Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Halogen bonding in the structures of pentaiodobenzoic acid and its salts

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Crystallographic data and refinement details for **1-5** are given in Table S1. The diffraction data were collected on a New Xcalibur (Agilent Technologies) diffractometer with MoK_α radiation (λ = 0.71073) by doing ϕ scans of narrow (0.5°) frames at 130 K. Absorption correction was done empirically using SCALE3 ABSPACK (CrysAlisPro, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET). Structures were solved by SHELXT [G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Adv.*, 2015, 71, 3–8] and refined by full-matrix least-squares treatment against $|F|^2$ in anisotropic approximation with SHELX 2014/7 [Sheldrick, G. M. (2015). Acta Cryst. C71, 3-8.] in ShelXle program [C. B. Hübschle, G. M. Sheldrick and B. Dittrich // J. Appl. Cryst., 44, (2011) 1281-1284.]. H-atoms coordinates (for COOH and OH groups) in the structure of **1** were localized directly from XRD experiment and refined with isotropic displacement parameters set to 1.2 Ueq of the attached atoms. H-atoms of H_2O molecules in the crystal structure of **2** were not localized. H-atoms in the structures of **3-5** were refined in calculated positions. Position of H-atom attached to N of NBu_3H^+ cation in **5** was found from the XRD experiment and its coordinates were refined with isotropic displacement parameters set to 1.2 Ueq of the attached atom. The crystallographic data have been deposed in the Cambridge Crystallographic Data Centre under the deposition codes CCDC 1919375-1919379.

Table S1. Details of XRD experiments for 1-5

	1	**2**	**3**	**4**	**5**
Chemical formula	$C_9H_7I_5O_3$	$C_7H_2I_5KO_3$	$C_{13}H_{16}I_5NO_2$	$C_{19}H_{29}I_5N_2O_3$	$C_{19}H_{28}I_5NO_2$
M_r	797.65	807.69	852.77	967.94	936.92
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, *Cmca*	Orthorhombic, $Pna2_1$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1$
a, *b*, *c* (Å)	21.5195 (7), 8.8433 (3), 16.5517 (5)	37.861 (3), 9.2563 (5), 9.2740 (5)	17.9973 (6), 11.0540 (5), 10.3194 (4)	8.2333 (4), 15.4642 (9), 20.9533 (9)	8.3240 (4), 16.4369 (6), 9.5423 (4)
α, β, γ (°)	90, 90.697 (3), 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 98.004 (4), 90
V (Å^3)	3149.61 (18)	3250.1 (3)	2052.96 (14)	2667.8 (2)	1292.87 (10)
Z	8	8	4	4	2
μ (mm^{-1})	9.87	9.82	7.58	5.85	6.03
Crystal size (mm)	0.15 × 0.15 × 0.04	0.25 × 0.18 × 0.05	0.18 × 0.12 × 0.06	0.36 × 0.06 × 0.06	0.35 × 0.35 × 0.10
T_{min}, T_{max}	0.401, 1.000	0.422, 1.000	0.665, 1.000	0.664, 1.000	0.548, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14326, 7013, 5704	5040, 1852, 1683	14763, 4615, 4352	9747, 5491, 5001	9442, 5135, 4930
R_{int}	0.027	0.031	0.039	0.030	0.027
θ values (°)	θ_{max} = 29.0, θ_{min} = 3.4	θ_{max} = 29.0, θ_{min} = 3.5	θ_{max} = 29.0, θ_{min} = 3.5	θ_{max} = 29.0, θ_{min} = 3.4	θ_{max} = 28.8, θ_{min} = 3.5
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.682	0.683	0.682	0.682	0.679
Range of *h*, *k*, *l*	$-17 \le h \le 28$, $-11 \le k \le 8$, $-20 \le l \le 22$	$-50 \le h \le 48$, $-12 \le k \le 11$, $-6 \le l \le 11$	$-24 \le h \le 24$, $-14 \le k \le 11$, $-13 \le l \le 13$	$-10 \le h \le 11$, $-20 \le k \le 15$, $-19 \le l \le 28$	$-11 \le h \le 10$, $-22 \le k \le 22$, $-12 \le l \le 11$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.027, 0.055, 1.02	0.032, 0.086, 1.11	0.039, 0.087, 1.11	0.032, 0.061, 1.02	0.031, 0.070, 1.06
No. of reflections, parameters, restraints	7013, 321, 12	1852, 89, 0	4615, 193, 25	5491, 267, 0	5135, 250, 0
H-atom treatment	H atoms treated by a	H-atom parameters not	H-atom parameters	H-atom parameters constrained	H atoms treated by a

	mixture of independent and constrained refinement	defined	constrained		mixture of independent and constrained refinement
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0154P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0467P)^2 + 0.6426P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 11.3404P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0206P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma s^2(F_o^2) + (0.0314P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, -1.25	1.33, -1.18	1.33, -1.33	0.87, -0.87	0.98, -1.01
Absolute structure	–	–	Flack x determined using 1709 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 1785 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 1899 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	–	–	-0.03 (6)	-0.05 (3)	0.01 (3)

Computer programs: *CrysAlis PRO* 1.171.38.41 (Rigaku OD, 2015), *SHELXS2014* (Sheldrick, 2014), *SHELXL2014* (Sheldrick, 2014), ShelXle (Hübschle, 2011), CIFTAB-2014 (Sheldrick, 2014).

Table S2. Hydrogen bond parameters in **1**

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A	
O1-H1	0.860	1.728	173.23	2.583	O2	
O2-H7	0.987	1.786	173.16	2.769	O3	[-x+1, -y+1, -z+1]
O4-H4	0.731	1.938	172.05	2.664	O5	
O6-H6	0.793	1.687	163.86	2.458	O1	

Table S3. Halogen bonding parameters in **1-5.**

1		
Atoms	**Distance**	**Angle**
I68···O17	3.092	C-O-I = 120.77, C-I-O = 170.64
I117···O42	2.945	C-O-I = 129.28, C-I-O = 177.75
I21···I101	3.859	C-I-I = 96.85 and 177.02
I22···I130	3.873	C-I-I = 129.77 and 125.95
I22···I86	3.954	C-I-I = 128.93 and 126.87
3		
I13···O60	2.864	C-O-I = 124.75, C-I-O = 169.07
I12···O45	2.934	C-O-I = 133.46, C-I-O = 174.29
4		
I12···O77	3.008	C-O-I = 122.21, C-I-O = 178.45
I10···O47	2.920	C-O-I = 136.57, C-I-O = 174.99
I4···O66	2.886	C-O-I = 105.42, C-I-O = 172.57
5		
I65···O2	2.806	C-O-I = 116.94, C-I-O = 163.95
I81···I8	3.676	C-I-I = 126.62 and 166.08

Table S4. Hydrogen bonds in orto-iodinated carboxylic acids

No.	Acid	HB, Å	CSD refcode
1	2-iodobenzoic	1.899	OIBZAC
2	2-iodo-3-methylbenzoic	1.514	JONQAG
3	4-Pentanoyl-2-iodobenzoic	1.827	JOTJAD
4	4-chloro-2-iodobenzoic	2.197	LIKNUR
5	5-amino-2,4,6-triiodobenzene-1,3-dicarboxylic, methanol solvate	1.771	NIDDIQ
6	5-Hydroxy-2-iodobenzoic	1.907	OBIQUIB
7	2-Iodo-3,4,5-trimethoxybenzoic	1.809	TENPEJ

Computational details. The single point calculations based on the experimental X-ray geometries of **1** and **3**-**5** have been carried out at the DFT level of theory using the M06 functional [10.1007/s00214-007-0310-x] with the help of Gaussian-09 [M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, M. J. A.;, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, C. J.;, D. J. Fox, in Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT, 2010.] program package. The Douglas–Kroll–Hess 2nd order scalar relativistic calculations requested relativistic core Hamiltonian were carried out using the DZP-DKH basis sets [Barros, C. L.; de Oliveira, P. J. P.; Jorge, F. E.; Neto, A. C.; Campos, M. *Mol. Phys.* **2010**, *108*, 1965–1972. || Neto, A. C.; Jorge, F. E. *Chem. Phys. Lett.* **2013**, *582*, 158–162. || de Berredo, R. C.; Jorge, F. E. *Journal of Molecular Structure - Theochem* **2010**, *961*, 107–112. || Jorge, F. E.; Neto, A. C.; Camiletti, G. G.; Machado, S. F. *Journal of Chemical Physics* **2009**, *130*, 064108.] for all atoms. The topological analysis of the electron density distribution with the help of the atoms in molecules (QTAIM) method developed by Bader [10.1021/cr00005a013] has been performed by using the Multiwfn program [10.1002/jcc.22885]. The Wiberg bond indices were computed by using the Natural Bond Orbital (NBO) partitioning scheme [Glendening, E. D.; Landis, C. R.; Weinhold, F. *WIREs Computational Molecular Science*, **2012,** *2*, 1-42.]. The Cartesian atomic coordinates for model supramolecular associates are presented in **Table S5**.

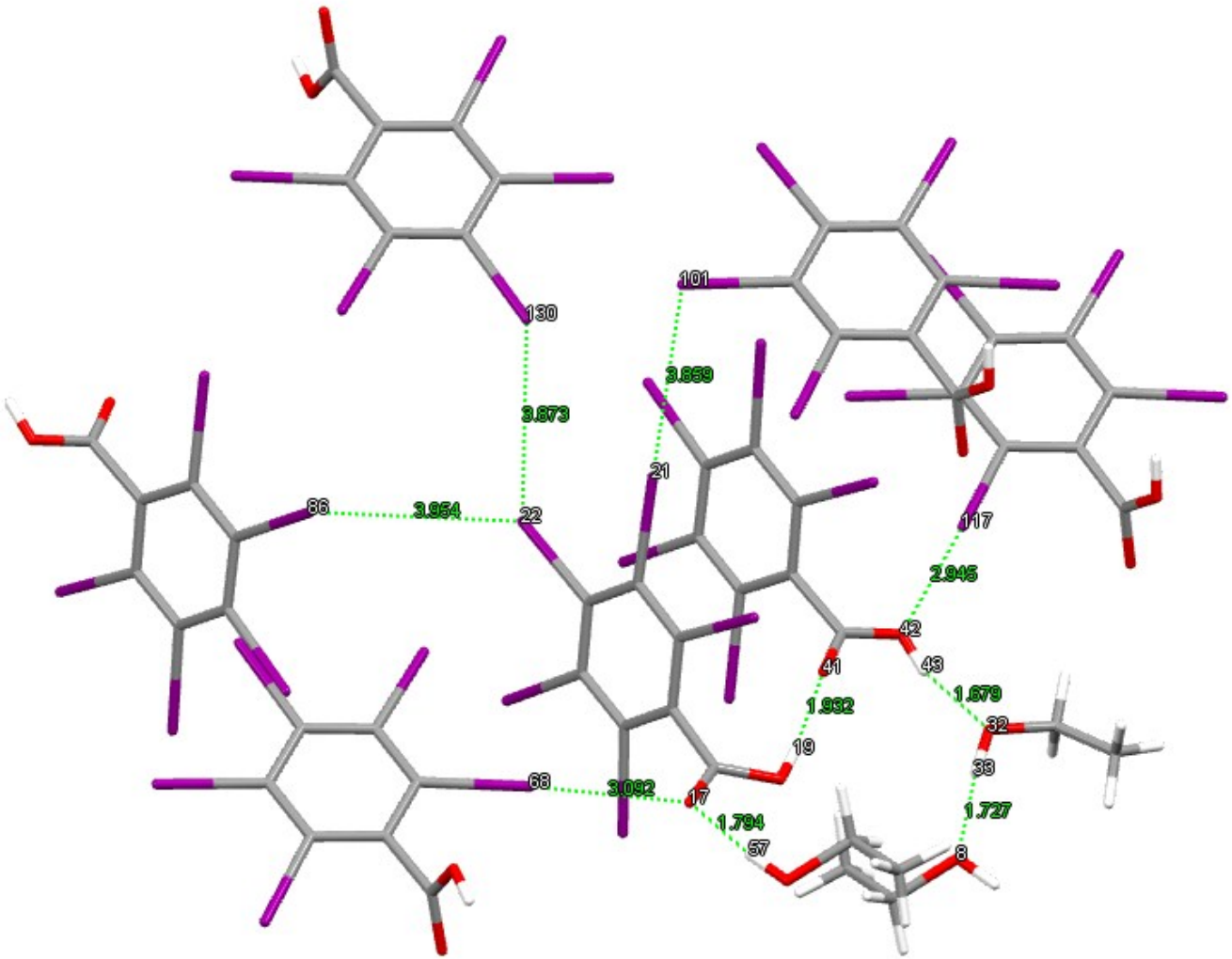

Figure S1. Non-covalent interactions in the structure of **1** (atom numbers are given in compliance with Table 1 in manuscript)

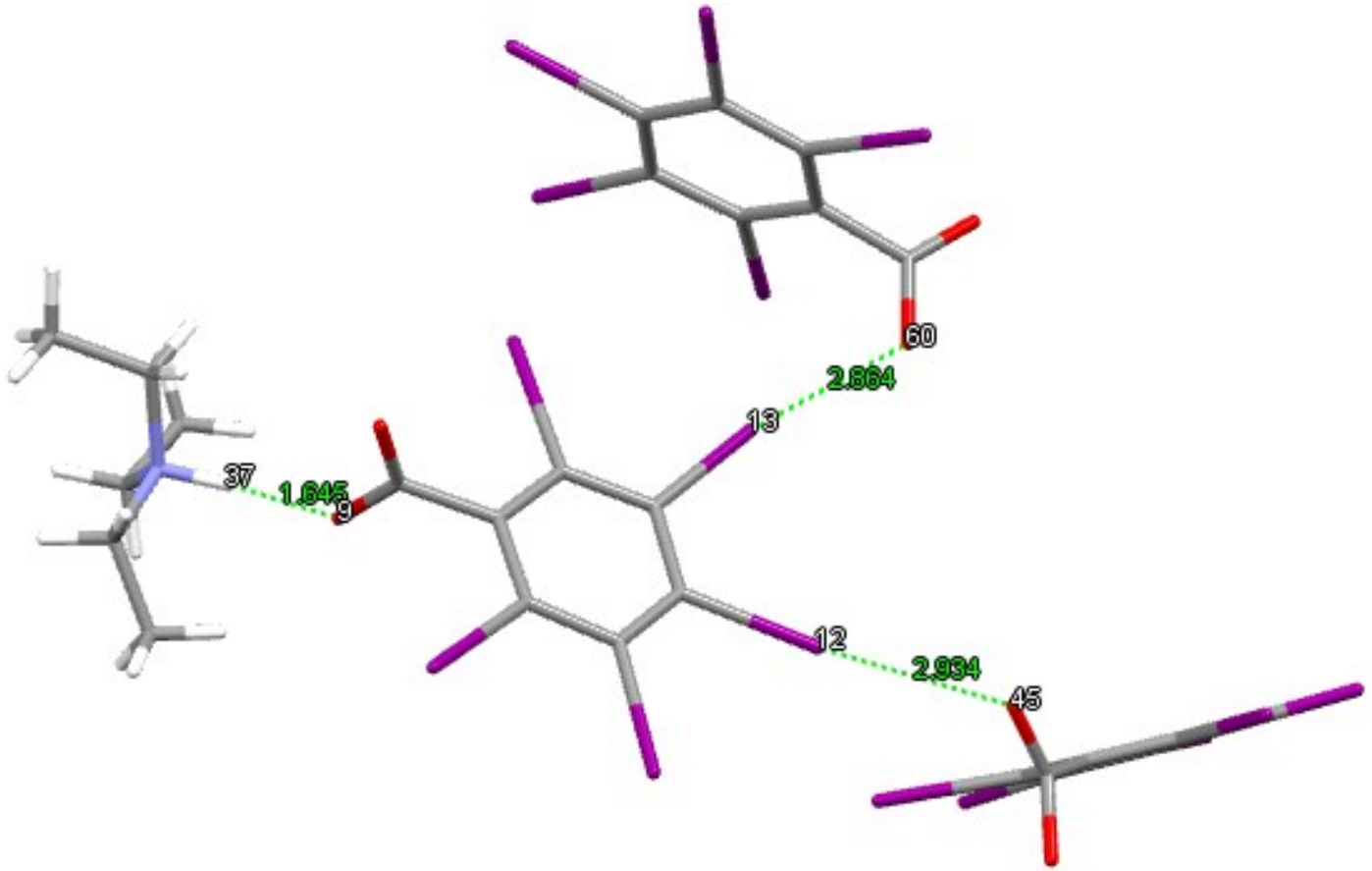

Figure S2. Non-covalent interactions in the structure of **3** (atom numbers are given in compliance with Table 1 in manuscript)

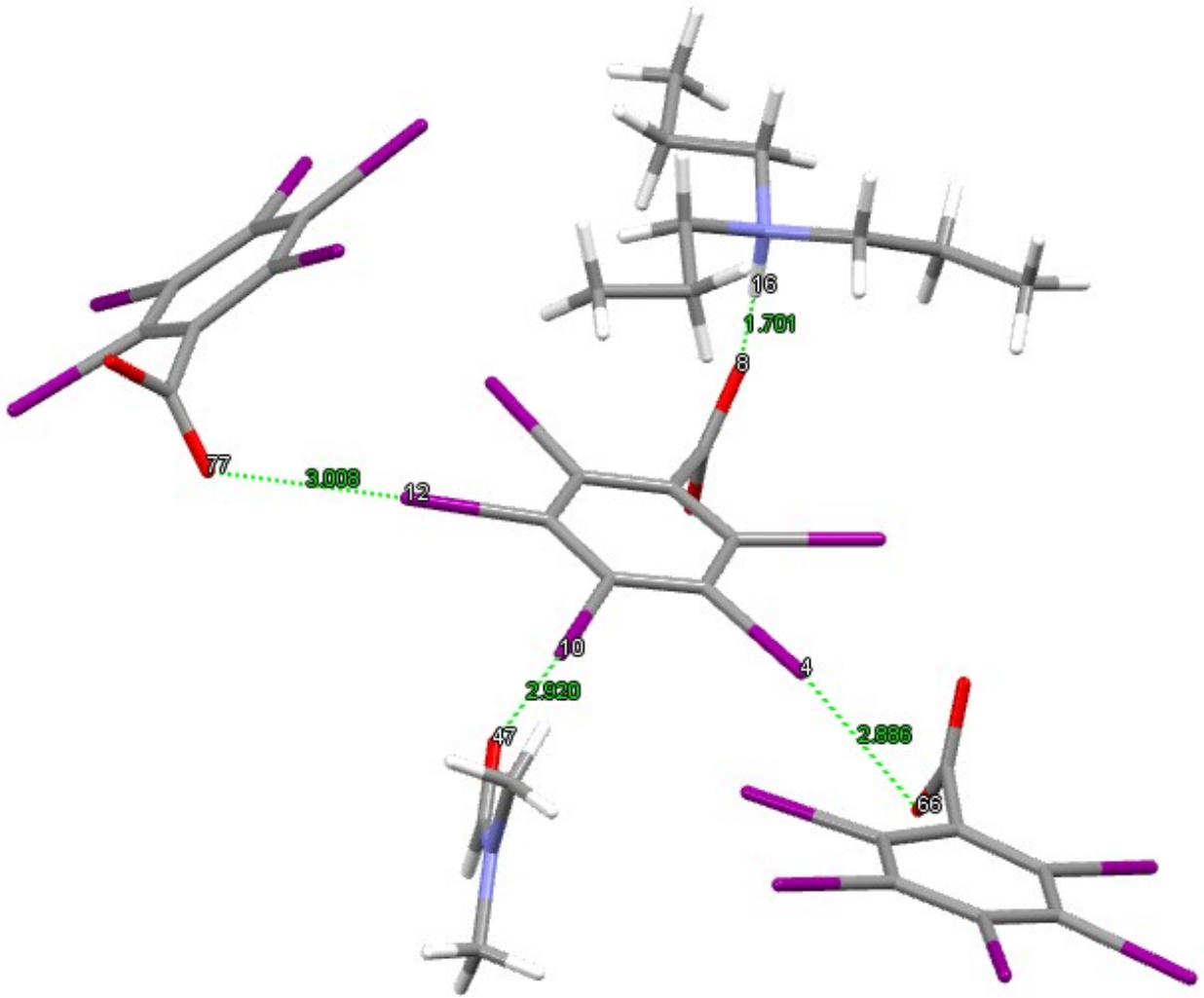

Figure S3. Non-covalent interactions in the structure of **4** (atom numbers are given in compliance with Table 1 in manuscript)

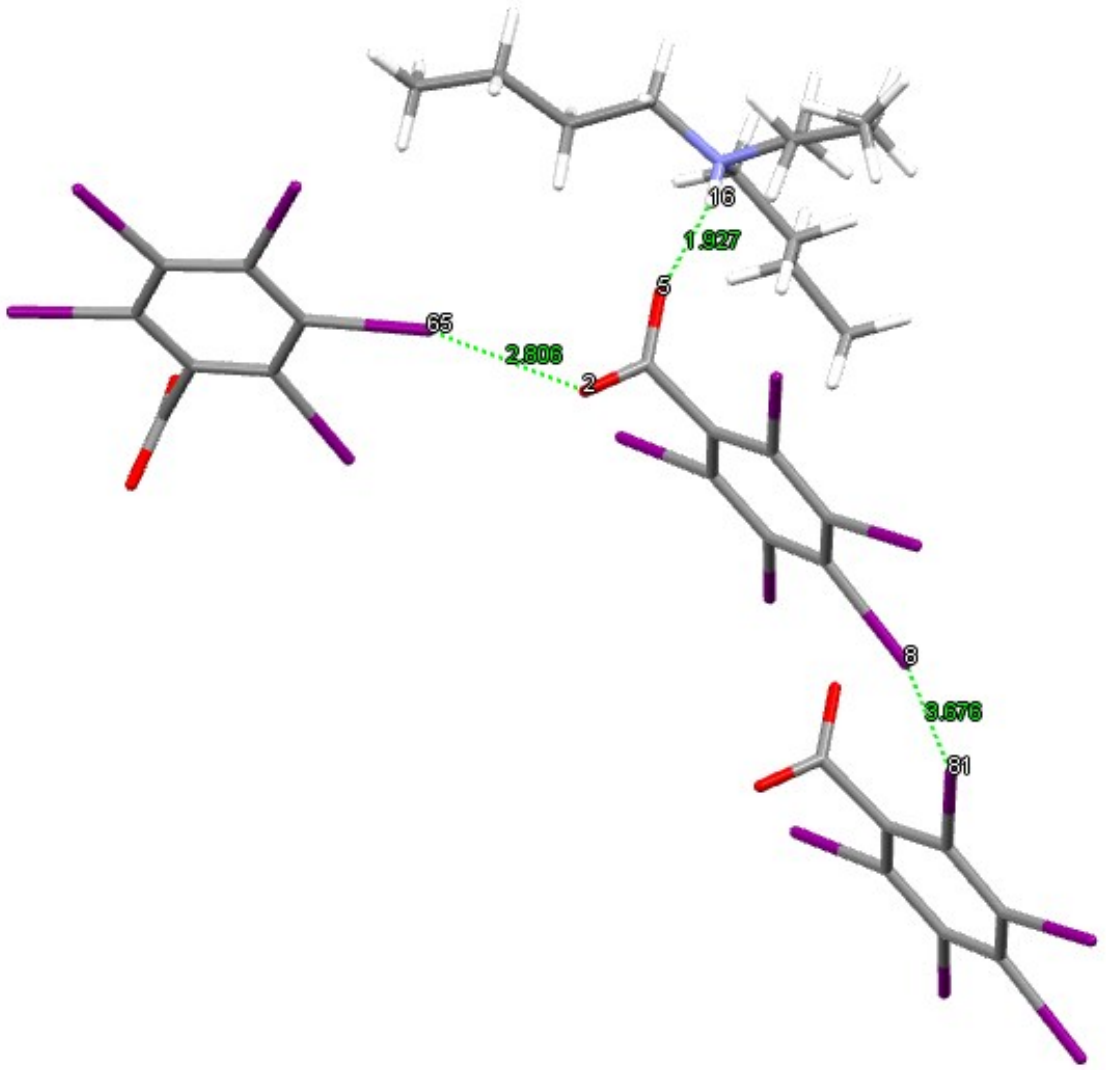

Figure S4. Non-covalent interactions in the structure of **5** (atom numbers are given in compliance with Table 1 in manuscript)

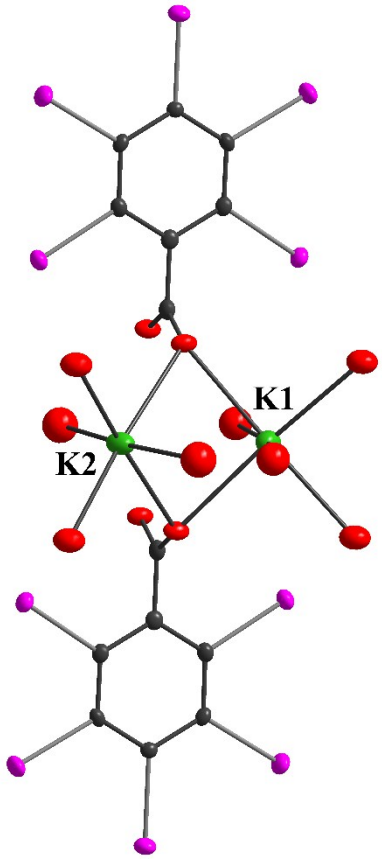

Figure S5. Disordering of K^+ cations over two closed positions marked as K1 and K2.

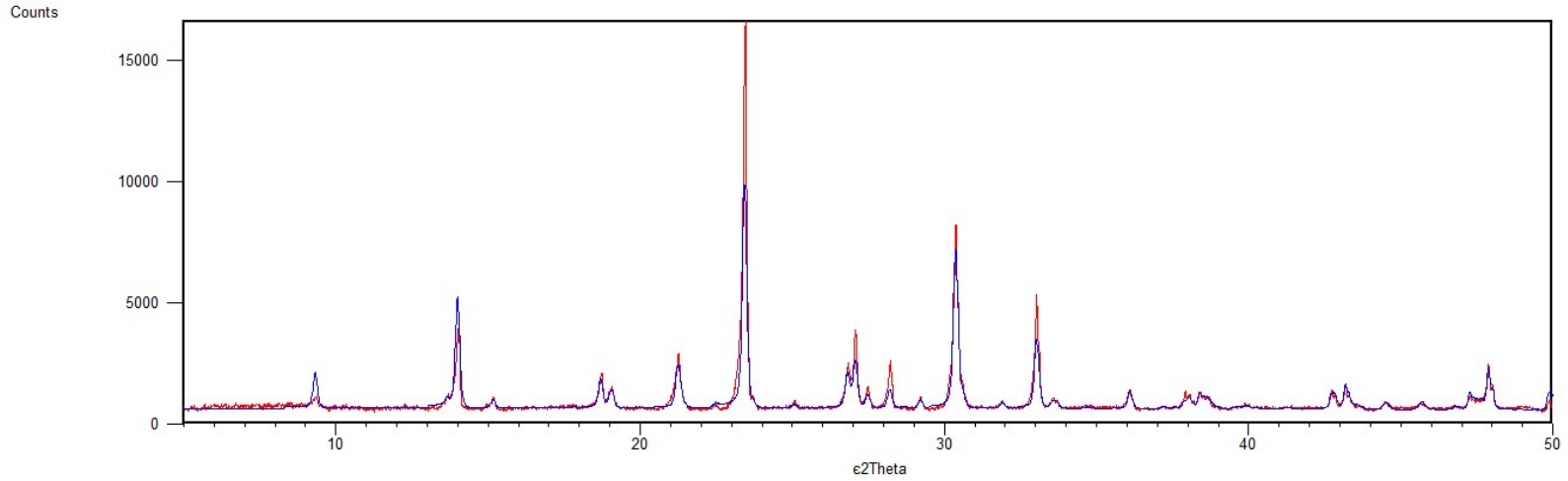

Figure S6. Theoretical PXRD pattern (blue) and experimental PXRD data (red) for **2**. The sample is pure

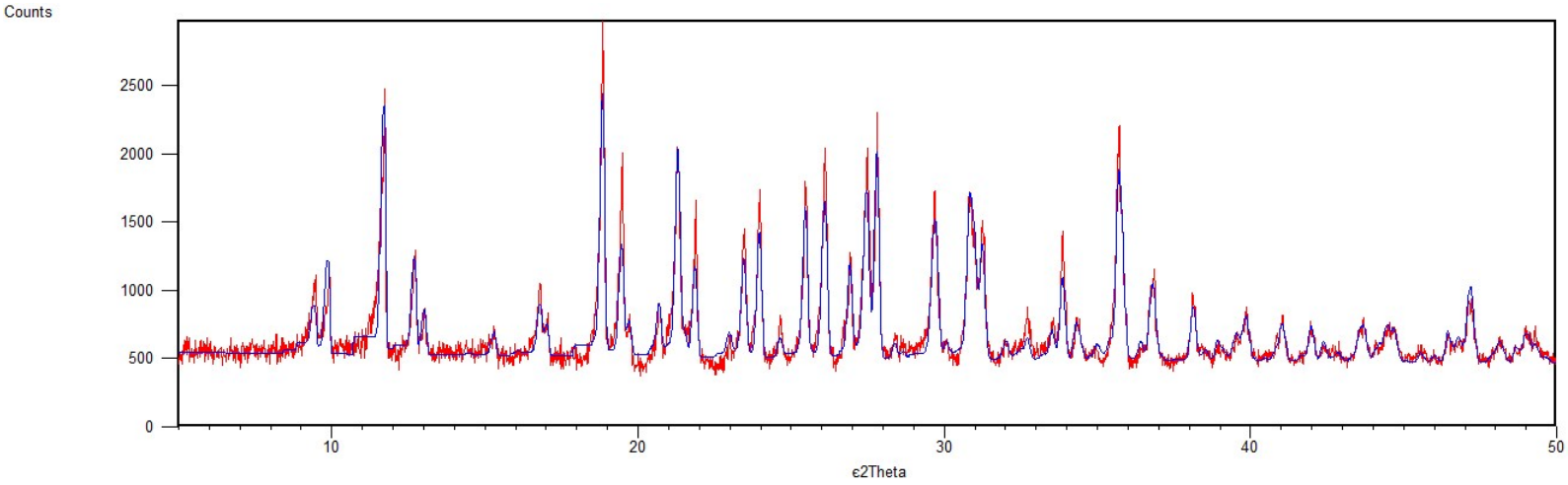

Figure S7. Theoretical PXRD pattern (blue) and experimental PXRD data (red) for **3**. The sample is pure

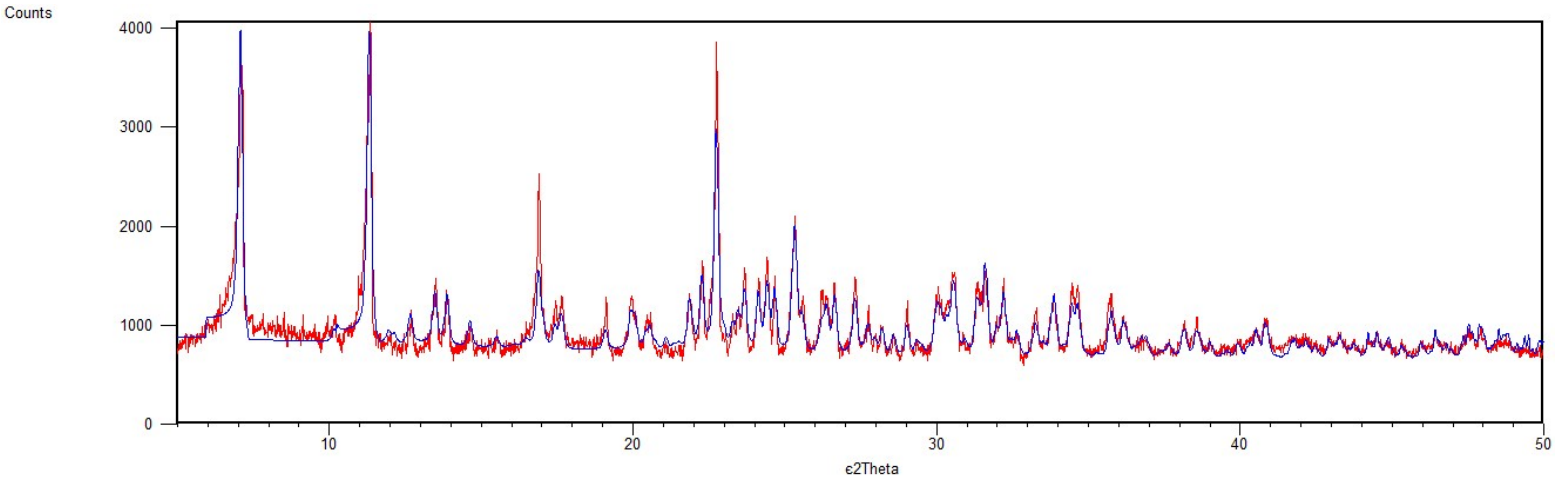

Figure S8. Theoretical PXRD pattern (blue) and experimental PXRD data (red) for **4**. The sample is pure

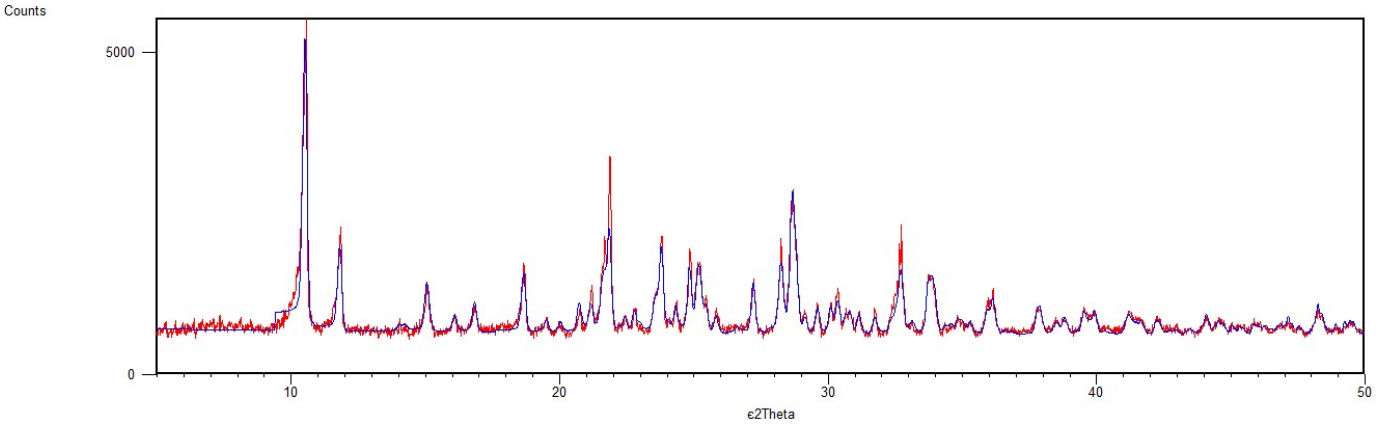

Figure S9. Theoretical PXRD pattern (blue) and experimental PXRD data (red) for **5**. The sample is pure

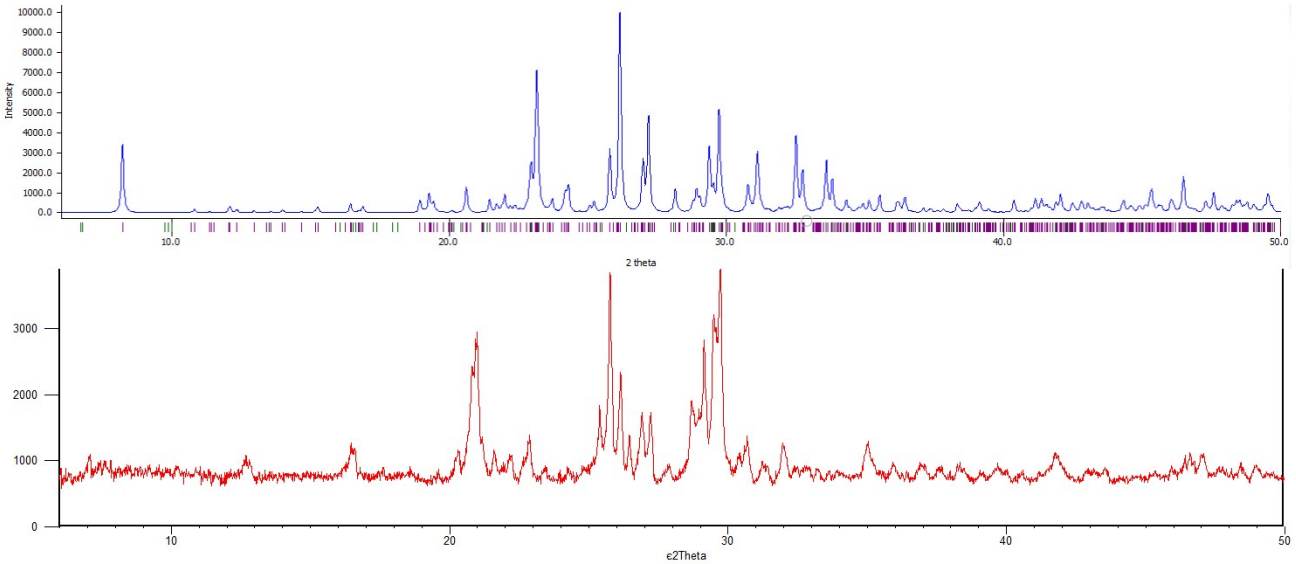

Figure S10. Theoretical PXRD pattern (blue) and experimental PXRD data (red) for **1**. The sample is not pure

Table S5. Cartesian atomic coordinates for model supramolecular associates.

Atom	X	Y	Z
1			
C	8.841429	7.387693	7.859821
H	8.266370	6.977815	8.538539
H	8.494805	7.178310	6.967336
H	8.853439	8.359952	7.985257

C	10.225674	6.853558	7.992225
H	10.236667	5.888975	7.771425
H	10.830112	7.324437	7.366236
O	10.663427	7.050763	9.332813
H	11.635283	6.959677	9.400670
C	7.484674	2.997879	7.944228
C	6.019433	3.089849	8.278548
C	5.527827	2.428370	9.418875
C	4.159987	2.451363	9.706854
C	3.286147	3.114610	8.834644
C	3.779764	3.781395	7.705901
C	5.140825	3.775205	7.444404
O	7.913625	2.178989	7.178107
O	8.285865	3.880440	8.508599
H	7.981196	4.271314	9.053110
I	6.928692	1.445880	10.626233
I	3.480605	1.518041	11.459053
I	1.223427	3.077203	9.212326
I	2.472235	4.761144	6.379546

I	5.982125	4.838081	5.843973
C	11.285536	8.272023	12.677664
H	11.429839	7.429663	13.155791
H	11.548041	9.022846	13.249913
H	11.824441	8.280733	11.859260
C	9.933854	8.392292	12.345000
H	9.417071	8.429425	13.188130
H	9.810921	9.261818	11.888008
O	9.369069	7.403611	11.540646
H	9.746375	7.304566	10.774359
C	6.486606	5.858686	11.269219
C	4.981384	5.750798	11.529061
C	4.483544	5.061905	12.651183
C	3.120229	5.030953	12.920956
C	2.235206	5.714540	12.083502
C	2.709737	6.368945	10.931589
C	4.070879	6.372482	10.663471
O	7.039730	5.103468	10.520310
O	7.004145	6.841177	11.906412

H	7.734591	7.030424	11.634984
I	5.898810	4.090557	13.877574
I	2.403169	3.925806	14.550847
I	0.200533	5.821191	12.579189
I	1.380461	7.333395	9.641645
I	4.844262	7.282811	8.932292
C	12.476725	1.455607	8.690655
H	13.051784	1.865485	8.011936
H	12.823349	1.664990	9.583139
H	12.464715	0.483348	8.565219
C	11.092480	1.989743	8.558251
H	11.081487	2.954325	8.779051
H	10.488043	1.518863	9.184239
O	10.654728	1.792537	7.217662
H	9.682872	1.883623	7.149805
C	6.587279	-1.437036	2.993981
C	5.082056	-1.329148	3.253823
C	4.584216	-0.640255	4.375946
C	3.220902	-0.609303	4.645718

C	2.335879	-1.292890	3.808264
C	2.810410	-1.947295	2.656351
C	4.171552	-1.950832	2.388234
O	7.140403	-0.681818	2.245072
O	7.104818	-2.419527	3.631174
H	7.835264	-2.608774	3.359746
I	5.999483	0.331093	5.602336
I	2.503842	0.495844	6.275609
I	0.301205	-1.399541	4.303951
I	1.481134	-2.911745	1.366407
I	4.944935	-2.861161	0.657054
C	-6.687951	2.984614	5.281257
C	-5.182729	3.092502	5.021414
C	-4.684889	3.781395	3.899292
C	-3.321575	3.812347	3.629519
C	-2.436552	3.128760	4.466973
C	-2.911083	2.474355	5.618886
C	-4.272225	2.470818	5.887004
O	-7.241075	3.739832	6.030166

O	-7.205491	2.002123	4.644063
H	-7.935937	1.812876	4.915491
I	-6.100156	4.752743	2.672902
I	-2.604515	4.917494	1.999628
I	-0.401878	3.022109	3.971287
I	-1.581807	1.509905	6.908830
I	-5.045607	1.560489	7.618184
C	7.384001	1.423771	16.219466
C	5.918760	1.331801	16.553785
C	5.427154	1.993280	17.694113
C	4.059315	1.970287	17.982091
C	3.185474	1.307040	17.109881
C	3.679091	0.640255	15.981139
C	5.040152	0.646445	15.719641
O	7.812952	2.242661	15.453344
O	8.185193	0.541210	16.783837
H	7.880523	0.150336	17.328348
I	6.828019	2.975770	18.901470
I	3.379932	2.903609	19.734290

I	1.122754	1.344447	17.487563
I	2.371562	-0.339494	14.654784
I	5.881452	-0.416431	14.119210
C	7.384001	10.267071	16.219466
C	5.918760	10.175101	16.553785
C	5.427154	10.836580	17.694113
C	4.059315	10.813587	17.982091
C	3.185474	10.150340	17.109881
C	3.679091	9.483555	15.981139
C	5.040152	9.489745	15.719641
O	7.812952	11.085961	15.453344
O	8.185193	9.384510	16.783837
H	7.880523	8.993636	17.328348
I	6.828019	11.819070	18.901470
I	3.379932	11.746909	19.734290
I	1.122754	10.187747	17.487563
I	2.371562	8.503806	14.654784
I	5.881452	8.426869	14.119210
C	-6.788624	1.437036	13.556494

C	-5.283402	1.329148	13.296652
C	-4.785562	0.640255	12.174530
C	-3.422248	0.609303	11.904757
C	-2.537225	1.292890	12.742211
C	-3.011756	1.947295	13.894124
C	-4.372898	1.950832	14.162242
O	-7.341748	0.681818	14.305403
O	-7.306163	2.419527	12.919301
H	-8.036609	2.608774	13.190729
I	-6.200828	-0.331093	10.948139
I	-2.705187	-0.495844	10.274866
I	-0.502551	1.399541	12.246524
I	-1.682480	2.911745	15.184068
I	-5.146280	2.861161	15.893421
3			
C	9.007649	2.948102	5.872771
C	7.996200	2.521417	5.030708
C	6.772384	3.259825	4.997685
C	6.619407	4.420495	5.746874

C	7.668650	4.828387	6.574490
C	8.879868	4.096612	6.671492
C	5.366795	5.237385	5.606530
O	4.393141	5.033992	6.353655
O	5.409988	6.073068	4.649922
I	5.131750	2.588405	3.862345
I	8.185712	0.848726	3.789696
I	10.812238	1.841596	5.985355
I	10.394881	4.694744	7.989899
I	7.353517	6.583210	7.714164
C	3.169325	6.047643	2.241374
H	3.507548	6.663605	1.557332
H	2.593069	5.376876	1.820249
H	3.924257	5.601570	2.679608
C	2.408039	6.791578	3.227908
H	1.848125	6.160671	3.747088
H	1.800936	7.420141	2.761595
C	3.930610	8.726028	3.548842
H	3.232819	9.378037	3.289825

H	4.383764	8.423513	2.722495
C	4.949258	9.422430	4.447661
H	4.483613	9.876727	5.176944
H	5.451382	10.079048	3.918544
H	5.568077	8.757421	4.813391
C	2.526821	7.768751	5.443483
H	3.130342	8.147428	6.130776
H	2.217609	6.885990	5.768029
C	1.340799	8.670758	5.291788
H	1.633687	9.541183	4.950846
H	0.907694	8.789887	6.163107
H	0.704360	8.270503	4.663110
N	3.291706	7.576412	4.187613
H	4.039638	6.955785	4.425908
C	18.006299	2.578898	5.872771
C	16.994850	3.005583	5.030708
C	15.771034	2.267175	4.997685
C	15.618057	1.106505	5.746874
C	16.667300	0.698613	6.574490

C	17.878518	1.430388	6.671492
C	14.365445	0.289615	5.606530
O	13.391791	0.493008	6.353655
O	14.408638	-0.546068	4.649922
I	14.130400	2.938595	3.862345
I	17.184362	4.678274	3.789696
I	19.810888	3.685404	5.985355
I	19.393531	0.832256	7.989899
I	16.352167	-1.056210	7.714164
C	8.989651	8.105898	11.032471
C	10.001100	8.532583	10.190408
C	11.224916	7.794175	10.157385
C	11.377893	6.633505	10.906574
C	10.328650	6.225613	11.734190
C	9.117432	6.957388	11.831192
C	12.630505	5.816615	10.766230
O	13.604159	6.020008	11.513355
O	12.587312	4.980932	9.809622
I	12.865550	8.465595	9.022045

I	9.811588	10.205274	8.949396
I	7.185062	9.212404	11.145055
I	7.602419	6.359256	13.149599
I	10.643783	4.470790	12.873864
4			
C	3.337780	13.831180	13.730697
I	4.183504	12.117438	16.280924
C	3.113011	12.343524	13.472972
I	4.407285	8.661189	15.459135
O	4.417989	14.267271	13.328394
C	2.539973	11.887331	12.287015
I	1.655552	13.363543	11.045323
O	2.441173	14.442016	14.357201
C	2.485633	10.532667	11.972716
I	3.121491	7.556427	12.333531
C	3.049614	9.604815	12.859040
I	1.575607	9.902191	10.169894
C	3.565842	10.006884	14.082713
C	3.559256	11.394023	14.378154

N	-0.008233	13.811077	15.222572
H	0.941626	13.860980	14.911709
C	1.079386	13.379626	18.853779
H	0.243821	12.999516	19.196722
H	1.471694	13.970389	19.529565
H	1.707463	12.655221	18.648772
C	0.792867	14.176032	17.586105
H	0.268471	14.986186	17.808922
H	1.643169	14.461548	17.167625
C	0.017290	13.310037	16.632730
H	0.410274	12.401608	16.639330
H	-0.914464	13.235608	16.958993
C	-0.721237	12.894050	14.292246
H	-0.502396	13.155132	13.362883
H	-1.696002	13.017702	14.415221
C	-0.392728	11.415672	14.472444
H	0.588969	11.294541	14.521182
H	-0.787853	11.085172	15.317721
C	-0.951769	10.626998	13.296964

H	-1.921455	10.762016	13.246425
H	-0.760633	9.674682	13.423229
H	-0.534671	10.938184	12.467402
C	-0.569744	15.205948	15.145045
H	-0.007064	15.809949	15.691570
H	-1.480290	15.207633	15.534379
C	-0.638904	15.744102	13.730697
H	-1.381737	15.307579	13.243470
H	0.204927	15.542062	13.255120
C	-0.865320	17.271965	13.766318
H	-1.718973	17.465237	14.206149
H	-0.882964	17.619801	12.850324
H	-0.136714	17.698019	14.263854
O	2.974691	4.715035	11.675179
N	3.578192	2.536129	11.725467
C	3.774145	3.805740	11.459360
H	4.605955	4.043502	11.066758
C	2.311911	2.078388	12.284920
H	1.878757	2.817546	12.761021

H	2.476799	1.340360	12.907128
H	1.727750	1.770744	11.559998
C	4.581831	1.523224	11.459360
H	5.358446	1.937077	11.028288
H	4.205636	0.838964	10.866256
H	4.858981	1.107299	12.302290
C	4.895520	6.099080	17.699253
I	4.049796	4.385338	15.149026
C	5.120289	4.611424	17.956978
I	3.826015	0.929089	15.970815
O	3.815311	6.535171	18.101556
C	5.693327	4.155231	19.142935
I	6.577748	5.631443	20.384627
O	5.792127	6.709916	17.072749
C	5.747667	2.800567	19.457234
I	5.111809	-0.175673	19.096419
C	5.183686	1.872715	18.570910
I	6.657693	2.170091	21.260056
C	4.667458	2.274784	17.347237

C	4.674044	3.661923	17.051796
C	-0.778870	9.365120	7.222603
I	0.066854	11.078862	4.672376
C	-1.003639	10.852776	7.480328
I	0.290635	14.535111	5.494165
O	0.301339	8.929029	7.624906
C	-1.576677	11.308969	8.666285
I	-2.461098	9.832757	9.907977
O	-1.675477	8.754284	6.596099
C	-1.631017	12.663633	8.980584
I	-0.995159	15.639873	8.619769
C	-1.067036	13.591485	8.094260
I	-2.541043	13.294109	10.783406
C	-0.550808	13.189416	6.870587
C	-0.557394	11.802277	6.575146
5			
I	0.612576	6.432581	7.291963
O	-0.496738	7.639871	4.012191
C	0.128257	8.468291	7.097401

C	-0.234608	9.267124	8.180296
O	1.674017	7.930804	4.279607
I	-0.233844	8.465497	10.131963
C	-0.607531	10.610019	7.955401
I	-1.328014	11.820268	9.513787
C	-0.526717	11.149149	6.670291
I	-0.962504	13.186010	6.283907
C	-0.099484	10.340454	5.609130
I	0.169935	11.092442	3.664077
C	0.173837	9.007421	5.790557
C	0.505457	8.100104	4.568757
N	4.316137	7.768079	4.427017
H	3.589140	7.906149	4.488438
C	4.145547	9.842416	2.982212
H	4.307311	9.327267	2.152759
H	3.173902	9.806896	3.169224
C	4.518348	11.237909	2.740309
H	5.502144	11.282863	2.637491
H	4.280000	11.766782	3.542143

C	3.903280	11.874017	1.567646
H	3.658038	11.187266	0.913921
H	4.540956	12.498569	1.162912
H	3.099956	12.362636	1.845636
C	4.872743	9.160284	4.115189
H	4.805914	9.723840	4.926292
H	5.830899	9.079776	3.880429
C	3.514316	3.277518	2.267842
H	4.185566	2.800092	2.798895
H	3.446439	2.864771	1.380955
H	2.645237	3.226629	2.718188
C	3.919480	4.714103	2.121377
H	3.275117	5.170161	1.524670
H	4.810153	4.753814	1.690969
C	3.978825	5.466913	3.457514
H	3.071266	5.528025	3.847347
H	4.556474	4.974332	4.093276
C	4.533895	6.854187	3.233565
H	4.099243	7.252174	2.437864

H	5.503953	6.789442	3.048660
C	4.387419	8.082024	9.407765
H	4.868086	8.934902	9.429036
H	4.595464	7.569094	10.217281
H	3.422797	8.250453	9.367776
C	4.812702	7.293053	8.188800
H	4.328668	6.428883	8.175495
H	5.781062	7.097338	8.249569
C	4.535549	8.037644	6.898020
H	5.052415	8.881662	6.891953
H	3.573907	8.269273	6.855838
C	4.906390	7.214155	5.669605
H	5.891698	7.191489	5.578939
H	4.590000	6.284912	5.793174
I	-1.941267	-1.785869	2.157379
O	-0.831953	-0.578579	5.437152
C	-1.456948	0.249841	2.351941
C	-1.094083	1.048674	1.269047
O	-3.002709	-0.287646	5.169735

I	-1.094847	0.247047	-0.682620
C	-0.721160	2.391569	1.493941
I	-0.000677	3.601818	-0.064445
C	-0.801974	2.930699	2.779052
I	-0.366187	4.967560	3.165435
C	-1.229207	2.122004	3.840213
I	-1.498626	2.873992	5.785265
C	-1.502528	0.788971	3.658785
C	-1.834149	-0.118346	4.880585
I	-0.716115	6.432581	16.741305
O	-1.825429	7.639871	13.461533
C	-1.200434	8.468291	16.546743
C	-1.563299	9.267124	17.629638
O	0.345326	7.930804	13.728949
I	-1.562536	8.465497	19.581305
C	-1.936223	10.610019	17.404743
I	-2.656705	11.820268	18.963129
C	-1.855409	11.149149	16.119633
I	-2.291196	13.186010	15.733249

C	-1.428175	10.340454	15.058472
I	-1.158756	11.092442	13.113419
C	-1.154854	9.007421	15.239899
C	-0.823234	8.100104	14.018099

Details of Hirshfeld surface analysis

The Hirshfeld molecular surfaces were generated by CrystalExplorer 3.1 program [Wolff, S. K.; Grimwood, D. J.; McKinnon, J. J.; Turner, M. J.; Jayatilaka, D.; Spackman, M. A. *CrystalExplorer (Version 3.1)* University of Western Australia: 2012; Spackman, M. A.; Jayatilaka, D., Hirshfeld surface analysis. *CrystEngComm* **2009,** 11, (1), 19–32.]. The normalized contact distances, d_{norm},[McKinnon, J. J.; Jayatilaka, D.; Spackman, M. A., Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. *Chemical Communications* **2007**, (37), 3814–3816.] based on Bondi's van der Waals radii,[Bondi, A., van der Waals Volumes and Radii of Metals in Covalent Compounds. *The Journal of Physical Chemistry* **1966,** 70, (9), 3006–3007.] were mapped into the Hirshfeld surface. In the color scale, negative values of d_{norm} are visualized by the red color indicating contacts shorter than the sum of van der Waals radii. The white color denotes intermolecular distances close to van der Waals contacts with d_{norm} equal to zero. In turn, contacts longer than the sum of van der Waals radii with positive d_{norm} values are colored with blue.

Table S6. Element analysis data for **1**-**5**

Compound	C, H, N, calcd (%)	C, H, N, found (%)
1*	13.5, 0.9, 0	12.9, 0.7, 0
2	10.4, 0.2, 0	10.5, 0.2, 0
3	18.3, 1.9, 1.6	18.5; 2.0, 1.7
4	23.6, 3.0, 2.9	23.4, 3.0, 2.8
5	24.3, 3.0, 1.5	24.5, 3.1, 1.6

*According to PXRD data, **1** was not isolated as pure phase. As follows from PXRD EA data, most likely, there occurs simultaneous formation of **1** and non-solvated phase.

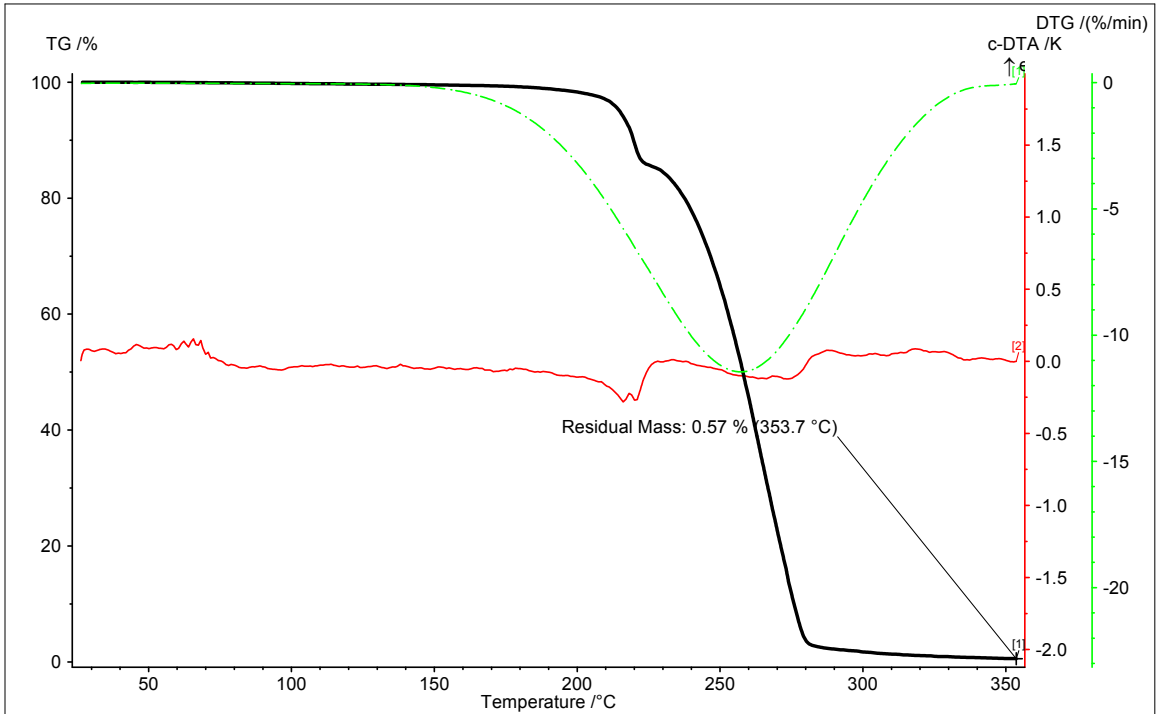

Figure S10. TGA data for **3**

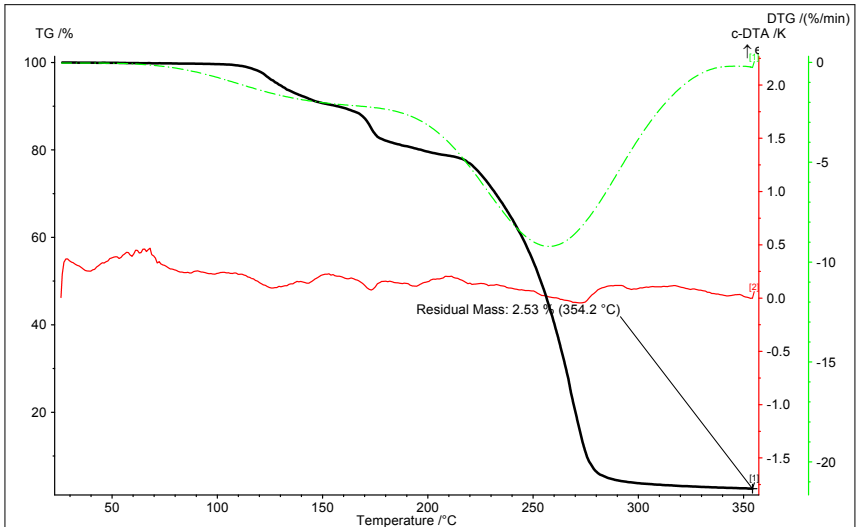

Figure S11. TGA data for **4**

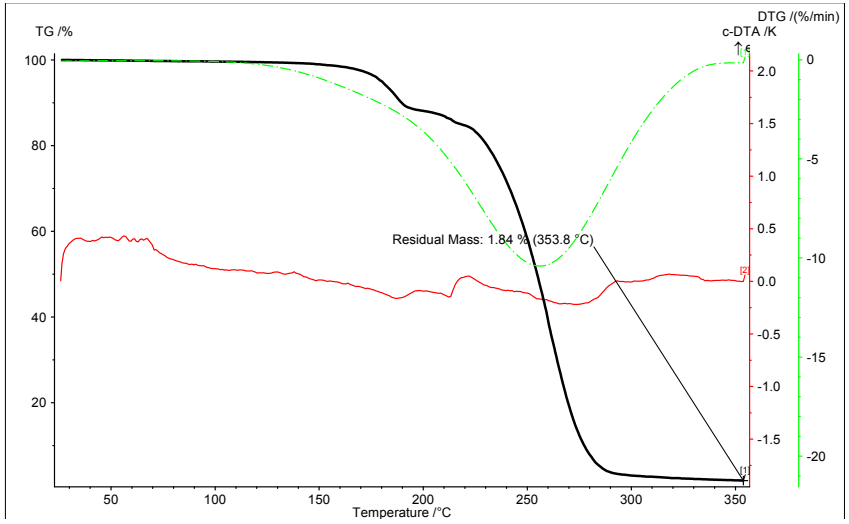

Figure S12. TGA data for **5**