Supplementary Material (ESI) for CrystEngComm

Supplementary Information for

Structures of Hydro-, Chloro-, and Bromo-substituted Maleimides and 2,6-Diaminopyridines, and of Some of their 1:1 Heterodimers

Tullio Pilati*

ISTM/CNR, c/o Dipartimento di Chimica Fisica ed Elettrochimica, Universita' degli Studi di Milano, via Golgi 19, I-20133, Milano, Italy

Franco Cozzi*

Dipartimento di Chimica Organica e Industriale, Universita' degli Studi di Milano, via Golgi 19, I-20133, Milano, Italy

Contents:

Supplementary Table 1.

Refcodes of structures containing a three parallel H-bonds as shown in Fig 1b (CCDC, version 5.31 updated at august 2010).

BUDWAY10	JICWIB10	QAFSOF	WEWZAA	YONNAQ
EWOBUN	JICWOH10	QOCTUX	WOMGIP	YONQAT
GOXCOL	LULQIS	RADKOX01	WULXUW	YONQEX
HECRIQ	MAWPUW	REGKIX	XAXPIW	ZUKXOS
HIMLUL	MCYTIM10	RUZMOO	XESSAQ	COWSUD
HIMMAS	MINVIP	SEPKON	XIMMOV	QOZFER
HIMMEW	MIWFUU	SEPNEG	XOJVUN	DUJCAN
JICTUK01	MOCNIC	TAZXAU	XUNCUE	
JICVAS10	ODOMIE	VIFKUR	XUNCUE01	
JICVOG20	PANLAS	VIXMOF	YAZRAS	
JICVUM10	POCPED	VIXNAS	YIHCOI	

Supplementary Table 2. Main geometric parameters for HBs and XBs in the monomers. Distances and angles are in Å and °, respectively. Estimated standard deviations of calculated H atoms are omitted, as are those relative to HMa and HPy data, not reported in the original papers.

Monomer	**Contact type**	**Contact A-H···B or A-X···B**	**A···B distance**	**H···B distance**	**A-H···B or A-X···B angle**
HMa	vertical	N1-H3···O2 $_{2-x,-y,-z}$	2.884	2.01	170
	lateral	C4-H2···O1 $_{3/2-x,1/2+y,-1/2-z}$	3.345	2.45	153
	lateral	C2-H1···O1 $_{1-x,-y,1-z}$	3.307	2.53	139
ClMa	vertical	N1-H1···O2 $_{1-x,-y,1-z}$	2.816(2)	1.96	172
	XB	C2-Cl1···O1 $_{-x,-1/2+y,-1/2-z}$	3.078(2)		158.7(6)
	XB	C3-Cl2···O1 $_{x,1+y,z}$	3.148(2)		170.5(7)
BrMa	vertical	N1-H1···O2 $_{-x,-1/2+y,-1/2-z}$	2.869(3)	2.02	169
	XB	C2-Br1···O1 $_{1-x,1/2+y,1/2-z}$	3.202(2)		158.7(7)
	XB	C3-Br2···O1 $_{x,1+y,z}$	3.038(2)		166.7(9)
HPy	vertical	N3-H6···N1 $_{1-x,1/2+y,1/2-z}$	2.982	1.98	170
	vertical	N2-H4···N2 $_{-1/2+X,1/2-Y,-Z}$	3.203	2.22	161
	lateral	N2-H5···N3 $_{3/2+x,1-y,-1/2+z}$	3.066	2.08	166
ClPy	vertical	N2-H2A···N1 $_{1-x,y,-1/2+z}$	3.136(2)	2.25(2)	172(2)
	vertical	N3-H3A···N1 $_{1-x,y,1/2+z}$	3.282(2)	2.45(2)	158(2)
	lateral	N3-H3B···N3 $_{x,-y,1/2+z}$	3.233(2	2.58(2)	136(2)
	lateral	N2-H2B···Cl1 $_{1/2-x,1/2-y,-1/2+z}$	3.491(2)	2.68(2)	159(2)
	XB	C4-Cl2···Cl2 $_{x,-y,1/2+z}$	3.4562(4)		83.4(3)
BrPy	vertical	N2-H2A···N1 $_{1-x,1-y,1-z}$	3.182(3),	2.35(2)	167(2)
	lateral	N2-H2B···Br1 $_{3/2-x,1/2-y,-1/2+z}$	3.765(2)	3.03(2)	147(2)
	XB	C2-Br2···N1 $_{3/2-x,1/2-y,-1/2+z}$	3.320(2)		156.9(7)

Supplementary Table 3.

The HBs in the **HMa/HPy** structure

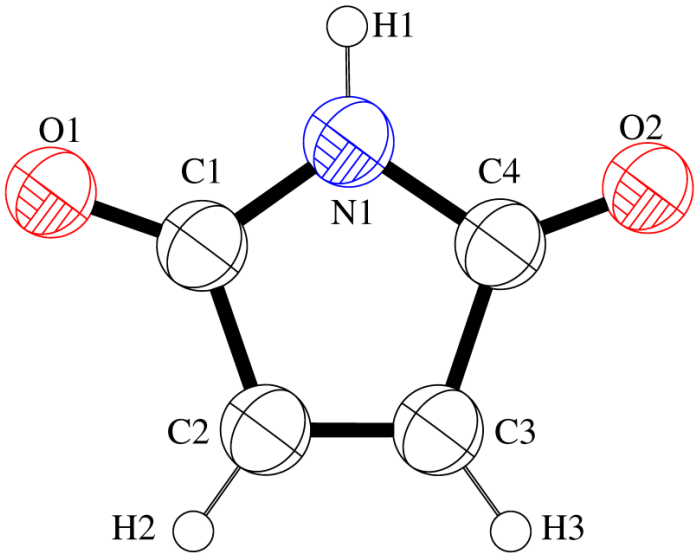
A-H•••B	d(A•••B) Å	d(H•••B) Å	Angle(A-H•••B) °
N4-H1N4•••N1	2.8346(17)	1.927(18)	179.43(17)
N2-H1N2•••O2	3.203(2)	2.31(2)	162.26(17)
N3-H1N3•••O1	3.124(2)	2.18(2)	170.08(17)
N8-H1N8•••N5	2.827(2)	1.926(18)	176.75(15)
N7-H1N7•••O4	3.022(2)	2.08(2)	177.66(18)
N6-H1N6•••O3	3.247(2)	2.31(2)	171.14(19)
N2-H2N2•••O4 $_{x,1/2-y,-1/2+z}$	3.071(2)	2.21(2)	170.84(17)
N3-H2N3•••O3 $_{-1+x,1/2-y,-1/2+z}$	3.121(2)	2.31(2)	164.97(17)
C7-H7•••O1 $_{-x,1-y,2-z}$	3.429(2)	2.499(18)	165.99(14)
N7-H2N7•••O2	2.970(2)	2.12(2)	162.76(18)
N6-H2N6•••N3 $_{1+x,y,z}$	3.447(2)	2.69(2)	147.98(17)
C11-H11•••O1 $_{1+x,y,z}$	3.446(2)	2.56(2)	160.13(16)

Supplementary Table 4. Main geometric parameters for halogenated heterodimers. MC_d is the centroid of a dimer calculated considering all its atoms and P_d is the relative mean least-squares molecular plane. Distances and angles are in in Å and °, respectively.

	ClMa/HPy	**BrMa/HPy**	**HMa/ClPy**	**ClMa/ClPy**	**BrMa/ClPy**
Vertical	H1•••N4	H1•••N4	H4•••N1	H4•••N1	H4•••N1
N•••N	2.779(3)	2.773(4)	2.844(3)	2.810(2)	2.796(2)
H•••N	1.87(3)	1.97(4)	2.06(4)	1.99(2)	1.90(3)
N-H•••N	177(2)	175(4)	175(4)	179(2)	179(2)
Vertical	H2A•••O1	H2A•••O1	H2A•••O1	H2A•••O1	H2A•••O1
N•••O	3.081(3)	3.084(4)	3.136(3)	3.107(2)	3.075(2)
H•••O	2.25(3)	2.19(5)	2.34(3)	2.29(2)	2.25(2)
N-H•••O	177(2)	176(4)	174(3)	175(2)	173(2)
Vertical	H3A•••O2	H3A•••O2	H3A•••O2	H3A•••O2	H3A•••O2
N•••O	3.093(3)	3.047(4)	3.132(3)	3.139(2)	3.147(2)
H•••O	2.28(3)	2.20(5)	2.35(4)	2.39(2)	2.31(2)
N-H•••O	174(2)	170(4)	166(3)	165(2)	175(2)
Lateral	H2B•••O1^{i}	H2B•••O1^{ii}	H2B•••O1^{iii}	H2B•••O1^{iv}	-
N•••O	2.903(3)	2.903 (4)	2.919(3)	3.210(2)	
H•••O	2.10(3)	2.12(4)	2.15(3)	2.50(2)	
N-H•••O	158(2)	163(4)	149(3)	143(2)	
Lateral	H3B•••O2^{v}	H3B•••O2^{vi}	H3B•••O2^{v}	H3B•••O2^{vii}	H3B•••O2^{iv}
N•••O	2.930(3)	2.847(4)	2.917(3)	3.080(2)	3.180(2)
H•••O	2.16(3)	2.00(4)	2.12(3)	2.25(2)	2.46(2)
N-H•••O	154(2)	155(4)	154(3)	147(2)	145(2)
Lateral				Cl1•••Cl4^{iii}	Cl1•••Brl^{vii}
Cl•••X	-	-	-	3.3470(6)	3.3607(7)
C-Cl•••X				150.57(5)	131.64(7)
Cl•••X-C				129.75(4)	149.34(6)
Lateral				Cl2•••Cl3^{vii}	Cl2•••Br^{iv}
Cl•••X	-	-	-	3.3068(5)	3.3915(6)
C-Cl•••X				156.81(4)	161.68(6)
Cl•••X-C				121.49(5)	115.72(6)
Vertical †			Cl1•••Cl1^{iii}		Cl1•••Cl1^{viii}
Cl•••Cl	-	-	3.395(2)	-	3.3536(9)
C-Cl•••Cl			145.52(9)		162.57(7)
Cl•••Cl-C			145.52(9)		162.57(7)
Vertical †			Cl2•••Cl2^{ix}		Cl2•••Br2^{x}
Cl•••X	-	-	3.335(2)	-	3.5476(7)
C-Cl•••X			149.42(9)		103.39(6)
Cl•••X-C			149.42(9)		158.72(6)
P_d•••P_d‡,	3.330(2)	3.281(2)	3.097(2)	3.218(2)	3.180(2)
			4.277(2)	3.248(2)	3.349(2)
MC_d•••MC_d‡	3.784(2)	3.822(2)	3.558(2)	3.588(2)	3.609(2)
			4.277(2)	4.607(2)	5.460(2)

‡ Calculated on all the atoms; only in the case of **ClMa/HPy** and **BrMa/HPy** the two centroids above and below the central one are equidistant from that. † Joning two parallel tapes of dimers. i =1-x, 1-y, -z; ii =1-x, 1-y, 1-z; iii = -x, 2-y, 2-z; iv = -x, -y, 1-z; v = -x, 1-y, 1-z; vi = -x, 1-y, 2-z; vii =2-x, 1-y, 1-z; viii = 2-x, -y, -z; ix = 2-x, 1-y, 2-z; x = x, -1+y, 1+z.

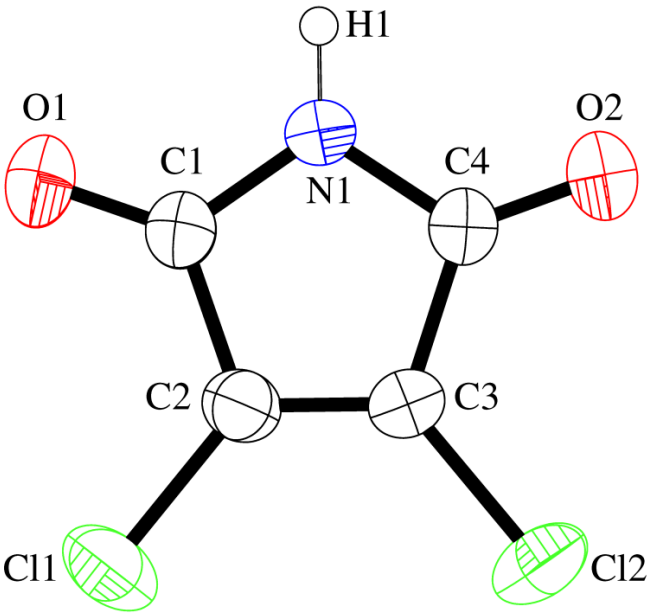
Figure S1.



ORTEP projection of **HMa** (CCDC refcode TEKQAB01) with numbering scheme.

ADPs at 50% level. H atoms not to scale.

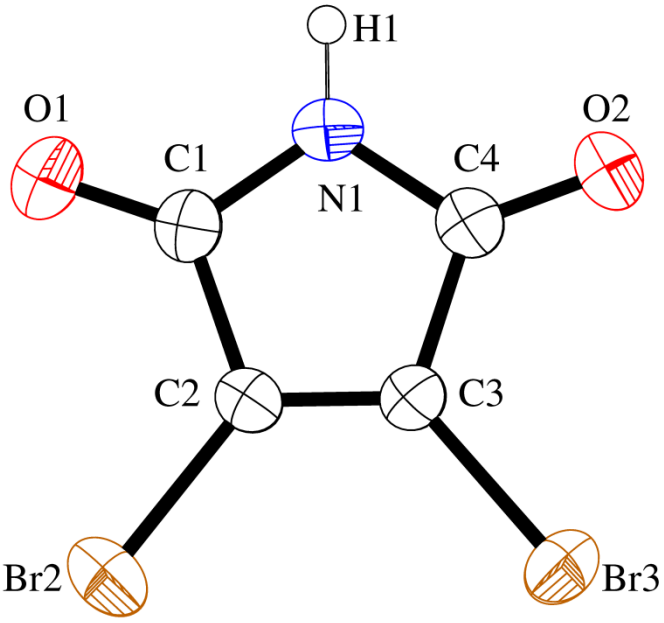
Figure S2.



ORTEP projection of α polymorph of **ClMa** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

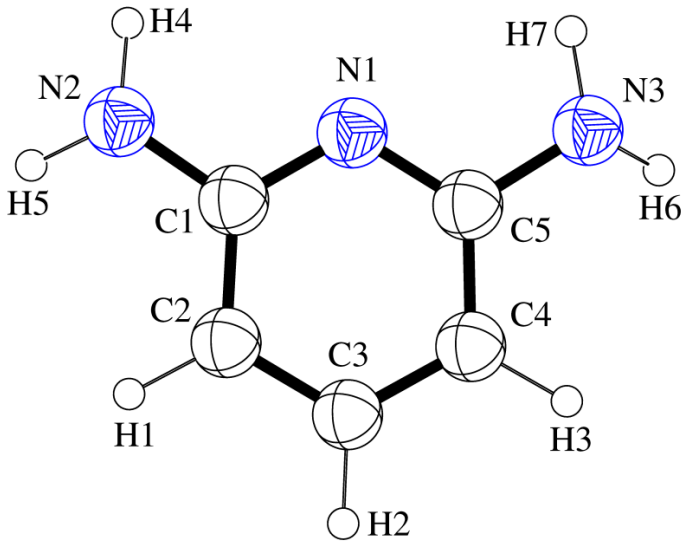
Figure S3.



ORTEP projection of **BrMa** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

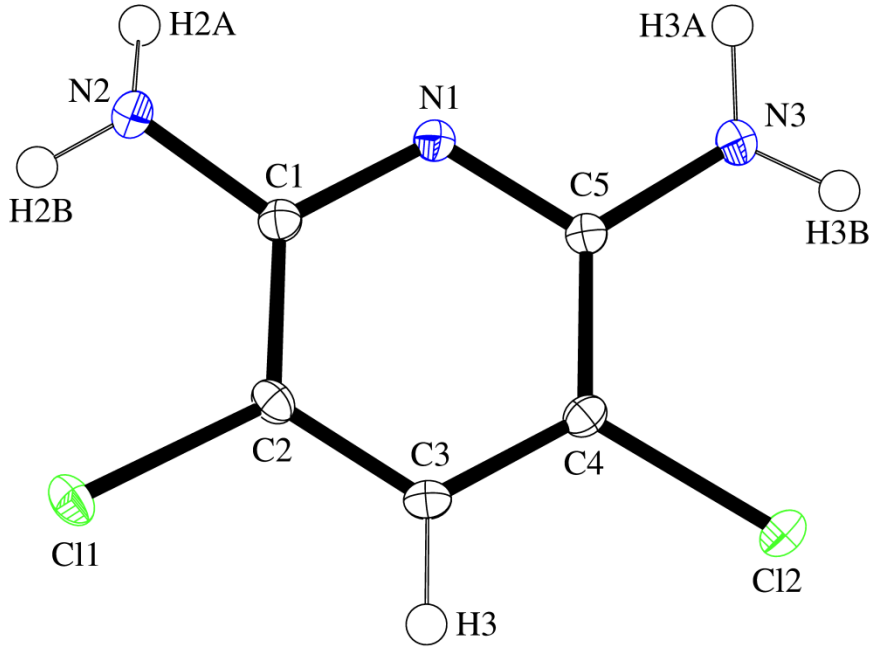
Figure S4.



ORTEP projection of **HPy** (CCDC refcode FOYLEK) with numbering scheme.

ADPs at 50% level. H atoms not to scale

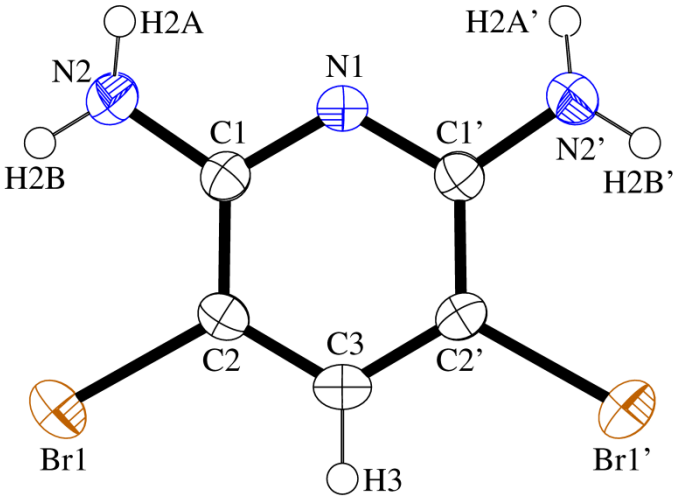
Figure S5.



ORTEP projection of **ClPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

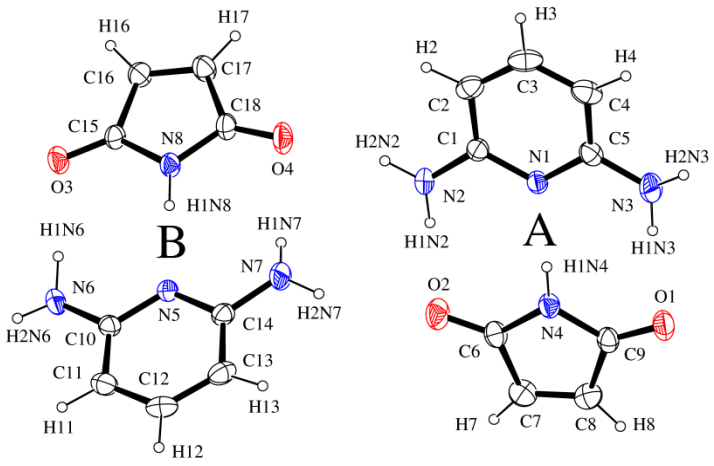
Figure S6.



ORTEP projection of **HPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

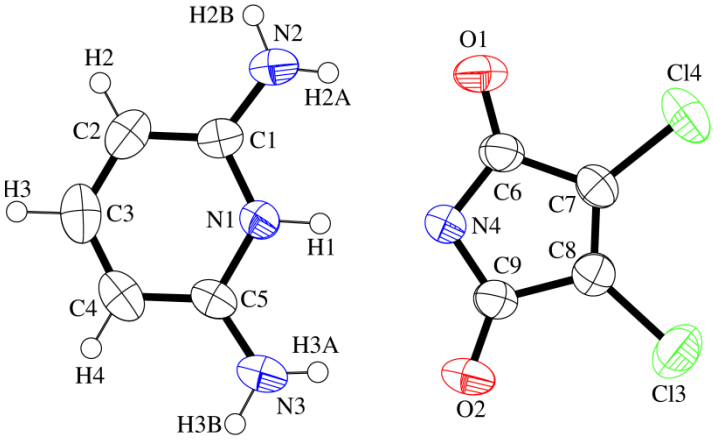
Figure S7.



ORTEP projection of **HMa/HPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale. **A** and **B** indicate the two independent dimers.

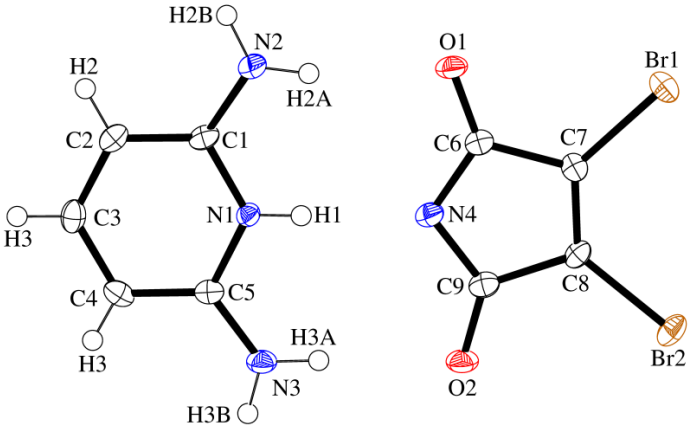
Figure S8.



ORTEP projection of **ClMa/HPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

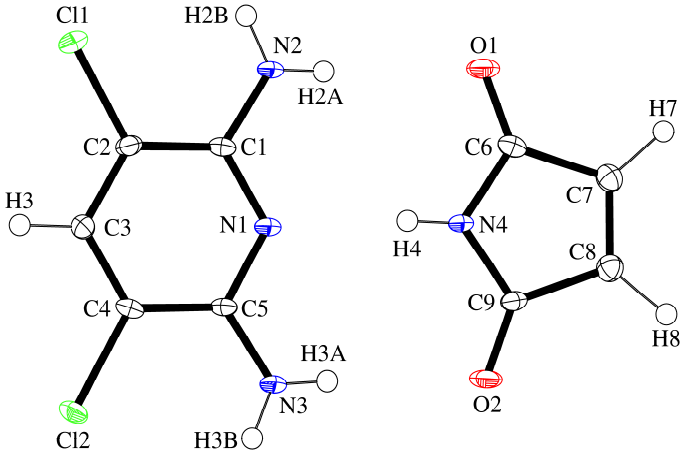
Figure S9.



ORTEP projection of **BrMa/HPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

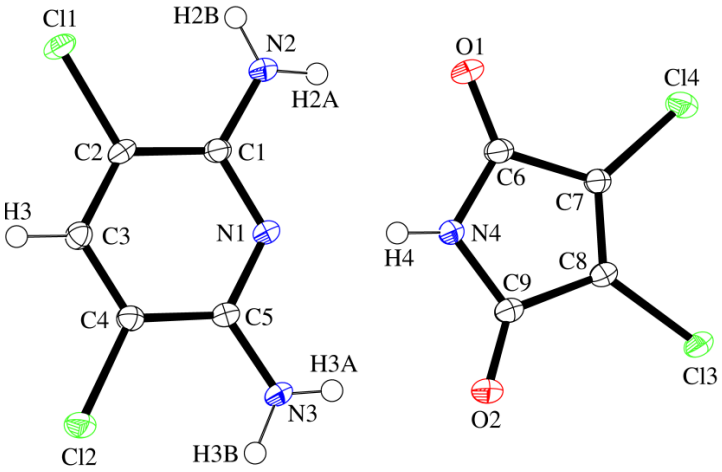
Figure S10.



ORTEP projection of **HMa/ClPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

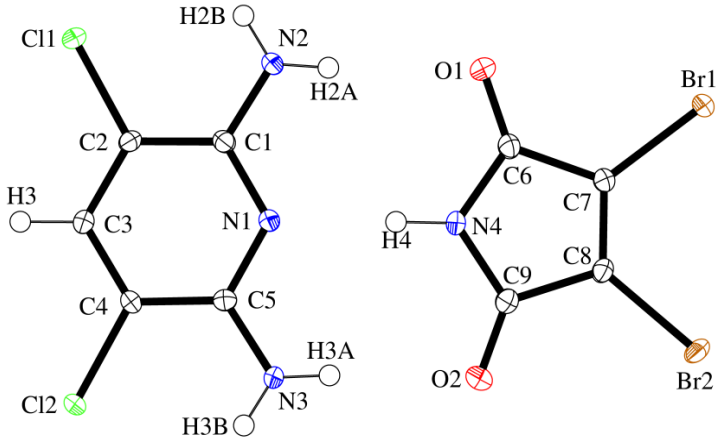
Figure S11.



ORTEP projection of **ClMa/ClPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

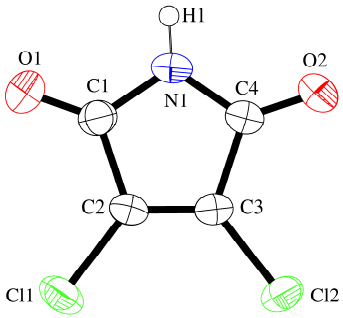
Figure S12.



ORTEP projection of **ClMa/HPy** with numbering scheme.

ADPs at 50% level. H atoms not to scale.

Figure S13.



ORTEP projection of the β polymorph of **ClMa** with numbering scheme.

ADPs at 50% level. H atoms not to scale.