

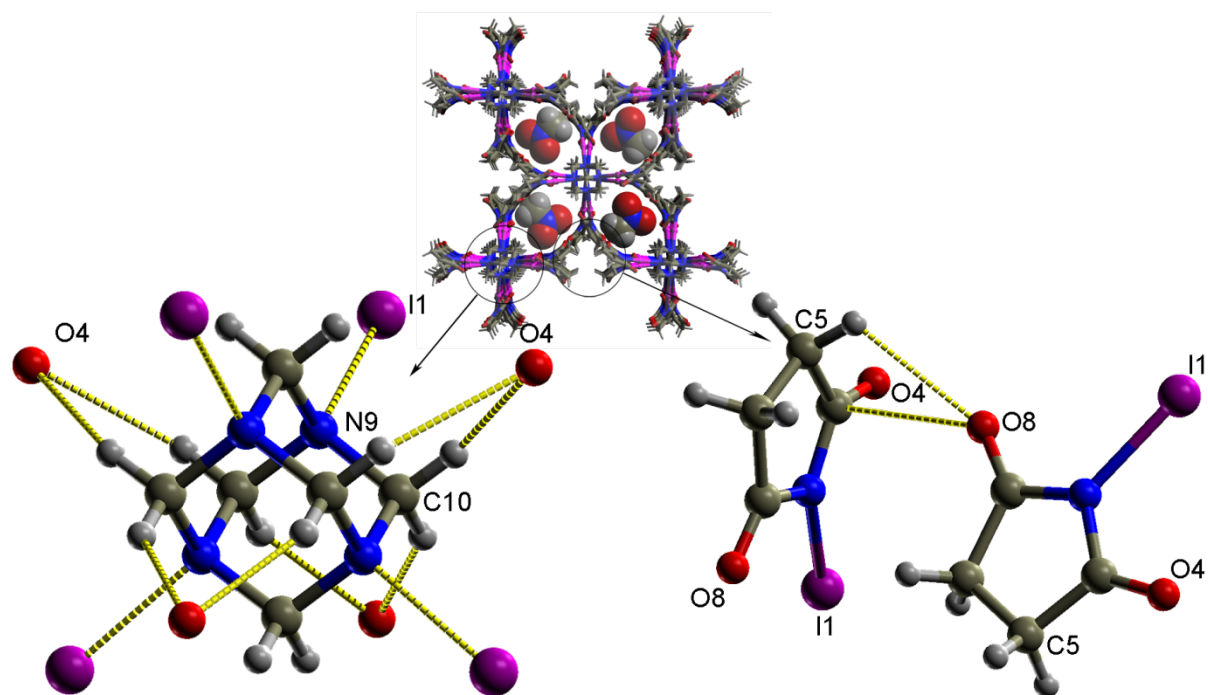
SUPPLEMENTARY INFORMATION

**Breathing Molecular Crystals: Halogen and Hydrogen Bonded Porous
Molecular Crystals with Solvent Induced Adaptation of the Nano-
sized Channels**

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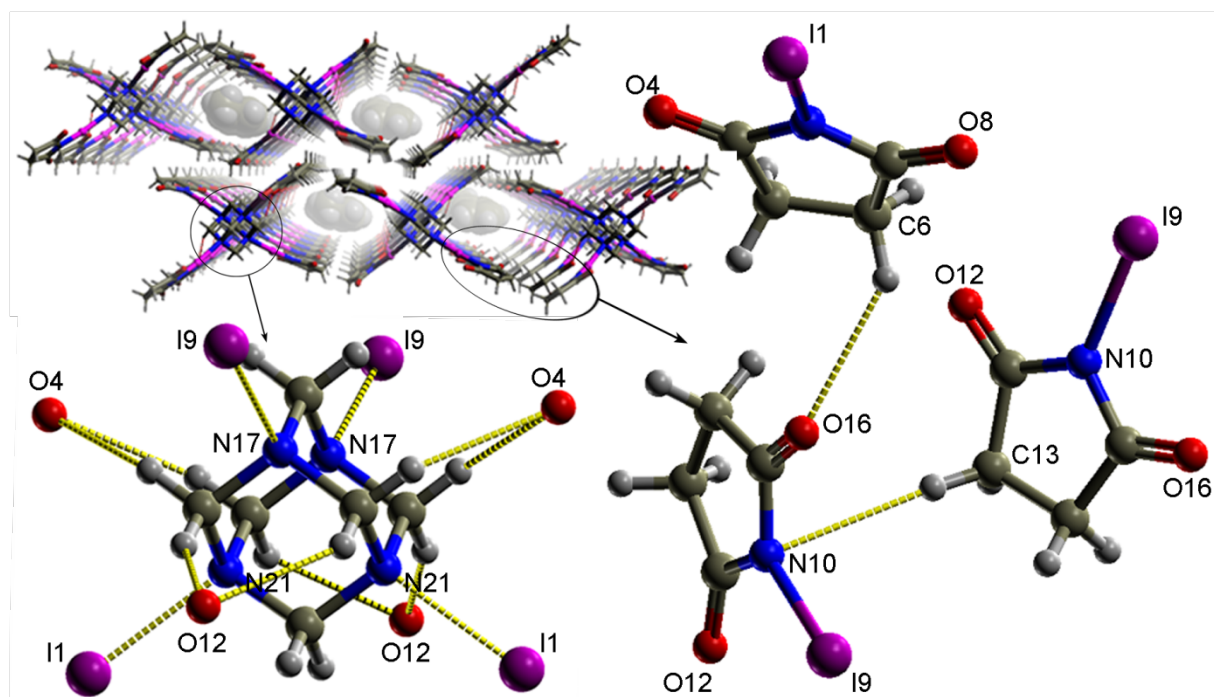
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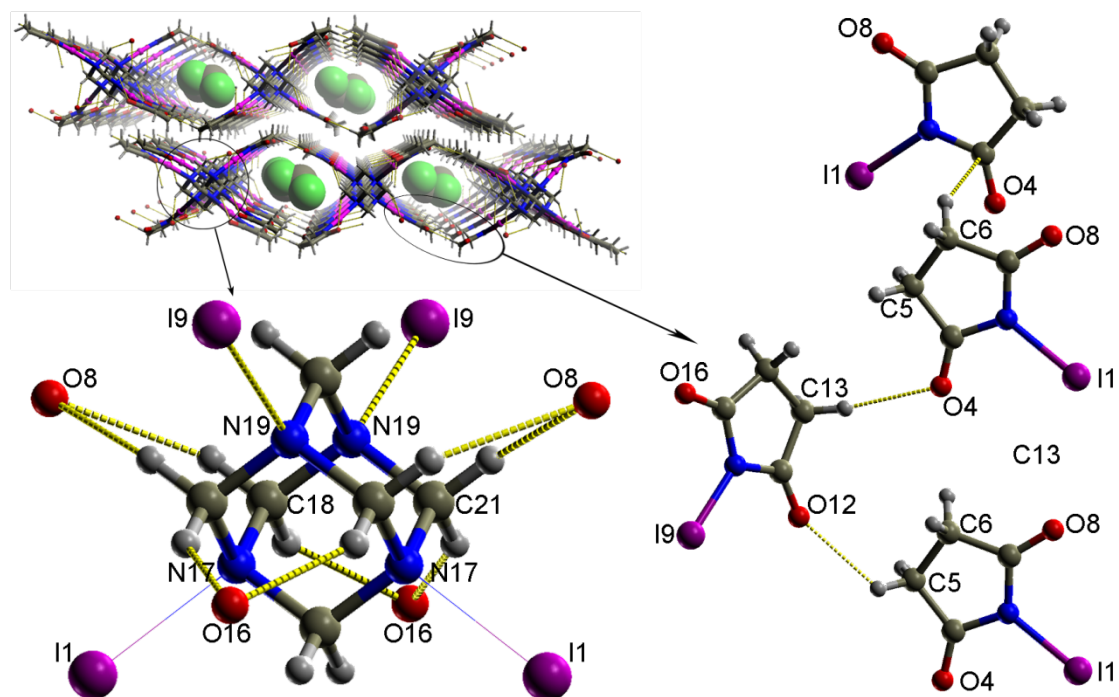
<i>H-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>	<i>X-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>
C10-H ... O4	3.189	152.2	N2-I1 ... N9	2.541	175.5
C10-H ... O4	3.333	144.8			
C5-H ... O8	3.134	114.3			

Scheme S1. Hydrogen and halogen bonding in II@CH₃NO₂



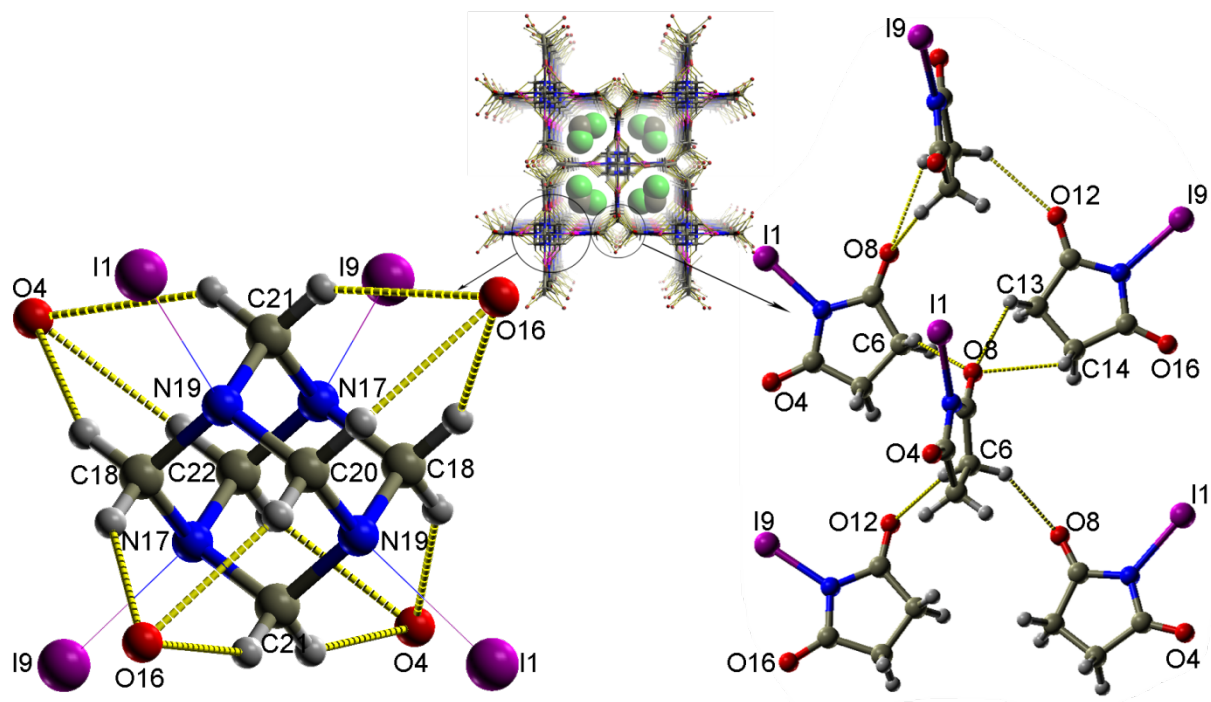
<i>H-bond</i>	<i>d [Å]</i>	<i>C-H ...O [°]</i>	<i>X-bond</i>	<i>d [Å]</i>	<i>C-H ...O [°]</i>
C19-H ...O4	3.345	139.8	N10-I9...N17	2.541	176.8
C20-H ...O4	3.062	155.1	N2-I1...N21	2.563	174.6
C19-H ...O12	3.314	148.2			
C20-H ...O12	3.335	148.1			
C13-H ...N10	3.689	169.2			
C6-H ...O16	3.408	136.0			

Scheme S2. Hydrogen and halogen bonding in I@C₆H₅CH₃



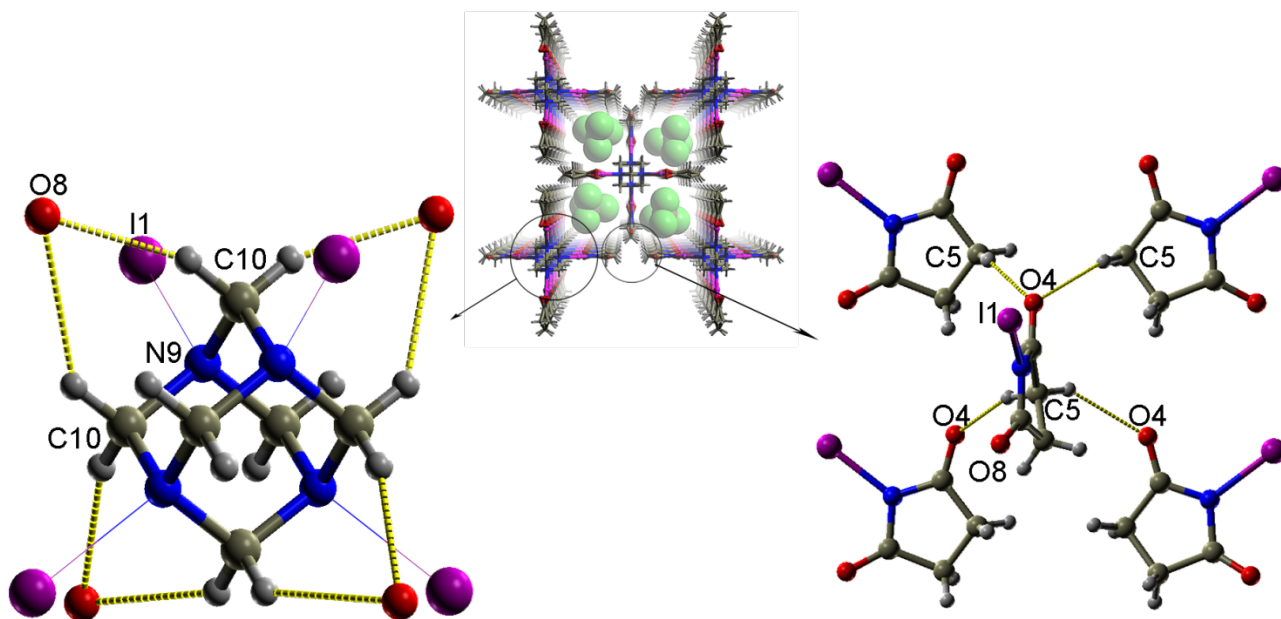
<i>H-bond</i>	<i>d [Å]</i>	<i>C-H ...O [°]</i>	<i>X-bond</i>	<i>d [Å]</i>	<i>C-H ...O [°]</i>
C21-H ...O8	3.223	148.8	N2-I1...N17	2.523	176.7
C18-H ...O8	3.290	145.5	N10-I9...N19	2.586	176.7
C21-H ...O16	3.185	144.6			
C18-H ...O16	3.135	146.9			
C13-H ...O4	3.323	172.0			
C5-H ...O12	3.088	120.1			

Scheme S3. Hydrogen and halogen bonding in I@CHCl₃



<i>H-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>	<i>X-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>
C22-H ... O4	3.240	146.3	N2-I1...N19	2.516	175.2
C21-H ... O4	3.427	138.2	N10-I9...N17	2.486	179.5
C18-H ... O4	3.223	147.0			
C18-H ... O16	3.223	146.6			
C20-H ... O16	3.267	145.3			
C21-H ... O16	3.383	140.4			
C6-H ... O8	3.275	146.6			
C6-H ... O12	3.364	162.8			
C13-H ... O8	3.270	126.2			
C14-H ... O8	3.261	126.0			

Scheme S4. Hydrogen and halogen bonding in **III**@CH₂Cl₂



<i>H-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>	<i>X-bond</i>	<i>d [Å]</i>	<i>C-H ... O [°]</i>
C10-H ... O8	3.079	153.7	N2-I1 ... N9	2.520	179.6
C10-H ... O8	3.329	140.2			
C5-H ... O4	3.394				

Scheme S5. Hydrogen and halogen bonding in **III@CCl₄**