	0	00
1	0	1	0	10
0	1	1	1	11
1	1	0	0	00

INPUT		OUTPUT		
X (K⁺)	Y (F⁻)	680 nm (Tr) Difference	670 nm (A) Borrow	X-Y
SDS	SDS	XOR	INH	
0	0	0	0	00
1	0	1	1	11
0	1	1	0	10
1	1	0	0	00

Figure S4- INHIBIT gates and half-subtractor true tables in the transmittance mode

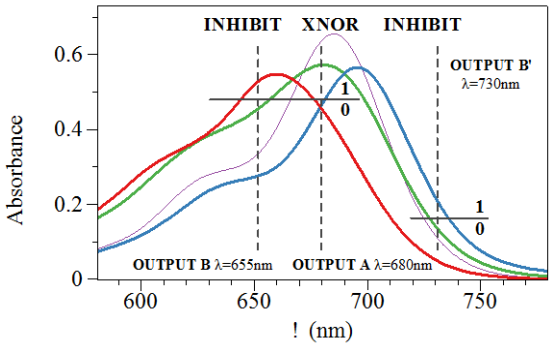


Figure S5- Other INHIBIT gates in the absorption mode, using K^+ or F^- as single inputs

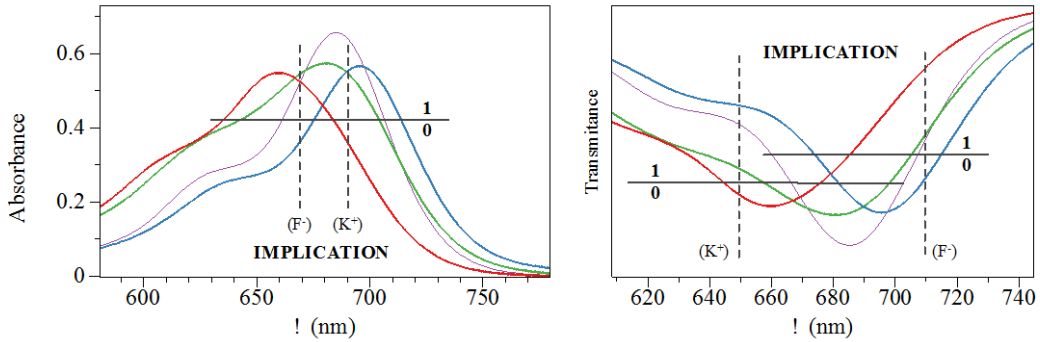


Figure S6- IMPLICATION gates operating both in absorbance or transmission modes, using K^+ or F^- as single inputs

Spectroscopic details: Steady-state absorption and fluorescence measurements were carried out using a Analytik Jena Specord 210 Plus spectrophotometer, a Spectronics Instrument 8100 spectrofluorometer and a Horiba Jobin–Yvon FluoroMax-4P spectrofluorometer. For all measurements, the temperature was kept constant at (298±1) K. Unless otherwise noted, only dilute solutions with an absorbance of less than 0.1 at the absorption maximum were used. Fluorescence experiments were performed with a 90° standard geometry, with polarisers set at 54.78 for emission and 08 for excitation. The fluorescence quantum yields (Φ_f) were determined relative to compound **3** of ref. S1 in acetonitrile (Φ_f= 0.10

± 0.01). The uncertainties of measurement were determined to ±5% (for Φ_f >0.2) and ±10% (for 0.2>Φ_f >0.02).

S1. Y.-H. Yu, A. B. Descalzo, Z. Shen, H. Röhr, Q. Liu, Y.-W. Wang, M. Spieles, Y.-Z. Li, K. Rurack and X.-Z. You, *Chem. Asian. J.*, 2006, **1**, 176–187.