Supplementary Material (ESI) for CrystEngComm

Co-crystal formation between 2-amino-4,6-dimethylpyrimidine and new p-xylylene-bis(thioacetic) acid

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The selected bond distances and angles are presented in Table S1 for the structures described in the present work.

Detailed peaks assignment for the free co-formers and each co-crystal is given in Table S2.

Table S1 Selected geometric parameters for ***p*-XBTA** acid and its co-crystals

***p*-XBTA**		**co-1**		**co-2**		**co-3**	
bond lenghts /Å							
C1–O1	1.322(2)	C1–O1	1.310(3)	C1–O1	1.309(3)	C1–O1	1.323(2)
C1–O2	1.222(2)	C1–O2	1.225(3)	C1–O2	1.222(3)	C1–O2	1.219(2)
C1–C2	1.504(2)	C1–C2	1.518(3)	C1–C2	1.513(4)	C1–C2	1.504(2)
C2–S1	1.815(1)	C2–S1	1.821(2)	C2–S1	1.820(3)	C2–S1	1.814(2)
C3–S1	1.827(1)	C3–S1	1.834(2)	C3–S1	1.832(3)	C3–S1	1.828(2)
C3–C4	1.504(2)	C3–C4	1.509(3)	C3–C4	1.512(4)	C3–C4	1.502(2)
		C7–N2	1.337(3)	C7–N2	1.344(4)	C7–N2	1.336(3)
		C7–N1	1.361(3)	C7–N1	1.355(3)	C7–N1	1.357(2)
		C7–N3	1.359(3)	C7–N3	1.362(4)	C8–N1	1.347(2)
		C8–N3	1.337(3)	C8–N3	1.345(3)	C8–C9	1.384(2)
		C8–C9	1.404(3)	C8–C9	1.395(4)	C8–C10	1.496(2)
		C8–C11	1.499(3)	C8–C11	1.501(4)		
		C9–C10	1.380(3)	C9–C10	1.388(4)		

		C10–N1	1.360(3)	C10–N1	1.356(3)		
		C10–C12	1.501(3)	C10–C12	1.495(4)		
bond angles /°							
O2–C1–O1	123.7(1)	O2–C1–O1	124.7(2)	O2–C1–O1	124.9(3)	O2–C1–O1	124.4(2)
O2–C1–C2	122.2(1)	O2–C1–C2	122.2(2)	O2–C1–C2	121.9(2)	O2–C1–C2	121.9(2)
O1–C1–C2	114.1(1)	O1–C1–C2	113.1(2)	O1–C1–C2	113.2(2)	O1–C1–C2	113.7(1)
C1–C2–S1	110.3(1)	C1–C2–S1	111.7(2)	C1–C2–S1	110.4(2)	C1–C2–S1	112.2(1)
C2–S1–C3	101.4(1)	C2–S1–C3	101.4(1)	C2–S1–C3	101.4(1)	C2–S1–C3	101.6(1)
C4–C3–S1	113.6(1)	C4–C3–S1	114.2(2)	C4–C3–S1	112.9(2)	C4–C3–S1	113.9(1)
C5–C4–C3	120.2(1)	C5–C4–C3	121.1(2)	C5–C4–C3	120.7(3)	C5–C4–C3	121.1(2)
C6–C4–C3	121.1(1)	C6^{i}–C4–C3	121.0(2)	C6–C4–C3	120.4(3)	C6^{ii}–C4–C3	120.4(2)
		N2–C7–N3	118.1(2)	N2–C7–N1	117.3(3)	N2–C7–N1	118.2(1)
		N2–C7–N1	118.0(2)	N2–C7–N3	118.4(3)	N1–C7–N1^{iii}	123.6(2)
		N3–C7–N1	123.9(2)	N1–C7–N3	124.3(3)	N1–C8–C9	121.1(2)
		N3–C8–C9	122.0(2)	N3–C8–C9	122.3(3)	N1–C8–C10	116.4(2)
		N3–C8–C11	117.5(2)	N3–C8–C11	116.5(3)	C9–C8–C10	122.5(2)
		C9–C8–C11	120.4(2)	C9–C8–C11	121.2(3)	C8–C9–C8^{iii}	118.3(2)
		C10–C9–C8	117.9(2)	C10–C9–C8	118.0(3)	C8–N1–C7	117.9(2)
		N1–C10–C9	120.6(2)	N1–C10–C9	120.4(3)		
		N1–C10–C12	116.4(2)	N1–C10–C12	117.1(2)		
		C9–C10–C12	122.9(2)	C9–C10–C12	122.5(3)		
		C10–N1–C7	118.1(2)	C7–N1–C10	118.3(2)		
		C8–N3–C7	117.4(2)	C8–N2–C7	116.7(4)		
torsion angles /°							
O1-C1-C2-S1	-97.1(1)	O1-C1-C2-S1	91.1(2)	O1-C1-C2-S1	91.3(2)	O1-C1-C2-S1	84.8(2)
C1-C2-S1-C3	-69.9(1)	C1-C2-S1-C3	-72.3(2)	C1-C2-S1-C3	-78.1(2)	C1-C2-S1-C3	-78.4(1)
C2-S1-C3-C4	-64.7(1)	C2-S1-C3-C4	-62.5(2)	C2-S1-C3-C4	-65.1(2)	C2-S1-C3-C4	-63.3(1)
S1-C3-C4-C5	97.1(1)	S1-C3-C4-C5	108.8(2)	S1-C3-C4-C6	99.0(3)	S1-C3-C4-C6^{ii}	102.6(2)
Symmetry codes: (i)*1-x, -y, 1-z ;* (ii)*1/2-x, 1/2-y, 1-z ;* (iii) *–x, y, z*							

Table S2 Bands in ATR-FTIR spectra of DMP, *p*-XBTA and co-crystals 1, 2 and 3

Proposed assignment	DMP	*p*-XBTA	co-1	co-2	co-3
ν(OH)+ν(C-H)	-	3200-2400	-	-	-
ν(OH)	-	-	-	3449	-
$\nu_{as}NH_2$	3396_m	-	3332	3324	3311
$\nu_{s}NH_2$	3306_m	-	3170	3192	3180
ν(NH)+ν(C-H)	3181	-	3170	3204	3179
$\nu(C_{ar}$-H)	3080_{vw}	3062_{vw}	3082	3090	-
$\nu_{as}CH_2$	-	2968	2964	2964	2965
$\nu_{s}CH_2$	-	2947	-	-	2940
$\nu_{as}CH_3$	2922	-	2919	2925	2923
$\nu_{s}CH_3$	2850	-	2853	2853	-
ν(OH)	-	$2656,2548_w$	-	-	-
ν(C=O)	-	1686_{vs}	1683_{vw}	1690_{vw}	1694_m
$\nu(C_{Ar}=C_{Ar})+\beta NH_{2scis}$	1632_s	-	1656_s	1646_s	1670_s
$\nu(C_{Ar}=C_{Ar})$	1590_{vs}	-	1597	1596	1596
ν(C=N)	1563_{vs}	-	1575	1575	1569
$\nu(C_{Ar}=C_{Ar})$	-	1510	1511	1509	1511
$\beta_{as}CH_3+\nu(C_{Ar}=C_{Ar})$	1463_{vs}	1468	-	1471	1464
$\beta_{s}CH_3$	1388_s	-	1389_{vw}	1385_{vw}	1380_{vw}
β(C-H)	1368_s	-	1373_{vw}	1372_{vw}	-
ν(C-N)	1338_s	-	1346	1348_w	1350
ν(C-O)+β(OH)	-	1280_{sb}	1311	1315	1302
βCH_3	1242	-	1247_w	1243_w	1248_w
β(C-H)	-	1153	1153	1150	1153
β(C-H)	-	1126	1128	1125	1131
β(C-H)	-	1104	1096		1099
$\beta(CH_3)_{rock}$	$1030_{m,}$ 1008	-	1032	1031	1023
βC-N	952_m	-	-	957	957
$\gamma(C_{Ar}$-H)	-	848, 839	847	846	843
γ(N-H)	815_w	-	-	-	816
γ(O-H)	-	916_{sb}	-	-	-
γ(C-H)	793_{vs}		790	790	801, 793,783
γ(C-H)	-	693	704	700	700
γ(C-H)	-	669	673	671	672

Abbreviations:
ν - stretching vibration
β - i*n-plane* deformation vibrations
γ - *out- of- plane* deformation vibrations
s: strong; m: medium; w:weak; v: very; b: broad