Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Co-crystals and molecular salts of pyridine complexes: Can calculated pK_a's predict proton transfer? A case study of 9 complexes

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SI1: Complete citation for reference 5:

Srinivasulu Aitipamula, Rahul Banerjee, Arvind K. Bansal, Kumar Biradha, Miranda L. Cheney, Angshuman Roy Choudhury, Gautam R. Desiraju, Amol G. Dikundwar, Ritesh Dubey, Nagakiran Duggirala, Preetam P. Ghogale, Soumyajit Ghosh, Pramod Kumar Goswami, N. Rajesh Goud, Ram R. K. R. Jetti, Piotr Karpinski, Poonam Kaushik, Dinesh Kumar, Vineet Kumar, Brian Moulton, Arijit Mukherjee, Gargi Mukherjee, Allan S. Myerson, Vibha Puri, Arunachalam Ramanan, T. Rajamannar, C. Malla Reddy, Nair Rodriguez-Hornedo, Robin D. Rogers, T. N. Guru Row, Palash Sanphui, Ning Shan, Ganesh Shete, Amit Singh, Changquan C. Sun, Jennifer A. Swift, Ram Thaimattam, Tejender S. Thakur, Rajesh Kumar Thaper, Sajesh P. Thomas, Srinu Tothadi, Venu R. Vangala, Narayan Variankaval, Peddy Vishweshwar, David R. Weyna, and Michael J. Zaworotko, Cryst. Growth Des., 2012, 12, 2147-2152.

SI2. Powder X-ray diffraction patterns for all complexes 1-9

Powder X-ray diffraction data were collected at 293 K on a Bruker D2 Phaser diffractometer which employed a sealed tube Cu X-ray source (λ = 1.5406 Å), operating at 30 kV and 10 mA, and LynxEye PSD detector in Bragg-Brentano geometry. Powder X-ray diffraction confirmed that the single crystal structures of all compounds were representative of the bulk material. The peak positions are shifted owing to the different temperatures at which the measured sample was carried out compared with the calculated pattern. The peak intensities vary, perhaps due to microcrystalline orientation and/or texture effects.

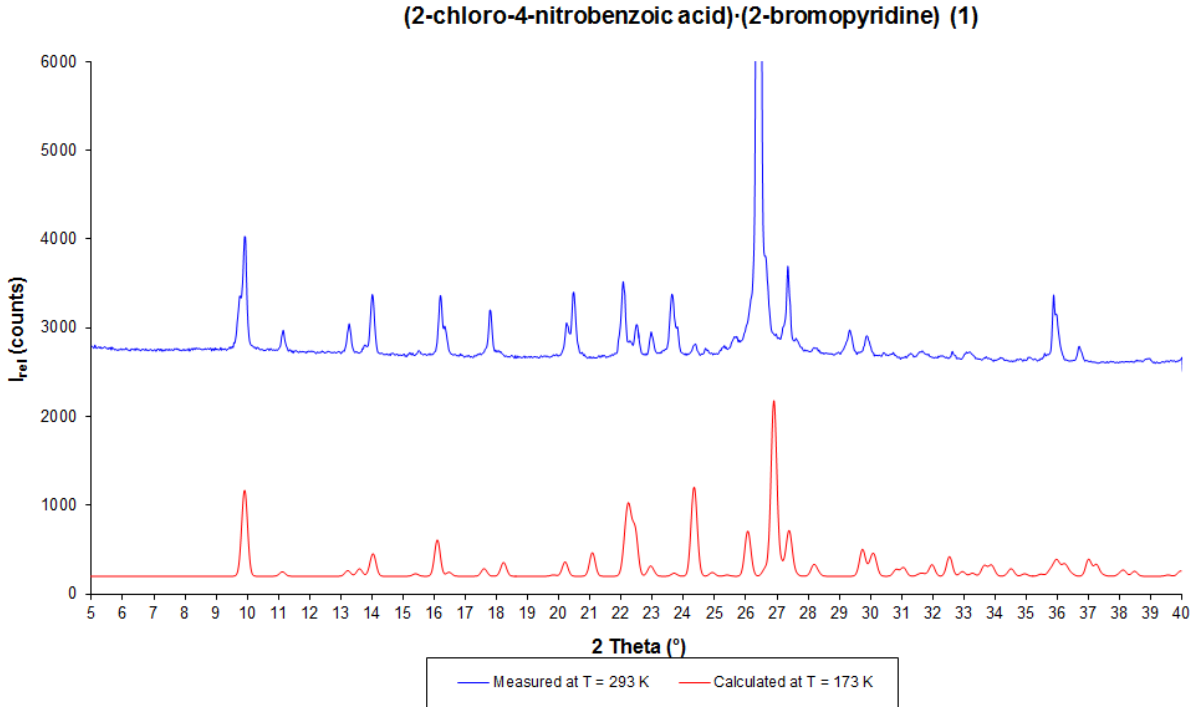

Figure S1: Measured PXRD of (**1**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

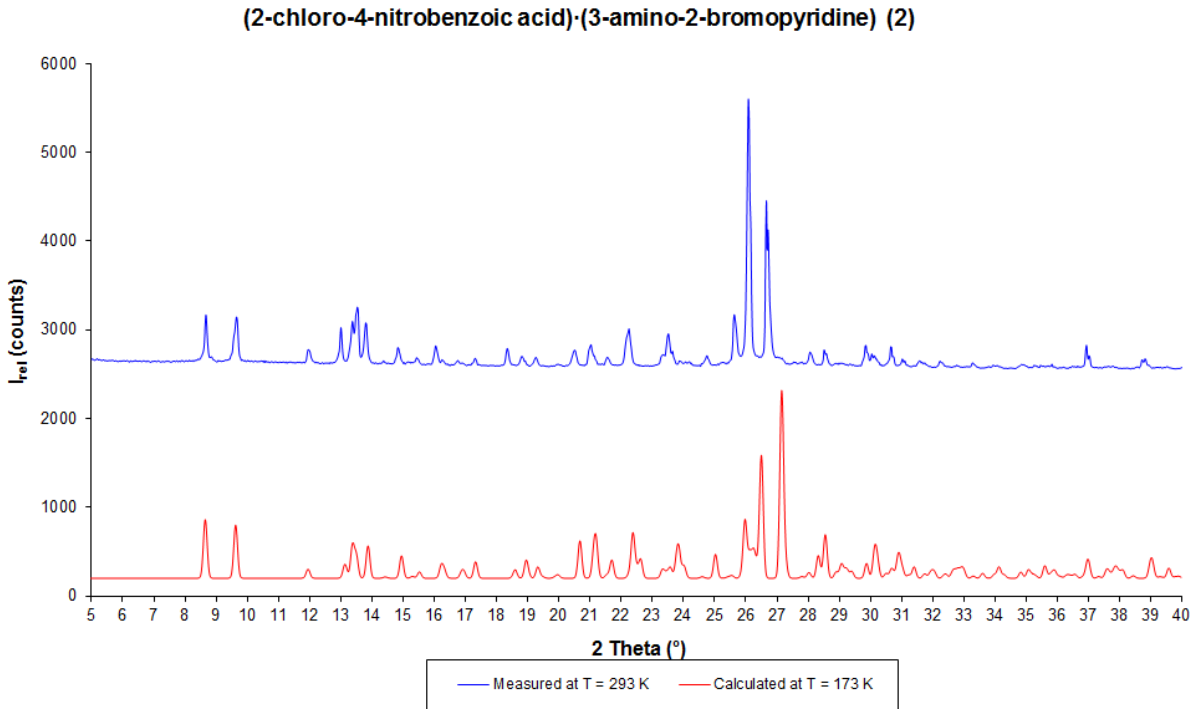

Figure S2: Measured PXRD of (**2**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

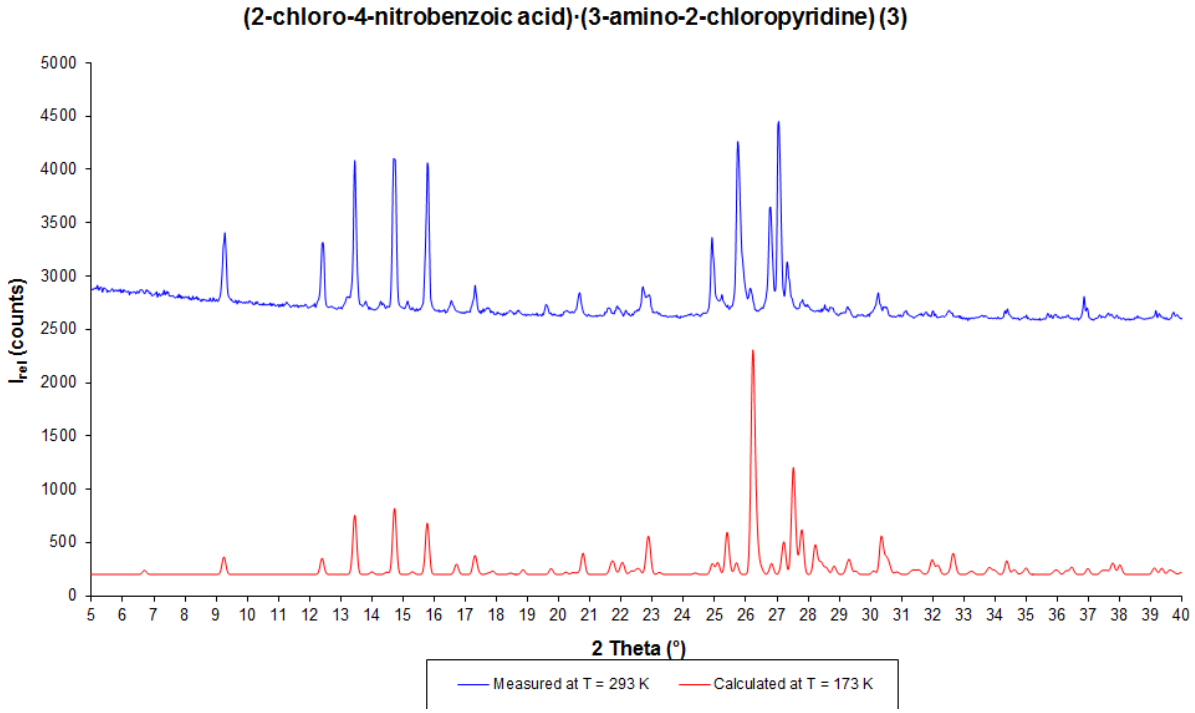

Figure S3: Measured PXRD of (**3**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

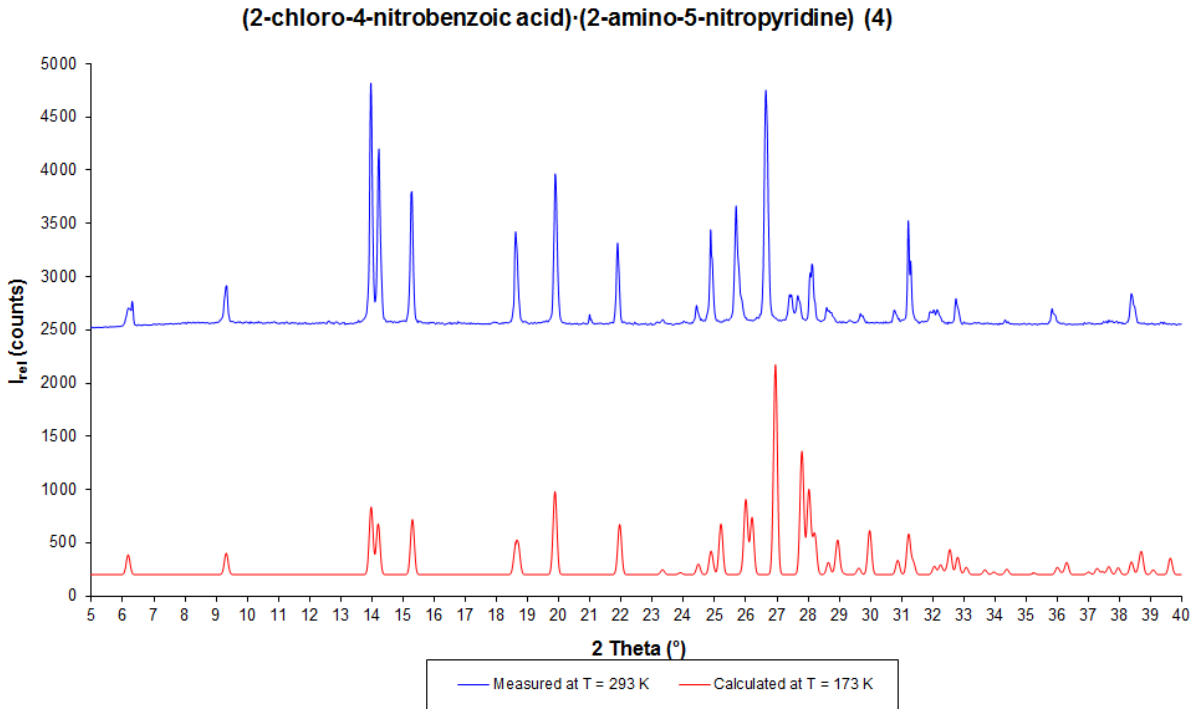

Figure S4: Measured PXRD of (**4**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

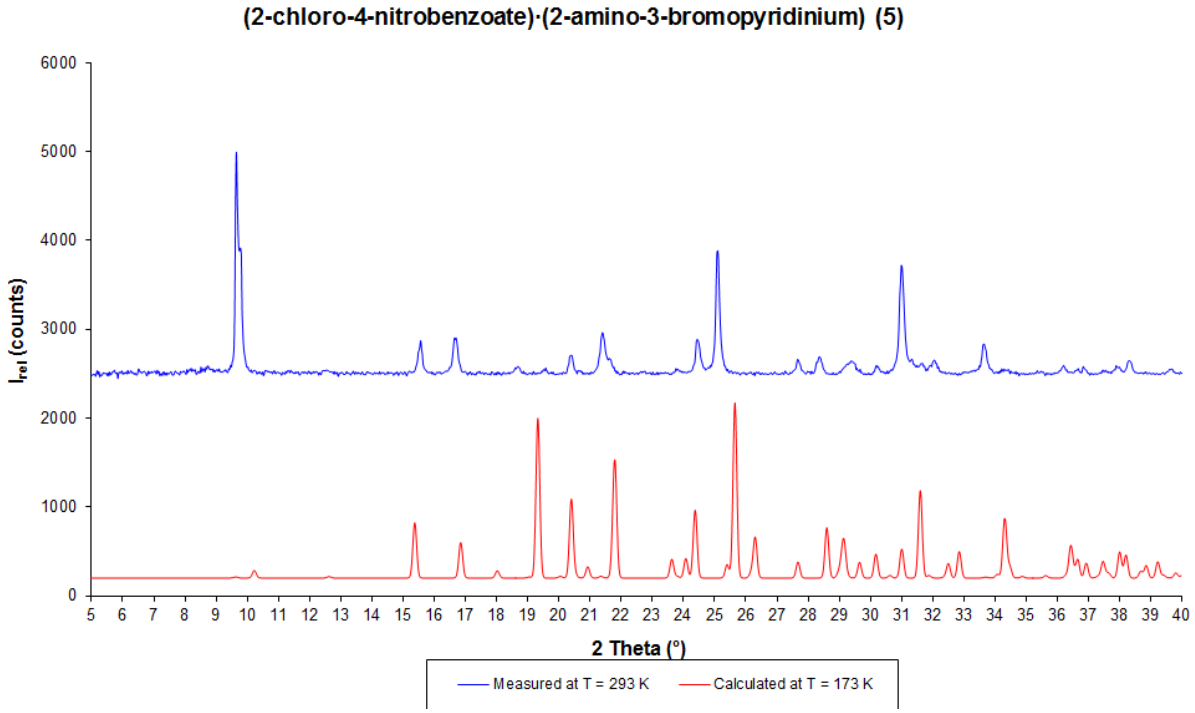

Figure S5: Measured PXRD of (**5**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

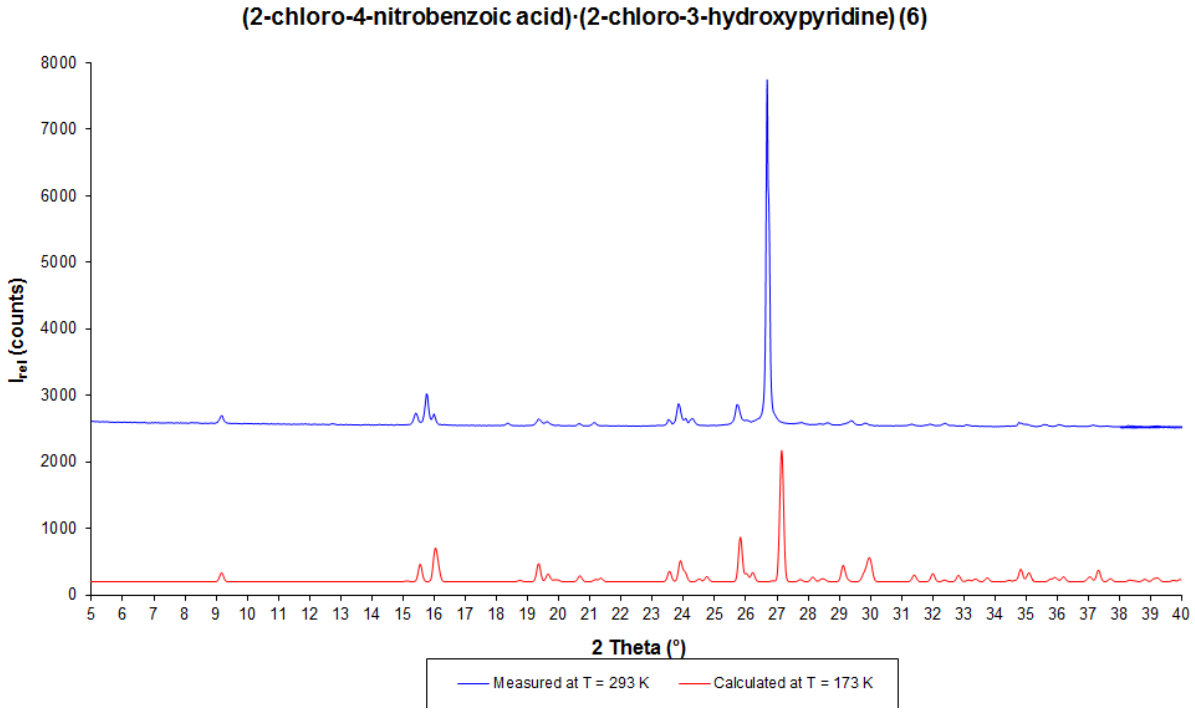

Figure S6: Measured PXRD of (**6**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

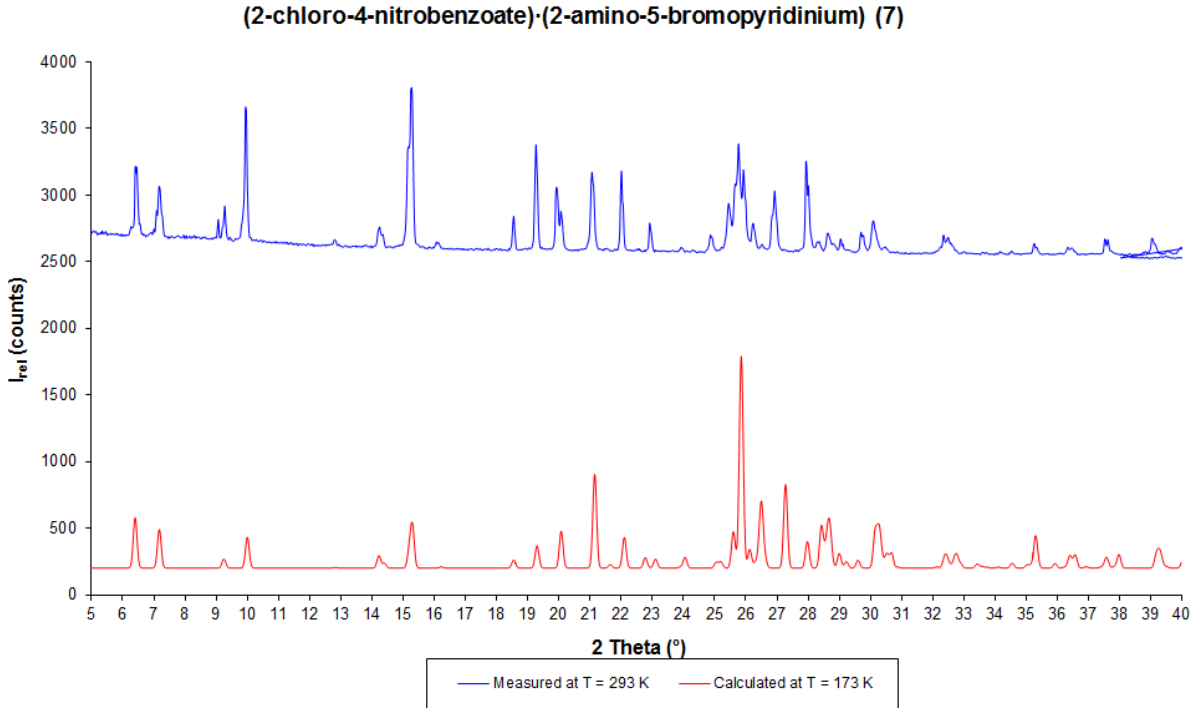

Figure S7: Measured PXRD of (**7**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

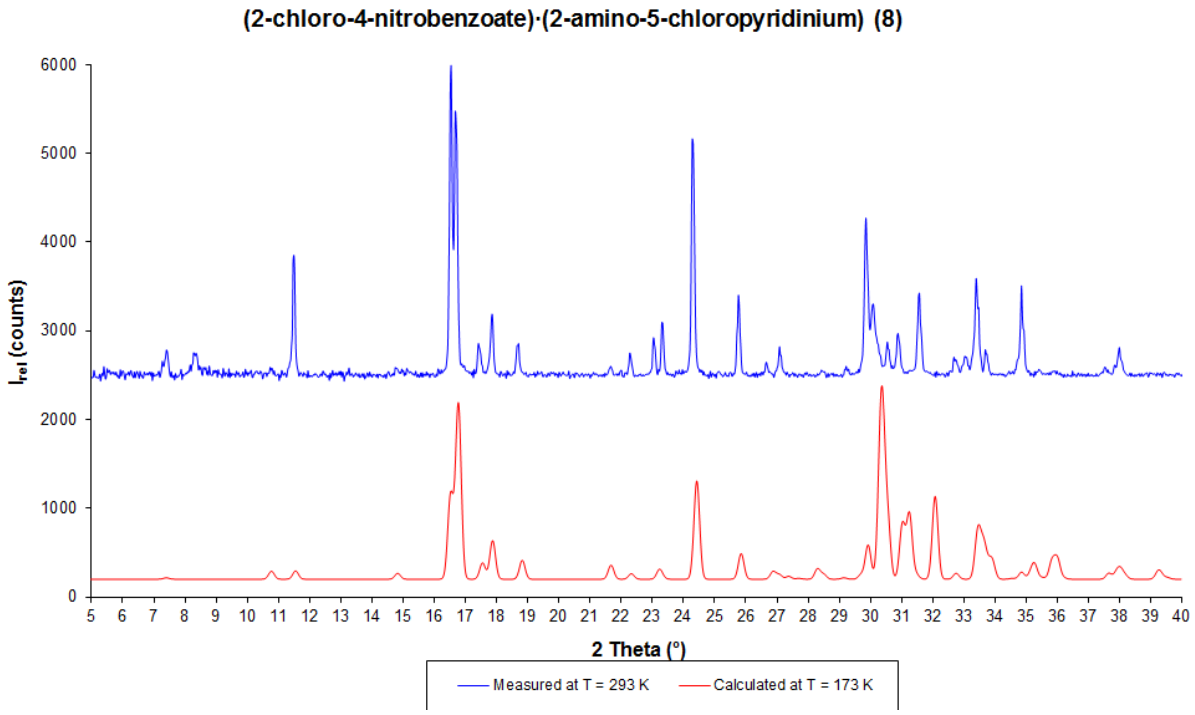

Figure S8: Measured PXRD of (**8**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

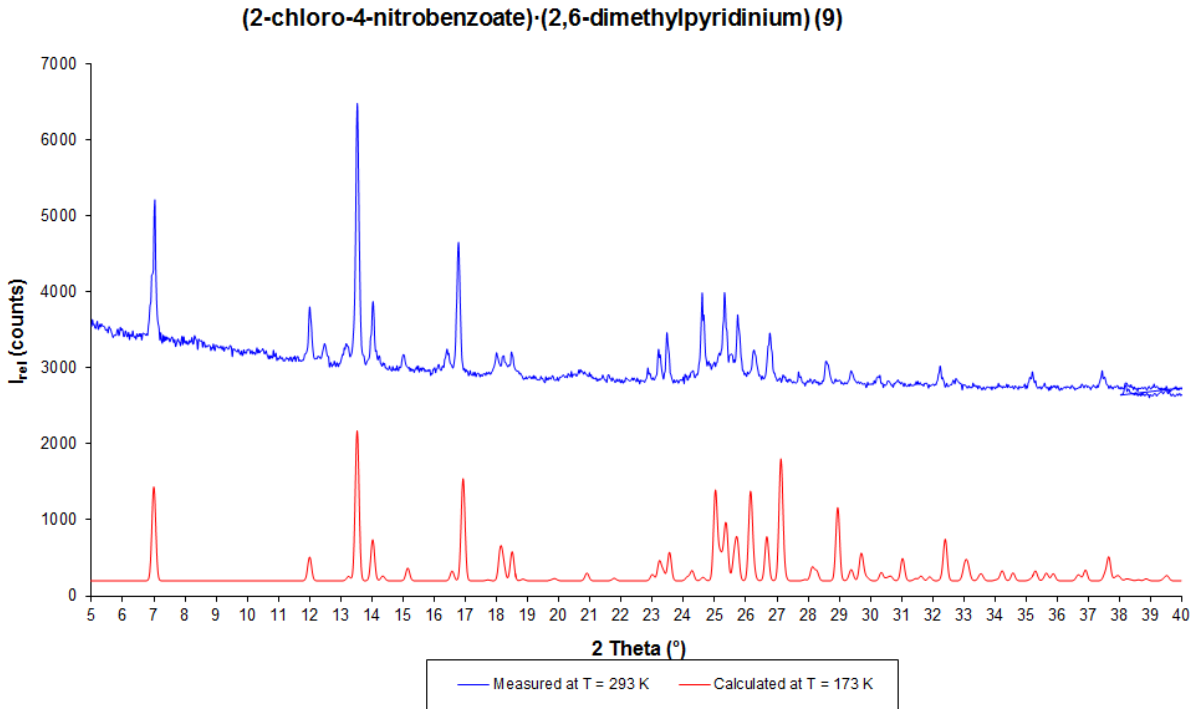

Figure S9: Measured PXRD of (**9**) compared to calculated PXRD of single crystal structure determination. The experimental pattern was measured at room temperature and the calculated pattern at 173 K.

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SI3. Crystallographic Data for all Compounds

Intensity data for all compounds were determined on a Bruker Venture D8 Photon CMOS diffractometer with graphite-monochromated MoKα_1 (λ = 0.71073 Å) radiation at 173 K using an Oxford Cryostream 600 cooler. Data reduction was carried out using the program *SAINT*+, version 6.02[1] and empirical absorption corrections for **1** and **4** were made using the program *SADABS*.[2] All other compounds had face-indexed[1] absorption corrections. Space group assignments were made using *XPREP*[1] on all compounds.

In all cases, the structures were solved in the *WinGX*[13] Suite of programs, using direct methods for all compounds using *SHELXS-97*[14] and refined using full-matrix least-squares/difference Fourier techniques on F^2 using *SHELXL-97*.[14] All non-hydrogen atoms were refined anisotropically. Thereafter, all hydrogen atoms attached to N and O atoms were located in the difference fourier map for all compounds structure, and their coordinates refined freely with isotropic parameters 1.5 times those of their parent atoms. All C-H hydrogen atoms were placed at idealized positions and refined as riding atoms with isotropic parameters 1.2 times those of their parent atoms.

Diagrams and publication material were generated using *ORTEP-3*,[16] *PLATON*,[17] *DIAMOND*.[18] Experimental details of the X-Ray analyses are provided in Tables S1-S9 below.

1 Bruker, SAINT+, Version 6.02 (Includes XPREP and SADABS), Bruker AXS Inc., Madison, Wisconsin, USA, 2004.
2 G. M. Sheldrick, Sadabs, Universität Göttingen, Germany, 2004.
3 L. J. Farrugia, *J. Appl. Crystallogr*., 1999, **32**, 837–838.
4 G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr*., 2008, **64**, 112–122..
6 L. J. Farrugia, *J. Appl. Crystallogr*., 1997, **30**, 565.
7 A. L. Spek, *J. Appl. Crystallogr*., 2003, **36**, 7–13.
8 K. Brandenburg, Diamond, Version 2.1e, Crystal Impact GbR, Bonn, Germany, 1996–2001.

Table S1. Crystal data and structure refinement for **1**. CCDC-1034733

Identification code	11a_sg24_p	
Empirical formula	C12 H8 Br Cl N2 O4	
Formula weight	359.56	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2583(7) Å	α= 88.094(5)°.
	b = 9.0938(7) Å	β= 77.372(5)°.
	c = 9.1385(7) Å	γ = 80.171(5)°.
Volume	659.86(9) $Å^3$	
Z	2	
Density (calculated)	1.810 Mg/m^3	
Absorption coefficient	3.331 mm^{-1}	
F(000)	356	
Crystal size	0.53 x 0.29 x 0.12 mm^3	
Theta range for data collection	2.27 to 27.99°.	
Index ranges	-10<=h<=10, -12<=k<=11, -12<=l<=11	
Reflections collected	8835	
Independent reflections	3168 [R(int) = 0.0675]	
Completeness to theta = 27.99°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6867 and 0.2703	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3168 / 0 / 185	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.1446	
R indices (all data)	R1 = 0.0727, wR2 = 0.1579	
Largest diff. peak and hole	1.282 and -0.590 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for **2**. CCDC-1034735

Identification code	11a_ks_f3_a	
Empirical formula	C12 H9 Br Cl N3 O4	
Formula weight	374.58	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8994(3) Å	α= 110.222(2)°.
	b = 11.9370(4) Å	β= 96.641(2)°.
	c = 13.4905(6) Å	γ = 107.0590(10)°.
Volume	1387.59(9) $Å^3$	
Z	4	
Density (calculated)	1.793 Mg/m^3	
Absorption coefficient	3.174 mm^{-1}	
F(000)	744	
Crystal size	0.676 x 0.383 x 0.122 mm^3	
Theta range for data collection	1.66 to 28.00°.	
Index ranges	-8<=h<=13, -15<=k<=12, -17<=l<=17	
Reflections collected	25750	
Independent reflections	6697 [R(int) = 0.0839]	
Completeness to theta = 28.00°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.7011 and 0.2945	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6697 / 0 / 403	
Goodness-of-fit on F^2	0.993	
Final R indices [I>2sigma(I)]	R1 = 0.0385, wR2 = 0.1038	
R indices (all data)	R1 = 0.0513, wR2 = 0.1081	
Largest diff. peak and hole	1.009 and -0.881 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for **3**. CCDC-1034737

Identification code	11a_sg3_a	
Empirical formula	C12 H9 Cl2 N3 O4	
Formula weight	330.12	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.0984(2) Å	α= 90°.
	b = 24.0534(7) Å	β= 93.424(2)°.
	c = 15.7748(5) Å	γ = 90°.
Volume	2688.59(14) $Å^3$	
Z	8	
Density (calculated)	1.631 Mg/m^3	
Absorption coefficient	0.502 mm^{-1}	
F(000)	1344	
Crystal size	0.761 x 0.096 x 0.076 mm^3	
Theta range for data collection	1.55 to 28.00°.	
Index ranges	-9<=h<=9, -31<=k<=31, -20<=l<=20	
Reflections collected	44874	
Independent reflections	6484 [R(int) = 0.0902]	
Completeness to theta = 28.00°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9791 and 0.8326	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6484 / 0 / 403	
Goodness-of-fit on F^2	0.985	
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0818	
R indices (all data)	R1 = 0.0516, wR2 = 0.0873	
Largest diff. peak and hole	0.326 and -0.290 $e.Å^{-3}$	

Table S14. Crystal data and structure refinement for **4**. CCDC-1034739

Identification code	12a_ks_g2_p	
Empirical formula	C12 H9 Cl N4 O6	
Formula weight	340.68	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 3.7370(3) Å	α= 90°.
	b = 12.6714(11) Å	β= 94.984(2)°.
	c = 14.3717(13) Å	γ = 90°.
Volume	677.97(10) $Å^3$	
Z	2	
Density (calculated)	1.669 Mg/m^3	
Absorption coefficient	0.323 mm^{-1}	
F(000)	348	
Crystal size	0.47 x 0.34 x 0.08 mm^3	
Theta range for data collection	1.42 to 28.00°.	
Index ranges	-4<=h<=4, -16<=k<=16, -18<=l<=18	
Reflections collected	5599	
Independent reflections	3133 [R(int) = 0.0628]	
Completeness to theta = 28.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9746 and 0.8630	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3133 / 1 / 217	
Goodness-of-fit on F^2	1.176	
Final R indices [I>2sigma(I)]	R1 = 0.1033, wR2 = 0.2886	
R indices (all data)	R1 = 0.1057, wR2 = 0.2908	
Absolute structure parameter	0.29(17)	
Largest diff. peak and hole	1.762 and -0.633 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for **5**. CCDC-1034741

Identification code	11a_mj6_a	
Empirical formula	C12 H9 Br Cl N3 O4	
Formula weight	374.58	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.4350(2) Å	α= 98.577(2)°.
	b = 10.3354(3) Å	β= 105.0740(10)°.
	c = 11.2546(4) Å	γ = 98.022(2)°.
Volume	702.11(4) $Å^3$	
Z	2	
Density (calculated)	1.772 Mg/m^3	
Absorption coefficient	3.136 mm^{-1}	
F(000)	372	
Crystal size	0.41 x 0.31 x 0.11 mm^3	
Theta range for data collection	1.91 to 28.00°.	
Index ranges	-8<=h<=8, -13<=k<=13, -14<=l<=13	
Reflections collected	16110	
Independent reflections	3389 [R(int) = 0.0544]	
Completeness to theta = 28.00°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.7242 and 0.3596	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3389 / 0 / 202	
Goodness-of-fit on F^2	0.986	
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0709	
R indices (all data)	R1 = 0.0333, wR2 = 0.0729	
Largest diff. peak and hole	0.766 and -0.637 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement for **6**. CCDC1034743

Identification code	11a_sg2_a	
Empirical formula	C12 H8 Cl2 N2 O5	
Formula weight	331.10	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.1583(2) Å	α= 83.332(2)°.
	b = 9.9176(2) Å	β= 76.2620(10)°.
	c = 11.1477(3) Å	γ = 77.0530(10)°.
Volume	643.14(3) $Å^3$	
Z	2	
Density (calculated)	1.710 Mg/m^3	
Absorption coefficient	0.529 mm^{-1}	
F(000)	336	
Crystal size	0.35 x 0.211 x 0.197 mm^3	
Theta range for data collection	1.88 to 28.00°.	
Index ranges	-7<=h<=8, -13<=k<=13, -14<=l<=14	
Reflections collected	8899	
Independent reflections	3089 [R(int) = 0.0358]	
Completeness to theta = 28.00°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.9399 and 0.8896	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3089 / 0 / 198	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0281, wR2 = 0.0723	
R indices (all data)	R1 = 0.0389, wR2 = 0.0783	
Largest diff. peak and hole	0.346 and -0.194 $e.Å^{-3}$	

Table S7. Crystal data and structure refinement for **7**. CCDC-1034745

Identification code	11a_ks_f2_a	
Empirical formula	C12 H9 Br Cl N3 O4	
Formula weight	374.58	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 3.9305(2) Å	α= 94.312(2)°.
	b = 12.4261(6) Å	β= 91.431(2)°.
	c = 13.8457(7) Å	γ = 96.374(2)°.
Volume	669.77(6) $Å^3$	
Z	2	
Density (calculated)	1.857 Mg/m^3	
Absorption coefficient	3.288 mm^{-1}	
F(000)	372	
Crystal size	0.61 x 0.14 x 0.09 mm^3	
Theta range for data collection	1.48 to 28.00°.	
Index ranges	-4<=h<=5, -16<=k<=16, -13<=l<=18	
Reflections collected	9646	
Independent reflections	3229 [R(int) = 0.0613]	
Completeness to theta = 28.00°	99.8 %	
Absorption correction	Integration	
Max. and min. transmission	0.7652 and 0.2386	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3229 / 0 / 202	
Goodness-of-fit on F^2	0.907	
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0661	
R indices (all data)	R1 = 0.0375, wR2 = 0.0689	
Largest diff. peak and hole	0.598 and -0.522 $e.Å^{-3}$	

Table S8. Crystal data and structure refinement for **8**. CCDC-1034747

Identification code	11a_ks_f5_a	
Empirical formula	C12 H9 Cl2 N3 O4	
Formula weight	330.12	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 3.8601(2) Å	α= 93.742(2)°.
	b = 12.3629(6) Å	β= 91.893(2)°.
	c = 13.9025(7) Å	γ = 96.066(2)°.
Volume	657.80(6) $Å^3$	
Z	2	
Density (calculated)	1.667 Mg/m^3	
Absorption coefficient	0.513 mm^{-1}	
F(000)	336	
Crystal size	0.802 x 0.053 x 0.032 mm^3	
Theta range for data collection	1.47 to 28.00°.	
Index ranges	-4<=h<=5, -16<=k<=16, -15<=l<=18	
Reflections collected	7798	
Independent reflections	3158 [R(int) = 0.1084]	
Completeness to theta = 28.00°	99.7 %	
Absorption correction	Integration	
Max. and min. transmission	0.9864 and 0.8542	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3158 / 0 / 202	
Goodness-of-fit on F^2	0.920	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.0896	
R indices (all data)	R1 = 0.0642, wR2 = 0.0978	
Largest diff. peak and hole	0.373 and -0.306 $e.Å^{-3}$	

Table S9. Crystal data and structure refinement for **9**. CCDC-1034749

Identification code	11a_sg5_a	
Empirical formula	C14 H13 Cl N2 O4	
Formula weight	308.71	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 15.5907(12) Å	α= 90°.
	b = 25.242(2) Å	β= 100.654(5)°.
	c = 7.1987(6) Å	γ = 90°.
Volume	2784.1(4) $Å^3$	
Z	8	
Density (calculated)	1.473 Mg/m^3	
Absorption coefficient	0.292 mm^{-1}	
F(000)	1280	
Crystal size	0.403 x 0.258 x 0.124 mm^3	
Theta range for data collection	1.55 to 27.99°.	
Index ranges	-20<=h<=16, -33<=k<=30, -6<=l<=9	
Reflections collected	8530	
Independent reflections	3366 [R(int) = 0.0317]	
Completeness to theta = 27.99°	99.9 %	
Absorption correction	Integration	
Max. and min. transmission	0.9794 and 0.9157	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3366 / 0 / 196	
Goodness-of-fit on F^2	0.982	
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0933	
R indices (all data)	R1 = 0.0591, wR2 = 0.1016	
Largest diff. peak and hole	0.418 and -0.292 $e.Å^{-3}$	

SI5. Hydrogen Bonding Details for all Compounds

Table S10. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(2)	0.95(5)	1.74(5)	2.686(4)	176(4)

Table S11. Hydrogen bonds and short contacts for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...N(3)	0.68(5)	2.06(5)	2.706(3)	159(5)
O(5)-H(5)...N(5)	0.67(4)	2.00(4)	2.664(3)	174(5)
N(4)-H(4A)...Br(2)#1	0.81(3)	2.81(3)	3.221(2)	113(3)
N(4)-H(4B)...O(3)#2	0.90(3)	2.30(3)	3.139(3)	156(3)
N(6)-H(6A)...Br(2)	0.91(5)	2.61(4)	3.089(3)	113(3)
N(6)-H(6B)...O(7)#3	0.79(5)	2.69(5)	3.370(4)	144(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x+1,y,z+1 #3 x-1,y,z-1

Table S12. Hydrogen bonds and short contacts for **3**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(2)...N(3)	0.95(3)	1.74(3)	2.6902(18)	176(2)
C(19)-H(19)...O(2)	0.95	2.73	3.342(2)	123
O(5)-H(5)...N(5)	0.90(2)	1.77(2)	2.6744(17)	175(2)
C(24)-H(24)...O(6)	0.95	2.69	3.342(2)	127
N(4)-H(4A)...O(7)	0.82(2)	2.48(2)	3.270(2)	162(2)
N(4)-H(4A)...Cl(3)	0.82(2)	2.59(2)	2.9826(18)	111(2)
N(4)-H(4B)...O(4)#1	0.88(3)	2.30(3)	3.157(2)	164(2)
N(4)-H(4B)...O(3)#1	0.88(3)	2.63(3)	3.391(2)	144(2)
N(6)-H(6A)...Cl(4)	0.86(2)	2.54(2)	2.9755(18)	113(2)
N(6)-H(6A)...Cl(3)#1	0.86(2)	2.62(2)	3.2196(17)	128(2)
N(6)-H(6B)...O(8)#1	0.82(2)	2.37(2)	3.161(2)	162(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1

Table S13. Hydrogen bonds for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(2)	0.84	1.80	2.605(7)	161
N(3)-H(3A)...O(2)	0.74(11)	2.41(11)	3.127(9)	164(11)
N(3)-H(3B)...O(5)#1	0.82(11)	2.58(11)	3.307(10)	149(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y+1/2,-z+2

Table **S14**. Hydrogen bonds for **5**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(2)	0.82(3)	1.93(3)	2.754(2)	175(3)
N(3)-H(3A)...O(1)	0.84(3)	1.92(3)	2.757(2)	175(2)
N(3)-H(3B)...O(1)#1	0.87(3)	2.05(3)	2.846(2)	151(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S15. Hydrogen bonds for **6**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(3)#1	0.77(2)	2.27(2)	2.9415(15)	146(2)
O(5)-H(5)...O(4)#1	0.77(2)	2.59(2)	3.3074(16)	154(2)
O(1)-H(1)...N(2)	0.82(2)	1.86(2)	2.6846(14)	175(2)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y+1,z-1

Table S16. Hydrogen bonds for **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)	0.92(3)	1.71(3)	2.620(2)	168(2)
N(3)-H(3A)...O(2)	0.83(3)	2.07(3)	2.897(3)	174(3)
N(3)-H(3B)...O(2)#1	0.82(3)	2.07(3)	2.854(2)	158(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S17. Hydrogen bonds for **8**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)	1.06(3)	1.53(2)	2.5817(19)	169(2)
N(3)-H(3A)...O(2)	0.92(2)	1.99(2)	2.910(2)	174(2)
N(3)-H(3B)...O(2)#1	0.80(2)	2.09(2)	2.856(2)	158(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S18. Hydrogen bonds for **9**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)	0.98(2)	1.61(2)	2.5822(17)	173(2)

SI4. ORTEP Diagrams Co-crystals 1-4 and 6

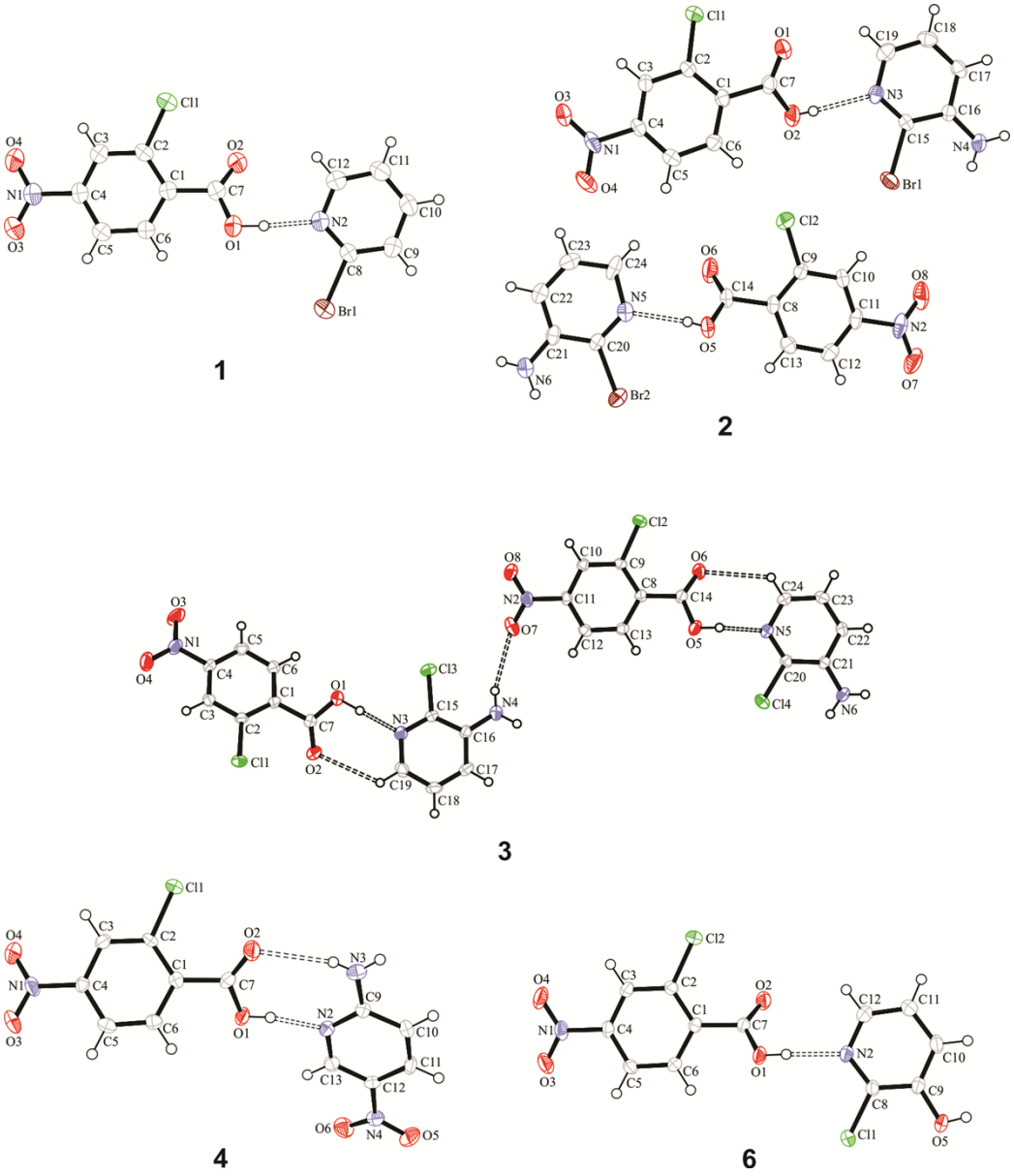

Figure S10: The complete asymmetric units of the co-crystals. Displacement ellipsoids are shown at the 50% probability level.

SI5. ORTEP Diagrams Molecular Salts 5, 7-9

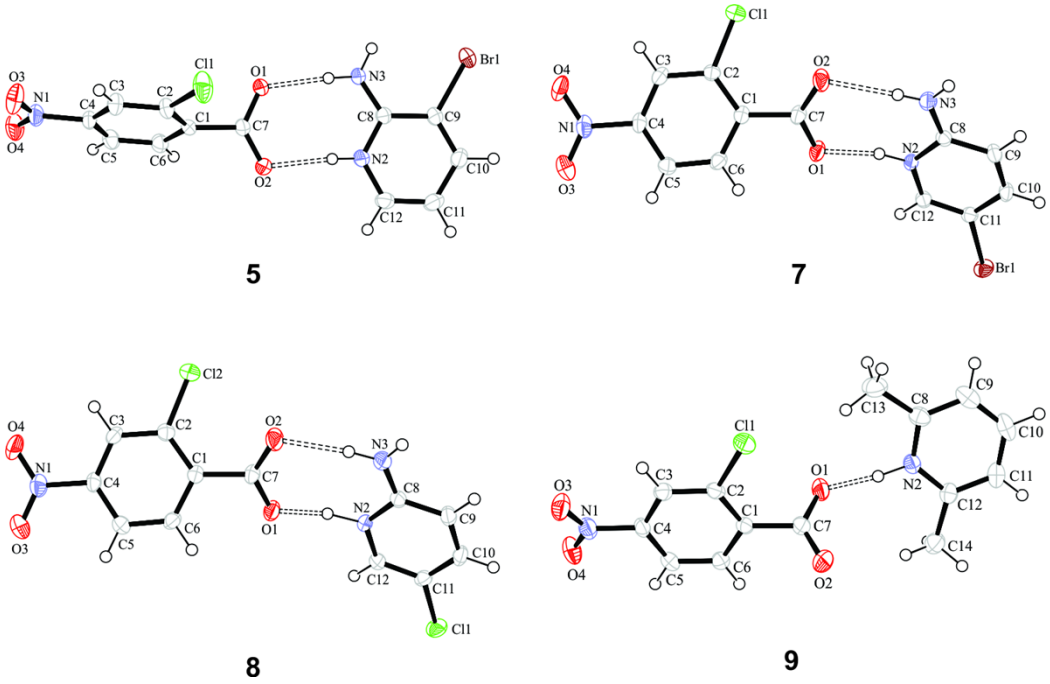

Figure S10: The complete asymmetric units of the co-crystals. Displacement ellipsoids are shown at the 50% probability level.