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Synthesis, structure and Hirshfeld surface analysis of a series of novel low melting salts without alkyl group

Shan-Shan Yu,[a] Hai-Rong Zhao,[b] Jian-Han Shi,[b] Hui Zhang*[a] and Hai-Bao Duan[a]

[a] Key laboratory of Advanced Functional Materials of Nanjing, Nanjing Xiaozhuang University, Nanjing 211171, P. R. China

[b] School of Environmental Science, Nanjing Xiaozhuang University, Nanjing 211171, P. R. China

Tel.: +86-25-86178437

E-mail: duanhaibao4660@163.com

Table S1 Crystal and structural refinement data of **1-4**

Compound	**1**	**2**	**3**	**4**
Chemical formula	$C_5H_7N_2I_3$	$C_{12}H_{10}N_2FI_3$	$C_{12}H_{10}N_2ClI_3$	$C_{12}H_{10}N_2BrI_3$
CCDC no.	2041337	2041338	2041339	2041340
Formula weight	475.83	581.92	598.37	642.82
Temperature (K)	100(2)	100(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	*P*-1	*C 2/c*	$P2_1/c$	$P2_1/c$
a(Å)	7.9381(6)	16.7765(14)	12.8734(5)	12.8074(5)
b(Å)	8.3518(9)	12.5959(7)	14.7359(6)	14.9333(6)
c(Å)	9.1264(9)	17.5833(16)	8.5326(3)	8.4726(3)
α(°)	79.736(9)	90	90	90
β(°)	88.578(7)	121.008(12)	91.977(3)	91.583(3)
γ(°)	64.587(9)	90	90	90
V(Å3) / Z	536.86(10)/2	3184.6(6)/8	1617.68(11)/4	1619.82(11)/4
Density ($g\cdot cm^{-3}$)	2.944	2.428	2.457	2.636
Abs coeff. (mm^{-1})	8.677	5.885	5.947	8.241
F(000)	420.0	2112.0	1088.0	1160.0
Data collect θ range	2.27-29.44	2.11-24.99	2.10-25.00	2.77-28.97
Index range	$-9 \le h \le 10$	$-17 \le h \le 19$	$-14 \le h \le 15$	$-15 \le h \le 12$
	$-10 \le k \le 9$	$-13 \le k \le 14$	$-17 \le k \le 13$	$-15 \le k \le 17$
	$-8 \le l \le 11$	$-17 \le l \le 20$	$-10 \le l \le 10$	$-10 \le l \le 8$
Independent reflns	2480	2815	2850	2839
Refinement method on F^2	Full-matrix least-squares			
Data/restraints/parameters	2480/0/92	2815/7/165	2850/0/163	2839/0/163
Goodness-of-fit on F^2	1.050	1.20	1.039	1.042
Final R indices [I > 2δ(I)]	R1 = 0.0302	R1 = 0.0870	R1 = 0.0243	R1 = 0.0284
	wR2 = 0.0369	wR2 =0.0930	wR2 =0.0304	wR2 = 0.0337
R indices (all data)	R1 = 0.0618	R1 = 0.2368	R1 = 0.0414	R1 = 0.0575
	wR2 = 0.0664	wR2 = 0.2431	wR2 = 0.0449	wR2 = 0.0605

$R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $wR_2 = \Sigma w(|F_0|^2-|F_c|^2)^2/\Sigma w\,(|F_0|^2)^2]^{1/2}$

Table S2 Crystal and structural refinement data of **5-8**

Compound	**5**	**6**	**7**	**8**
Chemical formula	$C_{12}H_{10}N_2FI_3$	$C_{12}H_{10}N_2ClI_3$	$C_{12}H_{10}N_2BrI_3$	$C_{12}H_{10}N_2I_4$
CCDC no.	2041341	2041342	2041343	2041428
Formula weight	581.92	598.37	642.82	689.82
Temperature (K)	100(2)	150(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	orthorhombic	monoclinic	triclinic	triclinic
Space group	*P212121*	$P2_1/c$	*P-1*	*P-1*
a(Å)	7.1679(3)	7.4762(5)	8.0318(12)	9.2552(5)
b(Å)	10.8199(4)	8.8528(7)	11.7511(7)	9.4866(7)
c(Å)	20.5129(9)	25.417(2)	18.3130(12)	11.8244(10)
α(°)	90	90	104.739(6)	67.613(7)
β(°)	90	104.563(6)	93.199(10)	79.570(6)
γ(°)	90	90	91.627(9)	61.575(7)
V(Å3) / Z	1590.90(11)/4	1628.2(2)/4	1667.3(3)/4	844.21(12)/2
Density ($g\cdot cm^{-3}$)	2.430	2.441	2.561	2.714
Abs coeff. (mm^{-1})	5.890	5.909	8.007	7.369
F(000)	1056.0	1088.0	1160.0	616.0
Data collect θ range	2.71-29.04	2.35-29.28	2.30-279.12	2.50-29.27
Index range	$-8 \le h \le 8$	$-10 \le h \le 9$	$-11 \le h \le 9$	$-10 \le h \le 10$
	$-12 \le k \le 12$	$-11 \le k \le 11$	$-16 \le k \le 16$	$-11 \le k \le 11$
	$-24 \le l \le 22$	$-33 \le l \le 26$	$-25 \le l \le 22$	$-14 \le l \le 14$
Independent reflns	2819	3776	4156	2966
Refinement method on F^2	Full-matrix least-squares			
Data/restraints/parameters	2819/0/163	3776/0/163	7775/0/325	2966/0/167
Goodness-of-fit on F^2	1.051	1.062	1.094	1.007
Final R indices [$I > 2\delta(I)$]	R1 = 0.0209	R1 = 0.0783	R1 = 0.0788	R1 = 0.0233
	wR2 = 0.0219	wR2 =0.1240	wR2 =0.0841	wR2 = 0.0270
R indices (all data)	R1 = 0.0419	R1 = 0.1812	R1 = 0.1844	R1 = 0.0403
	wR2 = 0.0424	wR2 = 0.2244	wR2 = 0.1920	wR2 = 0.0422

$R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $wR_2 = \Sigma w(|F_0|^2-|F_c|^2)^2/\Sigma w\,(|F_0|^2)^2]^{1/2}$

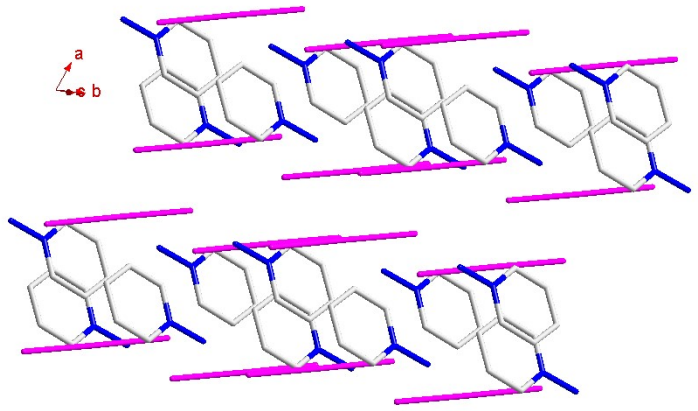

Figure S1 The crystal packing structure of **1** along the c-axis.

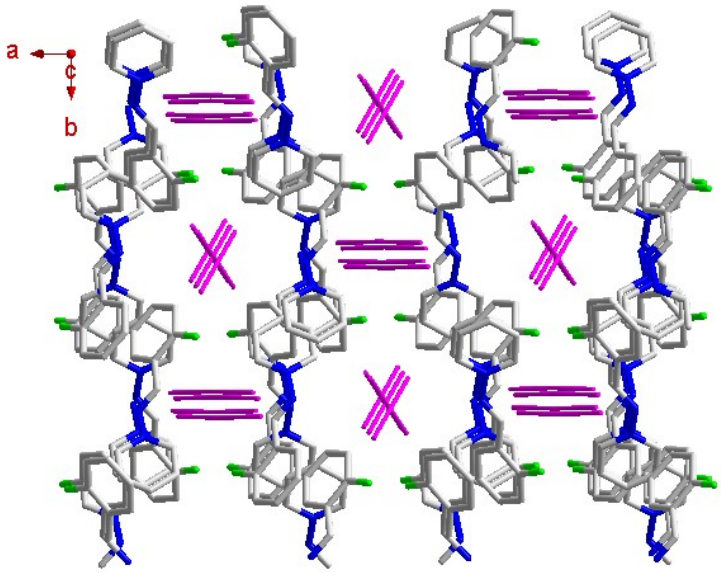

Figure S2 The parallelogram-like channels were formed by cations along the c-axis direction, and the crystallographically different I_3^- anion stacks are filled inside the supramolecular channels for 2.

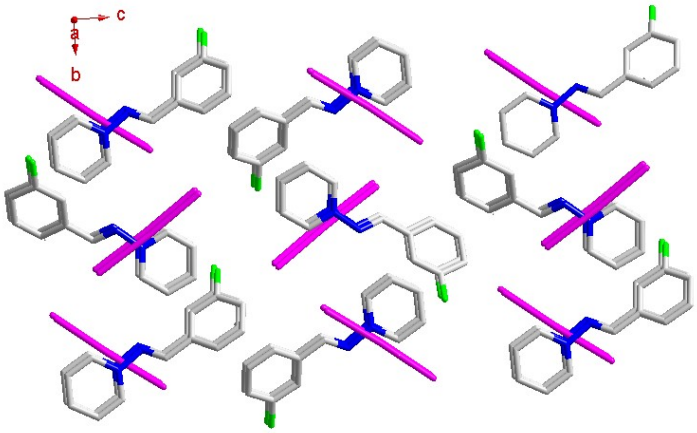

Figure S3. Along the a-axis direction, the anions and cations form mixed stack in **5**.

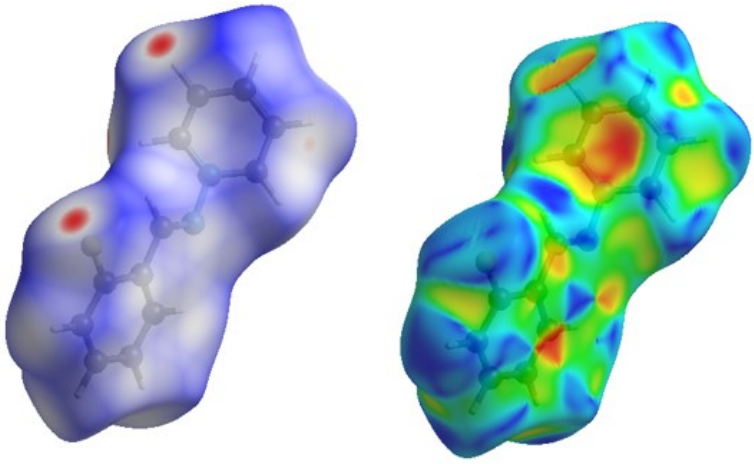

Figure S4. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **2**

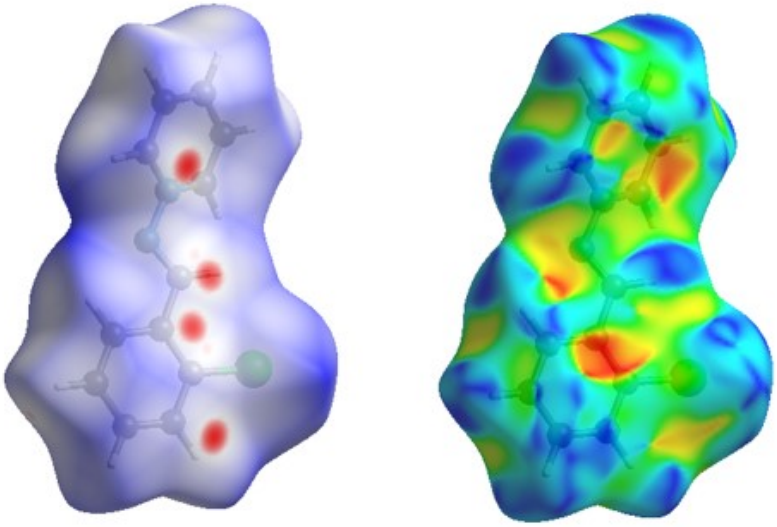

Figure S5. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **3**

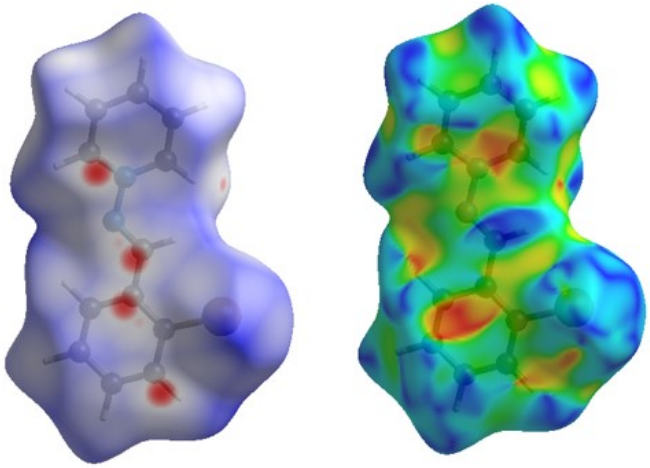

Figure S6. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **4**

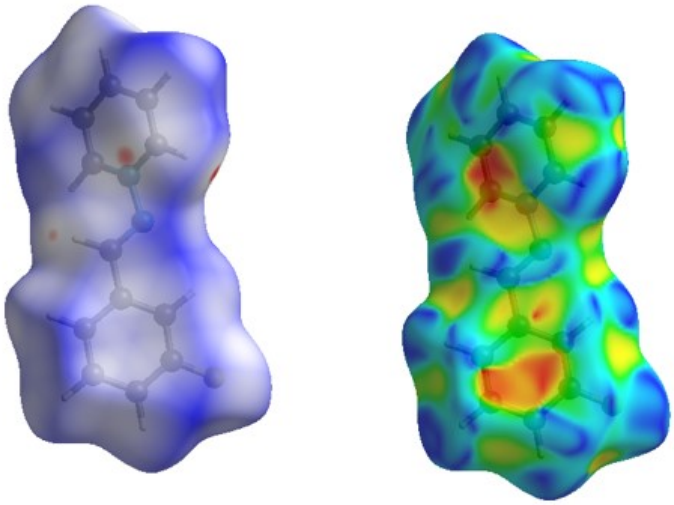

Figure S7. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **5**

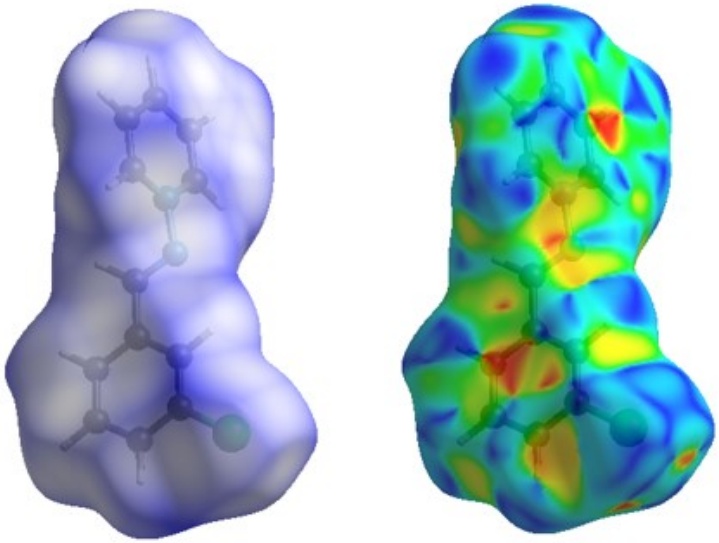

Figure S8. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **6**

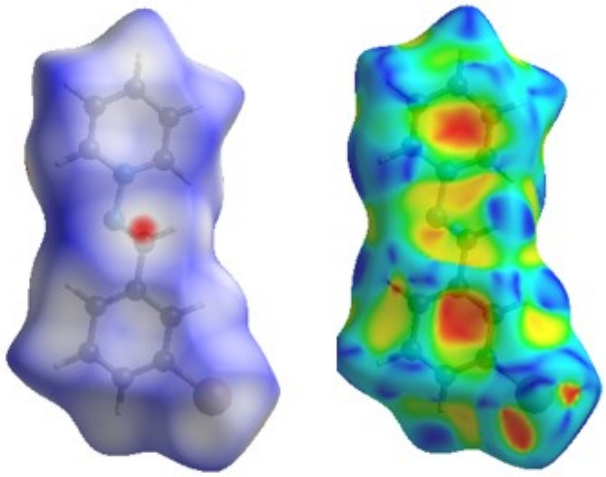

Figure S9. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **7**

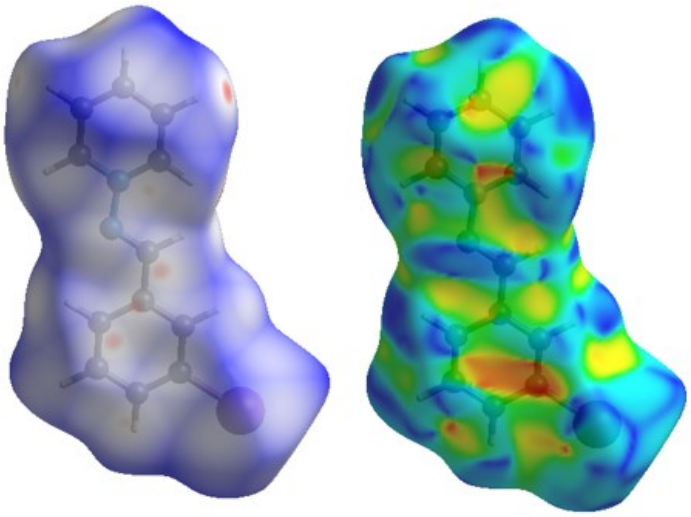

Figure S10. Hirshfeld surfaces mapped with (a) d_{normal} and (b) shape index of **8**