

Supporting Information

Multitopic Ligand Design: a New Concept for Single Source Precursors

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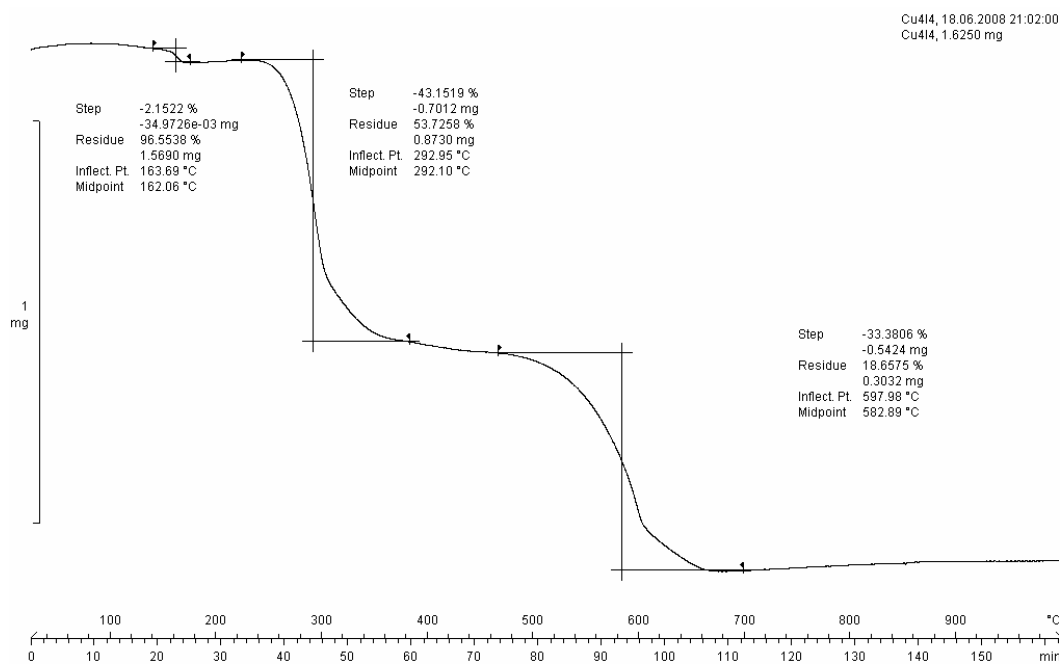


Figure S1. TGA analysis of compound **3**.

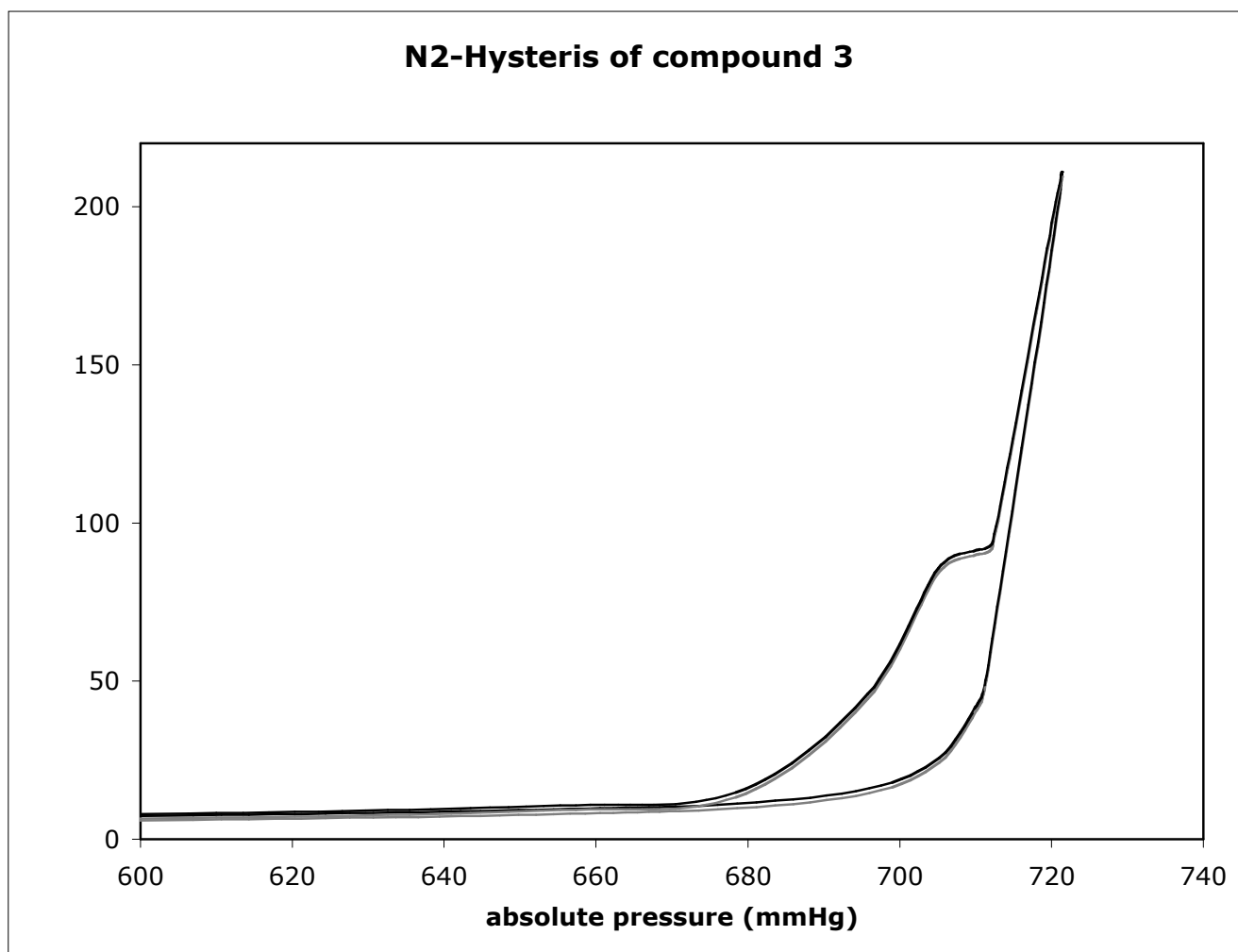


Figure S2. BET analysis:**3**: Hysteris curve of **3**.

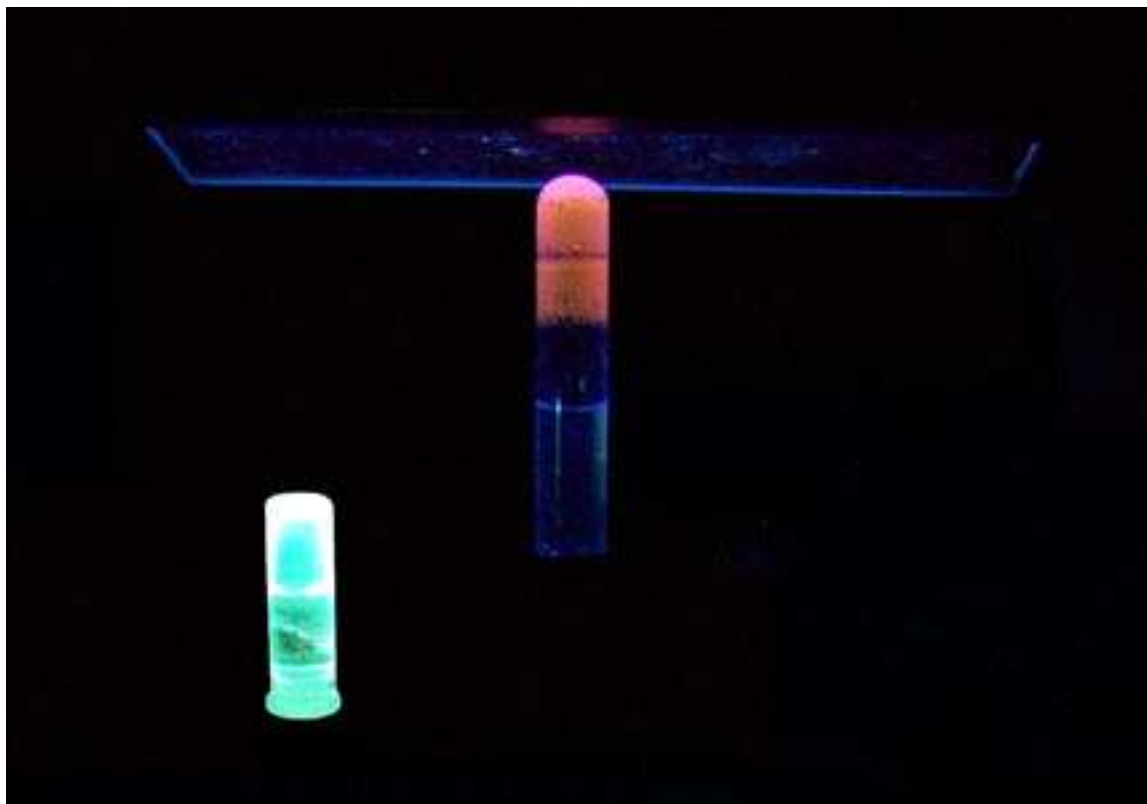


Figure S3. Picture of the fluorescence compound **3** and **3'**.

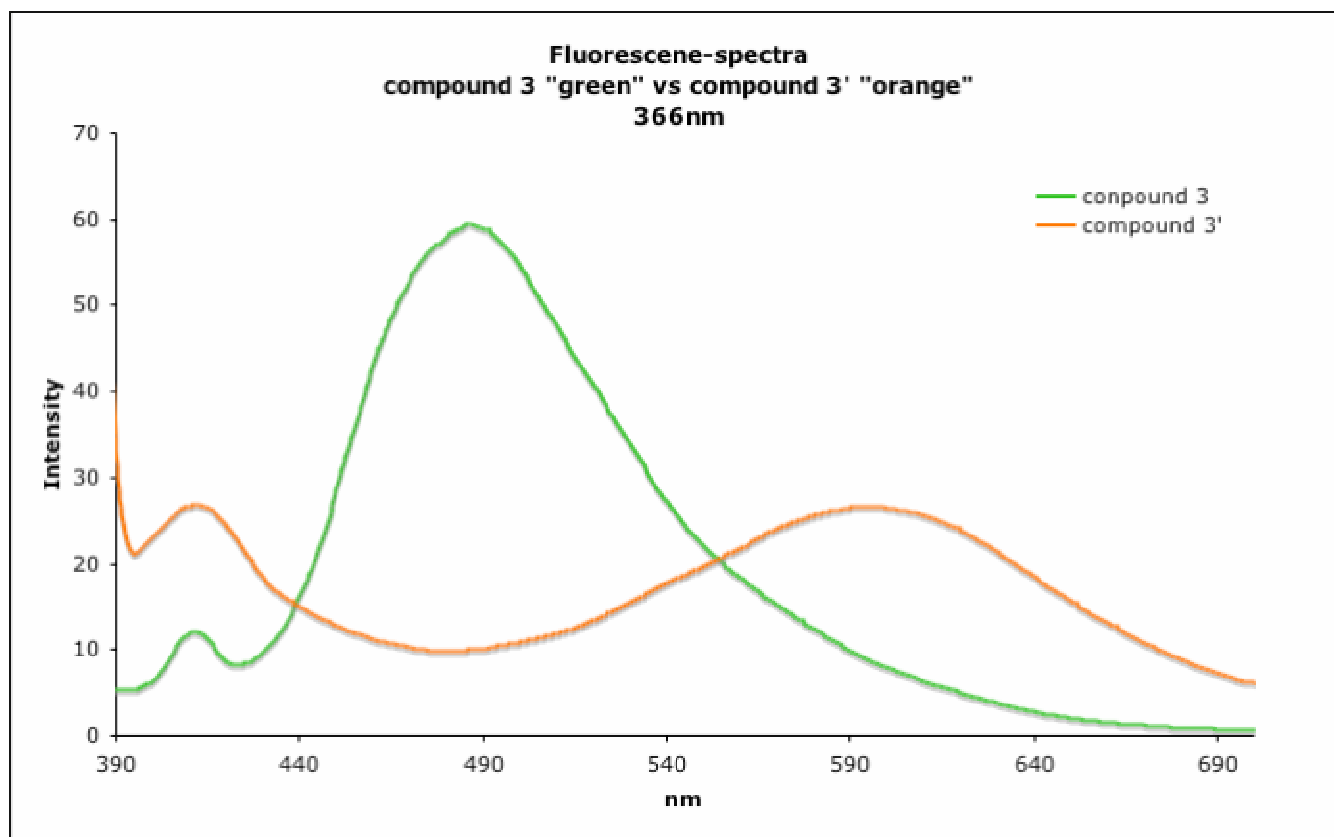


Figure S4. Fluorescence spectras of compound **3** and **3'**.

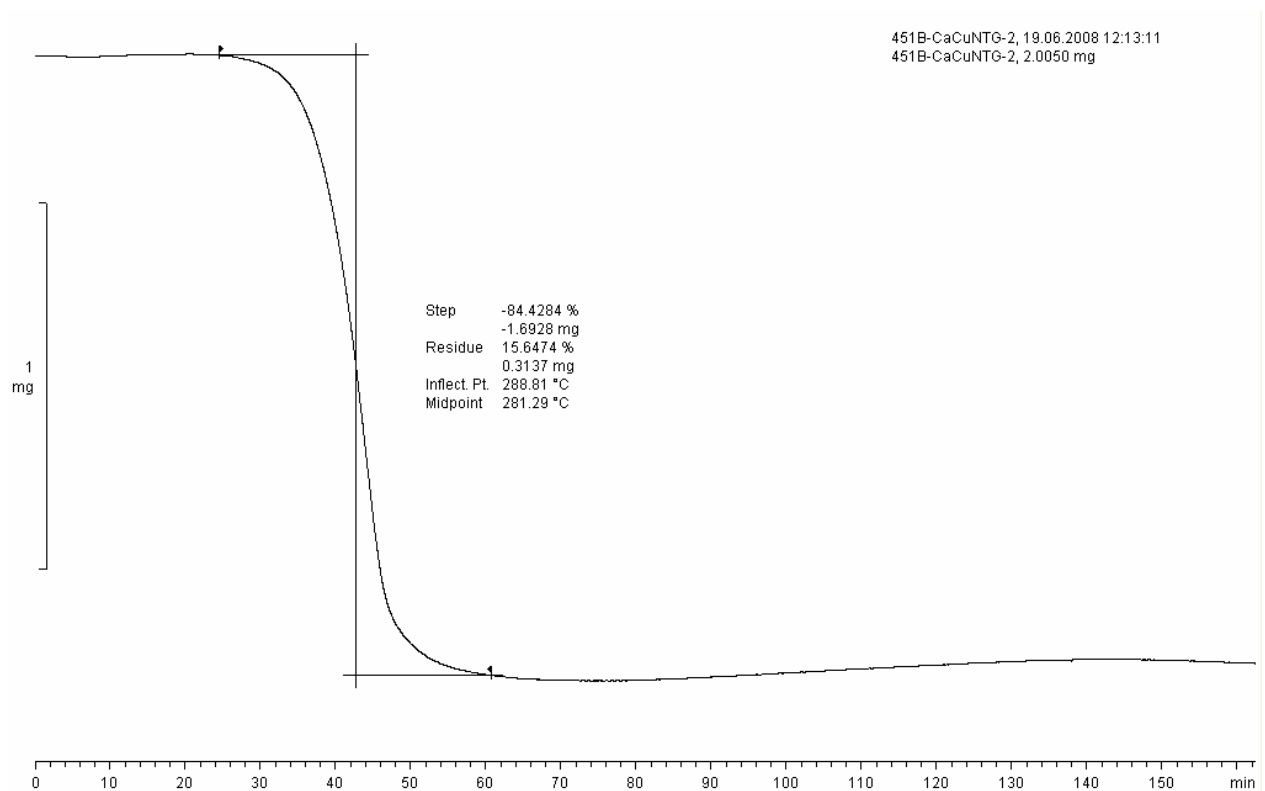


Figure S5. TGA analysis of compound **4**.

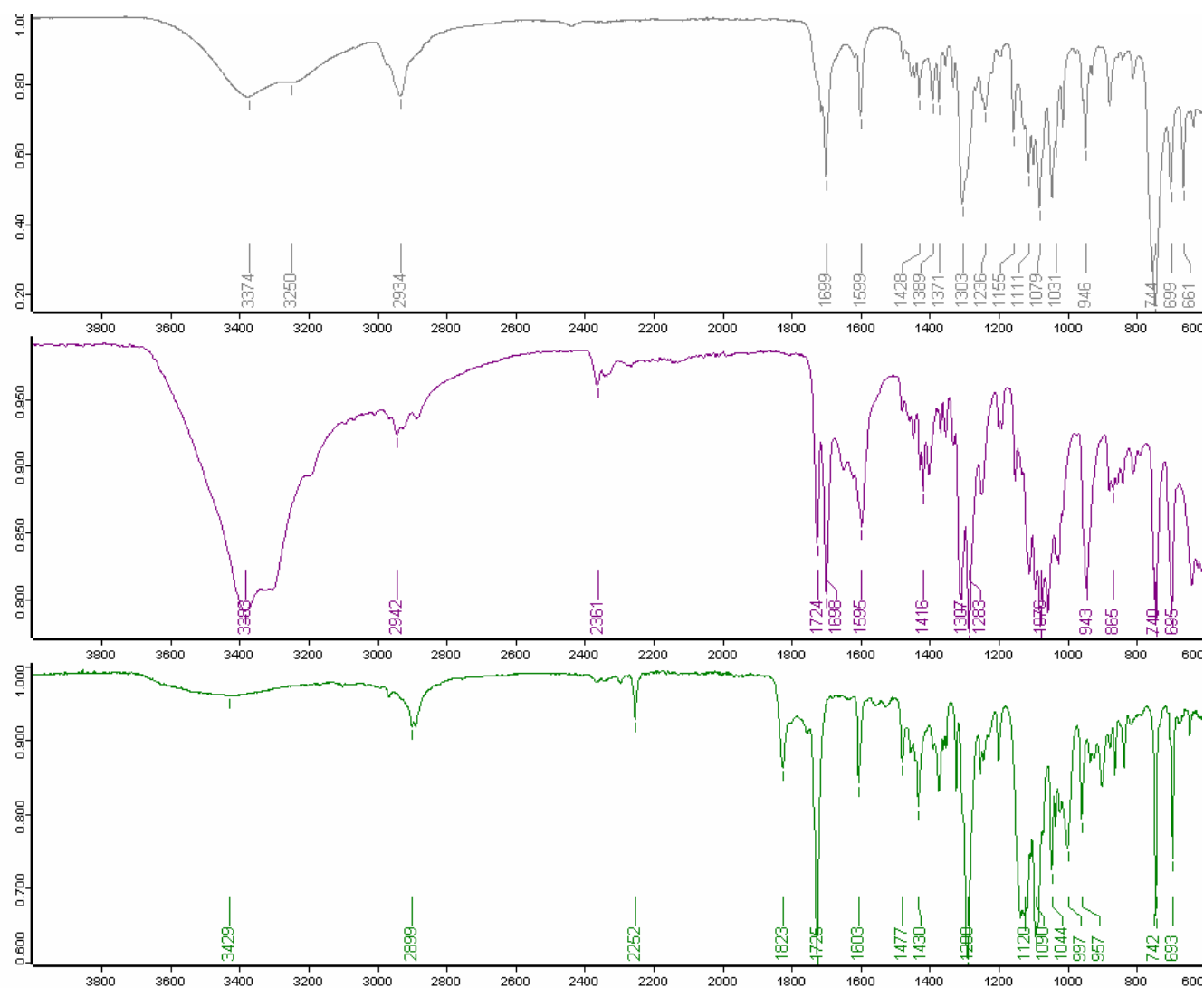


Figure S6. IR spectra of compound **2**, **1** and **5**.

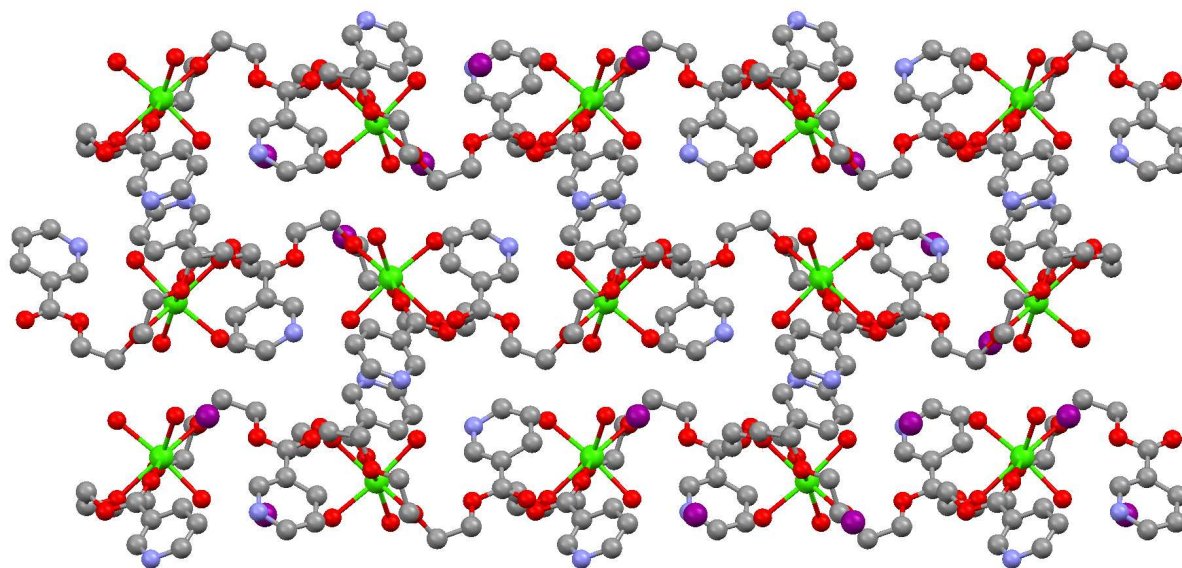


Figure S7. Packing along x -axis of compound **1**.

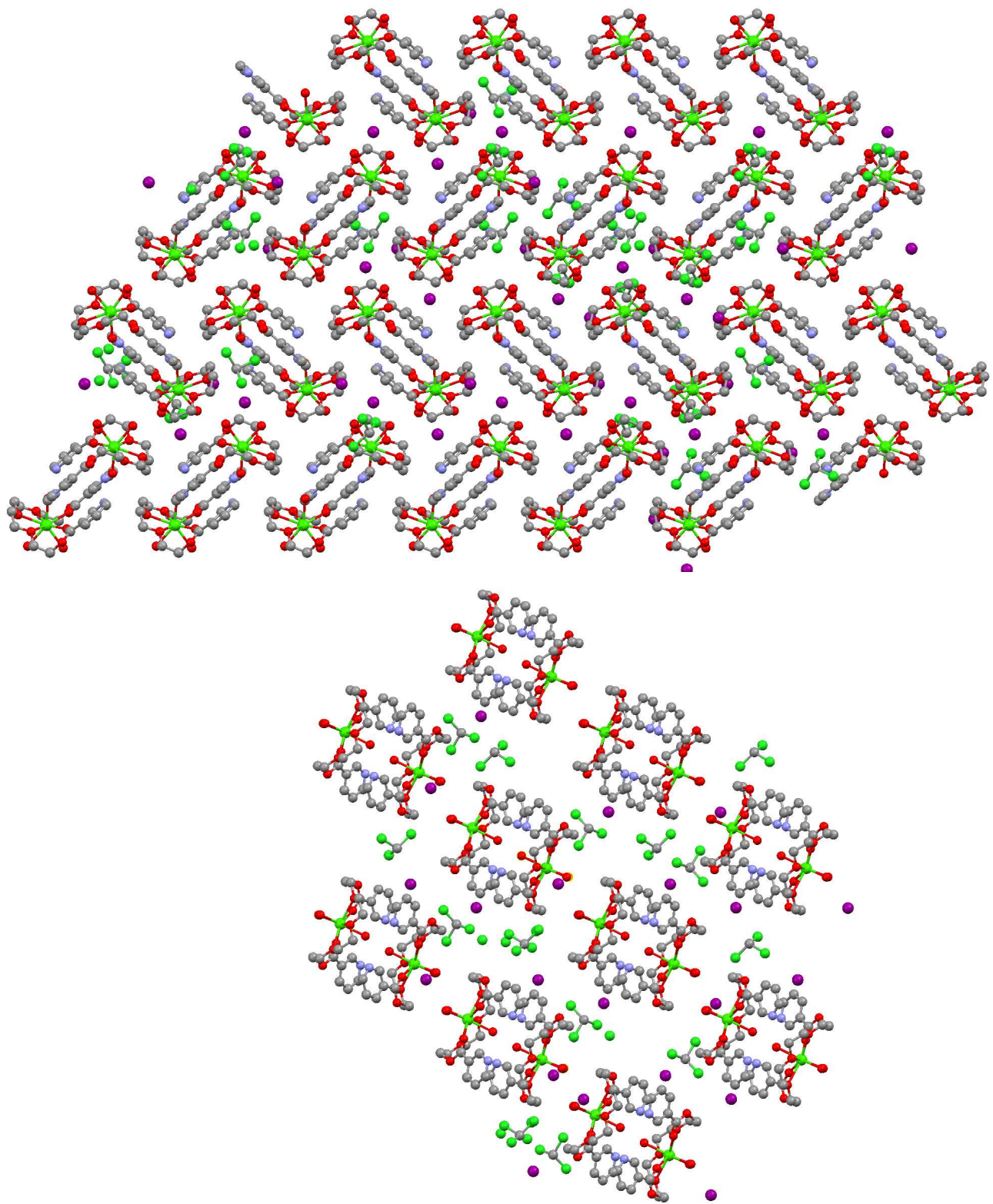


Figure S8. Packing of compound **2** a) along the *x*-axis, b) along the *y*-axis.

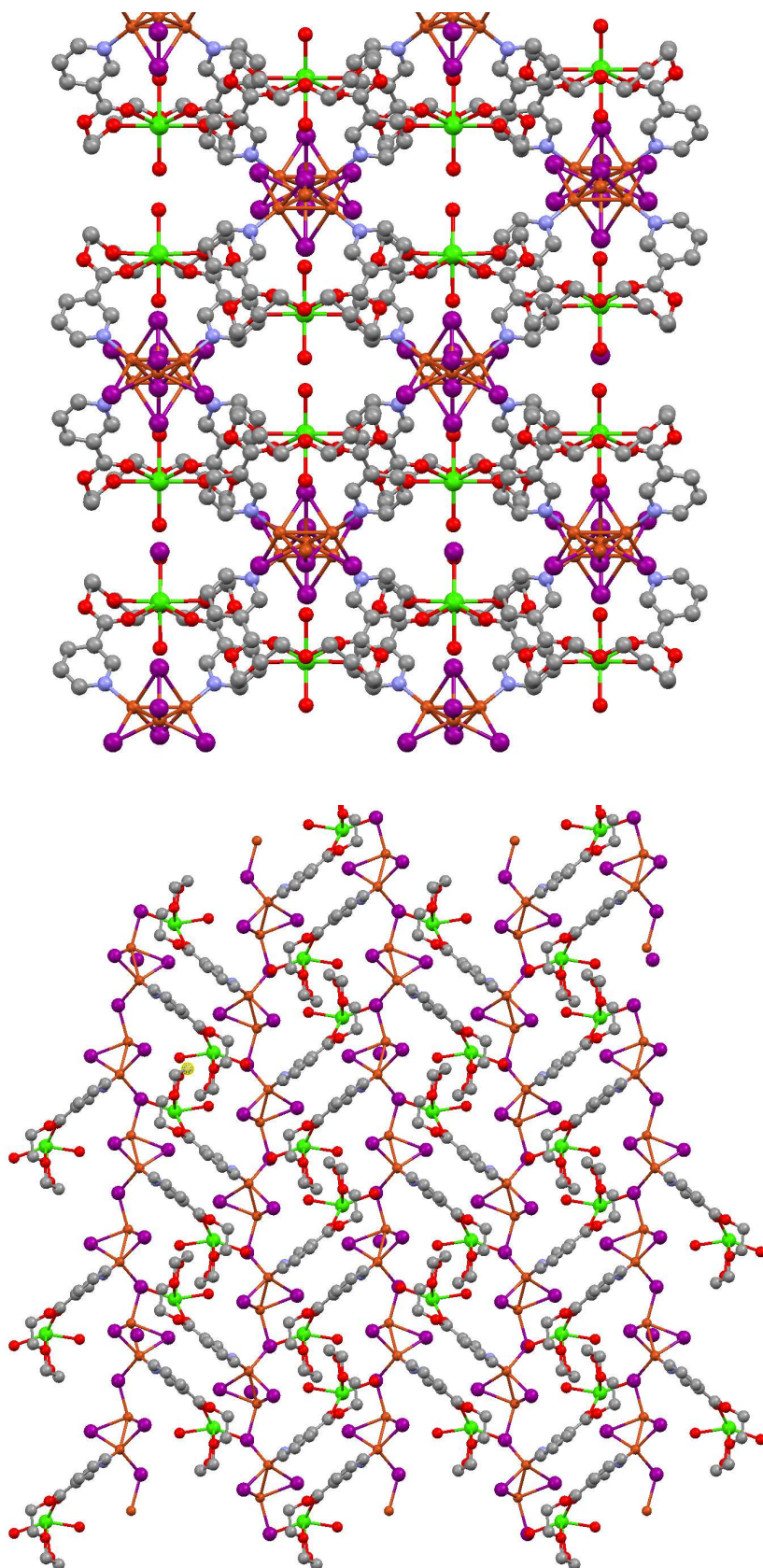


Figure S9. Packing of **4** a) along the *x*-axis, b) along the *y*-axis.

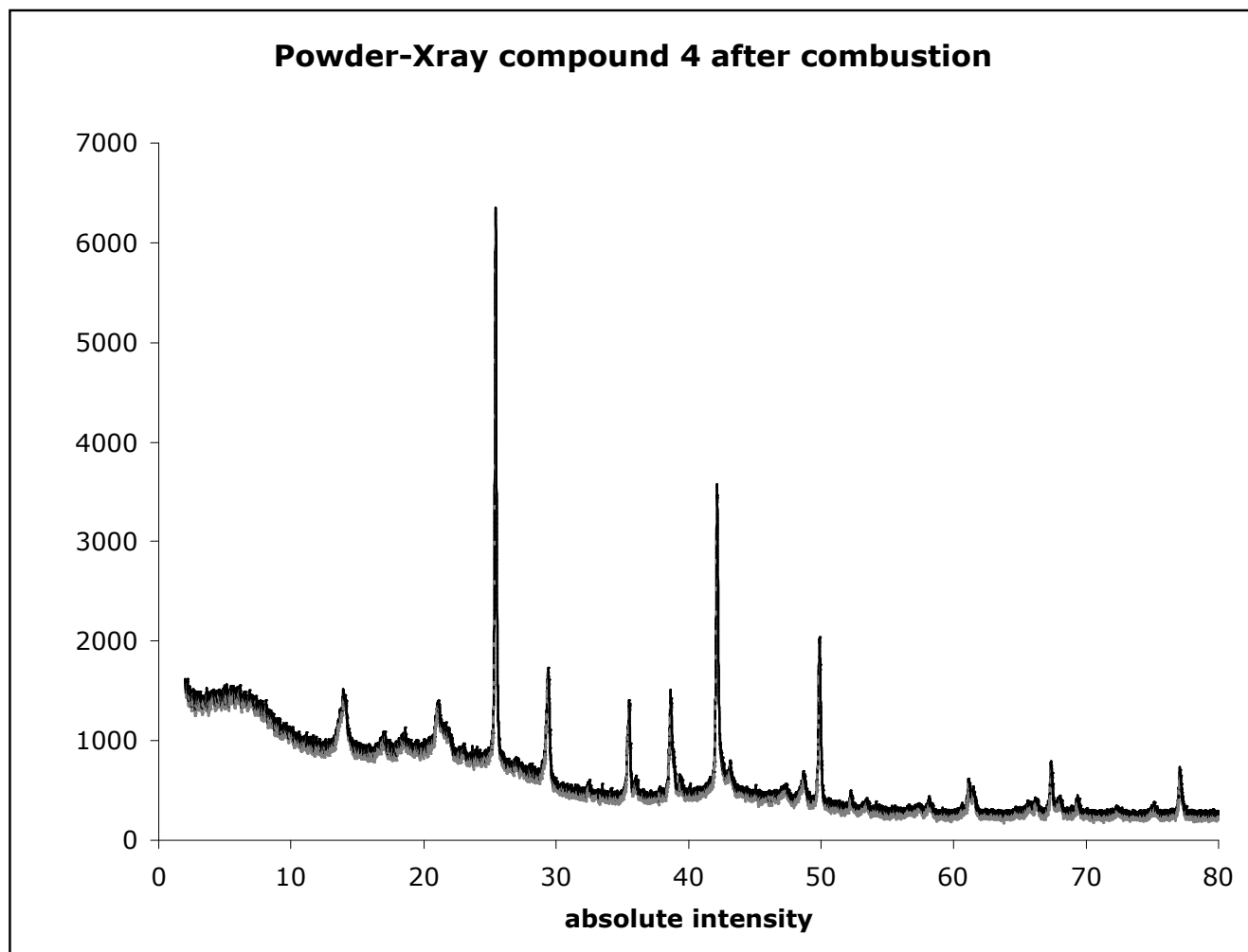


Figure S10. Powder-Xray-spectra of compound **4** after combustion.

Hydrogen bonds for compound **1** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(8)-H(21)...I(1)#1	0.85	2.62	3.470(9)	178.7
O(8)-H(22)...I(1)#2	0.87	2.63	3.499(10)	179.8
O(9)-H(23)...I(2)#3	0.98	2.64	3.595(9)	165.9
O(9)-H(24)...N(1)#1	0.74	2.23	2.778(15)	132.2
O(10)-H(25)...I(2)#4	0.99	2.88	3.446(10)	117.6
O(10)-H(26)...I(1)#2	0.99	2.66	3.531(11)	146.9

Symmetry transformations used to generate equivalent atoms:

#1 -x-1,-y,-z #2 x,y,z-1 #3 -x,-y,-z #4 x,-y+1/2,z-1/2

Hydrogen bonds for compound **2** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(8)-H(21)...N(1)#1	1.01	1.82	2.800(14)	162.4
O(8)-H(22)...N(2)#1	0.97	1.94	2.776(13)	143.1
O(9)-H(25)...I(1)	0.75	3.07	3.496(10)	119.1
O(9)-H(26)...I(1)#2	0.81	3.22	4.018(11)	171.1
O(10)-H(23)...I(1)#3	0.90	3.17	3.849(10)	133.6
O(10)-H(24)...I(1)	0.85	2.66	3.509(9)	179.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1 #2 -x+3/2,y-1/2,-z+1/2 #3 -x+3/2,y+1/2,-z+1/2

Hydrogen bonds for compound **4** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(51)...I(2)#2	0.96	2.86	3.433(11)	119.3
O(6)-H(61)...I(4)#6	1.00	3.04	3.521(17)	110.8

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z #2 x+1/2,y,-z+1/2 #3 x-1/2,y,-z+1/2
 #4 -x+1/2,-y+1,z+1/2 #5 -x+1/2,-y+1,z-1/2 #6 -x+1,-y+1,-z+1

Hydrogen bonds for compound **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(550)...O(4)#1	0.90(2)	2.53(2)	3.09(2)	120(12)
O(12)-H(550)...I(1)	0.90(2)	2.73(2)	3.46(2)	139(12)
O(6)-H(6z)...I(1)	0.93(7)	3.67(2)	4.60(3)	172.7(7)
O(6)-H(6z)...Cl(6)	0.93(7)	5.34(2)	5.74(1)	110.7(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x-1/2,y-1,-z #2 -x-1/2,y,-z #3 -x-1/2,y+1,-z

Figure S11. H-Bonds for **1**, **2**, **4** and **5**