SUPPORTING INFORMATION

Halogenide anions as halogen and hydrogen bond acceptors in iodopyridinium halogenides

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Table S1. Crystal data and refinement details for the prepared salts.

	(2IPyH$^+$)$_2$(Cl$^-$)(I$^-$)	**2IPy**HCl	**2IPy**HBr	**2IPy**HI
Molecular formula	$C_{10}H_{10}N_2I_3Cl$	C_5H_5NICl	C_5H_5NIBr	$C_5H_5NI_2$
M_r	574.35	241.45	285.91	508.97
Crystal system	triclinic	monoclinic	orthorhombic	orthorhombic
Space group	$P\,\bar{1}$	$P\,2_1/n$	P ca 2_1	P ca 2_1
Crystal data:				
a / Å	8.2027(6)	4.4564(3)	14.9620(7)	15.0849(7)
b / Å	8.8661(5)	10.8438(7)	4.5454(2)	4.7247(2)
c / Å	11.4800(7)	14.8824(11)	10.9014(5)	11.2538(4)
α / °	89.566(5)	90	90	90
β / °	70.547(6)	94.886(7)	90	90
γ / °	81.668(6)	90	90	90
V / Å^3	778.18(9)	716.57(9)	741.39(6)	802.08(6)
Z	2	4	4	4
D_{calc} / g cm^{-3}	2.451	2.238	2.561	2.757
λ(MoK_α) / Å	0.71073	0.71073	0.71073	0.71073
T / K	295	295	295	295
Crystal size / mm^3	0.28 x 0.24 x 0.22	0.50 x 0.21 x 0.10	0.48 x 0.28 x 0.12	0.42 x 0.22 x 0.24
μ / mm^{-1}	6.176	4.738	9.609	7.750
F(000)	520	448	520	592
Refl. collected/unique	5878 / 3374	5186 / 1550	4389 / 1548	6146 / 1695
Data/restraints/ parameters	145	73	75	74
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.662; –1.182	0.885; –0.653	0.538; –0.775	1.179; –2.195
$R[F^2 > 4\sigma(F^2)]$	0.0414	0.0413	0.0287	0.0191
w$R(F^2)$	0.0902	0.0748	0.0613	0.0413
Goodness-of-fit, S	0.902	0.800	0.880	0.871

Table S1. Continued.

	(**3IPy**HCl)$_2$ H_2O	**3IPy**HCl	**3IPy**HBr	**3IPy**HI
Molecular formula	$C_{10}H_{12}N_2I_2Cl_2O$	C_5H_5NICl	C_5H_5NIBr	$C_5H_5NI_2$
M_r	500.92	241.45	285.91	332.90
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	P –1	P 2/c	P 2_1/c	P 21/c
Crystal data:				
a / Å	8.0102(9)	10.5864(11)	4.5838(2)	4.6289(2)
b / Å	8.0918(10)	4.3468(5)	14.8642(5)	15.1319(8)
c / Å	14.0480(18)	15.0822(14)	10.6931(3)	11.0844(9)
α / °	90.722(10)	90	90	90
β / °	99.454(10)	90.518(8)	91.693(3)	91.478(7)
γ / °	119.570(13)	90	90	90
V / Å^3	776.53(19)	694.01(13)	728.25(5)	776.14(8)
Z	2	4	4	4
D_{calc} / g cm^{-3}	2.142	2.311	2.608	2.561
λ(MoK_α) / Å	0.71073	1.54184	0.71073	0.71073
T / K	295	295	295	295
Crystal size / mm^3	0.28 x 0.16 x 0.12	0.12 x 0.08 x 0.08	0.62 x 0.20 x 0.22	0.48 x 0.28 x 0.12
μ / mm^{-1}	4.381	38.942	9.782	8.009
F(000)	468	448.0	520	592
Refl. collected/unique	5112 / 3240	2838/1271	8044 / 1565	4872 / 1683
Data/restraints/ parameters	163	73	73	78
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.817; –0.840	1.530;-1.333	0.838; –1.093	1.228; –1.566
$R[F^2 > 4\sigma(F^2)]$	0.0297	0.0506	0.0290	0.0310
w$R(F^2)$	0.0687	0.1498	0.0651	0.0803
Goodness-of-fit, S	0.910	1.116	0.900	0.924

Table S1. Continued.

	4IPyHCl	**4IPy**HBr	**4IPy**HI
Molecular formula	C_5H_5NICl	C_5H_5NIBr	$C_5H_5NI_2$
M_r	241.45	285.91	332.90
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P\,2_1/m$	$P\,2_1/m$	P 21/c
Crystal data:			
a / Å	4.3369(8)	4.3789(3)	4.57920(10)
b / Å	8.4079(17)	8.5332(7)	21.7962(6)
c / Å	9.736(2)	9.9405(6)	8.1293(3)
α / °	90	90	90
β / °	94.120(18)	95.160(6)	101.885(3)
γ / °	90	90	90
V / Å^3	354.10(12)	369.93(5)	793.99(4)
Z	2	2	4
D_{calc} / g cm^{-3}	2.265	2.567	2.785
λ(MoK_α) / Å	0.71073	0.71073	0.71073
T / K	295	295	295
Crystal size / mm^3	0.22 x 0.14 x 0.12	0.36 x 0.12 x 0.08	0.66 x 0.42 x 0.36
μ / mm^{-1}	4.794	9.629	7.829
F(000)	224	260	592
Refl. collected/unique	1860 / 810	1659 / 855	12719 / 1717
Data/restraints/ parameters	44	30	61
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	3.451; –1.548	1.574; –2.093	0.808; –0.610
$R[F^2 > 4\sigma(F^2)]$	0.0811	0.0570	0.0281
w$R(F^2)$	0.2298	0.1573	0.0618
Goodness-of-fit, S	1.089	1.063	0.903

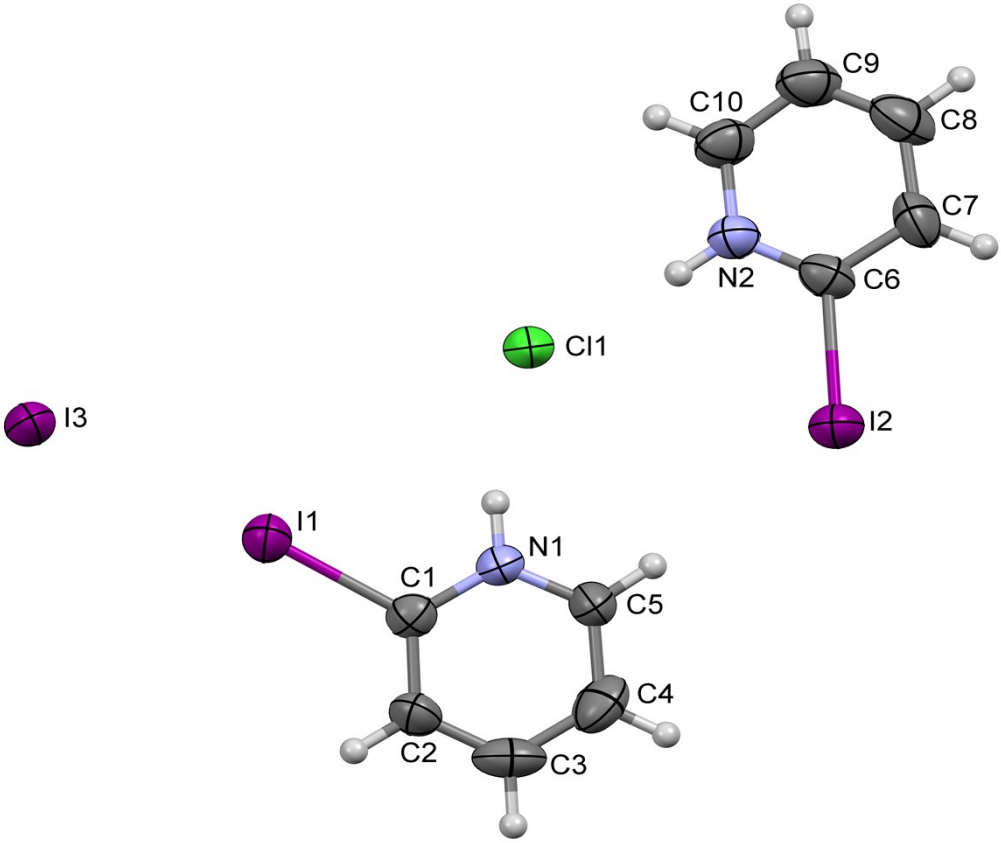

Figure S1. Ortep plot of the asymmetric unit of (**2IPy**H^+)$_2$(Cl^-)(I^-) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

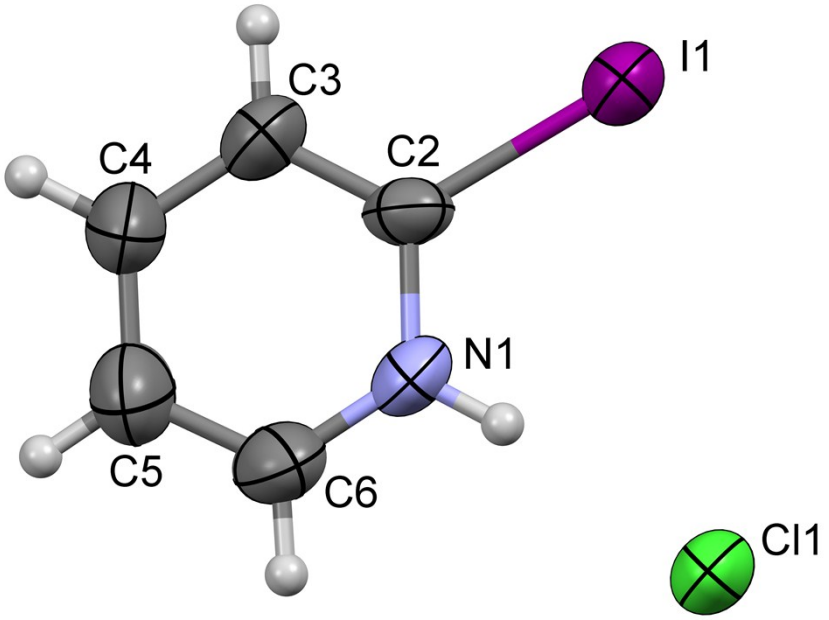

Figure S2. Molecular structure of **2IPy**HCl showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

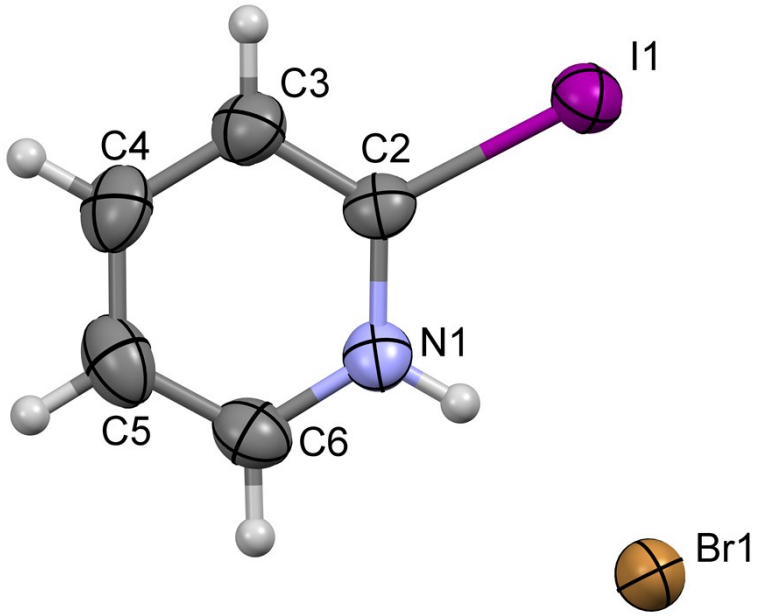

Figure S3. Molecular structure of **2IPy**HBr showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

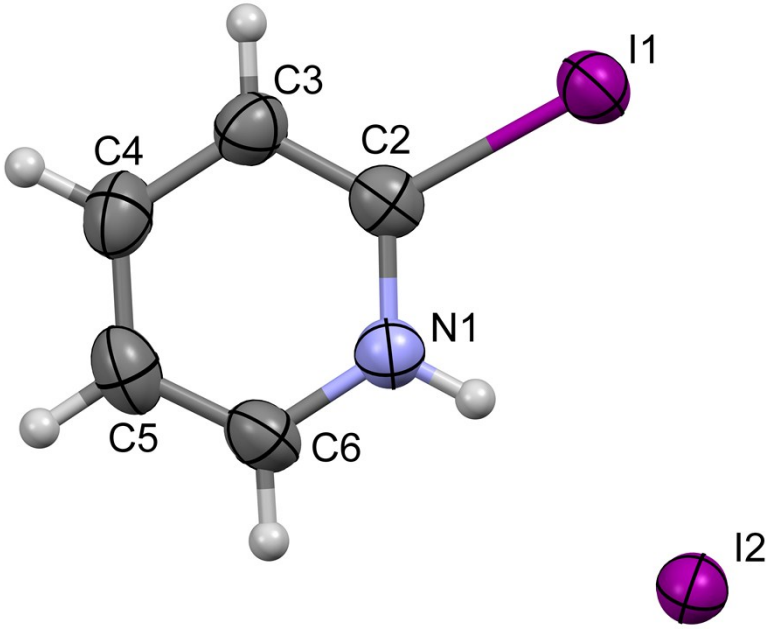

Figure S4. Molecular structure of **2IPy**HI showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

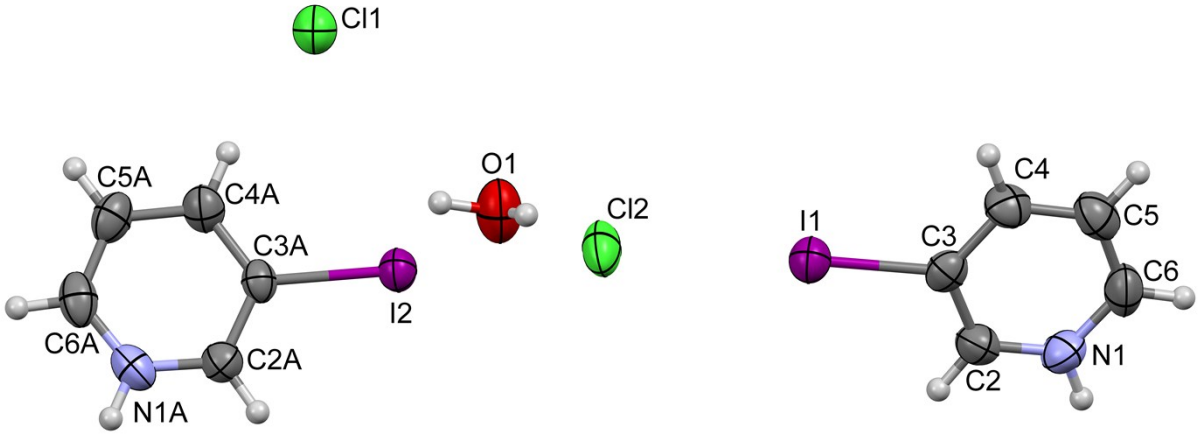

Figure S5. Molecular structure of (**3IPy**HCl)$_2$ H_2O showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

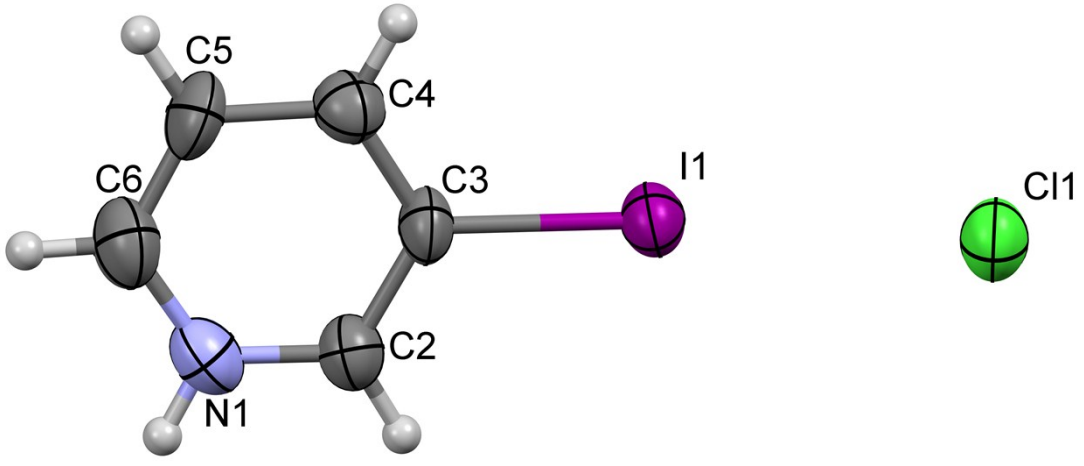

Figure S6. Molecular structure of **3IPy**HCl showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

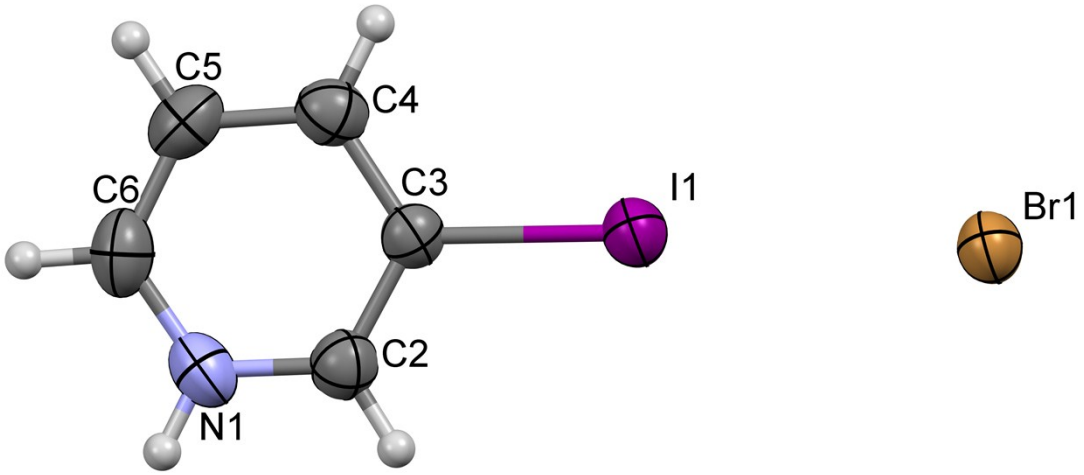

Figure S7. Molecular structure of **3IPy**HBr showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

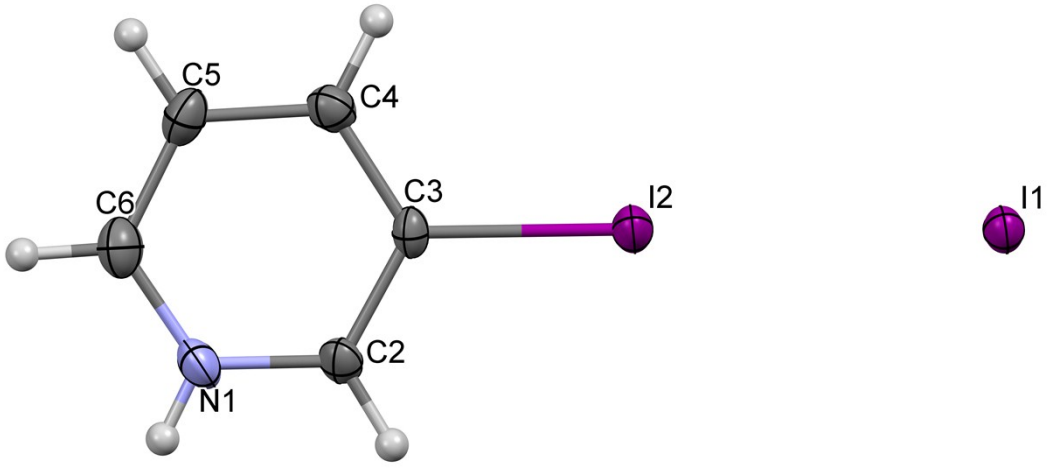

Figure S8. Molecular structure of **3IPy**HI showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

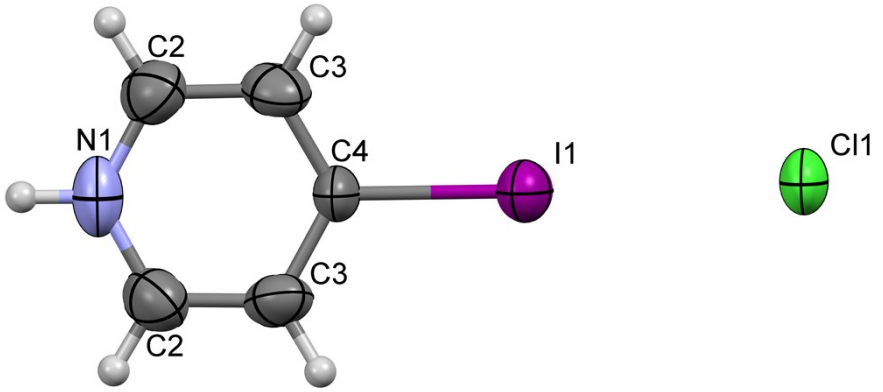

Figure S9. Molecular structure of **4IPy**HCl showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

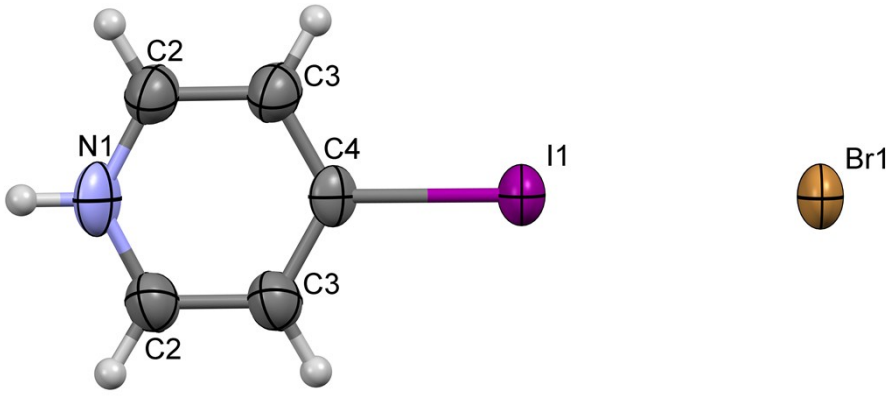

Figure S10. Molecular structure of **4IPy**HBr showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

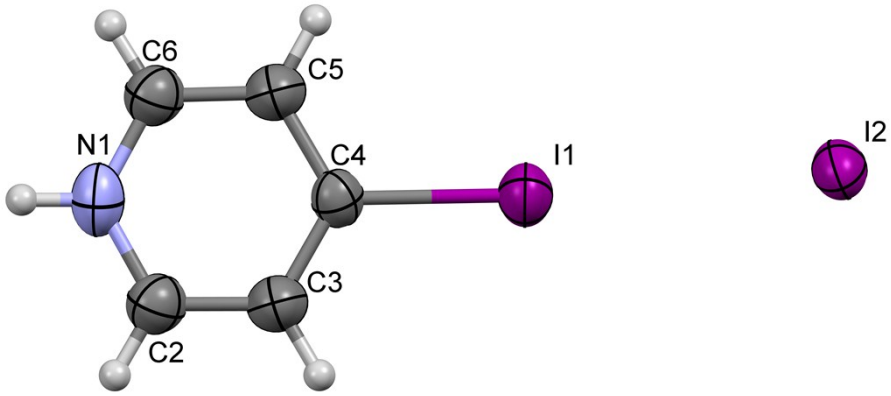

Figure S11. Molecular structure of **4IPy**HI showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50 % probability level, and H atoms are shown as small spheres of arbitrary radius.

Table S2. Hydrogen and halogen bond lengths, the corresponding relative shortening (*R.S.*) and angles in studyed iodopyridinium halogenides. (X = Cl^-, Br^-, I^-; *R.S.* (XB) = *R.S.* = 100 * $d(X^{-}\cdots I/N)/[r_{ion}(X^-) + r_{vdw}(I/N)]$)

Salt	d(C−I···X^-) / Å	*R.S.* (XB)[a] / %	∠(C−I···X^-) / °	d(N···X^-) / Å	*R.S.* (HB)[a] / %	∠(N−H···X^-) / °
2IPHCl	3.122	82,4	176.4	3.003	89,4	172.8
3IPHCl	3.267	85,5	174.7	3.173	90,3	165.1
4IPHCl	3.467	85,7	174.8	3.405	89,3	165.6
2IPHBr	3.240	83,1	171.83	3.033	90,7	160.33
3IPHBr	3.373	85,8	175.0	3.280	93,7	144.2
4IPHBr	3.516	85,3	176.4	3.503	90,9	146
2IPHI	3.248	83,7	166.8	3.00	91,8	179
3IPHI	3.352	84,9	170.8	3.182	94,4	175.5
4IPHI	3.533	85,3	176.1	3.510	94,6	153.6
(**3IP**HCl)$_2$ H_2O	3.165, 3.144	83.0, 83.5	174.8, 171.3	3.046, 3.058	90.7, 91.0	164.2, 160.7
(**2IPH**$^+$)$_2$(Cl^-)(I^-)	3.434, 3.514	82.9, 84.9	172.3, 163.7	3.011, 3.050	89.6, 90.8	157.7, 158.2

Weak C−H···X^- hydrogen bonds in presence of C/N−I···X^- halogen bond (X = Cl^-, Br^-, I)

We also made study on the simultaneous presence of weak C−H···X^- hydrogen and C/N−I···X^- halogen bond without presence of strong N/O−H···X^- hydrogen bonds, and have thus performed a CSD survey of structures which comprise a halogenide anion (chloride, bromide or iodide), and both C−H···X^- hydrogen bond and C/N−I···X^- halogen bond. Our search has yielded a total of 80 structures satisfying the above conditions which contained chloride, 89 with bromide and 179 with iodide. A search was also made for structures containing fluoride but, as only three datasets were recovered, it was excluded from further analysis.

On the one hand, as we can see from scatterplot of the HB angle *vs.* the percentage HB shortening (Fig. 12), there is no significant change in the weak C−H···X− hydrogen bond lengths with halogenide size. On the other hand, N/C−I···Cl^- halogen bonds in these structures are relatively shorter than halogen bonds with larger halogenide anions (Fig. 13). This trend is in agreement with the trend in case of simultaneous C/N−I···X^- halogen bonds and strong N/O−H···X^- hydrogen bonds, both established from our structures of iodopyridium halogenides and from CDS survey.

It can also be noticed that most of the angles between C−H···X^- contacts and C−I···X^- halogen bonds ((∠(I···X^-···H)) in these systems have values lower than 120° (Fig. 14). Since halogen bond is the strongest supramolecular interaction in these systems, these C−H···X^- supramolecular contacts can be classified as outcome of the close packing of the molecules.

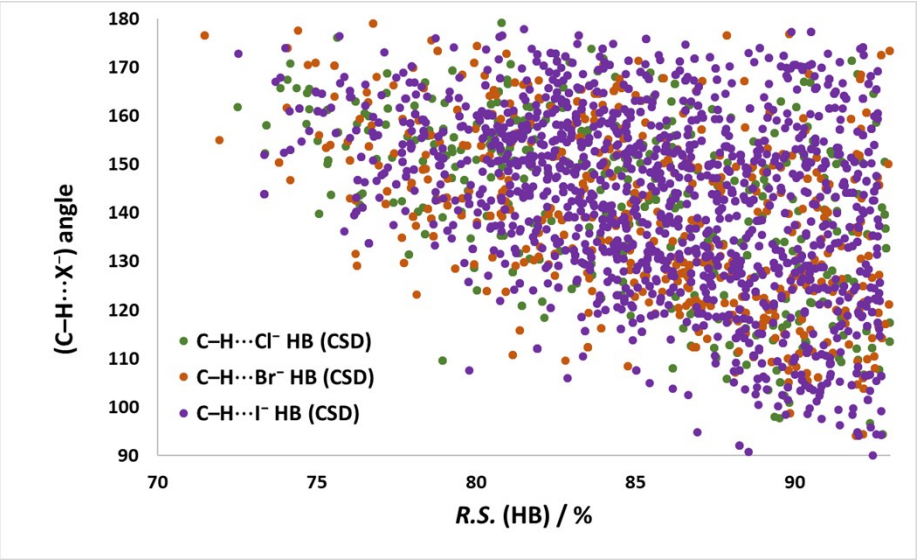

Figure S12. Scatterplot of the HB angle *vs.* the percentage HB shortening (*R.S.* / % = 100(d(C···X$^-$)/[r(C) + r(X$^-$)]) where r_{vdw}(N) and r_{ion}(X$^-$) are the radii of HB donor and acceptor.

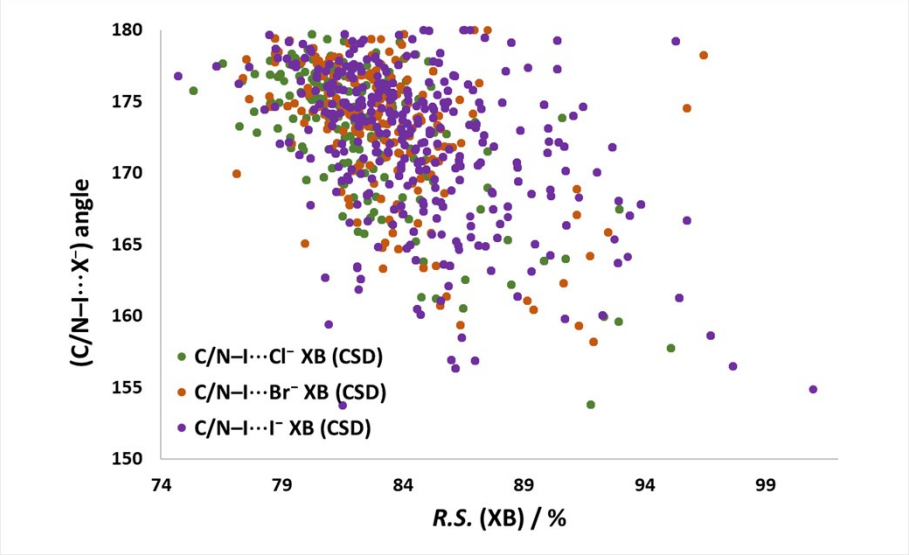

Figure S13. Scatterplot of the XB angle *vs.* the percentage XB shortening (*R.S.* / % = 100(d(I···X$^-$)/[r(I) + r(X$^-$)]) where r_{vdw} (I) and r_{ion} (X$^-$) are the radii of XB donor and acceptor. Y is defined as carbon or nitrogen.

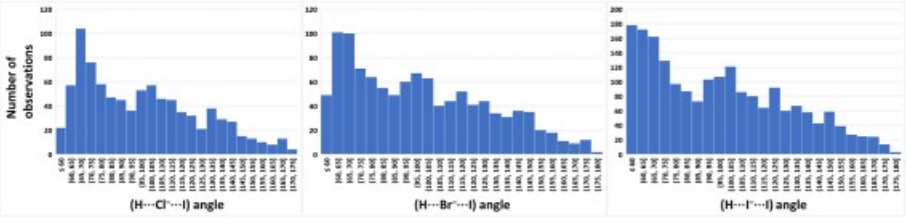

Figure S14. Distribution of angles between C-H···X$^-$ hydrogen and C-I···X$^-$ halogen bonds (X = Cl, Br, I)

Table S3. Refcodes of datasets from CSD comprising C−H···X$^-$ hydrogen bond and C/N−I···X$^-$ halogen bonds with corresponding geometrical parameters used for analysis (X = Cl, Br, I)

Chlorides		Bromides		Iodides			
ACEYAL	MUKJEJ	ACEXAK	IFIGEL	ABIHAU	GEPHAN	NEMYAI	SILRIR
ACEYUF	OHOVUD	ACEXEO	IFOHOC	ACEXOY	GUYNEV	NEMYEM	SUFLUC
ACEZUG	PAVZIV	ACEXIS	ISUNUH	ACEXUE	GUYNUL	NEMYIQ	SUSSOQ
ACIBAS	PAWBIY	ACEYIT	KAQSIG	ACEYOZ	HARXAZ	NEMYUC	TACPOE
ACIPIO	PESRUC	ACEZEQ	LOFDAM	ACEZIU	HEDGOM	NUKQIU	TEHQUT
ACIPOU	PUPLOD	ACIBEW	LOFDIU	ACEZOA	HEFCAW	NUKQOA	TEHRAA
ACIPUA	PUPZIL	ACICIB	NEDPAP	ACICAT	HEJLIR	NUKQUG	TEMJIG
AHUKIX	QAQSAF	ACIQAH	OHOWAK	AFEHAW	HIHXOO	NUPPEV	TEMJUS
AHULEU	QEHTEC	AHUKET	ORAVEK	AKIDEF	HINXEH	NUPPIZ	UDIPEE
AHULUK	RECSOJ	AHUKOD	PAVZOB	ANULIG	HIZFAZ	NUPPOF	UGULAK
BUYYAX	RENGUM	AHULIY	PAWBAQ	ASEWUS	HOBFEL	NUZKIC	UTOTUU
BUYYOL	SARMAC	AHULOE	PAWBOE	AYAWED	ICIKOW	OJIKAT	UVOJUM
CUJTIM	SASFAW	CUJTUY	PESREM	BEFVAL	ICIKUC	OJILIE	VOQLEV
CUJTOS	SERVIW	DAKVAO	PESRIQ	BEFVIT	ICOVEC	OMOPEN	VOQLIZ
DAKVES	SILREN	DAMPAK	PETTOZ	BIZVOX	IDIPUI	ONACOX	VOQLOF
DAMNOW	SIVYEC	DIQHET	PETVAN	BIZVUD	IDOSEB	ONACUD	VOQLUL
DATCOS	TACPIY	DIQHIX	PUPZEH	BURDID	IFOHES	ONADAK	VUFXUP
DATCUY	TUSCUH	DPIODB10	QAXXAQ	CAWSOJ	IFOHIW	ONADEO	WAWSIZ
DPIOCL	ULEKUT	EHOGIR	QEHTIG	CIZRUZ	IFOJAQ	ORATUY	WEDNOJ
EQUDUR	UYITAZ	EQUDOL	RIPQUE	CIZSAG	IHUQUX	ORAVIO	WOCTEQ
FOSGIF	VIBPEC	FEXYOY	SARLUV	CIZSEK	IHURAE	PESNUY	WODWIY
FOSGOL	WAWTAS	FICCAY	SILRAJ	CIZSIO	ISUPOD	PESRUA	WOMZOQ
FOSGUR	WEJZAN	FOFBOT	TACPEU	CIZSOU	IZAPEF	PIMCYP10	XAJVEM
FUBFAK	WEJZER	FOMYAJ	TACPUK	CIZSUA	IZAPIJ	POBTIM	XEBJIA
GIXFOI	WOMZUW	FOMYEN	TEMWIU	CODCEE	JEMKES	POBVEK	XEBJOG
GIXGAV	YUWJUX	FORDEX	TIDPOO	CODCII	JEMKIW	POKCIB	XEZREB
GODQAT	YUWKIM	FOSHAY	VIPQAP	CUNYEQ	JOHGAQ	PUJRAP	XONBUA
GUHYOZ	ZOVXAL	FOSHEC	WEJYUG	DAHKON	JUTXAZ	PUYBOC	XONCIP
GUYPEX		GARXAB	XERZID	DAMNUC	KAQSEC	QECYIJ	XONCUB
GUYPIB		GARYEG	XERZOJ	DAXGIT	KAZXIU	QEDCUA	XOTZOW
HEBWIV		GEWXAK	XERZUP	DOXTOA	KAZXOA	QEHTOM	XOVBEQ
HEBWUH		GIXFUO	XIVHUI	EDOTOH	KAZXUG	QEJTUX	XOVBOA
HEBXES		GIXGEZ	XOZBET	EHOGOX	KAZYAN	QIDTON	XOZBOD
HEBXUI		GIXGID	XOZBIX	EPIWOR	KAZYER	QIRZEY	XUPVIO
HIHXUU		HEBWOB	XULKEW	EPIWUX	KEWMIL	QIVTEW	YAMYUH
ICIROE		HEBXAO	YIHDIF	EPIXAE	KOBYIM	ROHPUZ	YODVUK
ISUNOB		HEBXIW	YILJIO	EQUJOR	KOFPUS	SAMXIQ	YODWEV
KABRUB		HEBXOC	YUVRAK	FASHAI	LINVEL	SARLIJ	YUVREO
LOFDEQ		HIHYIJ	YUWKEI	FASLEQ	LOFFUJ	SARLOP	YUWKAE
LOFDOA		IFIFUA	ZOMNEU	FASMIV	MAHBUU	SEZWAW	YUWKOS
				FASMOB	MAHCAB	SIHYOZ	ZOMWIH
				FIJBEG	MUHYUJ	SIHYUF	ZOYHAW
				FOMXUC			

Table S4. Dataset refcodes from CSD comprising O/N−H···X^- hydrogen bonds and C/N−I···X^- halogen bonds with corresponding geometrical parameters used for analysis (X = Cl, Br, I)

Chlorides			**Bromides**		**Iodides**		
ACEYAL	GEHFOR	PUPZIL	ACEXAK	MIRPIP	ABIHAU	GUYNOF	OXIVUN
ACEYUF	GUGNIG	QIQGEE	ACEXEO	MIRQEM	ACEXOY	GUYPAT	OXIWAU
ACEZUG	GUYPEX	QUNCLE	ACEYIT	PETTUF	ACIBIA	HIHXII	PESRUA
ACIBAS	HASQOJ	ROPYIH	ACEZAM	POPXAV	ACIBOG	HIHXOO	QIDTIH
BAGWUD	HEBXUI	RUWVUB	ACIBEW	PUPZEH	ACICAT	ICOVEC	QIDTON
BEXPOL	HOHVUY	RUWWIQ	AQUROV	QIQGAA	ACICEX	IDOSEB	QQQAHJ
BEXPUR	HOVVOF	SATJIG	CABWIL	SITRIZ	ACUTEZ	IFULEC	SAYTAP
BEXQAY	IDMEAN	TITYRN	CABXAE	SUPSON	ADOTES	ISUPET	TINMAF
BURCOI	IFUTEJ	ULEKUT	CACBOX	SUPSUT	AJENAG	IXOHOU	UFAJIU
BURDAV	IPLTYR10	VEXNAN	CACCIS	SUPTAA	CEWPIG	KAZYIV	UFAKAN
BURDUP	ISUPIX	VIDHEY	COGFAH	SUPTEE	CIZRUZ	KAZYOB	UGULAK
BURGAY	IZOLAM	VOCTOY	CUJTUY	SUPTII	CUJVAG	KAZYUH	UWEMUF
BUYYOL	JAQNAR	WOQREB	CUNXUF	SUPTOO	DAHKON	LIBSIZ	VEGTUY
BUZSOG	KAQSOM	WOQRIF	FORDEX	TACPUK	DAQMEN	MAZDAV	VIHFEY
CILZIJ	KEFNIU	WUWMAD	GINHAN	VIXKUK	DIQZOS	MICJEO	VOQLOF
COWTEN	KOBYEI	WUWMUX	GUHCAO	VOCTIS	DIZNUW	MIRQIQ	VOQLUL
CUJTOS	LOFDEQ	WUWNAE	HASQUP	WUWMEH	DOXTOA	NEMYAI	WARKIM
CUNYAM	LTYRXC	XEBRON	HEBWOB	XIVHUI	EPIWOR	NEMYEM	WEDNOJ
DATDAF	MEJKOB	XEZRAX	HIHYEF	XOGPER	EPIWUX	NEMYIQ	XALHEA
DUTRUF	MIDLTY	XOGPIV	HIHYIJ	YORZUC	EPIXAE	NEMYUC	XIDFUN
EPAZIF	MIRQAI	XUCLAK	JILKIB		ETIDUI	OHOVAJ	XIQNOB
EQOWAJ	MIRXOD	ZZZNXS	KOBZAF		GUYNEV	OHOVOX	YAMYUH
FOFBIN			MAHCEF		GUYNIZ	OJILIE	YICJUR

Table S5. Datasets from CSD comprising O/N−H···Cl^- hydrogen bonds and C/N−I···Cl^- halogen bonds with corresponding geometrical parameters used for analysis

Refcode	*ANG1 (A)*	*ANG2 (A)*	*ANG3 (A)*	*DIST1 (D)*	*DIST2 (D)*
BEXPOL	170,227	177,814	145,024	2,323	3,211
BEXPOL	170,227	111,991	88,08	2,323	4,037
BEXPOL	170,262	177,814	105,296	2,277	3,211
BEXPOL	170,262	111,991	155,399	2,277	4,037
BEXPOL	64,229	177,814	117,377	3,338	3,211
BEXPOL	64,229	111,991	148,894	3,338	4,037
BEXPOL	158,557	177,814	107,829	2,268	3,211
BEXPOL	158,557	111,991	75,714	2,268	4,037
BURCOI	172,248	166,272	90,914	2,279	3,436
BURCOI	157,907	166,272	67,472	2,394	3,436
BURCOI	171,616	166,272	164,829	2,311	3,436
BURDAV	172,213	168,01	118,885	2,253	3,249
BURDUP	158,787	176,373	71,704	2,461	3,23
BURDUP	158,787	177,217	126,259	2,461	3,318
BURDUP	172,972	176,373	141,368	2,27	3,23
BURDUP	166	173,694	115,049	2,382	3,14
BURDUP	168,759	173,694	78,107	2,413	3,14
BURDUP	172,972	177,217	125,121	2,27	3,318
BURDUP	166	172,063	170,987	2,382	3,563
BURDUP	168,759	172,063	114,689	2,413	3,563
BURGAY	171,308	172,505	78,635	2,323	3,313
BURGAY	86,09	172,505	141,502	3,187	3,313
BURGAY	141,122	172,505	164,295	2,514	3,313
CILZIJ	164,966	178,453	76,24	2,213	3,159
CILZIJ	164,966	176,091	99,557	2,213	3,163
CILZIJ	164,253	178,453	102,349	2,401	3,159
CILZIJ	164,253	176,091	83,601	2,401	3,163
CUJTOS	164,792	174,411	125,094	2,612	3,109
CUJTOS	164,792	167,466	67,889	2,612	3,305
CUJTOS	165,131	174,411	113,817	2,628	3,109
CUJTOS	165,131	167,466	72,336	2,628	3,305
CUNYAM	162,836	157,885	149,826	2,378	3,457
CUNYAM	171,148	157,885	68,529	2,424	3,457
DATDAF	168,996	173,805	93,774	2,249	3,219
DATDAF	173,089	173,805	113,28	2,282	3,219
DUTRUF10	172,312	167,422	96,95	2,459	3,249
EPAZIF	176,615	174,294	92,949	2,391	3,23
EPAZIF	176,615	174,108	106,332	2,391	3,222
EPAZIF	171,964	174,294	132,084	2,303	3,23
EPAZIF	171,964	174,108	87,73	2,303	3,222
EQOWAJ	172,991	172,698	89,433	2,47	3,37
EQOWAJ	179,026	172,698	67,209	2,512	3,37
EQOWAJ	176,381	172,698	133,122	2,514	3,37
FOFBIN	170,449	168,572	108,595	2,148	3,119

FOFBIN	170,449	173,08	108,635	2,148	3,138
FOFBIN	170,449	159,021	87,394	2,148	3,388
GEHFOR	148,797	176,812	141,708	2,267	3,344
GUGNIG	160,734	158,871	146,541	2,119	3,458
HASQOJ	164,308	175,894	83,512	2,289	3,33
HASQOJ	164,308	91,845	63,006	2,289	4,016
HASQOJ	155,744	175,894	79,542	2,36	3,33
HASQOJ	155,744	91,845	48,045	2,36	4,016
HASQOJ	173,606	175,894	168,65	2,201	3,33
HASQOJ	173,606	91,845	67,589	2,201	4,016
HASQOJ	171,121	175,894	90,058	2,271	3,33
HASQOJ	171,121	91,845	157,596	2,271	4,016
HOHVUY	154,475	169,284	150,757	2,302	3,349
HOHVUY	149,034	169,284	129,09	2,251	3,349
HOVVOF	149,996	161,945	159,775	2,354	3,634
HOVVOF	155,399	161,945	135,314	2,353	3,634
IFUTEJ	160,021	177,128	80,33	2,434	3,208
IFUTEJ	170,036	177,128	166,842	2,382	3,208
IFUTEJ	134,039	177,128	69,743	2,75	3,208
ISUPIX	155,348	176,825	109,804	2,315	3,417
ISUPIX	143,221	176,825	140,752	2,472	3,417
IZOLAM	164,694	175,884	167,717	2,157	3,172
IZOLAM	100,53	171,08	99,605	3,307	3,195
IZOLAM	166,064	171,08	76,436	2,246	3,195
IZOLAM	159,421	171,08	140,433	2,219	3,195
IZOLAM	148,546	175,884	112,992	2,322	3,172
JAQNAR	153,376	169,487	126,969	2,325	3,331
JAQNAR	153,376	169,487	99,127	2,325	3,331
KAQSOM	169,45	174,135	97,952	2,392	3,023
KAQSOM	169,45	60,189	136,195	2,392	3,937
KAQSOM	168,414	174,135	131,012	2,411	3,023
KAQSOM	168,414	60,189	73,458	2,411	3,937
KEFNIU	165,197	171,302	89,457	2,165	3,506
KEFNIU	164,254	171,452	91,618	2,185	3,573
KEFNIU01	159,069	171,313	93,344	2,172	3,569
KEFNIU01	160,351	171,005	91,973	2,189	3,508
MEJKOB	158	178,801	124,808	2,475	3,354
MEJKOB	158	173,284	117,83	2,475	3,386
MEJKOB	155,111	178,801	121,947	2,493	3,354
MEJKOB	155,111	173,284	123,635	2,493	3,386
MEJKOB	134,416	178,801	69,062	2,695	3,354
MEJKOB	134,416	173,284	131,639	2,695	3,386
MEJKOB	124,345	178,801	126,513	2,835	3,354
MEJKOB	124,345	173,284	66,51	2,835	3,386
MEJKOB	94,507	178,801	154,879	3,259	3,354
MEJKOB	94,507	173,284	69,475	3,259	3,386
MIRQAI	171,044	175,491	95,737	2,157	3,137
MIRXOD	158,706	176,598	94,077	2,198	3,022

QIQGEE	164,306	171,12	125,584	2,222	3,353
QIQGEE	148,727	171,12	101,812	2,298	3,353
QIQGEE	110,867	171,12	72,786	3,293	3,353
QIQGEE	166,501	171,12	80,808	2,462	3,353
ROPYIH	151,94	151,067	82,942	2,27	3,763
ROPYIH	164,004	151,067	176,33	2,213	3,763
RUWVUB	162,876	175,628	96,108	2,275	3,221
RUWVUB	162,876	168,67	107,792	2,275	3,289
RUWVUB	127,746	172,641	118,214	3,244	3,128
RUWVUB	127,746	170,513	94,797	3,244	3,216
RUWVUB	151,687	171,804	115,786	2,233	3,229
RUWVUB	151,687	173,858	101,136	2,233	3,159
RUWVUB	154,095	172,641	75,357	2,308	3,128
RUWVUB	162,453	172,641	76,38	2,386	3,128
RUWVUB	145,283	171,804	112,193	2,421	3,229
RUWVUB	154,095	170,513	119,47	2,308	3,216
RUWVUB	162,453	170,513	127,997	2,386	3,216
RUWVUB	145,283	173,858	104,289	2,421	3,159
RUWWIQ	173,622	178,207	110,877	2,264	3,117
RUWWIQ	166,294	179,778	114,277	2,246	3,087
RUWWIQ	177,848	178,207	120,425	2,329	3,117
RUWWIQ	178,454	179,778	110,767	2,307	3,087
RUWWIQ	179,219	179,778	73,709	2,356	3,087
SATJIG	169,728	166,131	128,309	2,223	3,361
SATJIG	72,63	166,131	157,422	3,225	3,361
SATJIG	149,559	166,131	135,04	2,236	3,361
ULEKUT	153,803	173,088	76,46	2,623	2,987
ULEKUT	153,922	173,088	95,824	2,607	2,987
ULEKUT	110,308	173,088	145,558	3,139	2,987
VEXNAN	152,869	171,649	110,993	2,251	3,363
VEXNAN	139,201	171,649	114,744	2,335	3,363
VEXNAN	69,935	171,649	122,968	3,312	3,363
VEXNAN	150,371	171,649	87,453	2,337	3,363
VIDHEY	176,927	169,324	71,101	2,312	3,489
VIDHEY	155,177	169,324	143,3	2,356	3,489
VOCTOY	172,111	177,838	117,409	2,167	3,109
VOCTOY	172,111	71,58	44,381	2,167	4,065
VOCTOY	162,363	177,838	111,664	2,221	3,109
VOCTOY	162,363	71,58	132,324	2,221	4,065
WOQREB	168,171	164,847	168,959	2,113	3,342
WOQREB	162,981	176,249	167,217	2,158	3,367
WOQRIF	174,835	160,383	78,258	2,131	3,422
WUWMAD	173,885	169,806	86,528	2,186	3,405
WUWMAD	158,641	169,806	139,899	2,238	3,405
WUWMAD	168,868	169,806	94,344	2,151	3,405
WUWMAD	68,06	169,806	127,307	3,326	3,405
WUWMUX	174,317	174,597	131,705	2,325	3,223
WUWMUX	178,607	174,597	141,201	2,359	3,223

WUWNAE	164,937	116,351	73,251	2,166	3,977
WUWNAE	163,011	113,025	75,686	2,182	3,957
WUWNAE	149,41	116,351	67,976	2,252	3,977
WUWNAE	145,946	113,025	66,625	2,29	3,957
WUWNAE	111,898	177,278	100,487	2,9	3,141
WUWNAE	111,898	174,265	74,732	2,9	3,189
WUWNAE	109,317	179,718	97,432	2,988	3,17
WUWNAE	109,317	173,751	74,459	2,988	3,227
WUWNAE	97,138	177,278	98,946	3,035	3,141
WUWNAE	97,138	174,265	80,392	3,035	3,189
WUWNAE	96,063	179,718	99,89	3,083	3,17
WUWNAE	96,063	173,751	77,303	3,083	3,227
WUWNAE	173,662	179,718	113,244	2,377	3,17
WUWNAE	173,662	173,751	72,593	2,377	3,227
XEBRON	161,573	153,175	102,745	2,48	3,628
XEBRON	161,573	153,175	66,527	2,48	3,628
XEBRON	146,272	153,175	140,558	2,64	3,628
XEBRON	146,272	153,175	57,841	2,64	3,628
XEZRAX	179,757	177,637	112,349	2,332	2,948
XEZRAX	179,58	177,637	168,715	2,394	2,948
XOGPIV	152,554	159,877	96,119	2,535	3,332
XOGPIV	151,845	149,479	106,235	2,235	3,162
XOGPIV	161,216	159,877	100,902	2,329	3,332
XOGPIV	154,719	137,369	88,853	2,528	3,487
XOGPIV	158,136	172,061	107,515	2,27	3,118
XOGPIV	156,736	137,369	109,088	2,419	3,487
XOGPIV	168,291	149,479	162,411	2,146	3,162
XOGPIV	127,712	137,369	100,792	2,934	3,487
XOGPIV	172,199	159,877	156,076	2,139	3,332
XOGPIV	119,343	172,061	145,554	2,925	3,118
XOGPIV	133,64	172,061	150,007	2,283	3,118
XOGPIV	115,84	159,877	97,233	3,16	3,332
XOGPIV	130,284	137,369	147,046	2,405	3,487
XOGPIV	121,605	149,479	151,888	3,174	3,162
XOGPIV	151,201	159,877	107,194	2,449	3,332
XOGPIV	149,64	137,369	99,669	2,37	3,487

Table S6. Datasets from CSD comprising O/N−H···Br^- hydrogen bonds and C/N−I···Br^- halogen bonds with corresponding geometrical parameters used for analysis

Refcode	*ANG1 (A)*	*ANG2 (A)*	*ANG3 (A)*	*DIST1 (D)*	*DIST2 (D)*
ACEXAK	175,36	173,075	89,022	2,534	3,224
ACEXAK	175,912	173,175	88,906	2,542	3,225
ACEXAK	175,36	175,178	75,203	2,534	3,263
ACEXAK	175,912	175,142	74,902	2,542	3,264
ACEZAM	164,451	170,963	131,998	2,363	3,318
ACEZAM	164,451	169,149	140,516	2,363	3,271
ACEZAM	164,451	171,666	126,102	2,363	3,328
ACEZAM	161,803	174,035	91,148	2,44	3,23
ACEZAM	161,803	170,735	156,199	2,44	3,316
ACEZAM	161,803	167,381	127,219	2,44	3,365
ACEZAM	145,432	169,149	110,726	2,401	3,271
ACEZAM	145,432	171,666	146,134	2,401	3,328
ACEZAM	166,541	171,645	120,049	2,479	3,246
ACEZAM	166,541	170,743	143,318	2,479	3,247
ACEZAM	166,541	167,039	122,933	2,479	3,327
ACEZAM	145,432	170,963	136,763	2,401	3,318
AQUROV	153,197	172,927	81,127	2,605	3,288
AQUROV	167,926	172,927	110,461	2,517	3,288
CABWIL	169,5	163,995	106,032	2,365	3,736
CABWIL	162,392	169,138	100,431	2,525	3,705
CABXAE	166,908	164,074	100,336	2,346	3,599
CABXAE	161,849	168,136	97,702	2,389	3,628
CACBOX	172,693	160,094	102,766	2,355	3,785
CACCIS01	152,402	163,265	104,335	2,417	3,658
CUJTUY	148,01	173,068	123,462	2,818	3,178
CUJTUY	148,01	170,835	60,929	2,818	3,359
CUJTUY	161,079	173,068	112,141	2,755	3,178
CUJTUY	161,079	170,835	73,241	2,755	3,359
CUNXUF	169,959	166,229	138,798	2,614	3,465
CUNXUF	74,972	166,229	127,17	3,446	3,465
CUNXUF	171,997	166,229	71,299	2,601	3,465
FORDEX	158,618	174,261	139,198	2,604	3,154
FORDEX	158,618	177,84	81,114	2,604	3,165
FORDEX	155,458	175,561	87,701	2,59	3,179
FORDEX	155,458	177,668	133,348	2,59	3,161
GINHAN	172,366	148,015	79,707	2,531	4,059
GINHAN	172,366	115,888	115,528	2,531	4,201
GINHAN	167,637	148,015	57,22	2,611	4,059
GINHAN	167,637	115,888	55,848	2,611	4,201
GINHAN	174,139	148,015	59,281	2,646	4,059
GINHAN	174,139	115,888	56,367	2,646	4,201
HASQUP	74,152	175,666	67,58	3,431	3,465
HASQUP	74,152	93,191	61,246	3,431	4,193
HASQUP	150,285	175,666	81,755	2,523	3,465

HASQUP	150,285	93,191	48,183	2,523	4,193
HASQUP	148,274	175,666	87,249	2,492	3,465
HASQUP	148,274	93,191	63,271	2,492	4,193
HASQUP	162,416	175,666	163,163	2,422	3,465
HASQUP	162,416	93,191	62,787	2,422	4,193
HASQUP	166,815	175,666	93,961	2,371	3,465
HASQUP	166,815	93,191	154,325	2,371	4,193
KOBZAF	171,709	167,182	110,162	2,416	3,407
KOBZAF	171,709	167,182	69,838	2,416	3,407
KOBZAF	173,485	167,182	103,4	2,354	3,407
KOBZAF	173,485	167,182	76,6	2,354	3,407
MIRPIP	154,701	175,75	90,458	2,36	3,165
MIRQEM	156,932	169,313	87,689	2,469	3,3
QIQGAA	164,633	75,124	64,268	2,427	4,221
QIQGAA	147,086	177,867	80,593	2,673	3,417
QIQGAA	147,086	174,654	115,082	2,673	3,448
QIQGAA	158,957	177,867	133,446	2,55	3,417
QIQGAA	158,957	174,654	62,252	2,55	3,448
QIQGAA	147,646	75,124	80,799	2,743	4,221
QIQGAA	156,157	177,867	71,025	2,642	3,417
QIQGAA	156,157	174,654	93,883	2,642	3,448
QIQGAA	155,389	75,124	150,433	2,26	4,221
QIQGAA	150,455	177,867	86,062	2,53	3,417
QIQGAA	150,455	174,654	86,007	2,53	3,448
SUPSON	168,531	169,637	161,324	2,369	3,316
SUPSON	101,592	169,637	154,38	3,294	3,316
SUPSON	152,548	169,637	109,717	2,704	3,316
SUPSON	128,419	169,637	111,46	2,693	3,316
SUPSUT	108,039	178,759	154,86	3,163	3,322
SUPSUT	155,75	178,759	138,165	2,425	3,322
SUPSUT	135,688	178,759	106,649	2,484	3,322
SUPSUT	150,995	178,759	125,545	2,65	3,322
SUPTAA	145,632	171,74	84,465	2,503	3,305
SUPTAA	105,023	171,74	160,726	3,224	3,305
SUPTAA	95,279	172,257	150,706	3,299	3,367
SUPTAA	171,66	176,519	161,722	2,29	3,339
SUPTAA	152,291	172,257	93,566	2,448	3,367
SUPTAA	165,278	172,257	98,003	2,404	3,367
SUPTAA	148,269	176,519	107,514	2,713	3,339
SUPTAA	141,241	172,257	99,193	2,53	3,367
SUPTAA	119,136	176,519	91,903	2,954	3,339
SUPTAA	108,571	176,493	90,163	3,387	3,319
SUPTAA	153,366	171,74	96,042	2,502	3,305
SUPTAA	163,54	176,493	157,97	2,326	3,319
SUPTAA	99,09	171,74	152,63	3,162	3,305
SUPTAA	150,488	176,493	106,054	2,711	3,319
SUPTAA	168,024	171,74	99,244	2,361	3,305
SUPTEE	124,812	172,077	94,616	3,207	3,325

SUPTEE	124,812	170,481	154,127	3,207	3,336
SUPTEE	158,775	161,672	125,551	2,332	3,306
SUPTEE	142,923	174,194	113,113	2,399	3,322
SUPTEE	131,894	175,338	127,521	2,773	3,382
SUPTEE	154,915	174,194	109,195	2,338	3,322
SUPTEE	120,765	172,077	107,248	3,084	3,325
SUPTEE	120,765	170,481	102,838	3,084	3,336
SUPTEE	137,403	174,194	103,22	2,578	3,322
SUPTEE	162,742	172,077	84,281	2,332	3,325
SUPTEE	162,742	170,481	164,234	2,332	3,336
SUPTEE	156,366	161,672	107,399	2,382	3,306
SUPTEE	147,779	172,077	118,545	2,714	3,325
SUPTEE	147,779	170,481	107,221	2,714	3,336
SUPTEE	126,284	175,338	91,59	2,977	3,382
SUPTEE	134,19	161,672	113,72	2,714	3,306
SUPTEE	162,409	175,338	154,374	2,355	3,382
SUPTII	157,66	170,665	131,055	2,359	3,355
SUPTII	162,324	177,113	148,011	2,319	3,41
SUPTII	172,091	175,053	171,974	2,315	3,265
SUPTII	102,516	177,113	169,648	3,437	3,41
SUPTII	154,758	177,113	117,419	2,454	3,41
SUPTII	156,237	175,053	100,055	2,316	3,265
SUPTII	128,255	177,113	89,968	2,778	3,41
SUPTII	146,215	170,665	106,238	2,491	3,355
SUPTII	97,405	170,665	159,742	3,32	3,355
SUPTII	151,147	170,665	118,486	2,42	3,355
SUPTII	135,978	175,053	102,74	2,72	3,265
SUPTII	123,402	175,053	137,379	3,403	3,265
SUPTOO	169,003	158,813	154,355	2,256	3,274
TACPUK	140,363	165,061	74,953	2,973	3,142
TACPUK	173,003	165,061	77,572	2,64	3,142
VIXKUK	174,306	173,683	141,588	2,491	3,407
VIXKUK	171,637	173,683	120,731	2,628	3,407
VOCTIS	167,458	177,666	111,593	2,333	3,228
VOCTIS	167,458	73,609	127,931	2,333	4,152
VOCTIS	158,108	177,666	115,358	2,356	3,228
VOCTIS	158,108	73,609	39,697	2,356	4,152
WUWMEH	143,696	154,13	104,059	2,519	3,834
WUWMEH	137,694	148,501	107,562	2,581	3,893
WUWMEH	137,694	148,501	72,438	2,581	3,893
WUWMEH	150,67	148,501	84,903	2,608	3,893
WUWMEH	150,67	148,501	95,097	2,608	3,893
WUWMEH	112,29	158,429	84,322	2,895	3,704
WUWMEH	112,29	141,942	105,545	2,895	4,053
WUWMEH	112,244	158,429	106,645	2,957	3,704
WUWMEH	112,244	141,942	66,861	2,957	4,053
WUWMEH	102,563	154,13	97,144	3,015	3,834
WUWMEH	172,4	158,429	85,964	2,361	3,704

WUWMEH	172,4	141,942	84,953	2,361	4,053
WUWMEH	174,713	154,13	85,018	2,387	3,834
WUWMEH	103,581	158,429	91,889	3,015	3,704
WUWMEH	103,581	141,942	95,727	3,015	4,053
WUWMEH	79,172	148,501	80,589	3,359	3,893
WUWMEH	79,172	148,501	99,411	3,359	3,893
WUWMEH	174,001	154,13	84,394	2,35	3,834
WUWMEH	148,96	158,429	88,764	2,629	3,704
WUWMEH	148,96	141,942	96,631	2,629	4,053
WUWMEH	109,996	154,13	106,797	2,91	3,834
WUWMEH	103,596	158,429	97,879	3,077	3,704
WUWMEH	103,596	141,942	79,894	3,077	4,053
WUWMEH	77,135	154,13	95,672	3,377	3,834
XOGPER	132,663	174,621	93,227	2,637	3,31
XOGPER	136,4	167,395	109,06	2,522	3,242
XOGPER	100,02	174,621	98,223	3,148	3,31
XOGPER	124,295	174,621	112,553	2,829	3,31
XOGPER	170,378	174,621	151,173	2,29	3,31
XOGPER	178,845	167,395	156,556	2,293	3,242
XOGPER	109,374	167,395	155,885	3,337	3,242
YORZUC	105,414	170,659	157,124	3,447	3,274
YORZUC	150,171	170,659	115,44	2,987	3,274
YORZUC	134,521	170,659	100,202	2,654	3,274
YORZUC	153,762	170,659	156,446	2,292	3,274

Table S7. Datasets from CSD comprising O/N−H···I⁻ hydrogen bonds and C/N−I···I⁻ halogen bonds with corresponding geometrical parameters used for analysis

Refcode	*ANG1 (A)*	*ANG2 (A)*	*ANG3 (A)*	*DIST1 (D)*	*DIST2 (D)*
ACIBIA	170,75	168,136	73,383	2,777	3,422
ACIBIA	170,75	177,153	87,538	2,777	3,397
ACIBIA	170,75	173,579	59,129	2,777	3,477
ACUTEZ	162,853	174,119	95,392	2,504	3,673
CEWPIG	167,155	132,654	67,595	2,817	4,317
CEWPIG	158,483	166,74	83,999	2,81	3,946
CEWPIG	158,483	69,173	86,323	2,81	4,286
CEWPIG	158,483	78,318	106,27	2,81	4,319
CEWPIG	155,696	132,654	78,662	2,889	4,317
CEWPIG	147,238	166,74	61,312	2,906	3,946
CEWPIG	147,238	69,173	48,51	2,906	4,286
CEWPIG	147,238	78,318	111,516	2,906	4,319
CEWPIG	167,026	166,74	62,456	2,799	3,946
CEWPIG	167,026	69,173	154,106	2,799	4,286
CEWPIG	167,026	78,318	133,681	2,799	4,319
CUJVAG	149,715	173,094	100,023	3,013	3,324
CUJVAG	149,715	169,616	60,313	3,013	3,543
CUJVAG	146,901	173,094	120,772	3,017	3,324
CUJVAG	146,901	169,616	57,519	3,017	3,543
DAQMEN	159,201	133,444	96,503	2,693	4,036
DIQZOS	153,474	175,564	126,154	2,695	3,515
DIQZOS	108,772	175,564	136,897	3,33	3,515
DIZNUW	152,42	165,408	111,816	2,745	3,531
DIZNUW	152,42	170,93	96,749	2,745	3,583
DIZNUW	152,42	165,964	69,566	2,745	3,604
DIZNUW	153,226	166,863	68,865	2,717	3,441
DIZNUW	153,226	176,374	114,261	2,717	3,463
ETIDUI	176,259	167,738	142,14	2,571	3,566
GUYNIZ	158,9	176,705	78,459	2,711	3,44
GUYNOF	168,209	172,322	131,67	2,584	3,469
GUYNOF	168,209	173,065	74,033	2,584	3,452
IFULEC	177,501	169,36	98,41	2,711	3,458
IFULEC	177,501	169,396	164,992	2,711	3,686
IFULEC	177,501	169	108,174	2,711	3,447
IFULEC	177,501	175,239	90,68	2,711	3,532
ISUPET	127,85	177,601	52,236	2,992	3,557
ISUPET	127,85	174,955	89,833	2,992	3,533
MAZDAV	151,317	173,206	143,294	2,66	3,574
MAZDAV	157,875	65,99	121,273	2,883	4,285
MAZDAV	168,131	65,99	113,936	2,783	4,285
MAZDAV	168,796	173,206	125,343	2,796	3,574
MAZDAV	162,255	65,99	112,422	2,826	4,285
MAZDAV	171,728	173,206	124,263	2,695	3,574
MICJEO	169,256	175,734	142,991	2,724	3,321
MIRQIQ	144,429	170,286	89,341	2,744	3,471

OHOVAJ	136,565	162,419	99,117	2,595	3,652
OHOVAJ	136,565	176,747	95,674	2,595	3,548
OHOVAJ	151,602	162,419	119,973	2,676	3,652
OHOVAJ	151,602	176,747	73,285	2,676	3,548
OHOVAJ	162,679	162,419	61,357	2,506	3,652
OHOVAJ	162,679	176,747	121,051	2,506	3,548
OHOVAJ01	121,103	143,089	61,628	3,204	4,158
OHOVAJ01	121,103	153,22	121,004	3,204	3,72
OHOVAJ01	120,233	143,089	117,998	3,357	4,158
OHOVAJ01	120,233	153,22	65,592	3,357	3,72
OHOVOX	171,294	164,151	89,451	2,668	3,501
OHOVOX	171,294	174,984	99,212	2,668	3,492
OXIVUN	159,128	173,035	129,523	2,642	3,652
QIDTIH	157,294	163,617	136,743	2,827	3,892
UFAJIU	157,224	170,161	65,078	2,766	3,692
UFAJIU	157,224	94,548	42,782	2,766	4,325
UFAJIU	176,406	170,161	79,418	2,634	3,692
UFAJIU	176,406	94,548	136,894	2,634	4,325
UFAJIU	164,209	170,161	81,644	2,682	3,692
UFAJIU	164,209	94,548	71,418	2,682	4,325
UFAKAN	151,831	174,378	68,151	2,661	3,924
UFAKAN	170,468	174,189	68,49	2,716	3,782
UFAKAN	80,124	174,378	73,342	3,55	3,924
UFAKAN	145,407	174,189	90,077	2,691	3,782
UFAKAN	179,021	174,378	164,5	2,707	3,924
UFAKAN	79,753	174,378	96,012	3,556	3,924
UWEMUF	178,595	160,493	122,003	2,608	3,777
UWEMUF	160,178	160,493	93,967	2,619	3,777
VIHFEY	98,621	175,706	78,095	3,481	3,616
VIHFEY	98,621	170,714	149,694	3,481	3,47
WARKIM	164,937	171,375	133,522	2,586	3,574
XALHEA	170,884	175,305	138,928	2,773	3,578
XALHEA	170,884	171,613	87,082	2,773	3,595
XALHEA	170,884	169,944	91,539	2,773	3,713
XALHEA	176,874	168,672	138,72	2,743	3,593
XALHEA	176,874	172,272	122,436	2,743	3,588
XALHEA	165,47	175,305	139,068	2,628	3,578
XALHEA	165,47	171,613	122,75	2,628	3,595
XALHEA	165,47	169,944	100,943	2,628	3,713
XALHEA	172,11	168,672	124,835	2,719	3,593
XALHEA	172,11	172,272	125,728	2,719	3,588
XIDFUN	155,272	174,838	82,941	2,905	3,483
XIDFUN	155,272	172,695	107,074	2,905	3,489
XIDFUN	155,272	179,375	159,021	2,905	3,49
YICJUR	169,927	177,594	80,662	2,63	3,541
YICJUR	169,927	177,594	157,203	2,63	3,541

Table S8. Distribution of functional groups as strong hydrogen bond donors which exist simultaneously with C/N−I···X^- halogen bonds in structures studied as part of database survey. (X = Cl^-, Br^-, I^-)

Functional group	Chlorides	Bromides	Iodides
Pyridine* (NH^+)	13	4	7
Primary amine / cation (RNH_2 / RNH_3^+)	6	4	2
Secondary amine / cation (RR'NH / RR'NH_2^+)	8	9	3
Tertiary amine /cation (RR'R''N / RR'R''NH^+)	6	0	3
Amide (CONH)	2	2	3
Alcohol (OH)	11	11	10
Water (H_2O)	16	8	4

*represents all aromatic nitrogen-containig functional groups.