

A zwitterionic 1D/2D polymer co-crystal and its polymorphic sub-components: a highly selective sensing platform for HIV ds-DNA sequences

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Table S1. Selected bond distances (Å) and angles (°) for complexes **1–4**.

Complex 1			
Na(1)-O(4)	2.2522(15)	Na(1)-O(1)#1	2.2625(19)
Na(1)-O(3)#2	2.300(2)	Na(1)-O(1W)	2.3095(15)
O(1)-C(7)	1.241(3)	O(1)-Na(1)#3	2.2625(19)
O(2)-C(7)	1.257(3)	O(3)-C(8)	1.250(3)
O(3)-Na(1)#4	2.300(2)	O(4)-Na(1)-O(1)#1	113.90(7)
O(4)-Na(1)-O(3)#2	103.55(7)	O(1)#1-Na(1)-O(3)#2	105.30(8)
O(4)-Na(1)-O(1W)	125.27(7)	O(1)#1-Na(1)-O(1W)	97.42(6)
O(3)#2-Na(1)-O(1W)	110.09(6)		
Complex 2			
Cu(1)-O(1)	1.9497(19)	Cu(1)#5-O(1)	1.9497(19)
Cu(1)#6-N(2)	1.996(2)	Cu(1)#7-N(2)	1.996(2)
Cu(1)#8-N(2)	1.996(2)		
O(1)#5-Cu(1)-O(1)	180.0	O(1)#5-Cu(1)#6-N(2)	88.98(9)
O(1)-Cu(1)#6-N(2)	91.02(9)	O(1)#5-Cu(1)#7-N(2)	91.02(9)
O(1)-Cu(1)#7-N(2)	88.98(9)	N(2)#6-Cu(1)#7-N(2)	180.0(2)
Complex 3			
Cu(1)-O(1)	1.968(3)	Cu(1)-O(5)	1.987(3)
Cu(1)-N(2)#9	2.010(3)	Cu(1)-N(4)#10	2.026(4)
Cu(1)-O(3)#11	2.159(3)	O(3)-Cu(1)#12	2.159(3)
N(2)-Cu(1)#10	2.010(3)	N(4)-Cu(1)#9	2.026(4)
O(1)-Cu(1)-O(5)	176.12(13)	O(1)-Cu(1)-N(2)#9	91.11(14)
O(5)-Cu(1)-N(2)#9	89.51(14)	O(1)-Cu(1)-N(4)#10	90.37(14)
O(5)-Cu(1)-N(4)#10	88.32(14)	N(2)#9-Cu(1)-N(4)#10	169.33(15)
O(1)-Cu(1)-O(3)#11	90.84(12)	O(5)-Cu(1)-O(3)#11	92.91(13)
N(2)#9-Cu(1)-O(3)#11	95.60(14)	N(4)#10-Cu(1)-O(3)#11	94.95(14)
Complex 4			
Cu(1)-N(2)	2.012(3)	Cu(1)-N(3)	2.002(3)
Cu(1)#13-O(7)	1.964(2)	Cu(1)#14-O(1)	2.005(3)
Cu(1)#15-O(6)	2.155(2)	Cu(1)-O(1)#16	2.005(3)
Cu(1)-O(6)#17	2.155(2)	Cu(1)-O(7)#14	1.964(2)
Cu(2)-N(7)	2.025(3)	Cu(2)-N(6)	2.027(3)
Cu(2)-O(1W)	2.187(5)		
O(7)#13-Cu(1)-N(3)	91.66(11)	O(7)-Cu(1)-O(1)#14	177.73(11)
N(3)-Cu(1)#14-O(1)	89.44(11)	O(7)#13-Cu(1)-N(2)	90.02(11)
N(3)-Cu(1)-N(2)	170.53(12)	O(1)#14-Cu(1)-N(2)	88.57(11)
O(7)#13-Cu(1)-O(6)#15	89.21(10)	N(3)-Cu(1)#15-O(6)	94.17(10)
O(1)#14-Cu(1)-O(6)#15	92.70(10)	N(2)-Cu(1)#15-O(6)	95.18(11)
N(7)-Cu(2)-N(6)	164.51(17)	N(7)-Cu(2)-O(1W)	100.17(16)
N(6)-Cu(2)-O(1W)	94.79(17)		

Symmetry transformations used to generate equivalent atoms: #1: $-x, y - 1/2, -z + 1/2$; #2: $-x + 1, y - 1/2, -z + 1/2$; #3: $-x, y + 1/2, -z + 1/2$; #4: $-x + 1, y + 1/2, -z + 1/2$; #5: $-x + 2, -y, -z$; #6: $-x + 1, -y, -z + 1$; #7: $x + 1, y, z - 1$; #8: $x - 1, y, z + 1$; #9: $x, y, z + 1$; #10: $x, y, z - 1$; #11: $x - 1, y, z$; #12: $x + 1, y, z$; #13: $x, y + 1, z$; #14: $x, y - 1, z$; #15: $x - 1, y + 1, z$; #16: $x, y + 1, z$; #17: $x + 1, y - 1, z$.

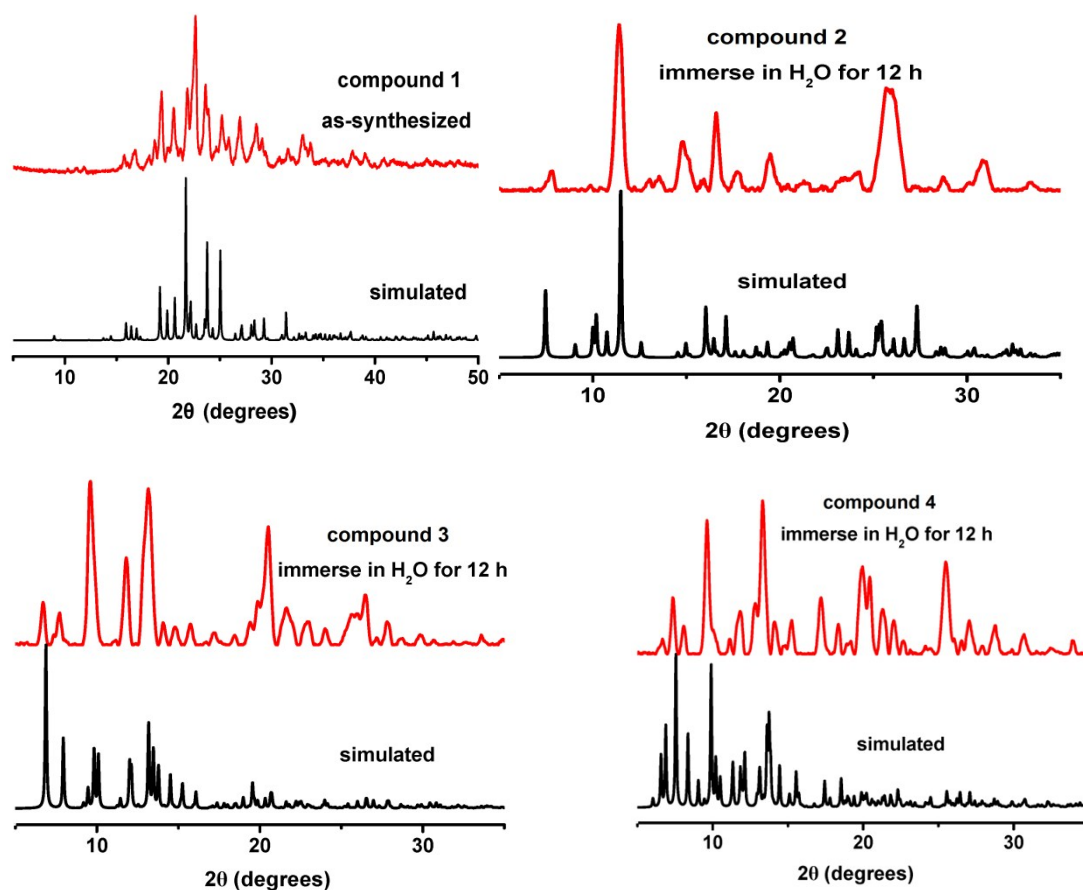


Figure S1. PXRD patterns of compounds 1–4 showing agreement between the simulated and as-synthesized for 1 (a), the simulated and immerse in H₂O for 12 h for 2–4 (b–d)

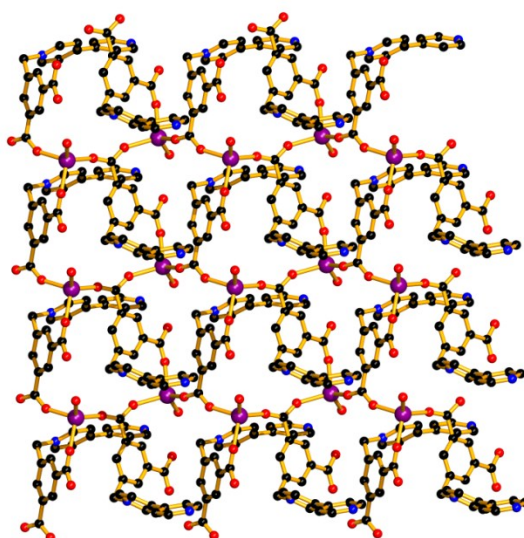


Figure S2. 2D network of [Na(dcbp)(H₂O)]_n (1) extended in the *ab* plane. Color codes: Na (violet), O (red), N (blue), C (black).

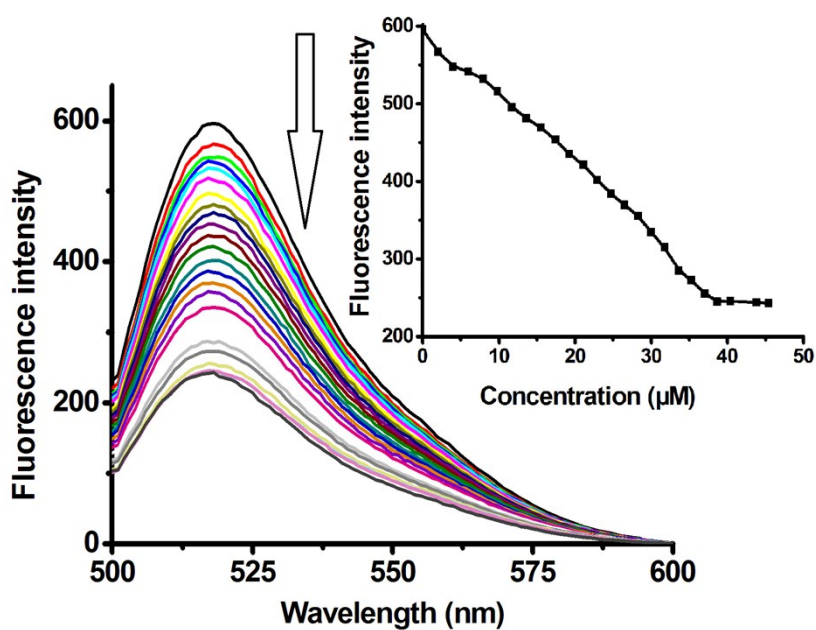


Figure S3. Fluorescence quenching of the probe DNA (70 nM) incubated with $\text{Cu}(\text{NO}_3)_2$ of varying concentrations at room temperature. Inset: Plot of fluorescence intensity versus the concentrations of $\text{Cu}(\text{NO}_3)_2$.

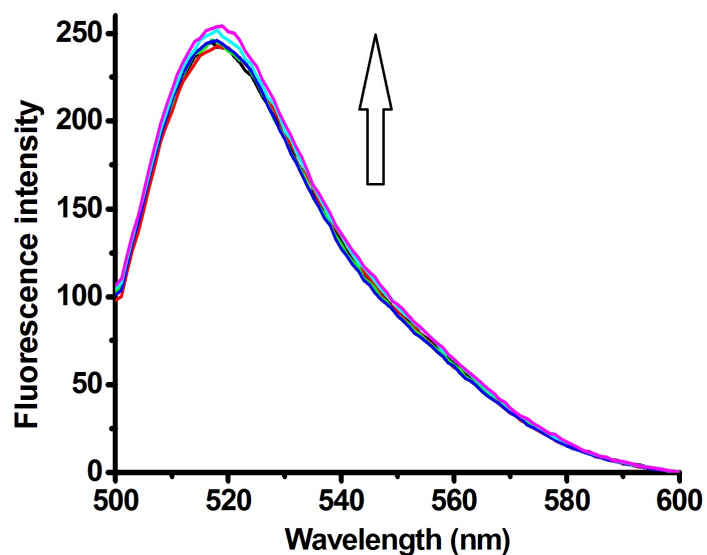


Figure S4. Fluorescent recovery of P-DNA@ $\text{Cu}(\text{NO}_3)_2$ system after incubation with varying concentrations of target HIV ds-DNA at room temperature.

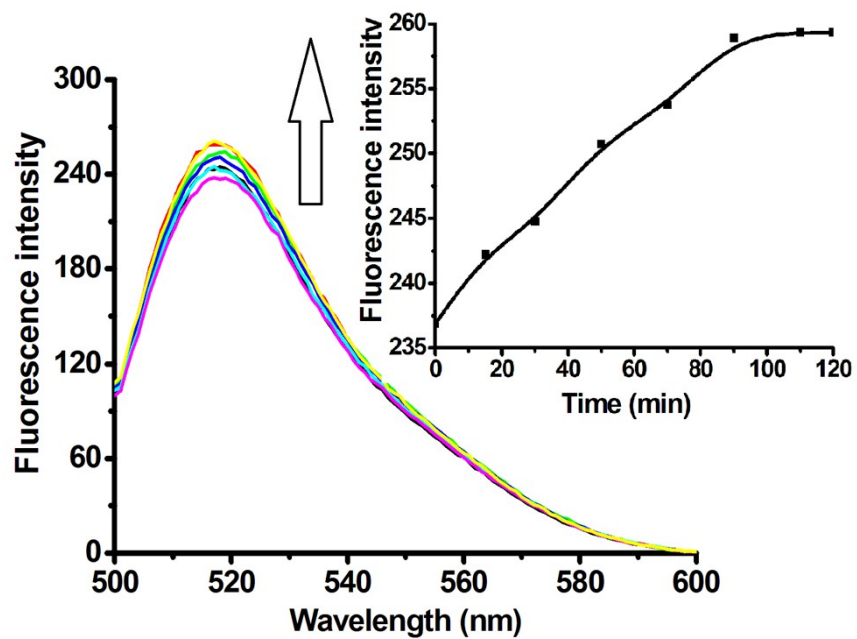


Figure S5. Influence of incubation time between the P-DNA@**3** system and the target ds-DNA on fluorescence intensity. Concentrations: target DNA, 20 nM; probe DNA, 70 nM; compound **3**, 24.7 μ M. The fluorescence intensity is collected at 518 nm.