Supramolecular Heterocatemers and Their Role in Co-crystal Design

Joanna A. Bis, Olga L. McLaughlin, Peddy Vishweshwar, Michael J. Zaworotko*

Department of Chemistry, University of South Florida, CHE205, 4202 East Fowler Avenue, Tampa, Florida, 33620

Supporting Information

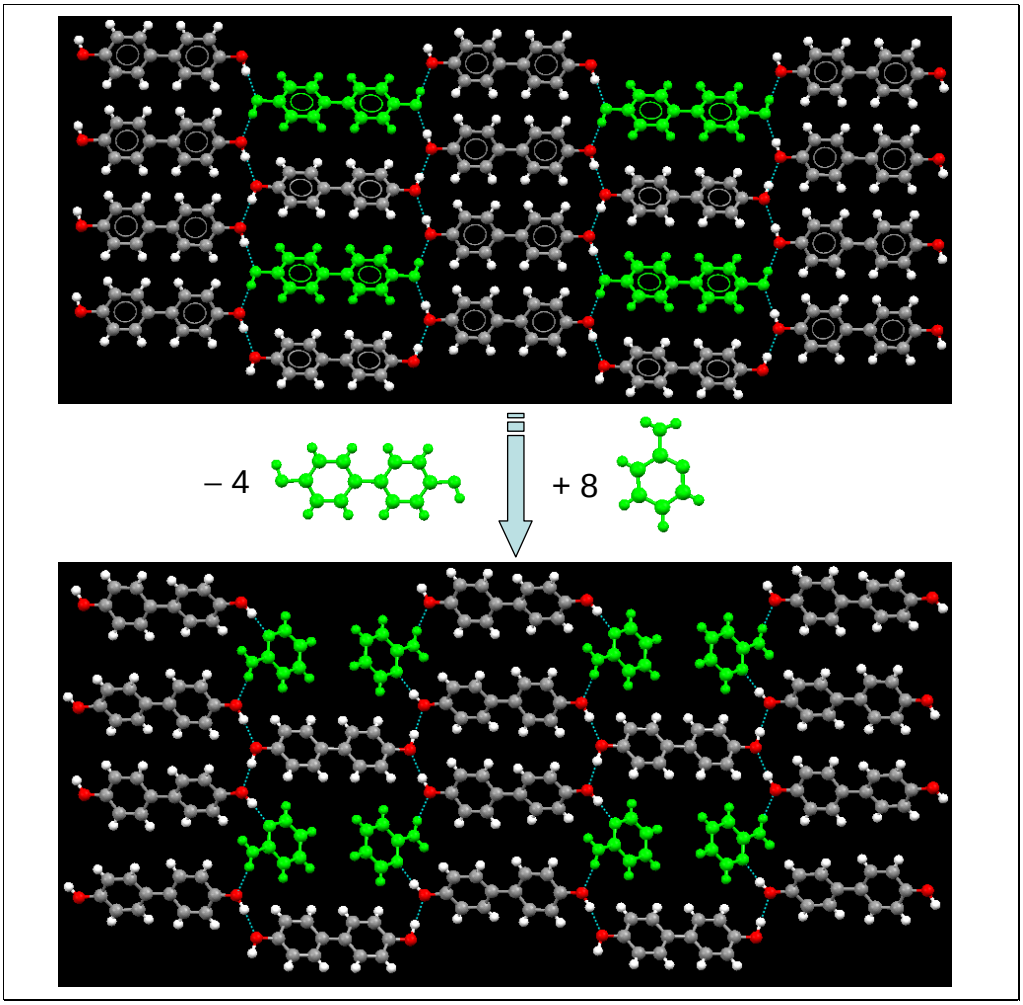


Figure S1. From "4,4'-biphenol crystal" to "(4,4'-biphenol)$_3$•(2-aminopyridine)$_2$, **1** co-crystal" through supramolecular heterocatemers. Notice that arrangement of molecules in pure 4,4'-biphenol and co-crystal **1** is similar.

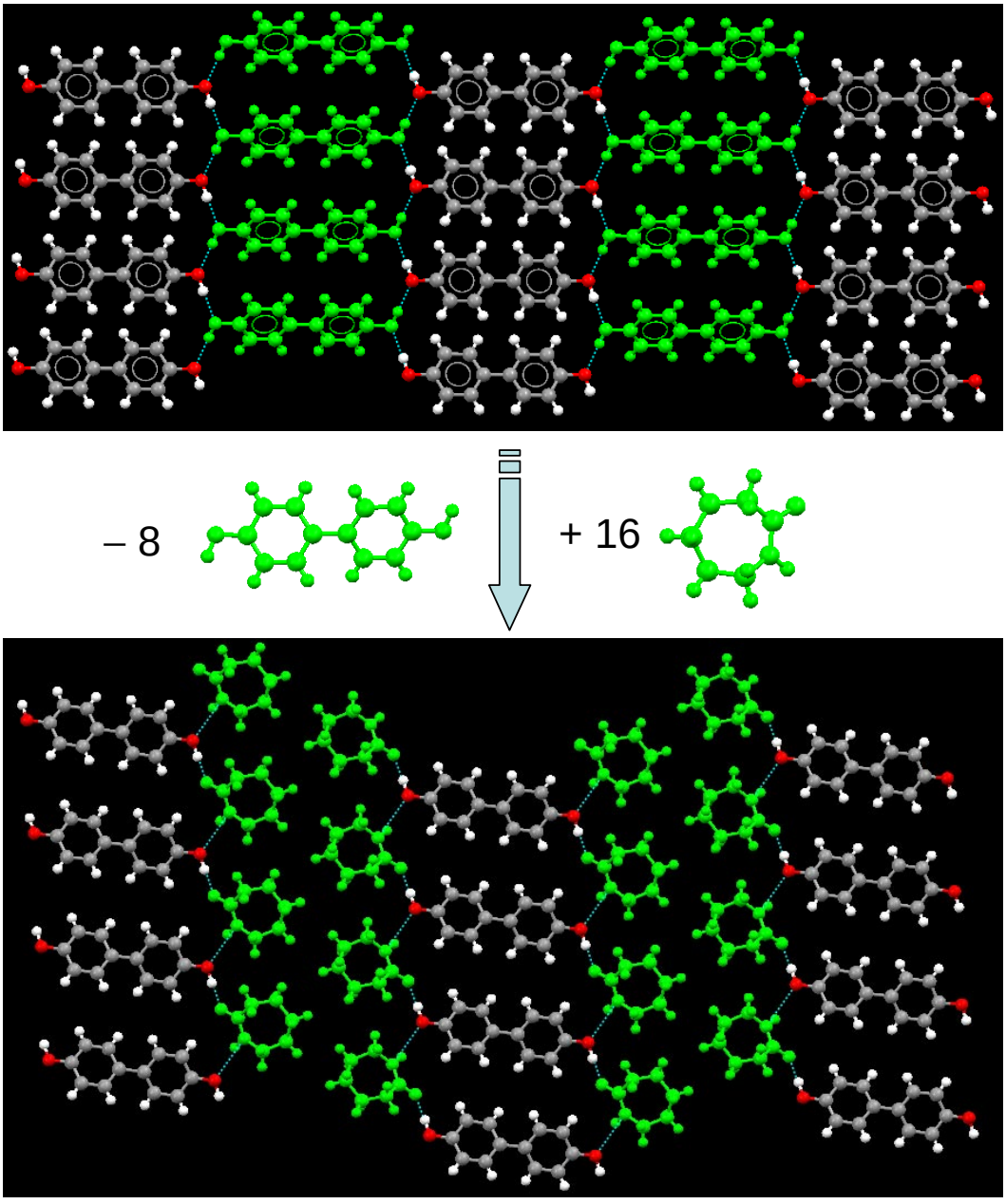


Figure S2. From "4,4'-biphenol crystal" to "(4,4'-biphenol)•(Caprolactam)$_2$, **2** co-crystal" through supramolecular heterocatemers. Notice that arrangement of molecules in pure 4,4'-biphenol and co-crystal **2** is similar.

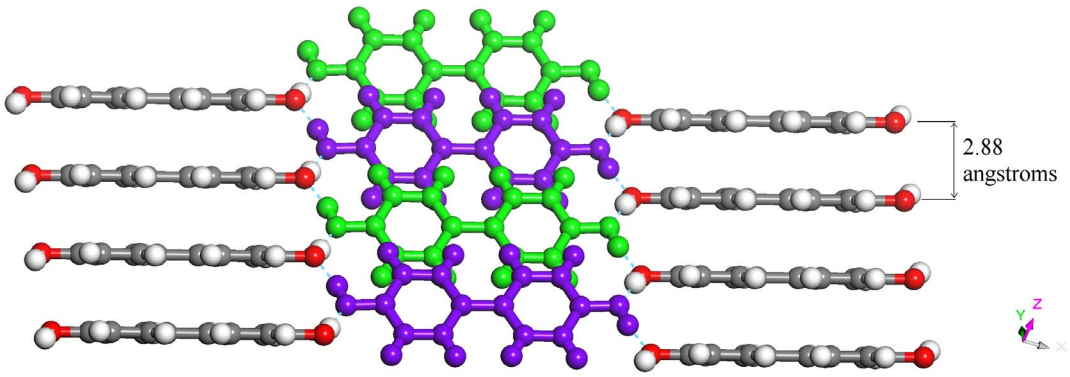
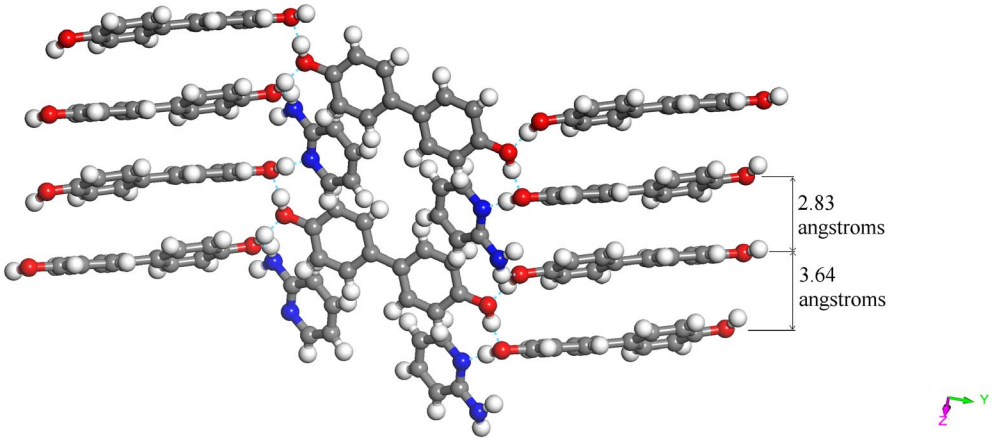
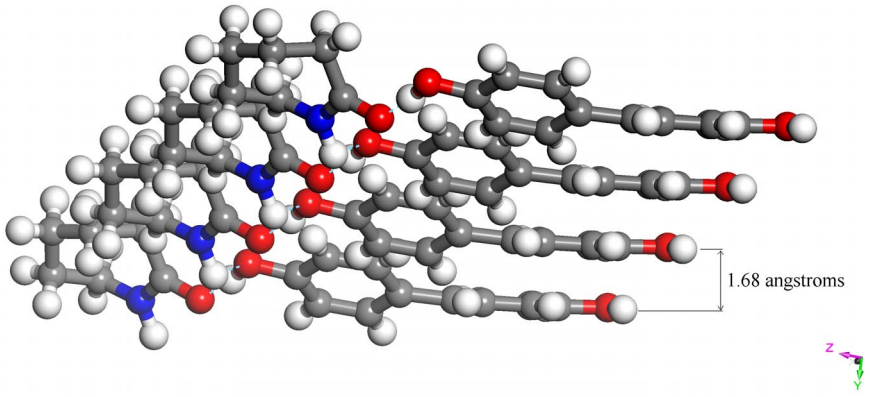


Figure S3. Figure 1 view down *b*-axis shows that adjacent 4,4'-biphenols along supramolecular homocatemer are separated by 2.88 Å.



(a)



(b)

Figure S4. (a) Crystal packing of co-crystal **1** along *a*-axis shows that 4,4'-biphenols are separated by 2.83 Å (with a 2-aminopyridine) and 3.64 Å (with a 4,4'-biphenol) in a supramolecular heterocatemer. (b) Crystal packing of co-crystal **2** shows that adjacent 4,4'-biphenols along supramolecular heterocatemer are separated by 1.68 Å.

Table 1. Hydrogen bonds for co-crystal **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(31)-H(31)...O(2)#2	0.96	1.84	2.788(2)	168.8
N(22)-H(22A)...O(1)#3	0.91	2.45	3.134(3)	131.8
O(2)-H(2)...N(21)#4	0.92	1.78	2.697(2)	171.9
O(1)-H(1)...O(31)#5	0.97	1.84	2.811(2)	173.8

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+2,-y+1,-z+1 #5 x,y,z-1

Table 2. Hydrogen bonds for co-crystal **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(11)#2	0.99	1.64	2.6285(14)	172.6
N(11)-H(11)...O(11)#3	1.07	1.98	3.0142(15)	161.8

Symmetry transformations used to generate equivalent atoms:

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

Table 3. Hydrogen bonds for co-crystal **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(21)#1	0.945	1.728	2.665	170.55
O(2)-H(2)...O(11)#2	1.020	1.686	2.674	161.68
N(11)-H(11)...O(11)#3	0.982	1.968	2.950	176.86
N(21)-H(21)...O(1)	0.860	2.136	2.956	159.28

Symmetry transformations used to generate equivalent atoms:

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