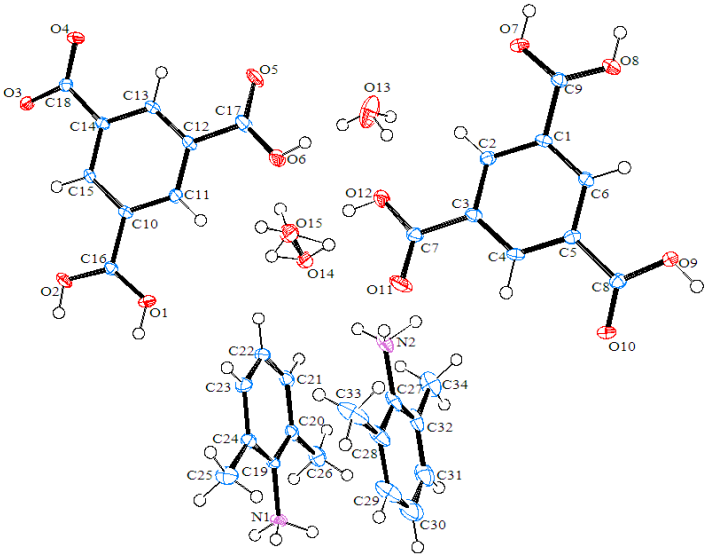
Supporting Information

X-ray Crystallography: X-ray crystal data were collected on Xcalibur Eos Oxford Diffraction Ltd. with Mo- K_α radiation (λ = 0.71073 Å). Temperature was controlled with an Oxford Cryojet HT instrument. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm were applied.[S1] Structure solution and refinement were performed with SHELX-97.[S2] One water molecule (O14 and O15) and one hydrogen (H13a, H13c) of the other water molecule (O13) are disordered over two sites with occupancy of 0.5 each. Each of the hydrogen atoms attached to O1, O2, O6-8 and O12 of the carboxyl groups is disordered over two positions and refined with occupancy of 0.5 each. Hydrogen atoms attached to the carbon atoms were placed in the calculated positions using riding model. All the hydrogen atoms attached to O atoms were refined with O–H = 0.85 Å and all other amino hydrogen atoms were refined freely. Hydrogen atoms (H2, H13C, H14A and H14B) attached to oxygens (O2, O13 and O14) in all the four structures and H12 attached to O12 in the structure BTA·DMA·H_2O–210 were refined with U_{iso}(H) = 1.5U_{eq}(O).


O4
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C16
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O13
O7
O8
C9
C2
C1
C6
O12
C3
C7
C4
C5
C8
O9
O11
O10
N2
C22
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C21
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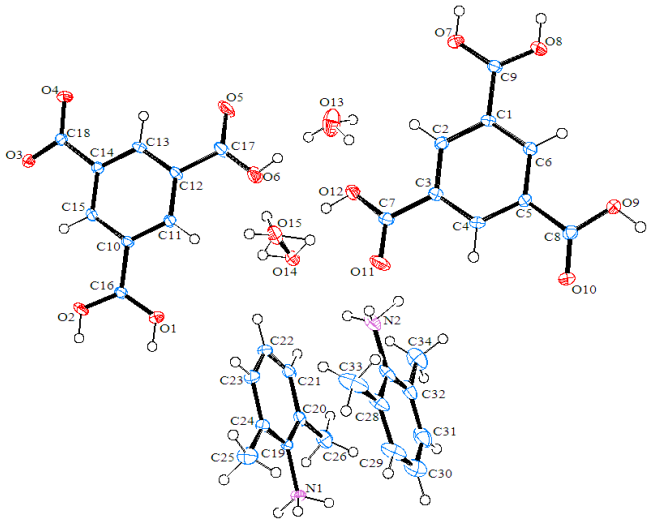
C30
N1

(a)


O4
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O11
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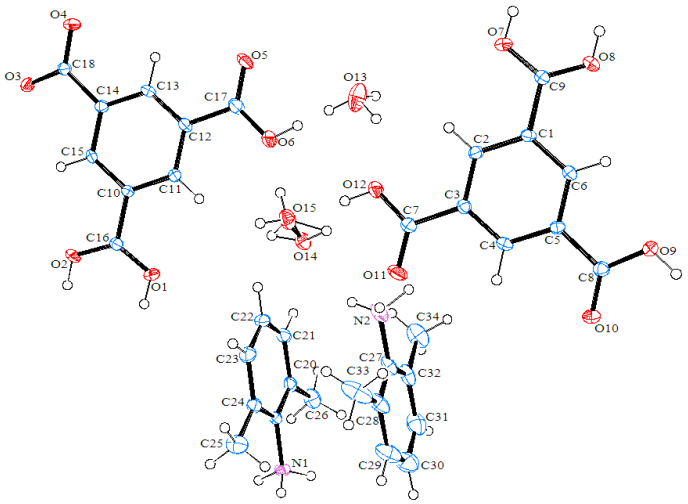
(b)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C6
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C5
C8
O9
O11
O10
N2
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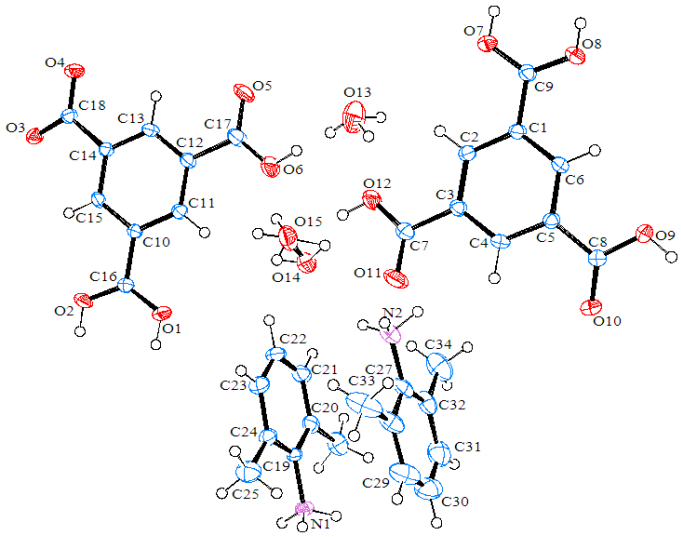
(c)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O9
O11
O10
N2
C34
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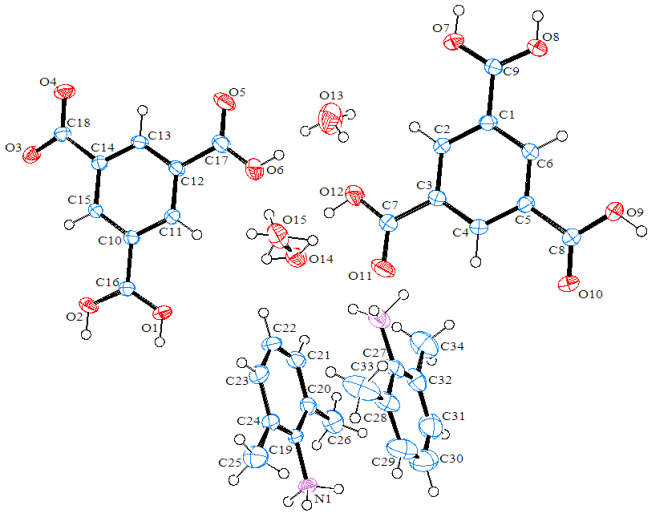
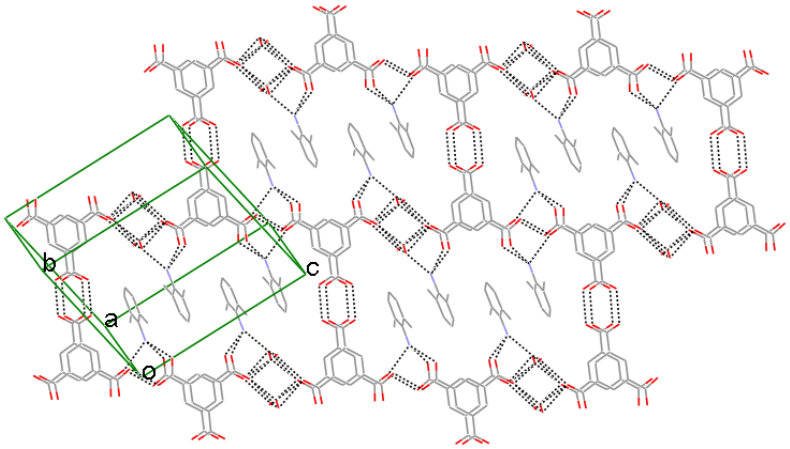
(d)

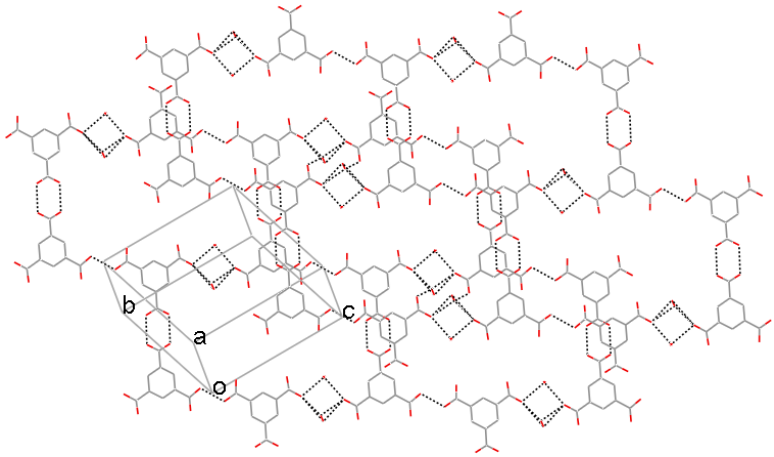


(e)

Fig. S1: ORTEP diagrams of the crystal structures of the data sets collected at (a) 120 K (AWAXEC), (b) 165 K, (c) 210 K, (d) 255 K, and (e) 300 K drawn at 45 % probability level.



(a)



(b)

Fig. S2. Interlayer interactions in the crystal structure of BTA·DMA·H_2O. (a) Hydrogen bond interactions within a bilayer and (b) hydrogen bond interactions between two adjacent layers of two consecutive bilayers.

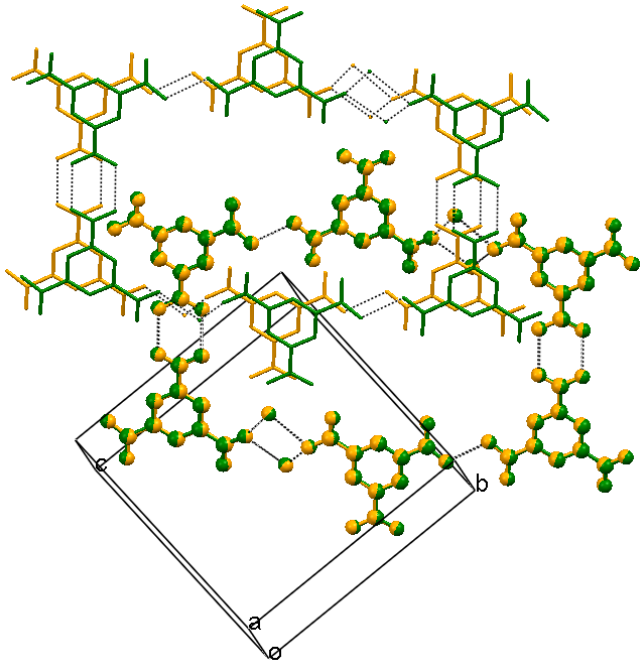


Fig. S3. This Fig. shows an overlay diagram of two layers of the brick wall nets obtained from the data sets collected at 120 K (orange) and at 300 K (green). It is evident from the diagram that

when the bottom layers (ball and stick model) are made to overlap, the relative positions of the top layers (wireframe model) are quite different. This indicates that there is no significant change in the intralayer geometry but there is a considerable difference in the interlayer hydrogen bond interactions which causes sliding of layers.

Table S1. Crystallographic details of the **BTA•DMA•H_2O** system at different temperatures.

Complex	**BTA•DMA•H_2O -120 (AWAXEC)**	**BTA•DMA•H_2O -165**	**BTA•DMA•H_2O – 210**	**BTA•DMA•H_2O -255**	**BTA•DMA•H_2O -300**
Formula	$C_9H_6O_6$, $C_8H_{11}N$, H_2O	$C_9H_6O_6$, $C_8H_{11}N$, H_2O	$C_9H_6O_6$, $C_8H_{11}N$, H_2O	$C_9H_6O_6$, $C_8H_{11}N$, H_2O	$C_9H_6O_6$, $C_8H_{11}N$, H_2O
*M*r	349.33	349.33	349.33	349.33	349.33
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
a (Å)	8.3651(4)	8.3768(13)	8.4027(12)	8.4236(5)	8.4373(3)
b (Å)	13.7509(5)	13.7290(10)	13.7129(10)	13.6964(8)	13.6980(5)
c (Å)	14.4816(4)	14.5547(10)	14.6157(8)	14.6918(7)	14.7629(6)
α (°)	90.155(3)	90.157(6)	90.126(5)	90.012(4)	89.956(3)
β (°)	102.153(3)	102.521(9)	102.668(8)	102.972(4)	103.262(3)
γ (°)	95.522(3)	95.439(9)	95.329(9)	95.368(5)	95.312(3)
V (Å^3)	1620.44(11)	1626.2(3)	1635.6(3)	1644.14(16)	1653.21(11)
T (K)	120(2)	165 (2)	210(2)	255(2)	300(2)
Z	4	4	4	4	4
F(000)	736	736	736	736	736
μ (mm^{-1})	0.112	0.112	0.111	0.111	0.110
Ref.collected/ unique	13564/7439	13511/8974	13391/8853	13341/8983	18052/ 9020
Parameters	530	540	539	540	540
Final R	R_1= 0.0473	R_1= 0.0478	R_1= 0.0487	R_1= 0.0556	R_1= 0.0524

indices [I>2σ(I)]					
R indices (all data)	wR_2= 0.1221	wR_2= 0.1177	wR_2= 0.1217	wR_2= 0.1395	wR_2= 0.1363
Goodness of fit on F^2	1.009	0.997	0.958	0.982	1.006

Table S2. Hydrogen bond interaction geometries in the crystal structures of BTA•DMA•H_2O system at different temperatures.

Interactions		**120 K (AWAXEC)**	**165 K**	**210 K**	**255 K**	**300 K**
O1–H1···O8	O–H *d* *D* θ	0.84(3) 1.78(3) 2.6237(18) 178(2)	0.85(3) 1.78(3) 2.6213(18) 179(4)	0.85(3) 1.78(4) 2.6261(19) 173(3)	0.85(4) 1.78(4) 2.630(2) 177(5)	0.85(3) 1.79(3) 2.636(2) 175(3)
N1–H1A···O3	N–H *d* *D* θ	0.92(2) 1.89(2) 2.7352(18) 152.1(19)	0.97(2) 1.84(2) 2.7373(18) 152.3(17)	0.98(2) 1.86(2) 2.741(2) 149.6(17)	1.01(3) 1.83(3) 2.743(2) 150(2)	1.02(3) 1.80(3) 2.751(2) 152(2)
N1–H1B···O10	N–H *d* *D* θ	0.98(2) 1.96(2) 2.8751(18) 155(2)	0.95(2) 1.98(2) 2.8743(18) 156(2)	0.92(2) 2.02(2) 2.8790(19) 155.2(17)	0.93(3) 2.00(3) 2.876(2) 155(3)	0.94(2) 2.03(2) 2.885(2) 150(2)
N1–H1C···O4	N–H *d* *D* θ	0.92(2) 1.83(2) 2.708(2) 157.7(18)	0.95(2) 1.81(2) 2.705(2) 156.4(18)	0.98(3) 1.79(2) 2.710(2) 155.2(17)	0.99(3) 1.79(3) 2.709(2) 154(2)	0.99(3) 1.78(2) 2.711(2) 154.9(18)
O2–H2···O7	O–H *d* *D* θ	0.84(3) 1.78(3) 2.6172(17) 171(3)	0.85(3) 1.78(3) 2.6163(17) 168(3)	0.85(3) 1.79(4) 2.6249(19) 170(3)	0.85(4) 1.78(4) 2.624(2) 173(4)	0.86(4) 1.78(4) 2.629(2) 177(3)
N2–H2A···O14	N–H *d* *D* θ	0.86(3) 2.28(3) 2.858(3) 125(2)	0.83(3) 2.32(2) 2.859(3) 123(2)	0.84(3) 2.33(3) 2.861(3) 121(2)	0.82(4) 2.30(4) 2.872(5) 127(4)	0.84(3) 2.28(3) 2.896(5) 130(3)
N2–H2B ···O5	N–H *d* *D* θ	0.99(2) 1.73(2) 2.704(2) 167(2)	1.05(3) 1.68(2) 2.697(2) 161(2)	1.06(3) 1.67(3) 2.699(2) 162(3)	0.98(3) 1.74(3) 2.702(3) 165(3)	1.05(3) 1.70(3) 2.694(3) 158(3)
N2–H2C···O11	N–H *d* *D*	0.98(3) 1.93(3) 2.854(2)	0.94(2) 1.99(2) 2.866(2)	0.90(2) 2.02(2) 2.871(2)	0.95(3) 1.99(3) 2.884(3)	0.95(3) 2.02(3) 2.900(3)

	θ	158(2)	155(2)	158(2)	156(3))	155(3)
O6–H6···O13	O–H *d* *D* *θ*	0.85(2) 1.85(3) 2.693(2) 174(5)	0.850(16) 1.854(19) 2.696(2) 171(4)	0.84(3) 1.88(3) 2.704(2) 167(4)	0.85(3) 1.85(3) 2.702(3) 177(6)	0.85(3) 1.85(2) 2.700(3) 175(2)
O7–H7···O2	O–H *d* *D* *θ*	0.85(3) 1.77(3) 2.6172(17) 178(4)	0.85(4) 1.77(4) 2.6163(17) 175(4)	0.85(3) 1.78(3) 2.6249(19) 175(2)	0.85(5) 1.79(5) 2.624(2) 166(4)	0.85(4) 1.78(4) 2.629(2) 172(3)
O8–H8 ···O1	O–H *d* *D* *θ*	0.86(4) 1.78(4) 2.6237(18) 171(4)	0.85(4) 1.79(4) 2.6213(18) 168(4)	0.85(5) 1.80(5) 2.6261(19) 164(4)	0.85(5) 1.81(5) 2.630(2) 164(4)	0.85(4) 1.80(4) 2.636(2) 170(4)
O9–H9···O3	O–H *d* *D* *θ*	0.875(14) 1.654(15) 2.5253(15) 174(2)	0.884(15) 1.636(16) 2.5199(15) 177.9(19)	0.887(15) 1.641(15) 2.5282(16) 179(3)	0.875(16) 1.652(16) 2.526(2) 178(3)	0.875(17) 1.652(17) 2.5262(19) 177(2)
O12–H12···O14	O–H *d* *D* *θ*	0.85(3) 1.97(2) 2.714(3) 144(4)	0.86(2) 1.96(2) 2.722(3) 147(3)	0.887(15) 1.641(15) 2.5282(16) 179(3)	0.85(3) 2.02(3) 2.746(5) 142(4)	0.86(3) 2.01(3) 2.750(3) 144(4)
O12–H12···O15	O–H *d* *D* *θ*	0.85(3) 1.71(2) 2.548(3) 166(4)	0.86(2) 1.70(2) 2.548(3) 168(3)	0.86(3) 1.71(2) 2.554(3) 167(4)	0.85(3) 1.73(3) 2.547(5) 161(4)	0.86(3) 1.74(3) 2.552(5) 159(4)
O13–H13A···O6	O–H *d* *D* *θ*	0.855(15) 1.87(3) 2.693(2) 160(6)	0.849(17) 1.87(2) 2.696(2) 163(5)	0.84(3) 1.86(3) 2.704(2) 175(5)	0.85(3) 1.88(5) 2.702(3) 163(8)	0.84(5) 1.87(5) 2.700(3) 168(10)
O14–H14A···O12	O–H *d* *D* *θ*	0.855(12) 1.872(17) 2.714(3) 168(5)	0.855(12) 1.882(14) 2.722(3) 167(4)	0.860(12) 1.884(15) 2.723(3) 165(4)	0.853(16) 1.902(16) 2.746(5) 170(5)	0.855(13) 1.906(15) 2.750(3) 169(5)

S1. CrysAlisPro, Oxford Diffraction Ltd.,Version 1.171.33.66, 2010.

S2. Sheldrick, G. M. SHELXS-97 and SHELXL-97, Programs for the Solution and Refinement of Crystal Structures, University of Göttingen, Germany, 1997.