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Supporting information for article:

Testing the tools for revealing and characterizing the iodine–iodine halogen bond in crystals

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Table S1 Interatomic distances (Å) after optimization of atomic positions in crystals and calculated values at bond critical points (a. u.) for I–I and I…I interactions

Refcode in CSD	Name of compound	Sort of bonding	$d_{I,I}$	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	$P(\mathbf{r}_{bcp})$	$\eta(\mathbf{r}_{bcp})$
DOWMAF	$C_{12}H_{11}INS^+\cdot I_3^-$	[I–I–I]$^-$	2.973	0.044	0.039	–0.218	0.491
$P\bar{1}$	1-(Iodomethyl)-1,2-dihydro[1,3]thiazolo[3,2-a]quinolin-10-ium tri-iodide		3.029	0.040	0.041	–0.259	0.436
			4.149	0.006	0.016	–0.623	0.036
	(Bartashevich *et.al.*, 2014)	I...I	4.798	0.002	0.006	–0.605	0.013
			4.389	0.005	0.012	–0.612	0.027
DOWMEJ	$(C_{12}H_{11}INS^+\cdot I_3^-)\cdot I_2$	I–I	2.856	0.055	0.026	–0.115	0.621
$P\bar{1}$	1-(Iodomethyl)-1,2-dihydro[1,3]thiazolo[3,2-a]quinolin-10-ium tri-iodide diiodine	[I–I–I]$^-$	2.936	0.046	0.038	–0.207	0.505
			3.016	0.039	0.043	–0.270	0.421
			3.441	0.019	0.037	–0.477	0.157
	(Bartashevich *et.al.*, 2014)		3.741	0.012	0.027	–0.589	0.069
		I...I	4.241	0.005	0.013	–0.650	0.026
			4.628	0.003	0.008	–0.626	0.016
			4.954	0.003	0.006	–0.624	0.013
			4.020	0.008	0.022	–0.637	0.045
DULZOZ01	$C_4H_{12}N^+\cdot I_5^-$	I–I	2.861	0.054	0.029	–0.134	0.601
C2/c	Tetramethylammonium pentaiodide	I...I	3.221	0.027	0.044	–0.407	0.250
	(Filguieras *et.al.*, 2001)						
EJUPOQ	$C_{12}H_8ClINO^+\cdot I_3^-$						
$P2_1/n$	(3E)-8-chloro-3-iodomethylidene-2,3-dihydro-1,4-oxazino[2,3,4-ij]quinolin-4-ium triiodide	I–I	2.923	0.049	0.033	–0.170	0.554
	(Bartashevich *et.al.*, 2016)	I...I	3.180	0.030	0.043	–0.353	0.308
HAFLAC	$C_7H_{10}N_2OS\ I_2$	I–I	2.901	0.050	0.031	–0.155	0.573
$P2_1/c$	(6-Propyl-thiouracil) diiodine	I...I	5.096	0.002	0.004	–0.581	0.009
	(Antoniadis *et. al.*, 2003)		3.969	0.007	0.019	–0.626	0.041
I_2	I_2	I–I	2.796	0.061	0.021	–0.085	0.655
Cmca	(Bertolotti *et.al.*, 2014)	I...I	3.470	0.018	0.037	–0.510	0.135
			4.357	0.005	0.012	–0.667	0.021
IVOVOG	$C_{22}H_{17}I_2N_2S_2^+\cdot I_3^-$						
C2/c	(E)-8-((2,3-diiodo-4-(quinolin-8-ylthio)but-2-en-1-yl)thio)quinolin-1-ium triiodide	I–I	2.995	0.042	0.040	–0.238	0.465
	(Bartashevich *et.al.*, 2016)	I...I	3.722	0.011	0.027	–0.606	0.066

NULBUR	$C_8H_6N_2\ I_2$						
Pbca	Quinoxaline diiodine	I–I	2.808	0.061	0.016	–0.066	0.676
	(Bailey *et.al.*, 1997)						
NUTSOL	$C_{12}H_{30}N_2^{2+}2I^-\ I_2$						
C2/m	Hexane-1,6-bis(trimethylammonium) iodine diiodide	I–I	2.881	0.053	0.028	–0.132	0.606
	(Abate *et. al.*, 2010)	I...I	3.455	0.019	0.035	–0.465	0.161
NUTSUR	$C_{12}H_{30}N_2^{2+}2I_5^-$	I–I	2.880	0.052	0.031	–0.146	0.583
C2/m	Hexane-1,6-bis(trimethylammonium) bis(pentaiodide)	I–I	2.862	0.054	0.029	-0.136	0.594
	(Abate *et. al.*, 2010)		3.155	0.031	0.044	-0.357	0.306
			3.143	0.032	0.044	–0.343	0.323
			4.487	0.004	0.010	–0.643	0.019
		I...I	4.592	0.003	0.009	–0.639	0.016
			4.571	0.003	0.009	–0.625	0.018
			4.518	0.003	0.008	–0.632	0.017
			4.528	0.004	0.010	–0.611	0.022
QIRZEY	$C_{13}H_{13}INS^+\cdot I^-$		3.700	0.012	0.027	–0.568	0.079
$P2_1/c$	3-(Iodomethyl)-3-methyl-2,3-dihydro[1.4]thiazino[2,3,4-i]quinolin-4-ium iodide	I...I	4.207	0.006	0.015	–0.624	0.034
	(Batalov *et.al.*, 2013)		4.458	0.004	0.011	–0.655	0.021
SUFLUC	$C_{12}H_{11}NS^+\cdot I^-$						
$P2_1/n$	1-(Iodomethyl)-1,2-dihydro[1,3]thiazolo[3,2-a]quinolin-10-ium iodide	I...I	3.670	0.013	0.029	–0.556	0.086
	(Slepukhin, 2015)						
TIJLUU	$C_{17}H_{12}N_2O_4S_5\ I_2$						
$P\bar{1}$	4,5-bis(2-nitrobenzylsulfanyl)-1,3-dithiole-2-diiodothione	I–I	2.853	0.055	0.028	–0.128	0.602
	(Skabara *et.al.*, 2007)						
YUSYUH	$C_5H_7N_2^+0.5I_2\cdot I^-$	I–I	2.879	0.053	0.029	–0.138	0.594
$P\bar{1}$	1-Methylpyrazin-1-ium iodide diiodine	I...I	3.386	0.022	0.038	–0.442	0.190
	(Nelyubina *et.al.*, 2010)						
ZOJPAR	$C_{12}H_9INO^+I_3^-0.5I_2$	I–I	2.830	0.058	0.022	–0.097	0.644
$P\bar{1}$	(E)-3-(iodomethylene)-2,3-dihydro-[1,4]oxazino[2,3,4-ij]quinolin-4-ium triiodide diiodine	$[I–I–I]^-$	2.940	0.047	0.038	–0.204	0.508
			3.027	0.040	0.043	–0.267	0.425
		I...I	3.504	0.017	0.034	–0.497	0.135

(Batalov *et.al.*, 2014)	3.604	0.013	0.032	–0.601	0.080
	3.991	0.008	0.021	–0.629	0.046
	4.048	0.007	0.019	–0.645	0.037
	4.150	0.007	0.017	–0.642	0.034
	4.277	0.005	0.014	–0.669	0.025
	4.526	0.004	0.009	–0.650	0.017
	4.782	0.003	0.006	–0.600	0.014
	4.488	0.004	0.011	–0.620	0.022
	4.489	0.004	0.010	–0.624	0.021

Table S2 Experimental and calculated Raman data for structures with bound diiodine molecule and triiodide ions

Refcode in CSD	Calculated wave number, ν(I_2), cm^{-1}	Experimental wave number ν(I_2), cm^{-1}	References of Raman data
DOWMAF	113 ν_{sym} (I_3^-)	116 ν_{sym} (I_3^-)	(Yushina *et.al.*, 2015)
DOWMEJ	114 ν_{sym} (I_3^-)	108 ν_{sym} (I_3^-)	(Yushina *et.al.*, 2016)
EJUPOQ	165 148	165 149	(Bartashevich *et.al.*, 2016)
IVOVOG	117 ν_{sym} (I_3^-)	116 ν_{sym} (I_3^-)	(Bartashevich *et.al.*, 2016)
ZOJPAR	115 ν_{sym} (I_3^-)	113 ν_{sym} (I_3^-)	(Yushina *et.al.*, 2015)
NUTSOL	168 158	172 161	(Abate *et. al.*, 2010)
DULZOZ01	165	155	(Nour *et.al.*, 1986)
HAFLAC	141	151	(Antoniadis *et. al.*, 2003)
TIJLUU	162	160	(Skabara *et.al.*, 2007)
NULBUR	182	182	(Bailey *et.al.*, 1997)
I_2	179	180	(Congeduti *et.al.*, 2000)

Table S3 The disagreement R-factors for the multipolar refinements

DOWMAF	DOWMEJ	EJUPOQ	IVOVOG	ZOJPAR	DULZOZ01	QIRZEY	SUFLUC
0.0011	0.0009	0.0020	0.0013	0.0010	0.0009	0.0017	0.0015

Figure S1 Typical residual density maps corresponding to the structures on the Fig. 3, yellow-brown lines are positive values, blue are negative ones, the step is 0.05 e/Å^3, zero level is omitted: a) polyiodide fragment in crystal DOWMEJ; b) polyiodide fragment in crystal EJUPOQ

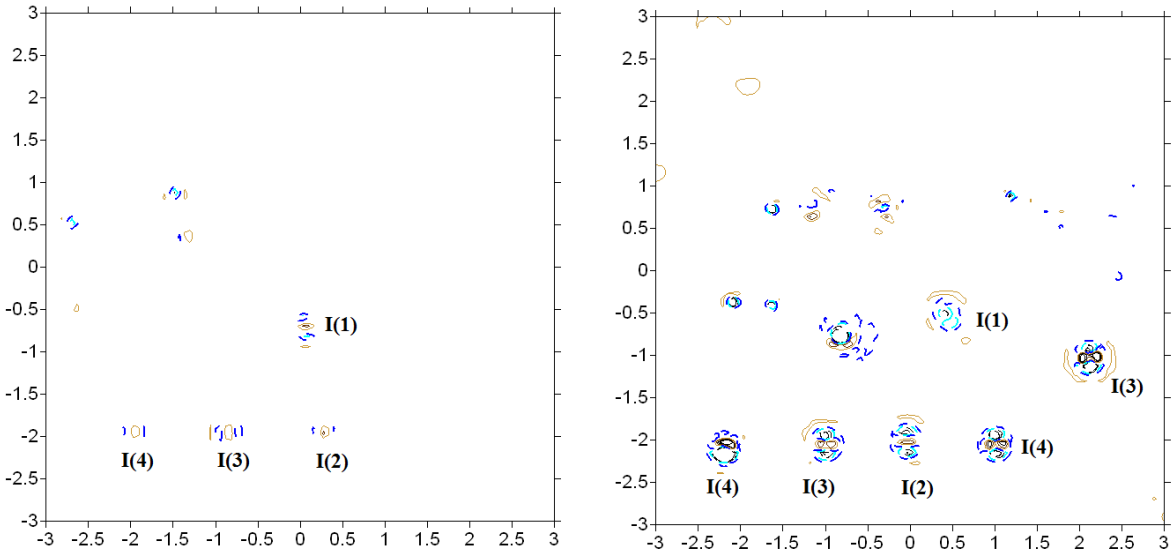

Table S4 The minima (top line) and maxima of the one-electron potential P(**r**) (bottom line), Å, represented using relativistic analytical wave functions

DOWMEJ	Halogen-bond donor		0.039	0.129	0.361	1.099
I_3^-…I–I		0.022	0.077	0.236	0.687	1.632
3.431 Å	Halogen-bond acceptor		0.039	0.129	0.361	1.117
		0.022	0.077	0.236	0.679	1.795
ZOJPAR	Halogen-bond donor		0.040	0.128	0.363	1.110
I_3^-…I–I		0.018	0.075	0.239	0.686	1.698
3.530 Å	Halogen-bond acceptor		0.040	0.128	0.363	1.119
		0.018	0.075	0.239	0.677	1.835
SUFLUC	Halogen-bond donor		0.041	0.127	0.363	1.130
I^-…I–C		0.018	0.078	0.239	0.685	1.791
3.670 Å	Halogen-bond acceptor		0.041	0.127	0.363	1.121
		0.018	0.078	0.239	0.680	1.879

QIRZEY	Halogen-bond donor		0.037	0.129	0.361	1.135
I^-…I–C		0.019	0.079	0.236	0.685	1.806
3.700 Å	Halogen-bond acceptor		0.037	0.129	0.361	1.121
		0.019	0.079	0.236	0.681	1.894
EJUPOQ	Halogen-bond donor		0.038	0.129	0.359	1.125
I_3^-…I–C		0.020	0.077	0.239	0.690	1.849
3.826 Å	Halogen-bond acceptor		0.038	0.129	0.359	1.140
		0.019	0.077	0.239	0.685	1.978
EJUPOQ	I(1) Type I interaction		0.041	0.127	0.360	1.137
I_3^-…I–C		0.020	0.076	0.239	0.680	2.009
4.054 Å	I(3) Type I interaction		0.041	0.127	0.360	1.147
		0.020	0.076	0.239	0.685	2.045

Table S5 The minima (top line) and maxima of the one-electron potential P(**r**) (bottom line), Å, represented using Clementi and Roetti wave functions

DOWMEJ	Halogen-bond donor		0.039	0.133	0.365	1.117
I_3^-…I–I		0.022	0.082	0.241	0.700	1.645
3.431 Å	Halogen-bond acceptor		0.039	0.133	0.365	1.121
		0.022	0.082	0.241	0.691	1.787
ZOJPAR	Halogen-bond donor		0.040	0.133	0.367	1.128
I_3^-…I–I		0.022	0.080	0.239	0.699	1.707
3.530 Å	Halogen-bond acceptor		0.040	0.133	0.367	1.123
		0.022	0.080	0.239	0.690	1.827
SUFLUC	Halogen-bond donor		0.041	0.133	0.367	1.144
I^-…I–C		0.018	0.078	0.239	0.703	1.796
3.670 Å	Halogen-bond acceptor		0.041	0.133	0.367	1.125
		0.018	0.078	0.239	0.694	1.874
QIRZEY	Halogen-bond donor		0.042	0.134	0.366	1.149
I^-…I–C		0.019	0.079	0.241	0.704	1.811
3.700 Å	Halogen-bond acceptor		0.042	0.134	0.366	1.130
		0.019	0.079	0.241	0.695	1.890
EJUPOQ	Halogen-bond donor		0.038	0.134	0.364	1.140
I_3^-…I–C		0.019	0.081	0.239	0.704	1.858
3.826 Å	Halogen-bond acceptor		0.038	0.134	0.364	1.145
		0.019	0.081	0.239	0.694	1.968
EJUPOQ	I(1) Type I interaction		0.041	0.132	0.365	1.142
I_3^-…I–C		0.020	0.081	0.244	0.695	2.009
4.054 Å	I(3) Type I interaction		0.041	0.132	0.365	1.147
		0.020	0.081	0.239	0.690	2.045