Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Materials

A polar/π model of interactions explains face-to-face stacked quinoid rings: a case study in the crystal of potassium hydrogen chloranilate dihydrate

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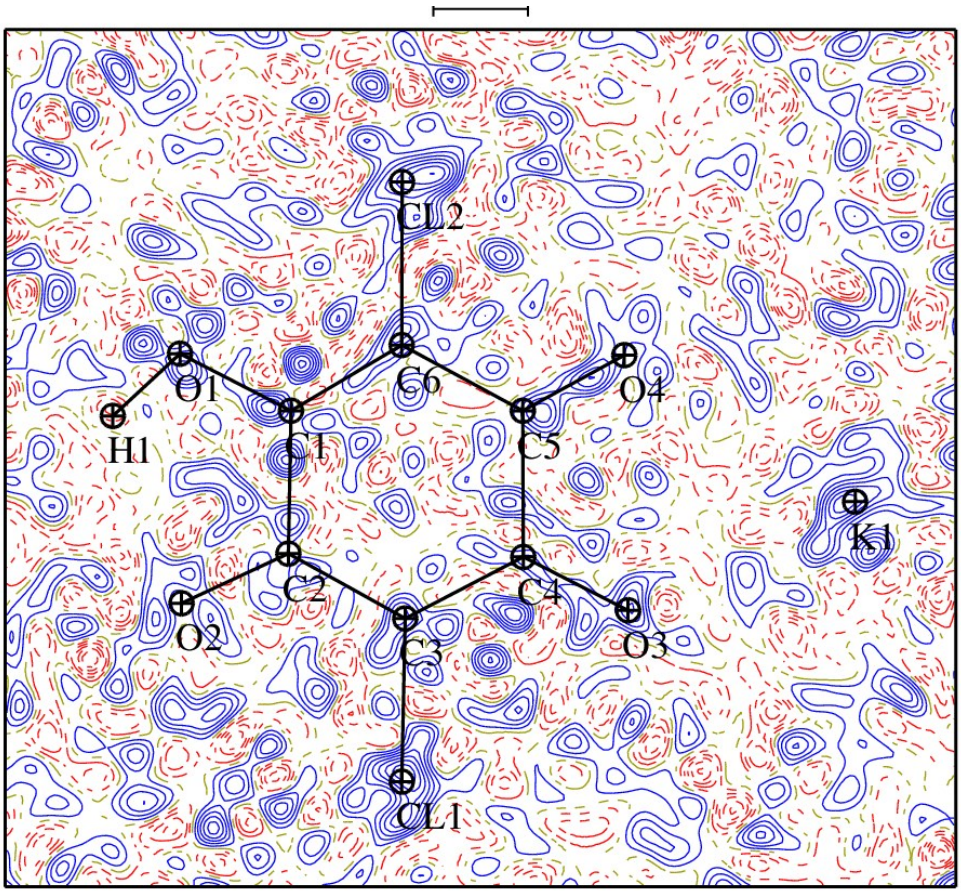

Figure S1 Fourier residual density in the plane of HCA^- anion using all reflections. Contours are drawn for 0.05 $eÅ^{-3}$, positive contours are blue, negative are red dotted and zero is dotted yellow line.

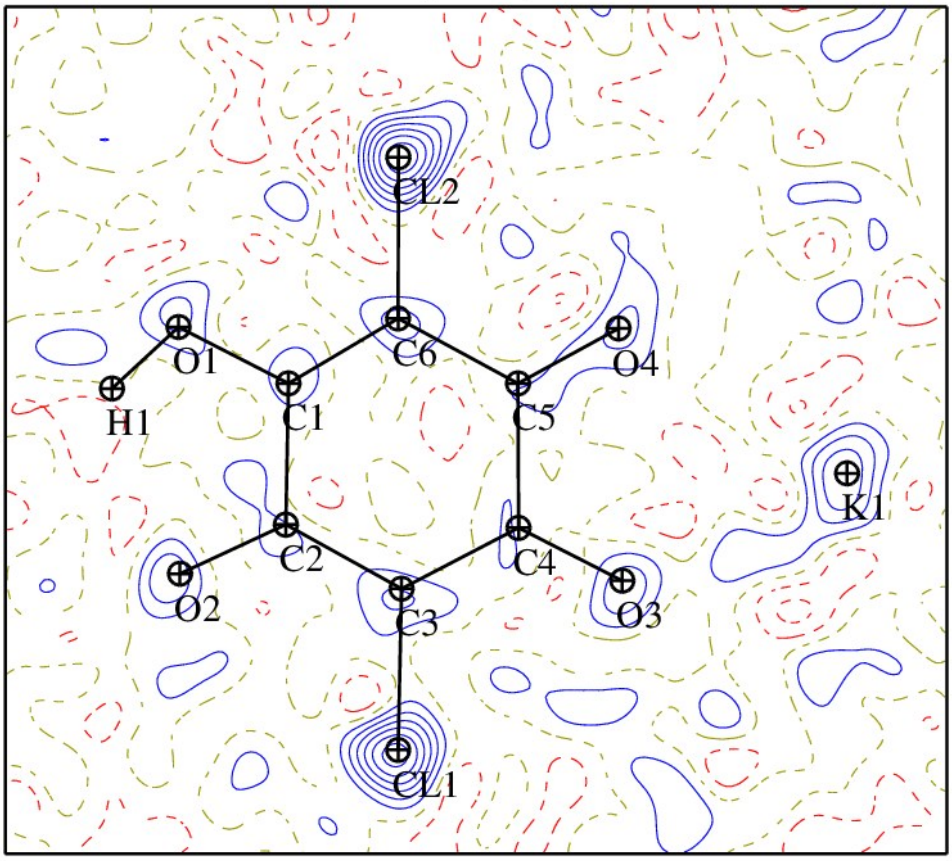

Figure S2 Fourier residual density in the plane of HCA^- anion using reflections up to s=0.7Å^{-1}. Contours are drawn for 0.05 eÅ^{-3}, positive contours are blue, negative are red dotted and zero is dotted yellow line.

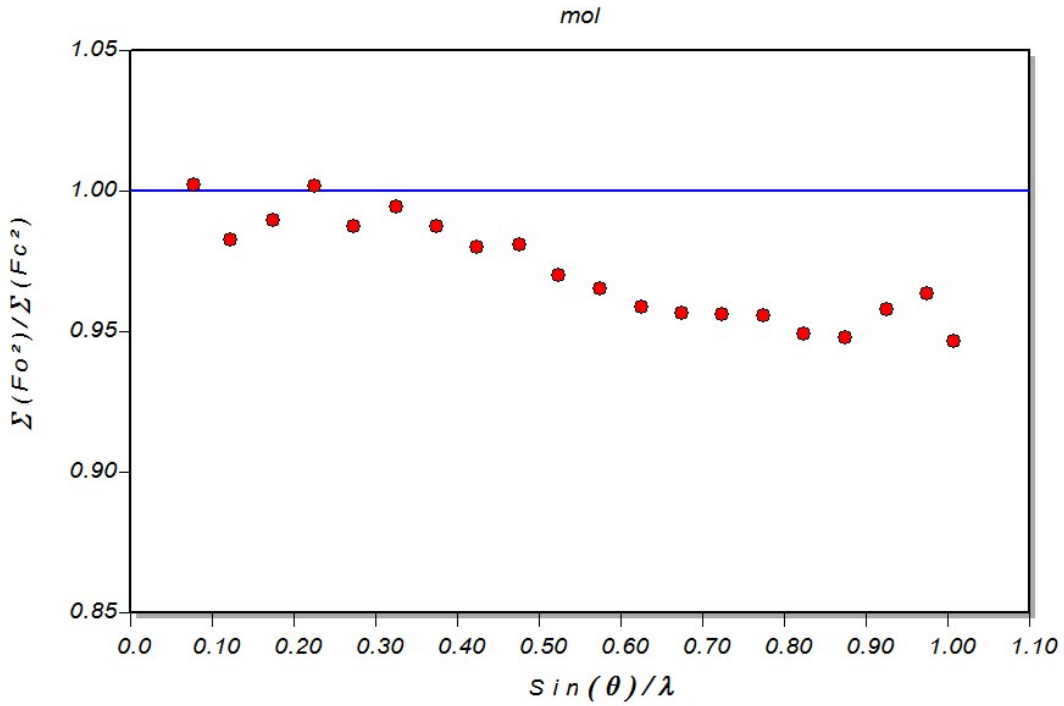

Figure S3 XDRK plot showing the expected and experimental data reduction profile.

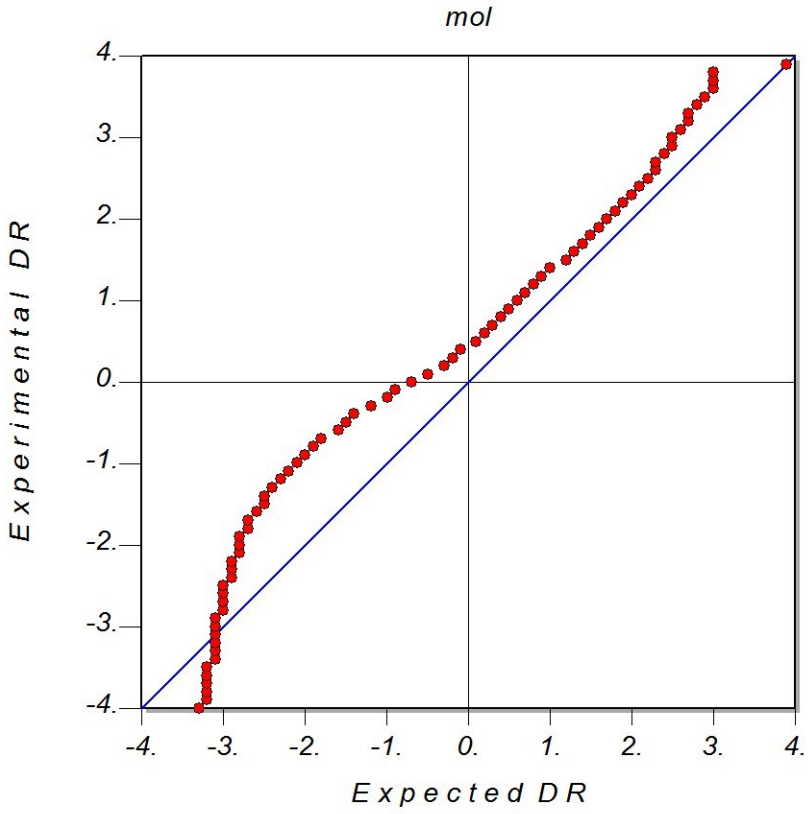

Figure S4 XDRK plot showing the fit of *Y*obs *vs Y*calc as a function of resolution.

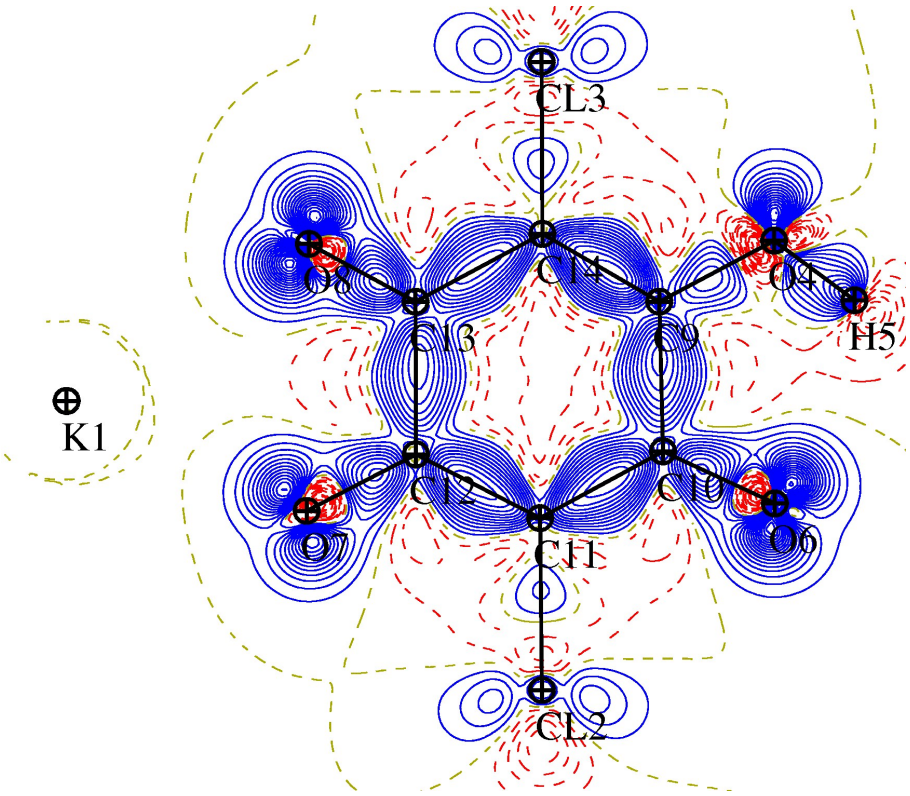

Figure S5 Theoretical deformation density map. Contours are drawn for 0.05 eÅ^{-3}, positive contours are blue, negative are red dotted and zero is yellow dotted line.

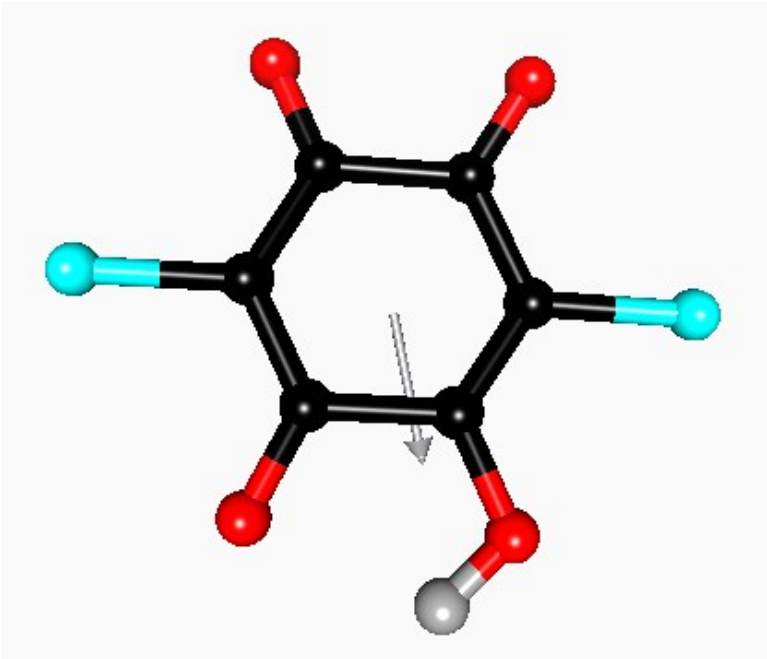

Figure S6.

Dipole moment of the HCA^- anion after global electro-neutralization.

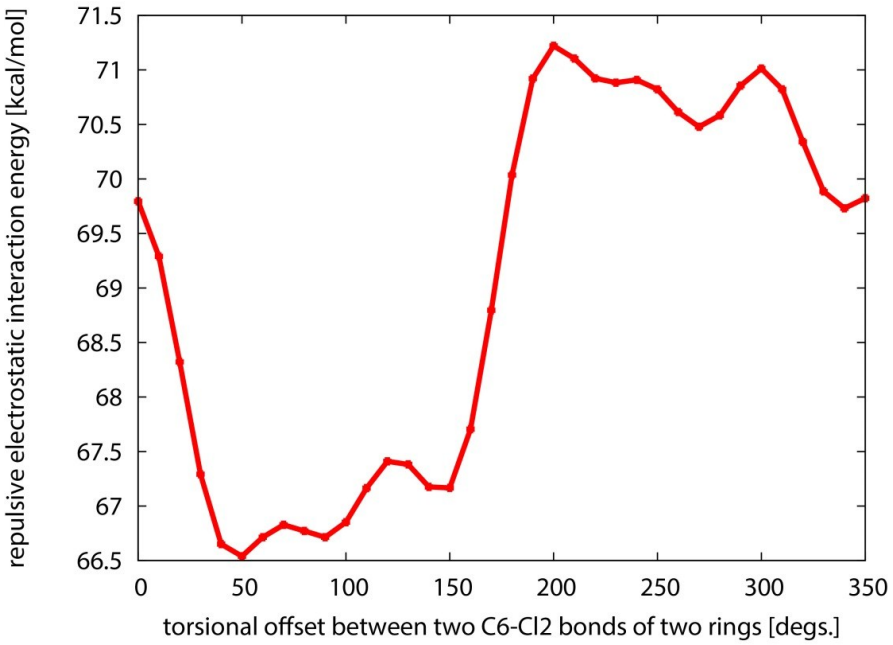

Figure S7. Electrostatic repulsion in a stacked pair of rings, using atomic charges derived by the M06-2X/6-311++G(2d,2p) calculation of the density and fitted to the electric potential according to the Merz-Kollman scheme.

Table S1 Saddle (3,-1) critical points within a pair of hydrogen chloranilate anions determined from experimental and theoretical electron density.

A···B	ρ tot		Laplacian ρ		type	Symm. operation on *A*
	exp	theo	exp	theo		
C3···C5	0.0560	0.0488	0.59	0.55	(3,-1)	$x, {}^{3}/_{2}- y, -½+z$
C3···C5	0.0527		0.56		(3,-1)	$x, {}^{3}/_{2} - y, ½ +z$
C6···C2	0.0550	0.0514	0.58	0.57	(3,-1)	$x, {}^{3}/_{2} - y, -½+z$
Cl1···O4	0.0431	0.0447	0.61	0.61	(3,-1)	$x, {}^{3}/_{2} - y, ½+ z$
Cl2···O2	0.0435	0.0439	0.59	0.60	(3,-1)	$x, {}^{3}/_{2} - y, - ½+ z$
Cl1···O4	0.0400	0.0391	0.49	0.51	(3,-1)	$x, {}^{3}/_{2} - y, -½+z$
Cl2···O2	0.0368	0.0405	0.57	0.56	(3,-1)	$x, {}^{3}/_{2} - y, ½+z$
C1···C3	0.0266	0.0212	0.29	0.26	(3,3)	$x, {}^{3}/_{2} - y, -½+z$