

Supporting Information

Layer-by-layer assembly of supramolecular hexagonal blocks driven by CH/ π and π - π interactions

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Table 1. Conditions Used for the Cultivation of Single Crystals.

No.	Solvents	Temperature	time	Self-Assembled
1	Ethyl Acetate	20 °C	6 h	Yes
2	Ethyl Acetate:CHCl ₃ (2:1)	20 °C	8 h	Yes
3	Ethyl Acetate:CH ₂ Cl ₂ (2:1)	20 °C	7 h	Yes
4	Acetone:CH ₂ Cl ₂ (2:1)	20 °C	9 h	Yes
5	CH ₃ CN:CH ₂ Cl ₂ (2:1)	20 °C	6 h	Yes
6	Ethyl Acetate:Ethanol (2:1)	20 °C	10 h	Yes
7	Ethanol:CHCl ₃ (1:1)	20 °C	8 h	Yes

Equimolar solutions of **1** and **2** were mixed in minimum amount of solvents at 20 °C, warmed the mixture to 35 °C. Filtered and kept the solution at 20 °C. Crystals suitable for X-ray diffraction analysis were collected.

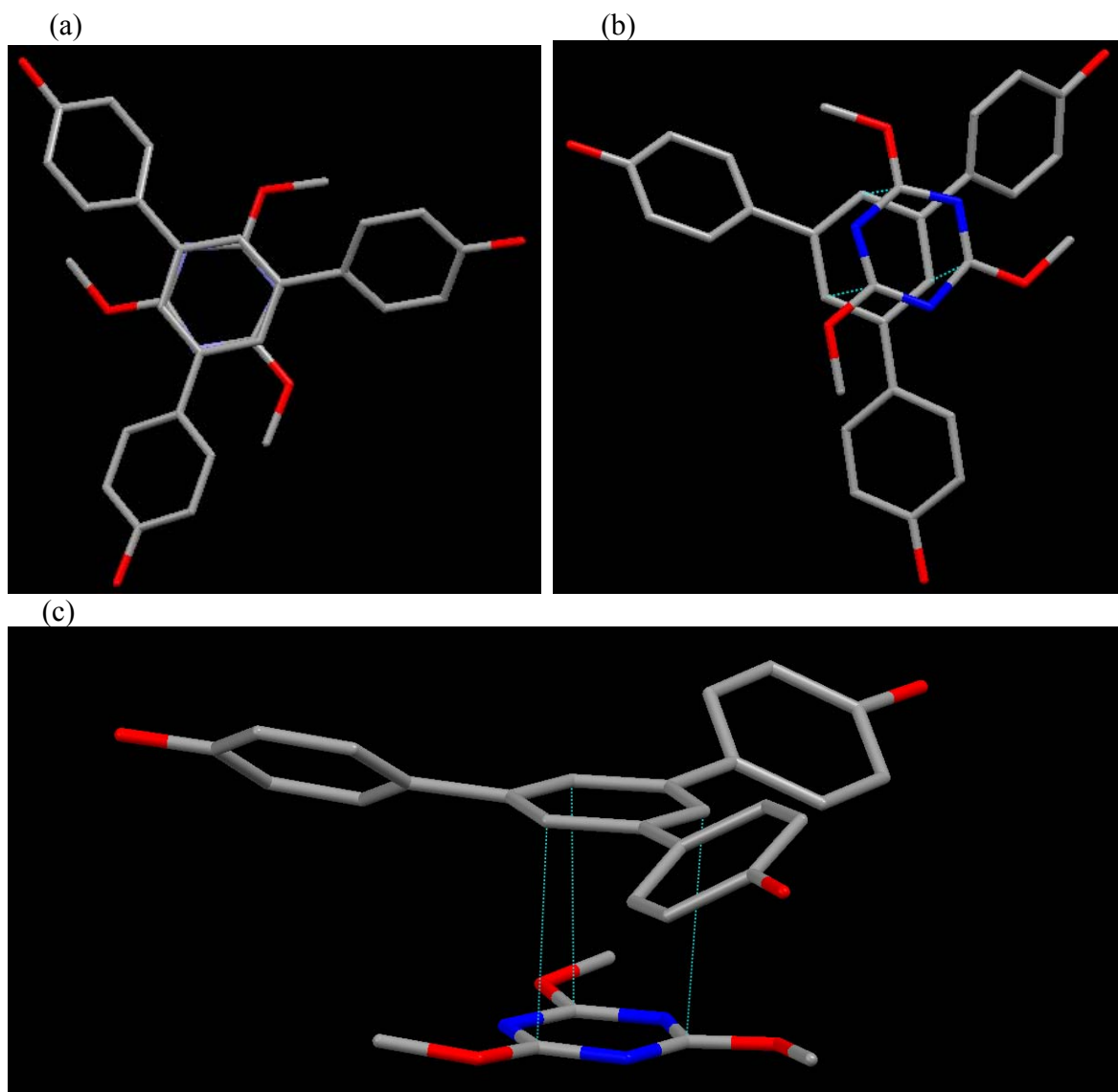
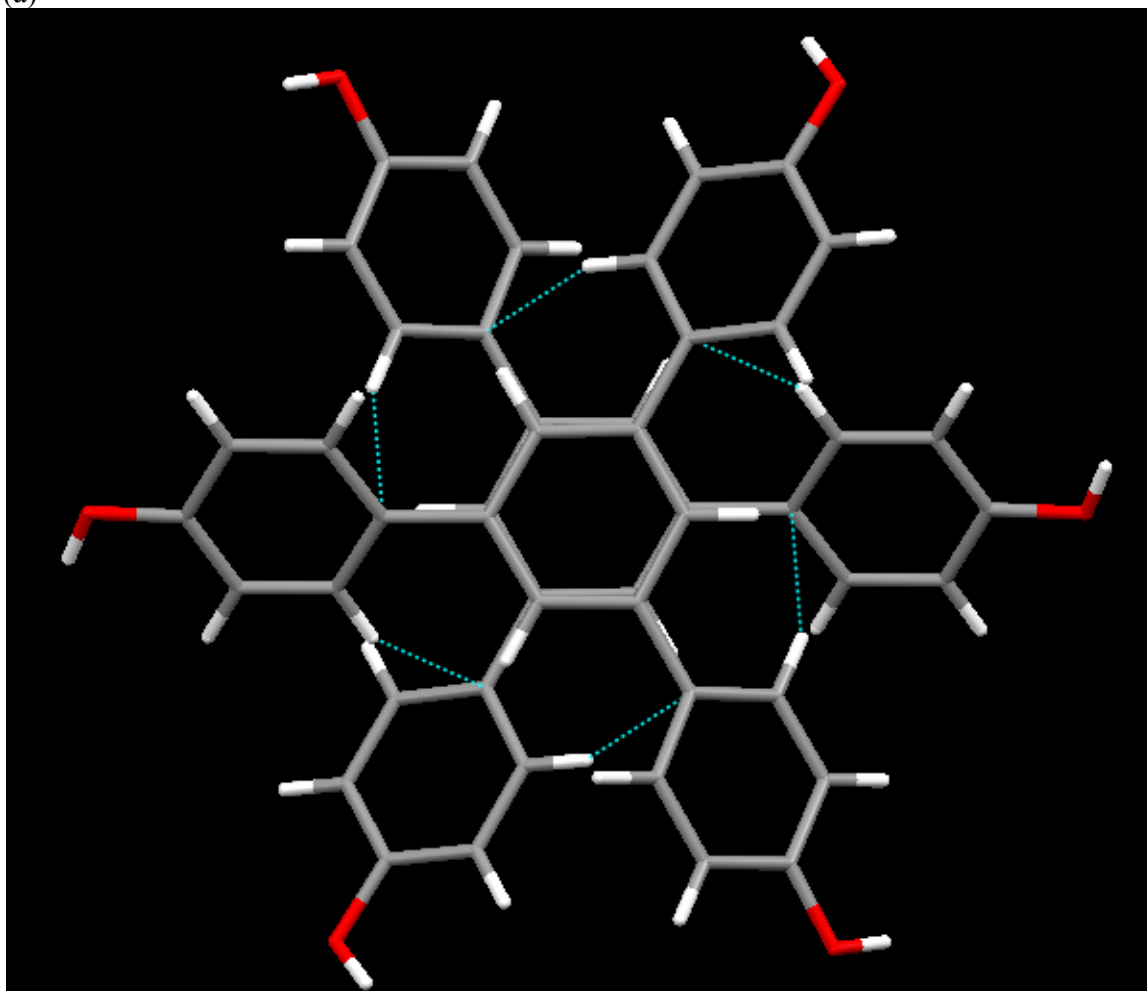


Fig. S1: (a,b) Top view showing staggered arrangement and (c) side view showing π - π stacking interactions between **1** and **2** of two successive layers. Hydrogen atoms are removed for the view point of clarity.

(a)



(b)

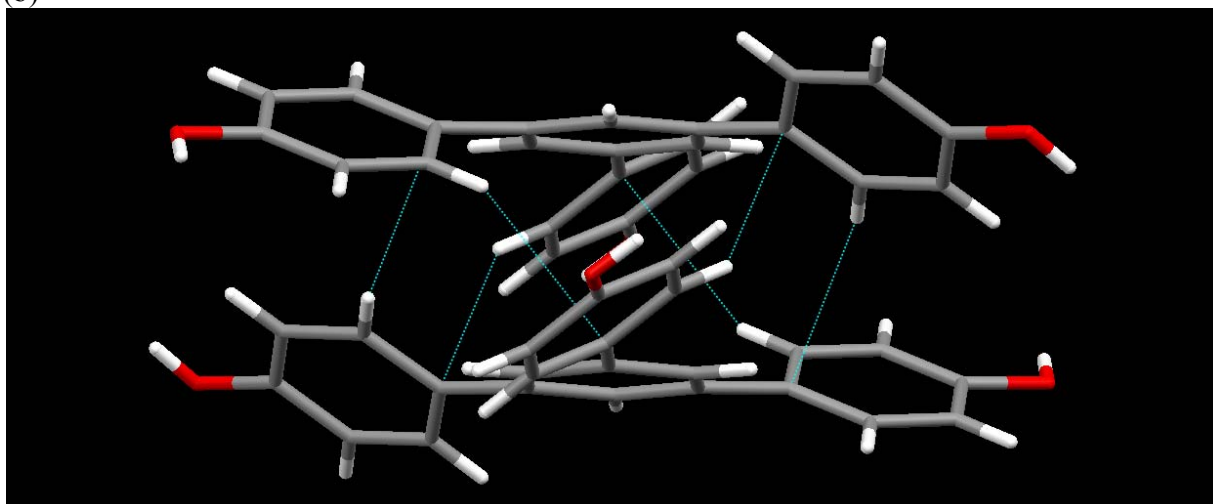


Fig. S2: (a) Top view showing staggered arrangement/piedfort unit of **2** and (b) side view showing CH- π interactions between **2** and **2** of two successive layers.

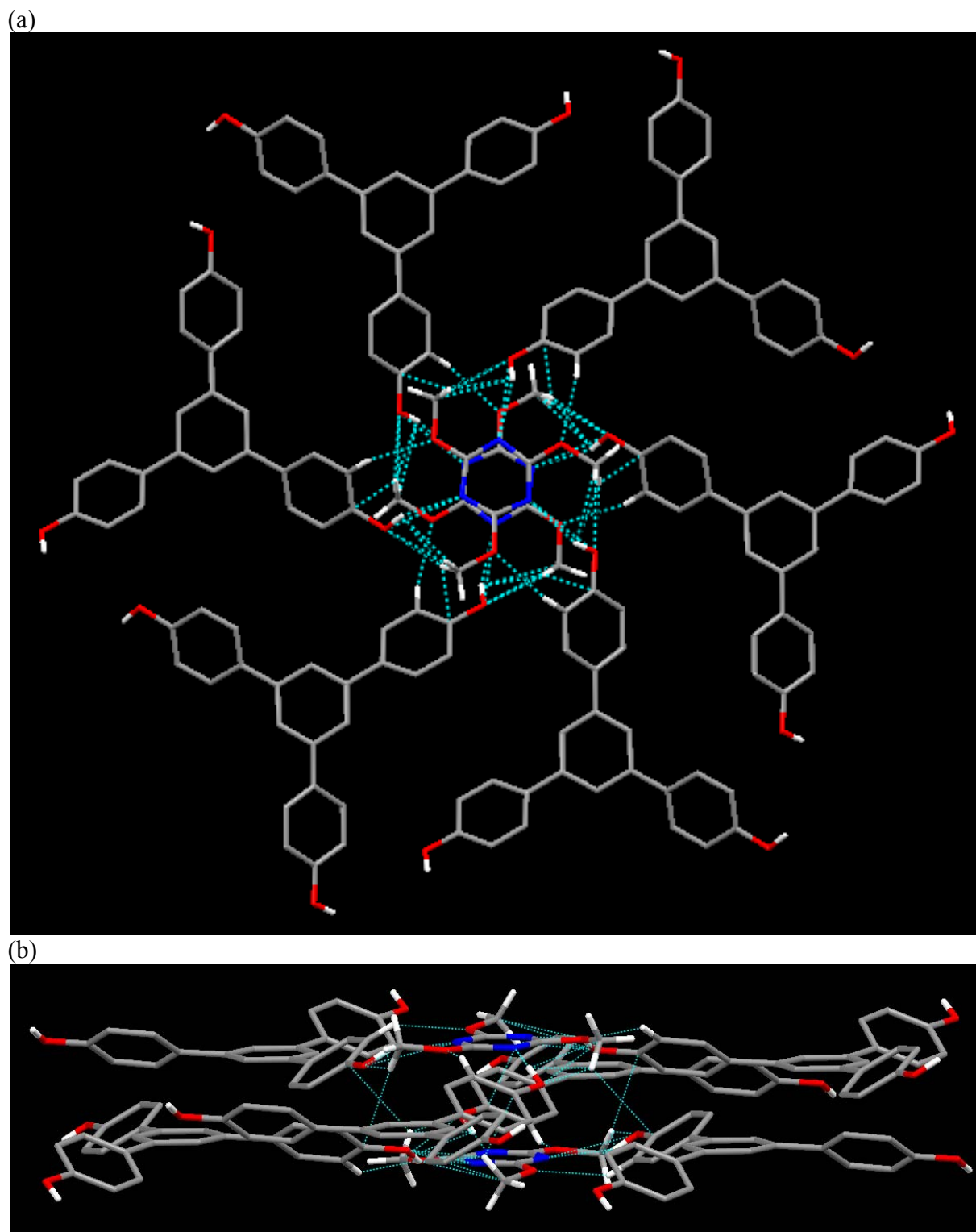


Fig. S3: (a) Top view showing staggered arrangement/piedfort unit of **1**, and (b) side view showing CH- π interactions between methoxy group of **1** and phenyl group of **2** of two successive layers.

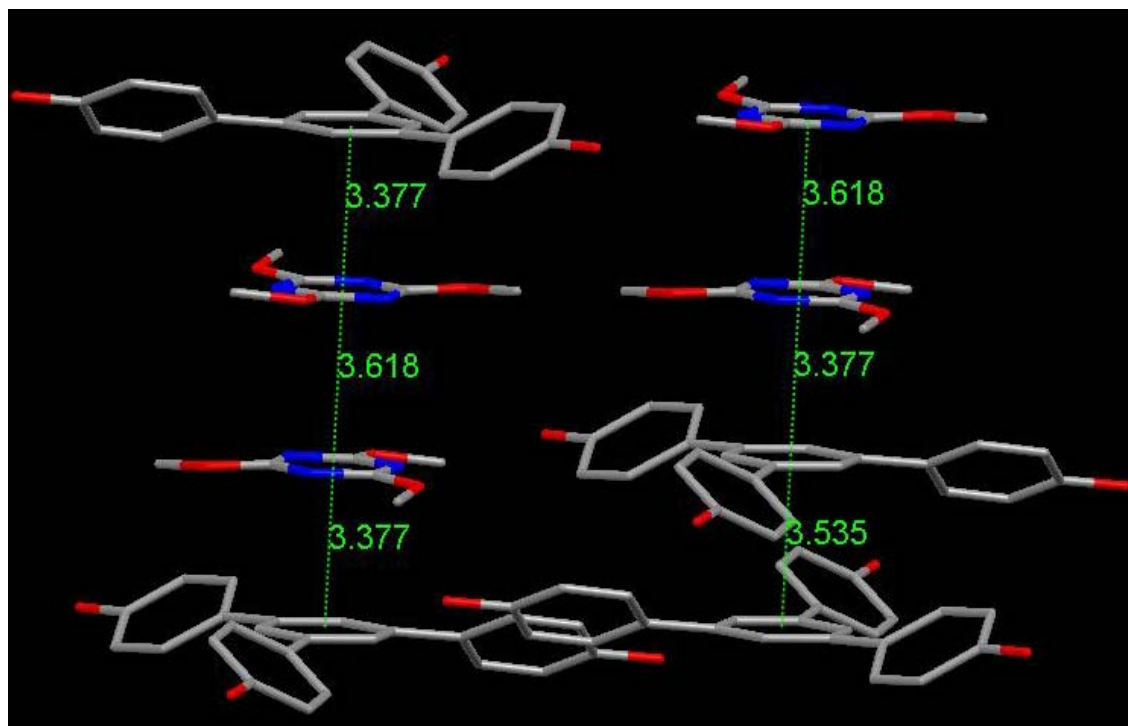


Fig. S4: (a) Side view showing distances between different aromatic units.

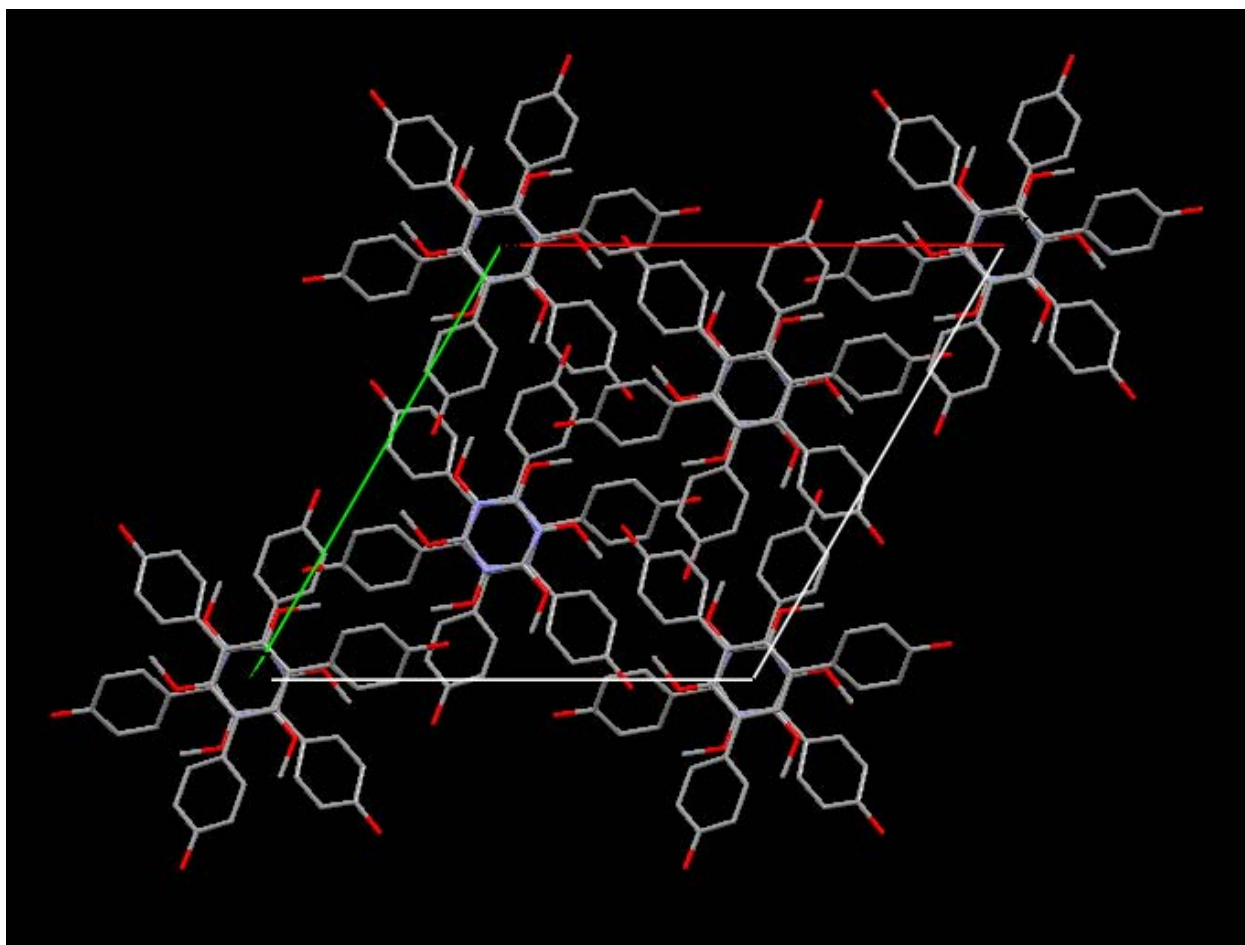


Fig. S5: A unit cell: viewed along the crystallographic c-axis

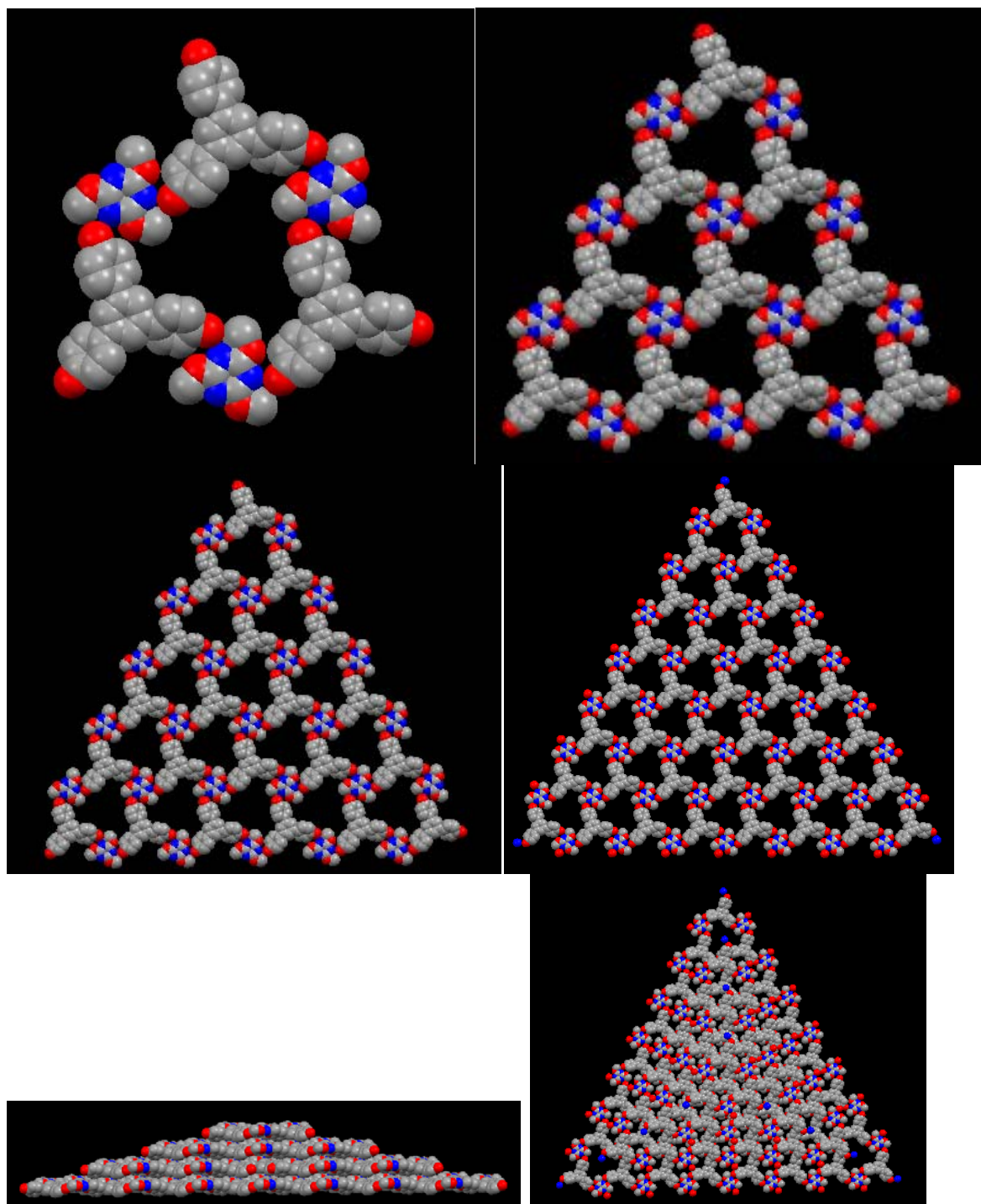


Fig. S6: A spacefill pyramid depiction of layered structure to better view the packing and staggered arrangement of hexagonal blocks in crystal packing.