Supplementary Information for

About the Influence of Hydrogen Bonding on a Planar Arrangement of Melamine in Crystal Structures of its Solvates, Cocrystals and Salts

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Table of Contents:

A) Crystallographic tables for Melamine dimethylsulfoxide solvate 1 CCDC 741063

Table 1 Crystal data and structure refinement for 1 CCDC 741063.

Identification code	1 CCDC 741063
Empirical formula	$C_5H_{12}N_6OS$
Formula weight	204.27
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.4296(6)
b/Å	12.3333(11)
c/Å	11.9384(11)
α/°	90
β/°	114.070(6)
γ/°	90
Volume/Å^3	998.81(16)
Z	4
ρ_{calc}mg/mm^3	1.358
m/mm^{-1}	0.299
F(000)	432.0
Crystal size/mm^3	0.283 × 0.035 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	4.988 to 52.82°
Index ranges	$-8 \le h \le 9$, $-15 \le k \le 15$, $-14 \le l \le 14$
Reflections collected	11113
Independent reflections	2035 [R_{int} = 0.0682, R_{sigma} = 0.0496]
Data/restraints/parameters	2035/0/166
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.0774
Final R indexes [all data]	R_1 = 0.0662, wR_2 = 0.0868
Largest diff. peak/hole / e Å^{-3}	0.29/-0.38

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1 CCDC 741063. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	6369(3)	2739.0(14)	5140.8(16)	15.3(4)
N2	5356(2)	1091.3(14)	3977.4(15)	16.2(4)
N3	6610(3)	2572.7(14)	3210.2(16)	16.1(4)
N4	5232(3)	1285.9(17)	5856.5(18)	20.1(4)
N5	5446(3)	1043.4(17)	2070.3(18)	20.5(4)
N6	7663(3)	4110.7(15)	4371.3(19)	18.2(4)
C1	6873(3)	3103.7(17)	4246.5(19)	14.6(5)
C2	5800(3)	1581.9(17)	3114.1(19)	15.0(5)
C3	5669(3)	1716.9(17)	4968.9(19)	15.1(5)
S1	11847.5(8)	3828.8(5)	2906.3(5)	23.99(17)
O1S	10755(3)	4498.0(15)	3474.1(16)	34.2(5)
C1S	10746(5)	4142(3)	1315(3)	37.6(7)
C2S	10936(4)	2474(2)	2803(3)	35.6(7)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 1 CCDC 741063. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	19.2(9)	14.1(9)	14.6(9)	0.2(7)	9.0(8)	-0.6(7)
N2	19.8(9)	15.1(9)	14.8(9)	-0.6(8)	8.3(7)	-2.4(8)
N3	21.1(10)	14.4(9)	15.9(9)	-0.2(7)	10.8(8)	-0.9(7)
N4	34.3(11)	15.9(11)	15.4(10)	-1.1(8)	15.6(9)	-5.1(9)
N5	31.9(11)	15.9(10)	17.8(10)	-4.7(8)	14.1(9)	-8.3(9)
N6	25.1(11)	15.8(10)	17.9(10)	-3.3(8)	13.1(9)	-5.6(8)
C1	12.4(10)	15.4(11)	14.9(11)	1.5(9)	4.4(9)	2.3(8)
C2	14.4(11)	15.6(11)	16.6(11)	0.5(8)	8.0(9)	2.6(8)
C3	13.9(10)	16.8(11)	15.1(11)	1.6(9)	6.5(9)	2.2(8)
S1	17.3(3)	32.5(3)	21.7(3)	-1.9(3)	7.5(2)	-3.7(3)
O1S	38.5(11)	38.8(11)	37.1(11)	-18.9(8)	27.6(9)	-16.6(8)
C1S	35.5(16)	53(2)	23.8(14)	-3.3(13)	11.9(13)	-13.8(14)
C2S	24.4(15)	32.2(15)	48.5(19)	0.3(14)	13.0(14)	-0.9(12)

Table 4 Bond Lengths for 1 CCDC 741063.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.345(3)	N4	C3	1.338(3)
N1	C3	1.347(3)	N5	C2	1.340(3)
N2	C2	1.347(3)	N6	C1	1.356(3)
N2	C3	1.351(3)	S1	O1S	1.4995(17)
N3	C1	1.342(3)	S1	C1S	1.778(3)
N3	C2	1.346(3)	S1	C2S	1.788(3)

Table 5 Bond Angles for 1 CCDC 741063.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C3	114.03(18)	N5	C2	N3	116.14(19)
C2	N2	C3	113.91(18)	N1	C3	N2	125.84(19)
C1	N3	C2	114.44(18)	N4	C3	N1	117.02(19)
N1	C1	N6	117.87(19)	N4	C3	N2	117.13(19)
N3	C1	N1	125.85(19)	O1S	S1	C1S	105.37(14)
N3	C1	N6	116.25(19)	O1S	S1	C2S	106.61(13)
N3	C2	N2	125.66(19)	C1S	S1	C2S	97.65(15)
N5	C2	N2	118.19(19)				

Table 6 Torsion Angles for 1 CCDC 741063.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	N1	C3	N2	-3.7(3)	C2	N3	C1	N1	-1.4(3)
C1	N1	C3	N4	176.77(18)	C2	N3	C1	N6	-179.22(18)
C1	N3	C2	N2	-3.6(3)	C3	N1	C1	N3	4.7(3)
C1	N3	C2	N5	177.57(19)	C3	N1	C1	N6	-177.50(18)
C2	N2	C3	N1	-0.4(3)	C3	N2	C2	N3	4.4(3)
C2	N2	C3	N4	179.08(18)	C3	N2	C2	N5	-176.76(19)

B) Crystallographic tables for melamine theobromine cocrystal 2 CCDC 995318

Table 7 Crystal data and structure refinement for 2 CCDC 995318 .

Identification code	2 CCDC 995318
Empirical formula	$C_{24}H_{30}N_{18}O_6$
Formula weight	666.66
Temperature/K	150.15
Crystal system	monoclinic
Space group	*C*2/*c*
a/Å	14.3308(8)
b/Å	16.2228(10)
c/Å	13.1104(10)
α/°	90
β/°	109.388(7)
γ/°	90
Volume/Å^3	2875.2(3)
Z	4
ρ_{calc}mg/mm^3	1.540
m/mm^{-1}	0.990
F(000)	1392.0
Crystal size/mm^3	0.3657 × 0.1922 × 0.0903
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	8.514 to 133.408°
Index ranges	-17 ≤ h ≤ 16, -19 ≤ k ≤ 16, -15 ≤ l ≤ 15
Reflections collected	10236
Independent reflections	2523 [R_{int} = 0.0473, R_{sigma} = 0.0290]
Data/restraints/parameters	2523/0/265
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0685, wR_2 = 0.2050
Final R indexes [all data]	R_1 = 0.0839, wR_2 = 0.2244
Largest diff. peak/hole / e Å^{-3}	0.32/-0.39

Table 8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2 CCDC 995318 . U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	5000	4790(2)	7500	47.5(8)
C2	4179.3(17)	5247(2)	7026(2)	44.8(7)
N3	4131.4(15)	6065.9(16)	7009.3(18)	45.6(6)
C4	5000	6458(3)	7500	43.8(9)
N5	3345.7(16)	4826.1(17)	6526(2)	55.7(7)
N6	5000	7266(3)	7500	47.1(9)
N11	2717.1(16)	8036.8(16)	3926.5(19)	48.9(7)
C12	2679.5(19)	7202(2)	3804(2)	48.9(7)
N13	3574.5(18)	6788.9(19)	4225(2)	52.6(7)
C13	3574.5(18)	6788.9(19)	4225(2)	52.6(7)
C14	4423(2)	7236(2)	4759(2)	52.5(8)
C15	4405.0(19)	8068(2)	4879(2)	55.0(8)
N15	4405.0(19)	8068(2)	4879(2)	55.0(8)
C16	3523.0(19)	8538(2)	4468(2)	51.0(8)
N17	5367(2)	8237(3)	5447(3)	51.0(9)
N17A	3960(15)	6132(12)	4385(15)	71(5)
C18	5873(3)	7535(3)	5601(3)	55.1(10)
C18A	4951(8)	6147(9)	4858(10)	55.1(10)

N19	5323.1(17)	6877.6(18)	5176(2)	55.8(7)
O20	3439.2(14)	9277.3(15)	4536(2)	64.6(7)
O21	1899.7(15)	6842.3(13)	3333.6(17)	54.9(6)
C22	3604(5)	5877(4)	4136(5)	56.2(14)
C22A	5346(13)	8689(13)	5506(13)	56.2(14)
C23	5754(3)	9054(3)	5838(5)	67.9(13)
C23A	3344(10)	5418(11)	4019(15)	67.9(13)
N31	10000	7968(2)	7500	46.7(8)
C32	9091.3(19)	7585(2)	6994(2)	47.3(7)
C33	9120(2)	6740(2)	6989(2)	56.5(8)
N33	9120(2)	6740(2)	6989(2)	56.5(8)
C34	10000	6314(3)	7500	56.5(11)
N35	8553(6)	6086(4)	6696(6)	57.1(17)
C36	9048(5)	5378(5)	6969(6)	70(2)
N37	10000	5497(3)	7500	64.7(11)
O38	8335.6(13)	8003.0(14)	6595.7(17)	53.1(6)
C39	7498(7)	6182(5)	6076(7)	75(2)
C40	8129(7)	6295(6)	6363(8)	59(2)

Table 9 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2 CCDC 995318 . The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	28.4(15)	66(2)	42.0(17)	0	4.0(13)	0
C2	27.0(13)	69(2)	34.9(14)	2.1(12)	5.1(10)	-1.3(12)
N3	26.4(12)	65.4(17)	40.1(12)	1.9(10)	4.6(10)	0.0(9)
C4	26.3(17)	69(3)	34.4(19)	0	7.9(14)	0
N5	26.6(11)	64.6(16)	62.8(16)	6.9(12)	-2.9(10)	-1.4(10)
N6	26.3(16)	64(2)	45.9(19)	0	5.4(14)	0
N11	24.7(11)	69.5(17)	48.1(14)	9.1(11)	6.2(10)	2(1)
C12	31.3(14)	74(2)	39.3(15)	6.0(13)	9.7(12)	1.8(13)
N13	36.5(14)	73(2)	46.3(15)	5.0(12)	10.8(11)	10.1(12)
C13	36.5(14)	73(2)	46.3(15)	5.0(12)	10.8(11)	10.1(12)
C14	32.9(15)	84(2)	40.2(15)	7.5(14)	11.1(12)	8.6(14)
C15	26.1(13)	93(2)	42.3(15)	11.9(14)	6.2(11)	2.8(13)
N15	26.1(13)	93(2)	42.3(15)	11.9(14)	6.2(11)	2.8(13)
C16	29.7(14)	70(2)	48.4(16)	11.8(14)	6.7(12)	0.9(13)
N17	26.5(15)	72(2)	49.1(19)	8.9(19)	4.5(13)	-3.5(17)
N17A	80(13)	68(11)	62(10)	-27(7)	19(9)	-2(9)
C18	27.8(18)	86(3)	48(2)	9(2)	7.7(15)	9.1(19)
C18A	27.8(18)	86(3)	48(2)	9(2)	7.7(15)	9.1(19)
N19	31.4(12)	84(2)	48.7(14)	3.7(13)	9.3(10)	11.4(13)
O20	31.6(10)	63.6(15)	83.6(17)	11.9(12)	-0.9(10)	-2.2(9)
O21	34.1(11)	71.0(14)	52.4(12)	-0.6(10)	4.9(9)	-0.4(9)
C22	55(4)	66(4)	44(3)	-6(3)	12(3)	4(3)
C22A	55(4)	66(4)	44(3)	-6(3)	12(3)	4(3)
C23	36(2)	73(3)	84(3)	7(3)	4(2)	-7(2)
C23A	36(2)	73(3)	84(3)	7(3)	4(2)	-7(2)
N31	32.1(17)	59(2)	46.5(18)	0	9.2(14)	0
C32	31.1(15)	71(2)	38.0(14)	-0.7(13)	8.8(12)	-1.6(12)
C33	47.6(17)	69(2)	55.3(17)	-4.7(14)	20.1(14)	-7.7(14)
N33	47.6(17)	69(2)	55.3(17)	-4.7(14)	20.1(14)	-7.7(14)
C34	52(3)	69(3)	51(2)	0	21(2)	0
N35	36(4)	71(5)	51(4)	1(3)	-4(3)	-4(3)

C36	47(4)	70(5)	77(5)	2(4)	0(3)	-6(3)
N37	51(2)	64(3)	69(3)	0	5.9(19)	0
O38	28.9(10)	69.9(14)	54.5(12)	-0.2(10)	5.6(9)	0.7(9)
C39	34(4)	97(6)	76(5)	4(4)	-7(4)	-10(4)
C40	28(5)	77(6)	62(5)	-8(4)	-1(4)	-10(4)

Table 10 Bond Lengths for 2 CCDC 995318 .

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C2[1]	1.354(3)	N17A	C18A	1.35(2)
N1	C2	1.354(3)	N17A	C23A	1.44(2)
C2	N3	1.330(4)	C18	N19	1.333(5)
C2	N5	1.343(4)	C18A	N19	1.310(15)
N3	C4	1.355(3)	N31	C32[2]	1.396(3)
C4	N3[1]	1.355(3)	N31	C32	1.396(3)
C4	N6	1.310(6)	C32	C33	1.371(5)
N11	C12	1.363(4)	C32	O38	1.237(3)
N11	C16	1.398(4)	C33	C34	1.398(4)
C12	N13	1.389(4)	C33	N35	1.314(8)
C12	O21	1.229(4)	C34	C33[2]	1.398(4)
N13	C14	1.389(4)	C34	N33[2]	1.398(4)
N13	C22	1.485(7)	C34	C36	2.006(8)
C14	C15	1.360(5)	C34	C36[2]	2.006(8)
C14	N19	1.354(4)	C34	N37	1.325(6)
C15	C16	1.420(4)	N35	C36	1.335(11)
C15	N17	1.360(4)	N35	C39	1.468(9)
C16	O20	1.212(4)	C36	N37	1.324(6)
N17	C18	1.328(6)	N37	C36[2]	1.324(6)
N17	C23	1.463(6)			

[1]1-X,+Y,1/2-Z; [2]2-X,+Y,1/2-Z

Table 11 Bond Angles for 2 CCDC 995318 .

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2[1]	N1	C2	113.6(4)	N19	C18	C14	40.29(18)
N3	C2	N1	125.9(3)	N17A	C18A	C14	69.6(10)
N3	C2	N5	117.9(2)	N19	C18A	C14	45.1(5)
N5	C2	N1	116.2(3)	N19	C18A	N17A	114.7(13)
C2	N3	C4	115.3(3)	C18	N19	C14	100.2(3)
N3	C4	N3[1]	124.0(4)	C18A	N19	C14	91.6(5)
N6	C4	N3[1]	118.0(2)	C32[2]	N31	C32	127.1(4)
N6	C4	N3	118.0(2)	C33	C32	N31	115.0(3)
C12	N11	C16	129.2(2)	O38	C32	N31	120.2(3)
N11	C12	N13	115.9(3)	O38	C32	C33	124.7(3)
O21	C12	N11	121.6(3)	C32	C33	C34	121.0(3)
O21	C12	N13	122.4(3)	N35	C33	C32	142.3(4)
C12	N13	C14	119.1(3)	N35	C33	C34	96.5(4)
C12	N13	C22	119.7(3)	C33[2]	C34	C33	120.8(4)
C14	N13	C22	121.1(3)	C33[2]	C34	C36	160.4(4)
N19	C14	C15	115.6(3)	C33	C34	C36[2]	160.4(4)
C14	C15	C16	122.5(3)	C33	C34	C36	78.8(3)
C14	C15	N17	102.0(3)	C33[2]	C34	C36[2]	78.8(3)
N17	C15	C16	135.4(4)	C36	C34	C36[2]	81.6(5)

N11	C16	C15	111.2(3)	N37	C34	C33	119.6(2)
O20	C16	N11	121.8(3)	N37	C34	C33[2]	119.6(2)
O20	C16	C15	126.9(3)	N37	C34	C36	40.8(2)
C15	N17	C14	39.0(2)	N37	C34	C36[2]	40.8(2)
C15	N17	C23	124.9(4)	C33	N35	C36	113.2(6)
C18	N17	C14	69.3(3)	C33	N35	C39	120.0(6)
C18	N17	C15	108.3(4)	C36	N35	C39	126.7(7)
C18	N17	C23	126.8(3)	N35	C36	C34	71.4(5)
C23	N17	C14	163.7(3)	N37	C36	C34	40.8(3)
C18A	N17A	C14	69.1(10)	N37	C36	N35	112.2(7)
C18A	N17A	C23A	127.1(18)	C36[2]	N37	C34	98.4(4)
C23A	N17A	C14	163.7(17)	C36	N37	C34	98.4(4)
N17	C18	C14	73.6(2)	C36	N37	C36[2]	163.2(8)
N17	C18	N19	113.9(3)				

[1]1-X,+Y,1/2-Z; [2]2-X,+Y,1/2-Z

Table 12 Hydrogen Bonds for 2 CCDC 995318 .

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N5	H5A	O20[1]	0.88	1.99	2.869(3)	178.4

[1] 1/2+X, -1/2+Y, Z

Table 13 Torsion Angles for 2 CCDC 995318 .

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	N3	C4	1.4(4)	C23	N17	C18	N19	178.2(4)
C2[1]	N1	C2	N3	-0.74(19)	C23A	N17A	C18A	C14	-178(2)
C2[1]	N1	C2	N5	178.9(3)	C23A	N17A	C18A	N19	-175.8(18)
C2	N3	C4	N3[1]	-0.64(16)	N31	C32	C33	C34	2.5(4)
C2	N3	C4	N6	179.37(16)	N31	C32	C33	N35	177.0(6)
N5	C2	N3	C4	-178.2(2)	C32[2]	N31	C32	C33	-1.26(18)
N11	C12	N13	C14	1.9(4)	C32[2]	N31	C32	O38	178.5(3)
N11	C12	N13	C22	179.6(4)	C32	C33	C34	C33[2]	-1.37(19)
C12	N11	C16	C15	3.3(4)	C32	C33	C34	N33[2]	-1.37(19)
C12	N11	C16	O20	-178.0(3)	C32	C33	C34	C36	177.8(3)
C14	C15	C16	N11	-1.1(4)	C32	C33	C34	C36[2]	-179.0(7)
C14	C15	C16	O20	-179.8(3)	C32	C33	C34	N37	178.63(19)
C14	C15	N17	C18	1.2(4)	C32	C33	N35	C36	-177.2(5)
C14	C15	N17	C23	-177.2(4)	C32	C33	N35	C39	6.1(11)
C14	N17	C18	N19	0.7(3)	C33[2]	C34	N37	C36[2]	-1.2(4)
C14	N17A	C18A	N19	2.5(10)	C33	C34	N37	C36	-1.2(4)
C14	C18	N19	C18A	-173(3)	C33	C34	N37	C36[2]	178.8(4)
C14	C18A	N19	C18	173(3)	C33[2]	C34	N37	C36	178.8(4)
C15	C14	N19	C18	1.8(4)	C33	N35	C36	C34	1.4(5)
C15	C14	N19	C18A	-179.5(6)	C33	N35	C36	N37	1.5(9)
C15	N17	C18	C14	-0.8(3)	N33[2]	C34	N37	C36[2]	-1.2(4)
C15	N17	C18	N19	-0.1(5)	N33[2]	C34	N37	C36	178.8(4)
C16	N11	C12	N13	-3.7(4)	C34	C33	N35	C36	-1.9(6)
C16	N11	C12	O21	177.3(3)	C34	C33	N35	C39	-178.7(6)
C16	C15	N17	C14	179.2(5)	C34	C36	N37	C36[2]	179.995(5)

C16	C15	N17	C18	-179.7(3)	N35	C33	C34	C33[2]	-178.0(4)
C16	C15	N17	C23	2.0(6)	N35	C33	C34	N33[2]	-178.0(4)
N17	C15	C16	N11	179.8(3)	N35	C33	C34	C36	1.2(4)
N17	C15	C16	O20	1.1(6)	N35	C33	C34	C36[2]	4.4(9)
N17	C18	N19	C14	-1.0(4)	N35	C33	C34	N37	2.0(4)
N17	C18	N19	C18A	-174(3)	N35	C36	N37	C34	-0.1(6)
N17A	C18A	N19	C14	-3.3(13)	N35	C36	N37	C36[2]	179.9(6)
N17A	C18A	N19	C18	170(2)	C36	C34	N37	C36[2]	180.001(2)
N19	C14	C15	C16	178.8(3)	C36[2]	C34	N37	C36	179.999(1)
N19	C14	C15	N17	-1.9(4)	O38	C32	C33	C34	-177.2(2)
O21	C12	N13	C14	-179.1(3)	O38	C32	C33	N35	-2.7(8)
O21	C12	N13	C22	-1.4(5)	C39	N35	C36	C34	177.9(8)
C23	N17	C18	C14	177.5(4)	C39	N35	C36	N37	178.0(7)

[1]1-X,+Y,1/2-Z; [2]2-X,+Y,1/2-Z

C) Crystallographic tables for dimelaminium ethylenediaminetetraacetate dihydrate 3 CCDC 741062

Table 14 Crystal data and structure refinement for 3 CCDC 741062.

Identification code	3 CCDC 741062
Empirical formula	$C_{16}H_{32}N_{14}O_{10}$
Formula weight	580.55
Temperature/K	296.15
Crystal system	triclinic
Space group	*P*-1
a/Å	7.0884(3)
b/Å	7.7150(2)
c/Å	11.6340(5)
α/°	80.755(3)
β/°	78.037(4)
γ/°	83.455(3)
Volume/Å^3	612.18(4)
Z	1
ρ_{calc}mg/mm^3	1.575
m/mm^{-1}	0.131
F(000)	306.0
Crystal size/mm^3	0.48 × 0.16 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.368 to 58.652°
Index ranges	$-9 \le h \le 9$, $-10 \le k \le 10$, $-15 \le l \le 15$
Reflections collected	13003
Independent reflections	2953 [R_{int} = 0.0241, R_{sigma} = 0.0378]
Data/restraints/parameters	2953/0/221
Goodness-of-fit on F^2	0.897
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.0832
Final R indexes [all data]	R_1 = 0.0655, wR_2 = 0.0892
Largest diff. peak/hole / e Å^{-3}	0.17/-0.23

Table 15 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3 CCDC 741062. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O11	10752.1(13)	1771.1(11)	98.9(8)	32.3(2)
O12	11153.1(14)	3886.9(12)	-1466.0(9)	39.0(3)
O21	5962.9(16)	2237.1(14)	3058.4(8)	46.8(3)
O22	7275.9(16)	-123.8(13)	2228.7(9)	46.1(3)
N11	7062.0(15)	1405.7(14)	-23.9(9)	26.4(3)
C11	10228.7(19)	2737.1(16)	-764.6(11)	27.3(3)
C12	8302.6(19)	2435.5(17)	-1050.4(11)	30.8(3)
C21	6546(2)	1409.2(19)	2195.3(12)	33.3(3)
C22	6338(2)	2451.9(17)	986.7(11)	32.0(3)
C31	5492.6(19)	698.5(17)	-459.8(11)	30.6(3)
N1	7881.4(16)	-435.1(15)	6709.1(10)	34.5(3)
N2	7677.4(18)	-673.2(19)	4758.1(11)	42.3(3)
N3	9008.6(17)	-3117.7(16)	5873.4(9)	37.3(3)
N4	9125(2)	-2875.6(19)	7771.1(11)	40.4(3)
N5	6547(2)	1879.7(19)	5538.2(15)	49.7(4)
N6	8746(2)	-3213(3)	3952.1(13)	57.3(4)
C1	8668.7(19)	-2117.1(18)	6758.5(11)	31.7(3)
C2	7363(2)	259.6(19)	5694.6(12)	36.7(3)

C3	8481(2)	-2346(2)	4874.9(12)	39.1(4)
O91	4938.2(19)	5872.0(18)	2640.6(12)	55.9(3)

Table 16 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3 CCDC 741062. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O11	33.2(5)	35.8(5)	29.6(5)	-6.5(4)	-11.6(4)	2.9(4)
O12	32.2(6)	37.5(5)	44.6(6)	1.9(4)	-4.8(5)	-7.4(4)
O21	58.0(7)	55.8(6)	27.2(5)	-7.4(5)	-5.0(5)	-11.7(5)
O22	51.2(7)	42.9(6)	40.3(6)	6.0(5)	-12.6(5)	2.9(5)
N11	24.6(6)	28.5(6)	25.0(5)	0.0(5)	-6.5(5)	-0.1(5)
C11	28.5(7)	28.8(6)	24.8(6)	-7.9(5)	-4.6(5)	2.0(5)
C12	29.9(7)	37.7(7)	24.1(6)	1.1(6)	-5.6(6)	-7.1(5)
C21	29.9(7)	40.5(8)	29.1(7)	-0.1(6)	-6.0(6)	-8.3(6)
C22	32.6(8)	33.0(7)	28.6(7)	-3.7(6)	-4.4(6)	0.7(6)
C31	27.6(7)	36.2(7)	29.2(7)	-1.0(6)	-9.9(6)	-4.1(5)
N1	33.0(7)	41.5(7)	29.6(6)	-4.4(5)	-8.4(5)	-2.2(5)
N2	37.4(8)	63.5(9)	24.4(6)	4.1(6)	-8.7(5)	-6.6(6)
N3	37.1(7)	50.8(7)	25.8(6)	-10.6(5)	-6.5(5)	-2.7(5)
N4	54.8(9)	41.4(7)	28.7(6)	-11.1(6)	-18.8(6)	9.4(6)
N5	46.6(9)	53.4(9)	44.5(9)	8.8(8)	-13.5(7)	1.2(7)
N6	63.5(11)	85.5(13)	27.1(7)	-18.3(8)	-12.4(7)	-2.7(9)
C1	25.6(7)	44.6(8)	25.7(7)	-6.1(6)	-4.7(5)	-5.6(6)
C2	26.2(7)	49.9(9)	31.9(7)	2.7(7)	-3.8(6)	-9.8(6)
C3	30.4(8)	62.2(10)	25.1(7)	-7.4(7)	-2.7(6)	-9.2(7)
O91	46.7(8)	50.6(7)	67.7(8)	-3.2(6)	-11.1(6)	-0.4(6)

Table 17 Bond Lengths for 3 CCDC 741062.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O11	C11	1.2462(15)	N1	C1	1.3502(17)
O12	C11	1.2492(15)	N1	C2	1.3216(18)
O21	C21	1.2495(17)	N2	C2	1.3673(19)
O22	C21	1.2337(17)	N2	C3	1.348(2)
N11	C12	1.4999(15)	N3	C1	1.3508(17)
N11	C22	1.5025(16)	N3	C3	1.3234(18)
N11	C31	1.5012(17)	N4	C1	1.3146(18)
C11	C12	1.5213(18)	N5	C2	1.318(2)
C21	C22	1.5302(18)	N6	C3	1.324(2)
C31	C31[1]	1.512(2)			

[1]1-X,-Y,-Z

Table 18 Bond Angles for 3 CCDC 741062.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	N11	C22	111.97(10)	C2	N1	C1	115.55(12)
C12	N11	C31	109.16(10)	C3	N2	C2	119.80(13)
C31	N11	C22	114.13(10)	C3	N3	C1	115.27(12)
O11	C11	O12	127.21(13)	N1	C1	N3	126.45(12)

O11	C11	C12	117.27(11)	N4	C1	N1	117.21(13)
O12	C11	C12	115.44(11)	N4	C1	N3	116.33(13)
N11	C12	C11	112.03(10)	N1	C2	N2	121.10(14)
O21	C21	C22	115.08(12)	N5	C2	N1	121.59(15)
O22	C21	O21	126.61(13)	N5	C2	N2	117.30(15)
O22	C21	C22	118.30(12)	N3	C3	N2	121.79(13)
N11	C22	C21	113.20(11)	N3	C3	N6	120.13(16)
N11	C31	C31[1]	111.27(13)	N6	C3	N2	118.07(16)

[1]1-X,-Y,-Z

Table 19 Hydrogen Bonds for 3 CCDC 741062.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N11	H11	O11[1]	0.866(16)	1.985(15)	2.7500(14)	146.7(14)
N4	H41	O12[2]	0.835(17)	2.053(18)	2.8445(17)	158.1(16)
N4	H42	O11[3]	0.902(16)	1.912(17)	2.7675(16)	157.7(14)

[1]2-X,-Y,-Z; [2]+X,-1+Y,1+Z; [3]2-X,-Y,1-Z

Table 20 Torsion Angles for 3 CCDC 741062.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O11	C11	C12	N11	17.94(15)	C1	N1	C2	N5	178.79(13)
O12	C11	C12	N11	-165.23(10)	C1	N3	C3	N2	0.5(2)
O21	C21	C22	N11	179.86(12)	C1	N3	C3	N6	-179.85(13)
O22	C21	C22	N11	0.69(18)	C2	N1	C1	N3	1.64(19)
C12	N11	C22	C21	-134.20(12)	C2	N1	C1	N4	-177.18(13)
C12	N11	C31	C31[1]	166.18(13)	C2	N2	C3	N3	-1.0(2)
C22	N11	C12	C11	69.27(13)	C2	N2	C3	N6	179.38(13)
C22	N11	C31	C31[1]	-67.69(16)	C3	N2	C2	N1	1.8(2)
C31	N11	C12	C11	-163.37(10)	C3	N2	C2	N5	-178.96(13)
C31	N11	C22	C21	101.16(13)	C3	N3	C1	N1	-0.9(2)
C1	N1	C2	N2	-2.00(19)	C3	N3	C1	N4	177.92(13)

[1]1-X,-Y,-Z

D) Crystallographic tables for dimelaminium sulfate 4 CCDC 741064

Table 21 Crystal data and structure refinement for 4 CCDC 741064.

Identification code	4 CCDC 741064
Empirical formula	$C_6H_{14}N_{12}O_4S$
Formula weight	350.35
Temperature/K	296.15
Crystal system	monoclinic
Space group	*C*2/*c*
a/Å	18.041(2)
b/Å	10.6373(14)
c/Å	14.289(2)
α/°	90
β/°	103.652(14)
γ/°	90
Volume/Å^3	2664.7(6)
Z	8
ρ_{calc}mg/mm^3	1.747
m/mm^{-1}	0.293
F(000)	1456.0
Crystal size/mm^3	0.15 × 0.082 × 0.041
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	4.646 to 57.96°
Index ranges	$-23 \le h \le 22$, $-14 \le k \le 13$, $-17 \le l \le 15$
Reflections collected	6922
Independent reflections	2897 [R_{int} = 0.0585, R_{sigma} = 0.2339]
Data/restraints/parameters	2897/14/258
Goodness-of-fit on F^2	0.771
Final R indexes [I>=2σ (I)]	R_1 = 0.0493, wR_2 = 0.0745
Final R indexes [all data]	R_1 = 0.2244, wR_2 = 0.0972
Largest diff. peak/hole / e Å^{-3}	0.34/-0.23

Table 22 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4 CCDC 741064. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N11	772(2)	6518(3)	1117(3)	33.9(13)
C12	1337(3)	5996(4)	814(4)	34.3(15)
N13	1373(2)	4732(3)	674(4)	32.5(13)
C14	831(3)	3971(4)	909(4)	33.8(15)
N15	246(2)	4443(3)	1201(3)	32.8(13)
C16	230(3)	5704(4)	1260(4)	35.7(16)
N17	-390(2)	6209(4)	1438(3)	42.0(13)
N18	1904(2)	6680(4)	646(3)	43.5(13)
N19	894(2)	2748(3)	807(3)	41.7(13)
N21	237.8(19)	1017(3)	3685(3)	24.8(11)
C22	835(2)	1430(4)	3377(4)	24.7(13)
N23	1367(2)	626(3)	3174(4)	29.7(13)
C24	1306(3)	-631(4)	3358(4)	31.8(15)
N25	730(2)	-1088(3)	3675(3)	30.5(12)
C26	188(3)	-240(4)	3763(4)	25.3(13)
N27	922(2)	2642(3)	3257(3)	34.6(12)
N28	1850(2)	-1387(4)	3227(4)	46.9(14)
N29	-431(2)	-692(4)	3977(3)	35.1(12)

S1	2499.1(10)	154.2(10)	1264.1(18)	34.2(3)
O1	1988.6(17)	955(3)	1633(3)	61.3(13)
O2	3018.8(17)	928(3)	873(3)	60.7(12)
O3	2061.4(19)	-641(3)	487(3)	57.0(12)
O4	2922.8(19)	-646(3)	2036(3)	65.2(13)

Table 23 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4 CCDC 741064. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	33(2)	23(2)	47(4)	-2(2)	13(2)	-0.2(17)
C12	32(3)	33(3)	39(5)	1(3)	11(3)	-1(2)
N13	25(2)	32(2)	44(4)	0(2)	15(2)	5.5(18)
C14	37(3)	24(3)	41(5)	6(3)	12(3)	2(2)
N15	28(2)	23(2)	52(4)	3(2)	18(3)	2.0(17)
C16	29(3)	33(3)	46(5)	-5(3)	11(3)	1(2)
N17	32(3)	27(2)	73(4)	1(3)	24(2)	2(2)
N18	40(3)	31(2)	67(4)	-5(2)	29(3)	-6(2)
N19	42(3)	25(2)	66(4)	1(2)	28(3)	5.9(18)
N21	26(2)	23.6(19)	28(3)	2.3(19)	13(2)	-0.6(15)
C22	16(3)	32(3)	23(4)	1(2)	-3(2)	-1.6(19)
N23	31(2)	26(2)	39(4)	3(2)	20(3)	-2.6(18)
C24	35(3)	28(3)	34(5)	1(3)	11(3)	2(2)
N25	20(2)	27(2)	48(4)	8(2)	14(2)	-1.8(15)
C26	18(3)	33(3)	24(4)	2(2)	3(3)	-4.0(19)
N27	39(3)	20(2)	52(4)	0(2)	24(2)	-6.0(18)
N28	38(3)	29(2)	84(5)	9(3)	35(3)	6.5(19)
N29	37(2)	26(2)	49(4)	5(2)	24(2)	-1(2)
S1	24.3(5)	31.0(6)	51.4(9)	-2.0(8)	17.2(5)	0.9(6)
O1	68(2)	46(2)	92(4)	24(2)	62(3)	27.0(17)
O2	58(2)	60(2)	80(4)	-29(2)	49(2)	-27.3(18)
O3	53(2)	50(2)	65(4)	-3(2)	7(2)	-16.1(17)
O4	62(3)	75(3)	56(4)	7(2)	8(2)	42(2)

Table 24 Bond Lengths for 4 CCDC 741064.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N11	C12	1.320(5)	C22	N23	1.366(5)
N11	C16	1.357(5)	C22	N27	1.315(5)
C12	N13	1.363(5)	N23	C24	1.372(5)
C12	N18	1.322(5)	C24	N25	1.320(5)
N13	C14	1.371(5)	C24	N28	1.317(5)
C14	N15	1.322(5)	N25	C26	1.357(5)
C14	N19	1.317(5)	C26	N29	1.317(5)
N15	C16	1.344(5)	S1	O1	1.443(3)
C16	N17	1.319(5)	S1	O2	1.455(3)
N21	C22	1.331(5)	S1	O3	1.470(4)
N21	C26	1.347(4)	S1	O4	1.459(4)

Table 25 Bond Angles for 4 CCDC 741064.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	N11	C16	114.8(4)	N27	C22	N23	118.4(4)
N11	C12	N13	122.0(4)	C22	N23	C24	118.5(4)
N11	C12	N18	121.2(4)	N25	C24	N23	122.0(4)
N18	C12	N13	116.8(4)	N28	C24	N23	118.2(4)
C12	N13	C14	119.1(4)	N28	C24	N25	119.9(4)
N15	C14	N13	121.4(4)	C24	N25	C26	115.4(4)
N19	C14	N13	118.1(4)	N21	C26	N25	126.1(4)
N19	C14	N15	120.4(4)	N29	C26	N21	117.3(4)
C14	N15	C16	115.4(4)	N29	C26	N25	116.6(4)
N15	C16	N11	126.9(4)	O1	S1	O2	109.35(17)
N17	C16	N11	116.3(4)	O1	S1	O3	109.9(2)
N17	C16	N15	116.7(4)	O1	S1	O4	109.5(3)
C22	N21	C26	115.4(3)	O2	S1	O3	108.4(3)
N21	C22	N23	121.8(4)	O2	S1	O4	110.5(3)
N27	C22	N21	119.8(4)	O4	S1	O3	109.14(18)

Table 26 Hydrogen Bonds for 4 CCDC 741064.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N13	H13	O2[1]	0.96(3)	1.93(4)	2.780(6)	147(4)
N17	H17B	O2[2]	0.85(3)	2.17(4)	2.809(5)	131(4)
N18	H18B	O3[3]	0.93(3)	1.98(3)	2.877(5)	162(4)
N19	H19B	O1	0.83(3)	2.16(4)	2.797(5)	133(4)
N23	H23	O1	0.95(3)	1.79(4)	2.720(5)	163(4)
N27	H27A	O4[4]	0.88(3)	2.02(3)	2.872(4)	161(4)

[1]1/2-X,1/2-Y,-Z; [2]-1/2+X,1/2+Y,+Z; [3]+X,1+Y,+Z; [4]1/2-X,1/2+Y,1/2-Z

Table 27 Torsion Angles for 4 CCDC 741064.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N11	C12	N13	C14	-4.0(8)	N21	C22	N23	C24	-4.6(8)
C12	N11	C16	N15	5.9(8)	C22	N21	C26	N25	8.8(8)
C12	N11	C16	N17	-171.3(5)	C22	N21	C26	N29	-173.8(5)
C12	N13	C14	N15	5.0(8)	C22	N23	C24	N25	3.7(7)
C12	N13	C14	N19	-177.1(5)	C22	N23	C24	N28	-175.1(5)
N13	C14	N15	C16	-0.8(7)	N23	C24	N25	C26	2.8(8)
C14	N15	C16	N11	-5.0(7)	C24	N25	C26	N21	-9.6(8)
C14	N15	C16	N17	172.2(6)	C24	N25	C26	N29	172.9(5)
C16	N11	C12	N13	-1.0(8)	C26	N21	C22	N23	-1.2(7)
C16	N11	C12	N18	-180.0(5)	C26	N21	C22	N27	178.4(4)
N18	C12	N13	C14	175.0(5)	N27	C22	N23	C24	175.8(4)
N19	C14	N15	C16	-178.6(5)	N28	C24	N25	C26	-178.4(5)

E) Crystallographic tables for melaminium dinitrate 5 CCDC 741065

Table 28 Crystal data and structure refinement for 5 CCDC 741065.

Identification code	5 CCDC 741065
Empirical formula	$C_3H_8N_8O_6$
Formula weight	252.17
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.7710(14)
b/Å	9.8924(18)
c/Å	12.186(2)
α/°	90
β/°	101.198(9)
γ/°	90
Volume/Å^3	918.9(3)
Z	4
ρ_{calc}mg/mm^3	1.823
m/mm^{-1}	1.516
F(000)	520.0
Crystal size/mm^3	0.08 × 0.04 × 0.04
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection	11.608 to 130.236°
Index ranges	$-8 \le h \le 9$, $-11 \le k \le 10$, $-9 \le l \le 14$
Reflections collected	5198
Independent reflections	1518 [R_{int} = 0.2218, R_{sigma} = 0.6454]
Data/restraints/parameters	1518/0/178
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0335, wR_2 = 0.0905
Final R indexes [all data]	R_1 = 0.3022, wR_2 = 0.1046
Largest diff. peak/hole / e Å^{-3}	0.42/-0.42

Table 29 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5 CCDC 741065. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
N1	6888.0(15)	3554.1(12)	5791.5(16)	13.8(4)
N2	7815.4(15)	1850.9(13)	4750.4(17)	15.6(5)
N3	8341.5(15)	4132.9(12)	4311.1(16)	13.7(5)
N4	6440.1(17)	1322.3(13)	6204.6(17)	18.2(5)
N5	9303.3(17)	2381.7(13)	3354.1(16)	15.9(5)
N6	7251.8(18)	5778.2(12)	5307.2(17)	18.1(5)
C1	7031.8(17)	2207.5(15)	5603.3(19)	14.6(6)
C2	8492.2(17)	2808.1(16)	4143(2)	13.5(5)
C3	7516.9(18)	4491.3(16)	5117.5(18)	13.9(5)
N10	5615.8(16)	8155.4(13)	6933.6(18)	14.5(5)
O11	5337.6(13)	6914.8(10)	7059.4(13)	18.9(4)
O13	5020.3(14)	9029.9(10)	7501.9(14)	20.3(4)
O12	6460.2(13)	8493.6(11)	6206.6(13)	22.9(5)
N20	1306.9(16)	3658.9(13)	1308.4(15)	15.6(5)
O21	1176.6(13)	2404.0(11)	1367.2(15)	19.7(4)
O22	777.2(13)	4410.4(10)	2006.9(13)	21.8(4)
O23	1957.1(15)	4163.4(10)	534.7(14)	25.9(4)

Table 30 Anisotropic Displacement Parameters ($Å^2×10^3$) for 5 CCDC 741065. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	15.6(7)	15.4(7)	12.1(13)	-0.9(7)	6.9(7)	0.4(5)
N2	15.2(7)	12.1(6)	20.8(15)	-1.3(7)	6.7(7)	0.7(5)
N3	13.7(6)	13.9(6)	14.3(13)	0.8(7)	4.6(6)	0.5(4)
N4	19.8(8)	16.1(7)	21.5(16)	0.1(8)	11.4(8)	0.1(5)
N5	20.0(7)	15.2(6)	15.3(14)	-0.1(7)	10.2(7)	-0.9(5)
N6	17.7(7)	15.0(6)	24.6(15)	0.2(8)	11.3(8)	0.3(5)
C1	7.8(8)	18.3(7)	17.2(17)	-2.7(10)	1.1(8)	-0.7(5)
C2	10.0(7)	14.5(6)	15.3(17)	1.4(8)	1.2(7)	1.0(5)
C3	8.7(7)	16.0(7)	15.6(16)	2.8(9)	-1.0(7)	-0.4(5)
N10	14.8(6)	14.4(6)	14.9(15)	-1.3(7)	4.2(7)	0.1(4)
O11	20.1(6)	13.7(5)	24.6(13)	1.3(6)	8.7(7)	-0.6(4)
O13	25.6(6)	17.7(6)	21.1(11)	-5.2(6)	13.5(6)	0.1(4)
O12	31.9(7)	18.3(6)	24.1(14)	2.0(6)	19.0(7)	-1.1(4)
N20	15.3(7)	17.0(6)	15.4(15)	-0.1(8)	4.8(8)	0.2(5)
O21	21.8(6)	13.4(5)	25.0(13)	2.6(6)	6.9(7)	-0.6(4)
O22	27.4(6)	16.7(5)	25.6(12)	-3.3(7)	15.3(7)	2.4(4)
O23	38.1(7)	19.4(5)	25.9(13)	2.1(7)	20.6(7)	-2.9(4)

Table 31 Bond Lengths for 5 CCDC 741065.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.360(2)	N6	C3	1.317(2)
N1	C3	1.389(2)	N10	O11	1.2607(18)
N2	C1	1.350(2)	N10	O13	1.2516(19)
N2	C2	1.369(2)	N10	O12	1.246(2)
N3	C2	1.335(2)	N20	O21	1.2487(18)
N3	C3	1.322(2)	N20	O22	1.2580(19)
N4	C1	1.283(2)	N20	O23	1.256(2)
N5	C2	1.317(2)			

Table 32 Bond Angles for 5 CCDC 741065.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C3	120.28(16)	N3	C3	N1	122.53(14)
C1	N2	C2	120.94(15)	N6	C3	N1	117.16(16)
C3	N3	C2	116.57(16)	N6	C3	N3	120.31(16)
N2	C1	N1	116.75(16)	O13	N10	O11	121.00(15)
N4	C1	N1	121.46(17)	O12	N10	O11	118.31(15)
N4	C1	N2	121.79(15)	O12	N10	O13	120.66(12)
N3	C2	N2	122.79(17)	O21	N20	O22	120.52(15)
N5	C2	N2	117.52(15)	O21	N20	O23	119.13(15)
N5	C2	N3	119.69(17)	O23	N20	O22	120.34(12)

Table 33 Hydrogen Bonds for 5 CCDC 741065.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N4	H41	O12[1]	0.96(2)	1.88(2)	2.7983(17)	161.3(16)

[1]+X,-1+Y,+Z

Table 34 Torsion Angles for 5 CCDC 741065.

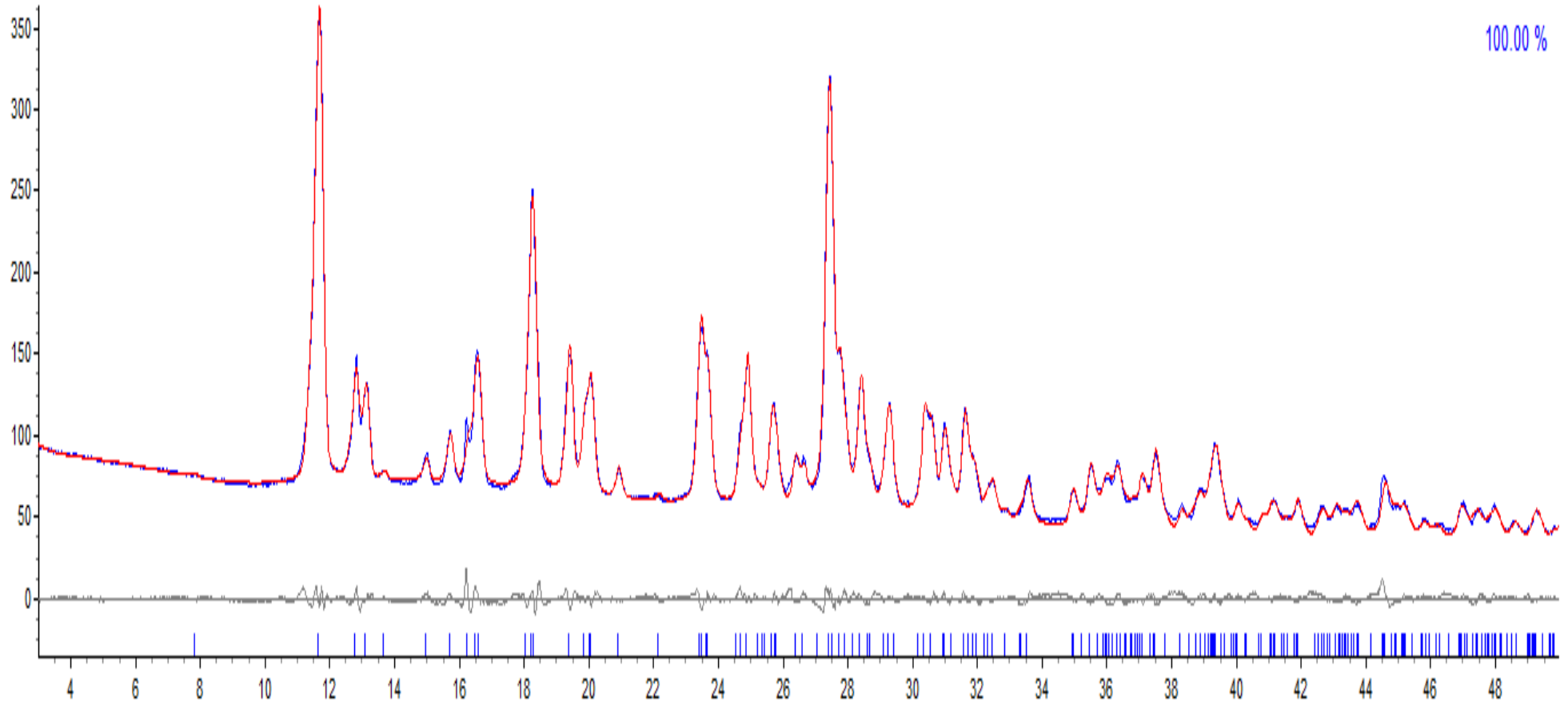
A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	N1	C3	N3	-3.2(3)	C2	N3	C3	N1	2.3(3)
C1	N1	C3	N6	176.45(19)	C2	N3	C3	N6	-177.28(18)
C1	N2	C2	N3	-3.6(3)	C3	N1	C1	N2	0.5(3)
C1	N2	C2	N5	177.17(17)	C3	N1	C1	N4	-179.05(16)
C2	N2	C1	N1	2.7(2)	C3	N3	C2	N2	1.0(3)
C2	N2	C1	N4	-177.73(19)	C3	N3	C2	N5	-179.82(16)

F) Crystallographic information of Rietveld refinements for crystalline powders of 3 and 5

Table 35. Crystallographic data for Rietveld refinement of 3 and 5

Compound	**3 CCDC 741062**	**5 741065**
Space Group	*P*-1	$P2_1/c$
***a* [Å]**	7.099(1)	7.905(1)
***b* [Å]**	7.720(1)	9.911(1)
***c* [Å]**	11.650(1)	12.270(1)
***α* [°]**	80.70(1)	90
***β* [°]**	78.095(1)	99.745(1)
***γ* [°]**	83.411(1)	90
V [Å^3]	614.41(1)	947.54(1)
Rwp	5.127	6.883

3 - Melamine-EDTA CCDC 741062 Rietveld Plot – Rwp = 5.127%



5 - Melaminium Dinitrate CCDC 741065 Rietveld Plot – Rwp = 6.883%