

Face-to-face π -stacking in the multicomponent crystals of chloranilic acid, alkali hydrogenchloranilates, and water

Supplement Data

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S1 Hydrogen bonding

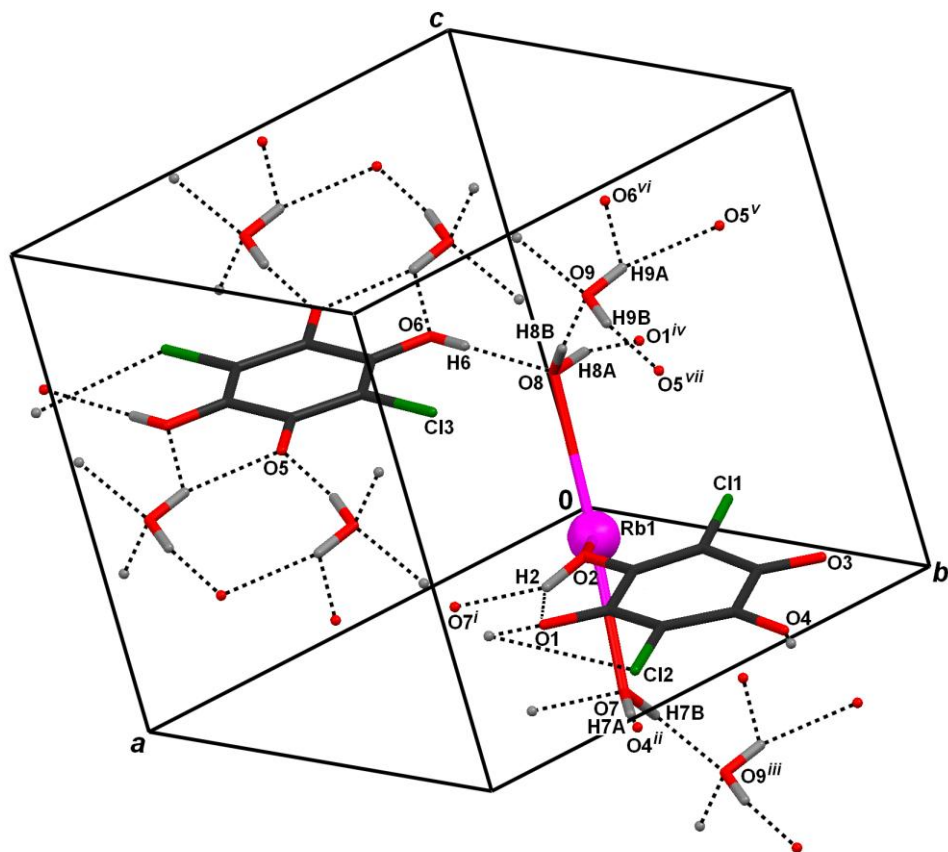


Figure S1 Hydrogen bonding in the isostructural packings of RbHCA·0.5H₂CA·3H₂O and CsHCA·0.5H₂CA·3H₂O. The alkali cation is arbitrarily scaled. Symmetry operators: *i*) 1 - *x*, 1 - *y*, -*z*; *ii*) 1 - *x*, 2 - *y*, -*z*; *iii*) *x*, *y*, -1 + *z*; *iv*) -1 + *x*, -1 + *y*, *z*; *v*) -1 + *x*, *y*, *z*; *vi*) -*x*, -*y*, 1 - *z*; *vii*) 1 - *x*, 1 - *y*, 1 - *z*.

Table S1 Geometric parameters of hydrogen bonds.

	<i>D</i> -H / Å	H··· <i>A</i> / Å	<i>D</i> ··· <i>A</i> / Å	<i>D</i> -H··· <i>A</i> / °	Symm. op. on <i>A</i>
CsHCA·0.5H₂CA·3H₂O					
O2-H2···O1	0.95	2.11	2.670(3)	116	<i>x</i> , <i>y</i> , <i>z</i>
O2-H2···O7	0.95	1.82	2.611(4)	139	1 - <i>x</i> , 1 - <i>y</i> , - <i>z</i>
O6-H6···Cl3	0.83	2.62	3.0899(18)	117	<i>x</i> , <i>y</i> , <i>z</i>
O6-H6···O8	0.83	1.75	2.505(3)	150	<i>x</i> , <i>y</i> , <i>z</i>

O7-H7A...O4	0.94	1.89	2.779(2)	156	$1 - x, 2 - y, -z$
O7-H7B...O9	0.95	1.90	2.831(3)	164	$x, y, -1 + z$
O8-H8A...O1	0.94	1.86	2.761(3)	159	$-1 + x, -1 + y, z$
O8-H8B...O9	0.94	1.85	2.784(3)	170	x, y, z
O9-H9A...O5	0.93	2.05	2.962(4)	163	$-1 + x, y, z$
O9-H9A...O6	0.93	2.32	2.949(3)	124	$-x, -y, 1 - z$
O9-H9B...O5	0.93	1.97	2.892(2)	172	$1 - x, 1 - y, 1 - z$
RbHCA·0.5H₂CA·3H₂O					
O2-H2...O1	0.94	2.13	2.680(4)	116	x, y, z
O2-H2...O7	0.94	1.80	2.606(4)	142	$1 - x, 1 - y, -z$
O6-H6...Cl3	0.82	2.63	3.089(3)	117	x, y, z
O6-H6...O8	0.82	1.76	2.505(4)	150	x, y, z
O7-H7A...O4	0.94	1.87	2.771(4)	160	$1 - x, 2 - y, -z$
O7-H7B...O9	0.94	1.92	2.849(4)	169	$x, y, -1 + z$
O8-H8A...O1	0.94	1.85	2.752(4)	162	$-1 + x, -1 + y, z$
O8-H8B...O9	0.93	1.86	2.783(4)	172	x, y, z
O9-H9A...O5	0.92	2.05	2.941(4)	162	$-1 + x, y, z$
O9-H9A...O6	0.92	2.32	2.941(4)	124	$-x, -y, 1 - z$
O9-H9B...O5	0.92	1.96	2.875(2)	172	$1 - x, 1 - y, 1 - z$
NaHCA·2(NH₂)₂CO					
N1-H1A...O6	0.89(4)	2.04(3)	2.934(4)	175(2)	$x, -1 + y, z$
N1-H1B...O4	0.83(3)	2.28(3)	3.054(3)	157(3)	x, y, z
O2-H2...O1	0.82(4)	2.21(4)	2.653(2)	114(3)	x, y, z
O2-H2...O6	0.82(4)	1.94(4)	2.704(2)	155(4)	$3/2 - x, -1/2 + y, 1/2 - z$
N2-H2A...O1	0.83(4)	2.33(4)	3.090(3)	154(4)	$-1/2 + x, 1/2 - y, -1/2 + z$
N3-H3A...Cl2	0.83(4)	2.89(4)	3.599(4)	144(4)	$2 - x, 1 - y, -z$
N3-H3B...O5	0.82(2)	2.48(3)	3.220(3)	150(3)	x, y, z
N4-H4A...O4	0.85(4)	2.10(3)	2.913(3)	158(4)	$2 - x, 1 - y, -z$
Cs₂CA·(NH₂)₂CO					
N1-H1A...O3	0.86	2.45	3.197(6)	146	$-x, -y, 1 - z$
N1-H1B...O1	0.86	2.17	2.849(7)	136	$-x, -y, 1 - z$

S2 Geometries of quinoid rings

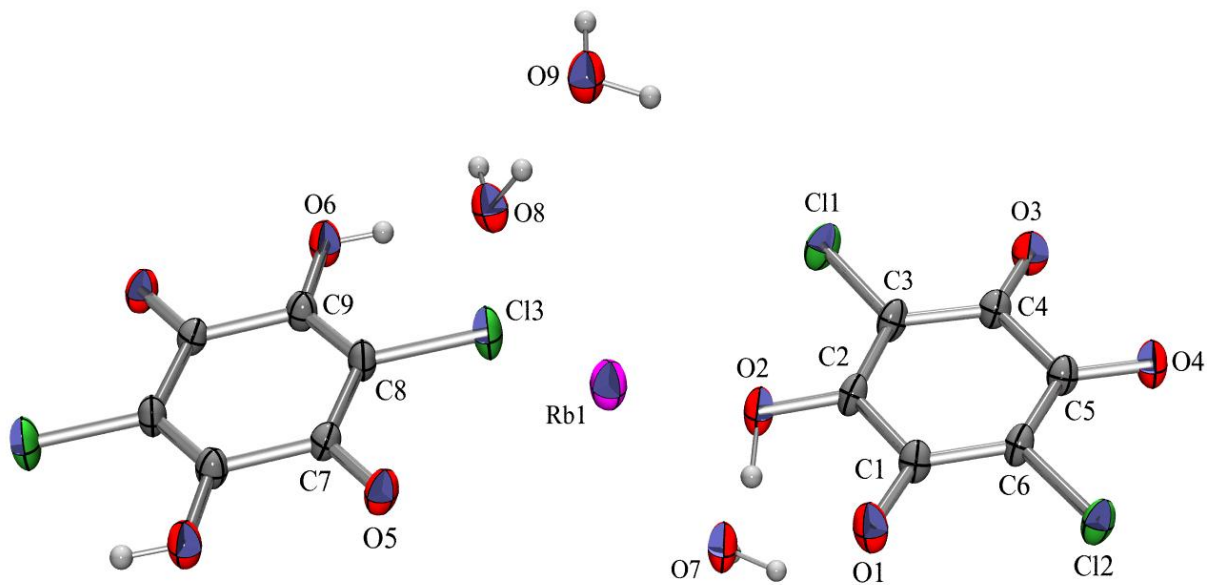


Figure S2 Asymmetric unit of RbHCA·H₂CA·3H₂O. Displacement ellipsoids are drawn at the 50 % probability and hydrogen atoms have been depicted as spheres of arbitrary radii.

Table S2 Bond lengths in molecules of chloranilic acid and hydrogen chloranilate anions in CsHCA·H₂CA·3H₂O and RbHCA·H₂CA·3H₂O.

	CsHCA·H₂CA·3H₂O	RbHCA·H₂CA·3H₂O
HCA⁻		
C1 – C2	1.518(3)	1.508(4)
C2 – C3	1.354(3)	1.364(4)
C3 – C4	1.451(3)	1.446(4)
C4 – C5	1.545(3)	1.544(4)
C5 – C6	1.408(3)	1.402(4)
C6 – C1	1.409(3)	1.410(4)
C1 – O1	1.243(3)	1.248(4)
C2 – O2	1.315(3)	1.314(4)
C4 – O3	1.217(3)	1.220(4)
C5 – O4	1.238(3)	1.243(4)
C3 – C11	1.719(2)	1.718(3)
C6 – C12	1.727(2)	1.730(3)
H₂CA		
C7 – C8	1.454(3)	1.455(4)
C8 – C9	1.359(3)	1.355(4)
C7 – C9 ⁱ	1.511(3)	1.516(4)
C7 – O5	1.220(3)	1.224(4)
C9 – O6	1.303(3)	1.300(4)
C8 – C13	1.719(2)	1.714(3)

Table S3 Bond lengths in hydrogen chloranilate mono anion in NaHCA[(NH₂)₂CO]₂.

C1 – C2	1.510(3)
C2 – C3	1.342(3)
C3 – C4	1.441(3)
C4 – C5	1.546(3)
C5 – C6	1.386(3)
C6 – C1	1.403(3)
C1 – O1	1.235(3)
C2 – O2	1.322(3)
C4 – O3	1.217(3)
C5 – O4	1.245(3)
C3 – Cl1	1.719(2)
C6 – Cl2	1.733(2)

Table S4 Bond lengths in chloranilate dianion in Cs₂CA•(NH₂)₂CO.

C1 – C2	1.413(7)
C2 – C3	1.408(7)
C1 – C3 ⁱ	1.524(7)
C1 – O1	1.242(6)
C3 – O2	1.252(6)
C2 – Cl1	1.730(5)

S2 Cation coordinations

Table S5 Geometry of cation coordination sphere in CsHCA·H₂CA·3H₂O and RbHCA·H₂CA·3H₂O (Å, °). Symmetry operators: *i*) $x, -1+y, z$; *ii*) $-x, 1-y, -z$; *iii*) $1-x, 1-y, -z$.

	CsHCA·H ₂ CA·3H ₂ O	RbHCA·H ₂ CA·3H ₂ O
M – O4 ^{<i>i</i>}	3.1006(18)	2.934(2)
M – O7	3.105(2)	2.949(3)
M – O3 ^{<i>i</i>}	3.0740(19)	2.952(2)
M – O3 ^{<i>ii</i>}	3.1851(19)	3.049(2)
M – O8	3.321(2)	3.167(3)
M – O2	3.2475(18)	3.201(2)
M – O1 ^{<i>iii</i>}	3.428(2)	3.424(3)
O4 ^{<i>i</i>} – M – O7	88.93(5)	87.74(7)
O4 ^{<i>i</i>} – M – O3 ^{<i>i</i>}	51.53(5)	54.33(6)
O4 ^{<i>i</i>} – M – O3 ^{<i>ii</i>}	136.61(5)	135.52(6)
O4 ^{<i>i</i>} – M – O8	87.20(5)	88.95(6)
O4 ^{<i>i</i>} – M – O2	79.56(5)	79.38(6)
O4 ^{<i>i</i>} – M – O1 ^{<i>iii</i>}	66.28(5)	65.95(6)
O7 – M – O3 ^{<i>i</i>}	117.51(5)	117.71(7)
O7 – M – O3 ^{<i>ii</i>}	94.93(5)	96.43(7)
O7 – M – O8	173.90(5)	172.96(7)
O7 – M – O2	77.46(5)	76.64(7)
O7 – M – O1 ^{<i>iii</i>}	54.25(5)	54.50(6)
O3 ^{<i>i</i>} – M – O3 ^{<i>ii</i>}	89.54(5)	85.61(6)
O3 ^{<i>i</i>} – M – O8	63.21(5)	64.80(6)
O3 ^{<i>i</i>} – M – O2	125.94(5)	128.55(6)
O3 ^{<i>i</i>} – M – O1 ^{<i>iii</i>}	65.14(5)	64.70(6)
O3 ^{<i>ii</i>} – M – O8	91.13(5)	90.29(6)
O3 ^{<i>ii</i>} – M – O2	143.40(5)	144.69(6)

O3 ⁱⁱ – M – O1 ⁱⁱⁱ	81.28(5)	80.75(6)
O8 – M – O2	97.19(5)	96.65(6)
O8 – M – O1 ⁱⁱⁱ	127.80(5)	129.19(6)
O2 – M – O1 ⁱⁱⁱ	119.10(5)	118.99(6)

Table S6 Geometry of sodium coordination sphere in NaHCA[(NH₂)₂CO]₂ (Å,°).
Symmetry operators: *i*) 1–*x*, 1–*y*, –*z*; *ii*) 3/2–*x*, 1/2+*y*, 1/2–*z*.

Na1 – O5 ⁱ	2.2863(18)
Na1 – O5	2.3323(18)
Na1 – O6	2.3346(19)
Na1 – O1 ⁱⁱ	2.389(2)
Na1 – O4	2.4240(18)
Na1 – O3	2.443(2)
O5 ⁱ – Na1 – O5	87.28(7)
O5 ⁱ – Na1 – O6	106.83(7)
O5 ⁱ – Na1 – O1 ⁱⁱ	91.87(7)
O5 ⁱ – Na1 – O4	158.44(7)
O5 ⁱ – Na1 – O3	92.68(7)
O5 – Na1 – O6	94.72(7)
O5 – Na1 – O1 ⁱⁱ	170.97(8)
O5 – Na1 – O4	99.97(8)
O5 – Na1 – O3	98.14(7)
O6 – Na1 – O1 ⁱⁱ	76.91(6)
O6 – Na1 – O4	92.89(7)
O6 – Na1 – O3	157.10(7)
O1 ⁱⁱ – Na1 – O4	84.03(7)
O1 ⁱⁱ – Na1 – O3	90.88(7)
O4 – Na1 – O3	66.31(6)

Table S7 Geometry of caesium coordination sphere in $\text{Cs}_2\text{CA}\cdot(\text{NH}_2)_2\text{CO}$ ($\text{\AA},^\circ$).
Symmetry operators: *i*) $1/2-x, -1/2+y, z$; *ii*) $x, 1-y, -1/2+z$; *iii*) $1/2-x, 1/2-y, -1/2+z$; *iv*) $-x, y, 1/2-z$.

Cs1 – O2 ⁱ	2.988(4)
Cs1 – O2 ⁱⁱ	2.989(5)
Cs1 – O1	3.070(4)
Cs1 – O3	3.157(4)
Cs1 – O1 ⁱⁱⁱ	3.399(5)
Cs1 – O1 ^{iv}	3.416(5)
Cs1 – Cl1 ⁱ	3.5270(15)
O2 ⁱ – Cs1 – O2 ⁱⁱ	139.18(5)
O2 ⁱ – Cs1 – O1	87.03(14)
O2 ⁱ – Cs1 – O3	106.13(10)
O2 ⁱ – Cs1 – O1 ⁱⁱⁱ	69.05(13)
O2 ⁱ – Cs1 – O1 ^{iv}	154.31(12)
O2 ⁱ – Cs1 – Cl1 ⁱ	53.81(9)
O2 ⁱⁱ – Cs1 – O1	100.85(12)
O2 ⁱⁱ – Cs1 – O3	114.69(10)
O2 ⁱⁱ – Cs1 – O1 ⁱⁱⁱ	81.26(11)
O2 ⁱⁱ – Cs1 – O1 ^{iv}	48.66(11)
O2 ⁱⁱ – Cs1 – Cl1 ⁱ	152.03(9)
O1 – Cs1 – O3	79.01(10)
O1 – Cs1 – O1 ⁱⁱⁱ	141.65(9)
O1 – Cs1 – O1 ^{iv}	67.60(16)
O1 – Cs1 – Cl1 ⁱ	104.97(9)
O3 – Cs1 – O1 ⁱⁱⁱ	135.27(10)
O3 – Cs1 – O1 ^{iv}	74.00(9)
O3 – Cs1 – Cl1 ⁱ	61.08(7)
O1 ⁱⁱⁱ – Cs1 – O1 ^{iv}	129.40(2)
O1 ⁱⁱⁱ – Cs1 – Cl1 ⁱ	85.10(8)
O1 ^{iv} – Cs1 – Cl1 ⁱ	134.94(7)

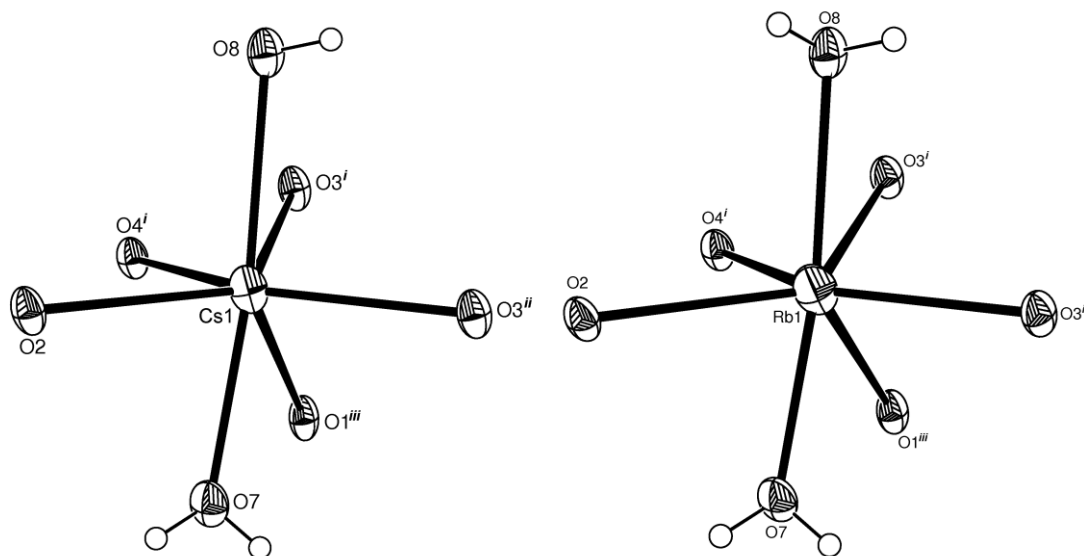


Figure S3 ORTEP-3 drawings of cation coordination spheres in $\text{CsHCA}\cdot\text{H}_2\text{CA}\cdot 3\text{H}_2\text{O}$ and $\text{RbHCA}\cdot\text{H}_2\text{CA}\cdot 3\text{H}_2\text{O}$. Both coordination polyhedra are distorted mono-capped octahedra. Symmetry operators: *i*) $x, -1+y, z$; *ii*) $-x, 1-y, -z$; *iii*) $1-x, 1-y, -z$.

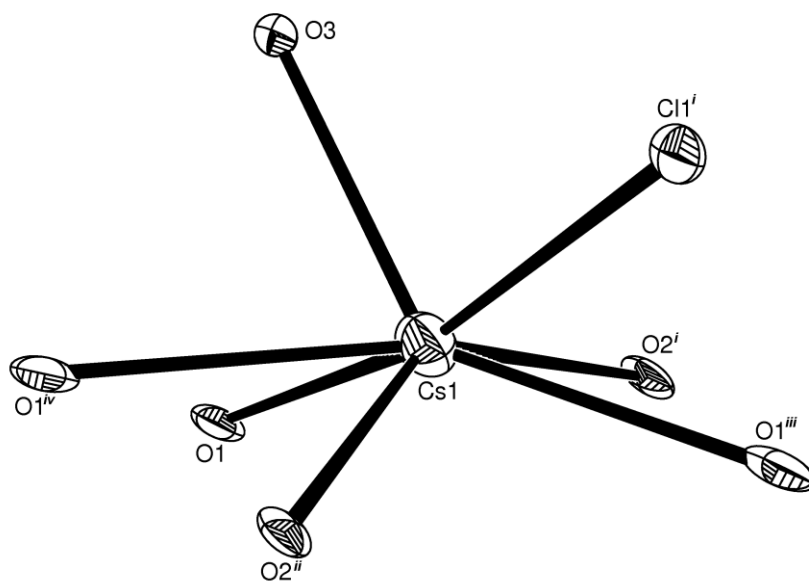


Figure S4 ORTEP-3 drawing of caesium coordination sphere in $\text{Cs}_2\text{CA}\cdot(\text{NH}_2)_2\text{CO}$. The coordination polyhedron can be described as a distorted mono-capped pentagonal prism. Symmetry operators: *i*) $1/2-x, -1/2+y, z$; *ii*) $x, 1-y, -1/2+z$; *iii*) $1/2-x, 1/2-y, -1/2+z$; *iv*) $-x, y, 1/2-z$.

S4 List of structures extracted from the CSD

Table S8 List of structures extracted from the CSD.

REFCODE	Compound	Reference
ABUHIO	1,2-bis(Pyrid-2-yl)acetylene 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone	Md.B.Zaman, M.Tomura and Y.Yamashita, <i>Org.Lett.</i> , 2000, 2 , 273
AJAGIB	Piperazine-2,5-dione chloranilic acid	Tzy-Jiun M.Luo and G.T.R.Palmore, <i>Cryst.Growth Des.</i> , 2002, 2 , 337
CAVYED	2,5-Dichloro-3,6-dihydroxy-p-benzoquinone bis(pyrimidine)	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 1999, 55 , 1714
CAVYIH	2,5-Dichloro-3,6-dihydroxy-p-benzoquinone bis(pyrazine)	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 1999, 55 , 1714
CLANAC10	Chloranilic acid	E.K.Andersen <i>Acta Crystallogr.</i> , 1967, 22 , 188
CLANAC11	2,5-Dichloro-3,6-dihydroxy-1,4-benzoquinone	G.Dutkiewicz, H.S.Yathirajan, Q.N.M.H.Al-arique, B.Narayana and M.Kubicki, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2010, 66 , o497
CLANDH	Chloranilic acid dihydrate	E.K.Andersen, <i>Acta Crystallogr.</i> , 1967, 22 , 191
EBAWAG	2,2'-Bipyrimidine chloranilic acid tetrahydrate	Md.B.Zaman, K.A.Udachin and J.A.Ripmeester, <i>Cryst.Growth Des.</i> , 2004, 4 , 585
GINKUK	Quinoxaline chloranilic acid	K.Gotoh, H.Nagoshi and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2007, 63 , o4295
HUFZUE	2,5-Dichloro-3,6-dihydroxy-1,4-benzoquinone 2-azaspiro[4.5]decan-3-one	J.P.Jasinski, R.J.Butcher, Q.N.M.H.Al-arique, H.S.Yathirajan and B.Narayana, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2010, 66 , o163
MAMPUM01	2,5-Dichloro-3,6-dihydroxy-1,4-benzoquinone phenazine	S.Horiuchi, R.Kumai and Y.Tokura, <i>J.Am.Chem.Soc.</i> , 2005, 127 , 5010
MAMPUM02	rac-(Phenazine chloranilic acid)	K.Gotoh, T.Asaji and H.Ishida, <i>Acta Crystallogr., Sect.C Cryst.Struct.Commun.</i> , 2007, 63 , o17
NIGQEA	4,4',5,4'-tetrakis(2-Pyrazinylmethylthio)tetrathiafulvalene bis(2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone)	S.-X.Liu, S.Dolder, A.Neels, G.Labat, H.Stoekli-Evans and S.Decurtins, <i>J.Phys.IV</i> , 2004, 114 , 679
NOQFUV	4,4'-Dimethyl-7,7'-bi[[1,2,5]thiadiazolo[3,4-b]pyridylidene) 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone	M.Tomura, K.Ono and Y.Yamashita, <i>Struct.Chem.</i> , 2008, 19 , 967,
PEZQAN	2,6-dimethylpyrazine chloranilic acid	M.Prager, W.Sawka-Dobrowolska, L.Sobczyk, A.Pawlukojc, E.Grech, A.Wischniewski and M.Zamponi, <i>Chem.Phys.</i> , 2007, 332 , 1
QUCKAB	Pyridine-3-carbonitrile chloranilic acid acetonitrile solvate	K.Gotoh and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2009, 65 , o2467
WATREP	Chloranilic acid tetramethylpyrazine	W.Sawka-Dobrowolska, G.Bator, L.Sobczyk, E.Grech, J.Nowicka-Scheibe and A.Pawlukojc, <i>Struct.Chem.</i> , 2005, 16 , 281
WATREPO1	2,3,5,6-Tetramethylpyrazine 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone	M.Prager, A.Pietraszko, L.Sobczyk, A.Pawlukojc, E.Grech, T.Seydel, A.Wischniewski and M.Zamponi, <i>J.Chem.Phys.</i> , 2006, 125 , 194525
WATREPO2	2,3,5,6-Tetramethylpyrazine 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone	M.Prager, A.Pietraszko, L.Sobczyk, A.Pawlukojc, E.Grech, T.Seydel, A.Wischniewski and M.Zamponi, <i>J.Chem.Phys.</i> , 2006, 125 , 194525
ABUHUA	1-(4-Pyridinio)-2-(pyrid-4-yl)acetylene 2,5-dichloro-6-hydroxy-1,4-benzoquinon-3-olate	Md.B.Zaman, M.Tomura and Y.Yamashita, <i>Org.Lett.</i> , 2000, 2 , 273
CIPSUQ	4,4'-Bipiperidinedi-ium bis(hydrogen chloranilate)	K.Gotoh, R.Ishikawa and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2007, 63 , o4518
DUJGER	3-Hydroxypyridinium hydrogen chloranilate monohydrate	K.Gotoh and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2009, 65 , o3060
GOMBEP	Pyridinium 2,5-dichloro-6-hydroxy-p-benzoquinone-3-olate monohydrate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 1999, 55 , 1149,
HOLPEE	2-Carboxypyridinium hydrogen chloranilate	K.Gotoh, H.Nagoshi and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2009, 65 , o614
IGAKUX	2-Aminopyrimidin-1-ium 2,5-dichloro-4-hydroxy-3,6-dioxo-1,4-cyclohexadien-1-olate monohydrate	Ping Su, Xue-Ying Huang and Xiang-gao Meng, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2008, 64 , o2217
JIQHAT	2-(2-(1,3-dithiol-2-ylidene)-1,3-dithiol-4-yl)-1H-imidazol-3-ium 2,5-dichloro-	T.Murata, Y.Morita, Y.Yakiyama, K.Fukui, H.Yamochi, G.Saito

	4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate monohydrate	and K.Nakasuji, <i>J.Am.Chem.Soc.</i> , 2007, 129 , 10837
KEQPEC	4-Aminopyrimidino-2(1H)-one 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone monohydrate	K.Gotoh, R.Ishikawa and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2006, 62 , o4738
KOQGEC	Ethylammonium chloranilate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2000, 56 , e202
KOQGIG	Diethylammonium chloranilate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2000, 56 , e202
MAJSUL	bis(eta ⁵ -Pentamethyl-cyclopentadienyl)-iron 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone monohydrate clathrate	M.B.Zaman, M.Tomura, Y.Yamashita, M.Sayaduzzaman and A.M.S.Chowdhury, <i>CrystEngComm</i> , 1999, 1 , 36
MAMPUM03	Phenazinium chloranilate	K.Gotoh, T.Asaji and H.Ishida, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2007, 63 , o17
NEQWEM	Benzimidazolium chloranilate monohydrate	De-Jun Yang and Shao-hua Qu, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2006, 62 , o4720
NIGQAW	4,5-bis(2-Pyridiniomethylthio)-4',5'-bis(2-pyridylmethylthio)tetrathiafulvalene bis(2,5-dichloro-6-hydroxy-1,4-benzoquinon-3-olate)	S.-X.Liu, S.Dolder, A.Neels, G.Labat, H.Stoekli-Evans and S.Decurtins, <i>J.Phys.IV</i> , 2004, 114 , 679
OMIXIR	Piperidinium hydrogen chloranilate	T.Fukunaga and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2003, 59 , o1793
PAGXOL	1,2,3,4-Tetrahydroquinolinium hydrogen chloranilate	H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2004, 60 , o1674
PAZHOO	3-Carboxypyridinium hydrogen chloranilate	Y.Tabuchi, A.Takahashi, K.Gotoh, H.Akashi and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2005, 61 , o4215
PAZHOO01	3-Carboxypyridinium hydrogen chloranilate	H.Ishida, Private Communication , , 2009
POVZEG	2-Carbamoylpyridinium hydrogen chloranilate	K.Gotoh, H.Nagoshi and H.Ishida, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2009, 65 , o273
POVZIK	3-Carbamoylpyridinium hydrogen chloranilate	K.Gotoh, H.Nagoshi and H.Ishida, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2009, 65 , o273
QIKGIA	Imidazolium hydrogen chloranilate acetonitrile solvate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect.C: Cryst.Struct.Commun.</i> , 2001, 57 , 476
SIYCAF	2,9-Dimethyl-1,10-phenanthrolium chloranilate	A.S.Gaballa, C.Wagner, S.M.Teleb, E.-M.Nour, M.A.F.Elmosallamy, G.N.Kaluderovic, H.Schmidt and D.Steinborn, <i>J.Mol.Struct.</i> , 2008, 876 , 301
SOMDOO	2,2'-(3,5-Di(pyridin-2-yl)pyrazine-2,6-diyl)dipyridinium bis(2,5-dichloro-4-hydroxy-3,6-dioxocyclohexanolate)	S.Horiuchi, R.Kumai, Y.Tokunaga and Y.Tokura, <i>J.Am.Chem.Soc.</i> , 2008, 130 , 13382
TIXTUQ	4-Cyanopyridinium hydrogen chloranilate	M.Tomura and Y.Yamashita, <i>Anal.Sci.: X-Ray Struct.Anal.Online</i> , 2008, 24 , x31
UHOTIV	Ammonium hydrogen chloranilate dihydrate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>CrystEngComm</i> , 2009, 11 , 1407
ULEHOI	4,6-bis(2-Pyridyl)-2-(2-pyridinio)-1,3,5-triazine 2,5-dichloro-6-hydroxy-1,4-benzoquinone-3-olate monohydrate	M.K.Kabir, H.Tobita, H.Matsuo, K.Nagayoshi, K.Yamada, K.Adachi, Y.Sugiyama, S.Kitagawa and S.Kawata, <i>Cryst.Growth Des.</i> , 2003, 3 , 791
WOGWUL	Pyridazin-1-ium hydrogen chloranilate	K.Gotoh and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2008, 64 , o2095
WUXYUJ	2,4-Dimethylpyridinium 2,5-dichloro-6-hydroxy-1,4-benzoquinone-3-olate	H.Ishida and S.Kashino, <i>Z.Naturforsch.,A: Phys.Sci.</i> , 2002, 57 , 829
WUXZAQ	2,5-Dimethylpyridinium 2,5-dichloro-6-hydroxy-1,4-benzoquinone-3-olate	H.Ishida and S.Kashino, <i>Z.Naturforsch.,A: Phys.Sci.</i> , 2002, 57 , 829
WUXZEU	2,6-Dimethylpyridinium 2,5-dichloro-6-hydroxy-1,4-benzoquinone-3-olate	H.Ishida and S.Kashino, <i>Z.Naturforsch.,A: Phys.Sci.</i> , 2002, 57 , 829
WUXZII	3,4-Dimethylpyridinium 2,5-dichloro-6-hydroxy-1,4-benzoquinone-3-olate	H.Ishida and S.Kashino, <i>Z.Naturforsch.,A: Phys.Sci.</i> , 2002, 57 , 829
YERXUP	4-Carboxypyridinium 2,5-dichloro-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate monohydrate	K.Gotoh, Y.Tabuchi, H.Akashi and H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2006, 62 , o4420
YERXUP01	4-Carboxypyridinium hydrogen chloranilate monohydrate	H.Ishida, Private Communication, 2009
ABUHOU	1,2-bis(3-Pyridinio)acetylene 2,5-dichloro-1,4-benzoquinone-3,6-diolate hydrate	Md.B.Zaman, M.Tomura and Y.Yamashita, <i>Org.Lett.</i> , 2000, 2 , 273
ACEWIP	bis(Trimethylpyridinium) chloranilate	H.Ishida, <i>Acta Crystallogr., Sect.E: Struct.Rep.Online</i> , 2004, 60 , o2005
AMCLAN10	Ammonium chloranilate monohydrate	E.K.Andersen, <i>Acta Crystallogr.</i> , 1967, 22 , 196
BALROV	bis(Anilinium) chloroanilate	Z.G.Aliev, S.I.Kondrat'ev, L.O.Atovmyan, M.L.Khidekel and V.V.Karpov, <i>Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)</i> , 1981, 487
BALRUB	Ammonium chloroanilate oxonium monohydrate	Z.G.Aliev, S.I.Kondrat'ev, L.O.Atovmyan, M.L.Khidekel and V.V.Karpov, <i>Izv.Akad.Nauk</i>

		<i>SSSR, Ser. Khim. (Russ.) (Russ. Chem. Bull.)</i> , 1981, 487
BARLOW	2,6-bis(Pyridinium-4-yl)benzene 2,5-di(4-pyridyl)benzene chloranilate hexahydrate	Md.Akhtaruzzaman, M.Tomura, K.Takahashi, J.Nishida and Y.Yamashita, <i>Supramol.Chem.</i> , 2003, 15 , 239
BEBJIC	4,4'-(Azinodimethylene)dipyridinium chloranilate dichloromethane solvate	A.R.Kennedy and F.R.N.Watson, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 2003, 59 , o613
CAHKUS	bis(4-(2-Pyridyl)pyridinium) 2,5-dichloro-3,6-dioxy-1,4-benzoquinone	M.B.Zaman, M.Tomura and Y.Yamashita, <i>J.Org.Chem.</i> , 2001, 66 , 5987
CAHLIH	Ethene-1,2-bis(4-pyridinium) 2,5-dichloro-3,6-dioxy-1,4-benzoquinone	M.B.Zaman, M.Tomura and Y.Yamashita, <i>J.Org.Chem.</i> , 2001, 66 , 5987
EWOWUI	bis(Pyrrolidinium) chloranilate	H.Ishida, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2004, 60 , o974
FAGZIW	Barium 3,6-dichloro-2,5-dihydroxy-p-benzoquinone trihydrate	C.Robl and A.Weiss, <i>Z.Naturforsch., B: Chem.Sci.</i> , 1986, 41 , 1495
FIBCIC	4,4'-Bipyridinium 2,5-dichloro-1,4-benzoquinone-3,6-diolate	Md.B.Zaman, M.Tomura and Y.Yamashita, <i>Chem.Commun.</i> , 1999, 999
FIBDEZ	trans-1,2-bis(2-Pyridinium)ethylene 2,5-dichloro-1,4-benzoquinone-3,6-diolate	Md.B.Zaman, M.Tomura and Y.Yamashita, <i>Chem.Commun.</i> , 1999, 999
GOMBIT	bis(1,2-Diazinium) 2,5-dichloro-6-hydroxy-p-benzoquinone-3-olate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 1999, 55 , 1149
IYESUA	bis(o-Toluidinium) 2,5-dichloro-1,4-benzoquinone-3,6-diolate	T.Fukunaga, N.Kumagai and H.Ishida, <i>Z.Naturforsch., A: Phys.Sci.</i> , 2003, 58 , 631
IYETAH	bis(m-Toluidinium) 2,5-dichloro-1,4-benzoquinone-3,6-diolate	T.Fukunaga, N.Kumagai and H.Ishida, <i>Z.Naturforsch., A: Phys.Sci.</i> , 2003, 58 , 631
IZIHAA	4,7-bis(4-Pyridinium)-2,1,3-benzothiadiazole chloranilate trihydrate	Md.Akhtaruzzaman, M.Tomura, J.Nishida and Y.Yamashita, <i>J.Org.Chem.</i> , 2004, 69 , 2953
JAVWUZ	bis(Hydrazinium) chloranilate	O.Kuhl and S.Goutal, <i>Cryst. Growth Des.</i> , 2005, 5 , 1875
JAXMEB	bis(4-Methylimidazolium) chloranilate	Zi-Liang Wang and Lin-Heng Wei, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2005, 61 , o3129
JIXCAU	bis(1,8-bis(Dimethylamino)naphthalene) chloranilic acid dihydrate	J.A.Kanters, A.Schouten, A.J.M.Duisenberg, T.Glowiak, Z.Malarski, L.Sobczyk and E.Grech, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 1991, 47 , 2148
JIXCAU01	bis(1,8-bis(Dimethylamino)naphthalene) chloranilic acid dihydrate	J.A.Kanters, A.Schouten, A.J.M.Duisenberg, T.Glowiak, Z.Malarski, L.Sobczyk and E.Grech, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 1991, 47 , 2148
OCANIQ	bis(3-Picolinium) chloranilate dihydrate	H.Ishida, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2004, 60 , o1900
ODAVUL	bis(Piperidinium) chloranilate	M.S.Refat, H.A.-D.Ahmed, L.A.El-Zayat, T.Fukunaga and H.Ishida, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2006, 62 , o1886
PEMJIB	bis(1H-1,2,3-benzotriazol-3-ium) chloranilate	Xiang-Gao Meng and Jin-Liang Qian, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2006, 62 , o4178
QIBLES	1,4-bis((4-pyridinium)ethynyl)benzene chloranilate	Md.Akhtaruzzaman, M.Tomura and Y.Yamashita, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2001, 57 , o353
QIKGAS	bis(Pyrazolium) chloranilate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 2001, 57 , 476
QIKGEW	bis(Imidazolium) chloranilate	H.Ishida and S.Kashino, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 2001, 57 , 476
QQQFJD01	Sodium 3,6-dichloro-2,5-dihydroxy-p-benzoquinone trihydrate	R.Benchekroun and J.-M.Savariault, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 1995, 51 , 186
SITBAZ	bis(2-Methyl-1H-imidazol-3-ium) chloranilate	Li-Hui Jia, Zong-E Mu and Zu-Li Liu, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2008, 64 , o32
TAWVAP	bis(S-Benzylthiuronium) chloranilate	D.V.Stergiou, S.Skoulika, N.P.Evmiridis and P.G.Veltsistas, <i>Chem.Mater.</i> , 2005, 17 , 1307
TINYIZ	Bis(adeninium) chloranilate dihydrate	K.Gotoh, R.Ishikawa and H.Ishida, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2007, 63 , o4433
ULEJAW	Tetrathiafulvalenium hemikis(2,5-dichloro-1,4-benzoquinone-3,6-diolate) hemikis(1,4-dichloro-2,3,5,6-tetrahydroxybenzene)	M.K.Kabir, H.Tobita, H.Matsuo, K.Nagayoshi, K.Yamada, K.Adachi, Y.Sugiyama, S.Kitagawa and S.Kawata, <i>Cryst. Growth Des.</i> , 2003, 3 , 791
WAKHAS	bis(3-Methylpyrazolium) chloranilate	H.Ishida, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 2004, 60 , o2506
AMCLAN11	Diammonium chloranilate monohydrate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>Croat.Chem.Acta</i> , 2009, 82 , 387
HUMNUZ	Sesqui-caesium hemi-sodium chloranilate monohydrate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>Croat.Chem.Acta</i> , 2009, 82 , 387

HUMPAH	Di-caesium chloranilate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>Croat.Chem.Acta</i> , 2009, 82 , 387
QQQFIP01	Di-potassium chloranilate monohydrate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>Croat.Chem.Acta</i> , 2009, 82 , 387
QQQFIS01	Di-rubidium chloranilate monohydrate	K.Molcanov, B.Kojic-Prodic and A.Meden, <i>Croat.Chem.Acta</i> , 2009, 82 , 387