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Supporting information for article:

Proton Transfer Compounds' Intermolecular Interactions : Synthesis, Crystal Structure and Hirshfeld Surface Analysis

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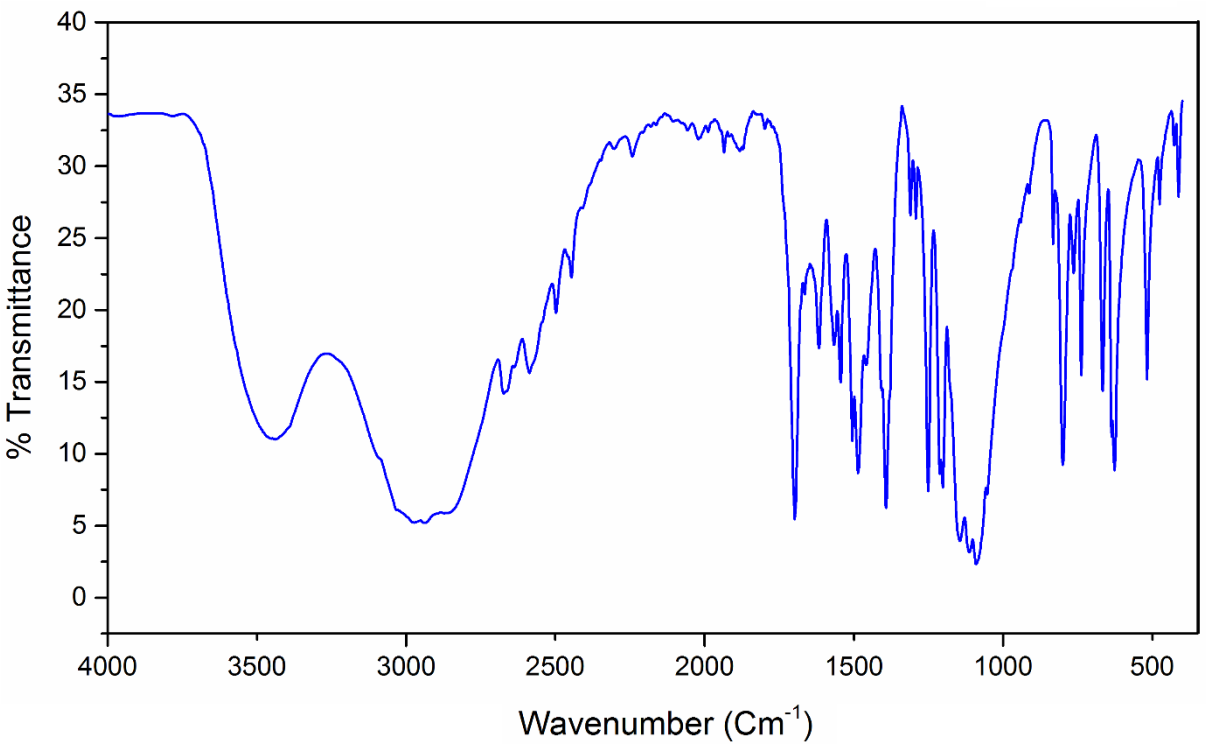
Supporting information

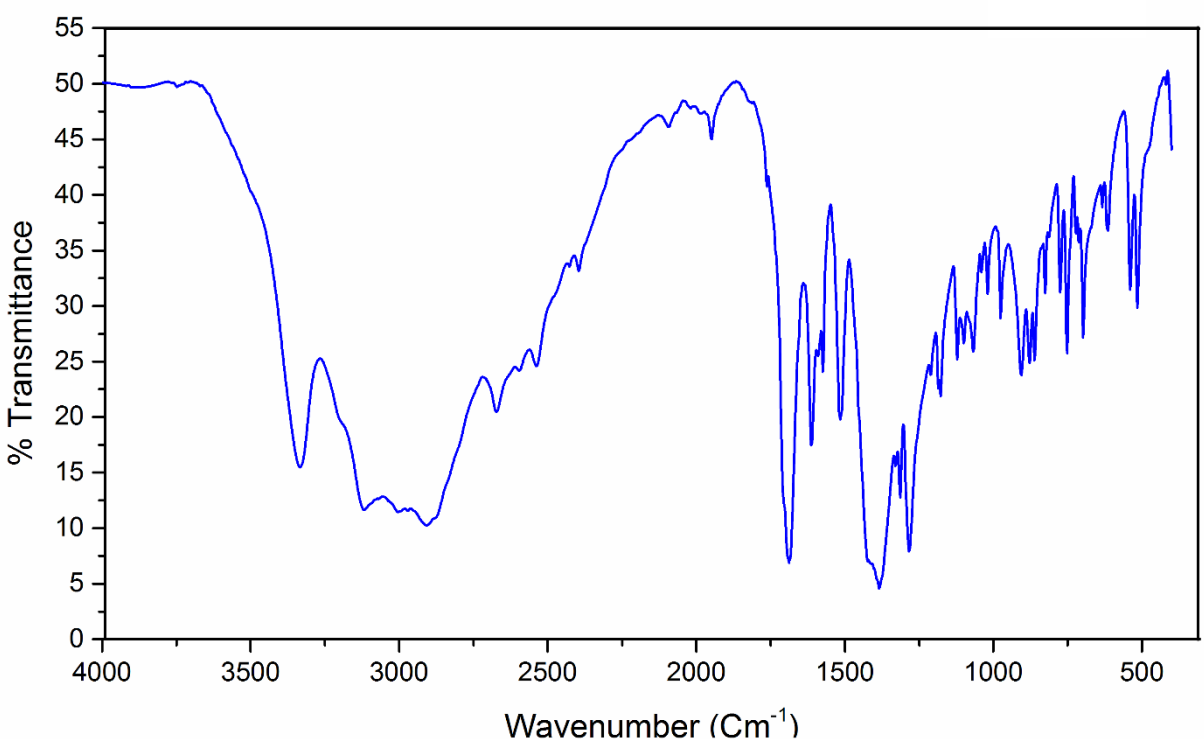
Table 1. Crystal data, full details of data collection and refinement statistics.

	(**1**)	(**2**)	(**3**)
Crystal data			
Chemical formula	$C_8H_{10}NO_2^+ \cdot ClO_4^-$	$C_8H_{10}NO_2^+ \cdot NO_3^-$	$C_8H_{10}NO_2^+ \cdot ClO_4^-$
M_r	251.62	214.18	251.62
Cell setting, space group	Monoclinic, $P2_1/a$	Monoclinic, $I2/a$	Triclinic, $P\text{-}1$
a, b, c (Å)	7.3914(2), 11.6712(10), 12.5913(9)	13.3114(10), 6.0032(4), 24.1094(15)	4.9634(4), 12.9992(11), 16.5405(17)
α, β, γ (°)	90, 91.455(4), 90	90, 101.854(5), 90	75.125(8), 88.907(7), 87.706(6)
V (Å^3)	1085.86(12)	1885.5(2)	1030.56(16)
Z	4	8	4
Radiation type		Mo $K\alpha$	
D_x (Mg.m^{-3})	1.539	1.509	1.622
μ (mm^{-1})	0.365	0.127	0.385
Temperature (K)		298	
Crystal form, colour	Prism, Yellow	Prism, Colourless	Prism, Colourless
Crystal size (mm)	0.2 × 0.2 × 0.2	0.35 × 0.3 × 0.1	0.25 × 0.125 × 0.05
Data collection			
Diffractometer		Bruker-Nonius KappaCCD diffractometer	
No. of measured reflections	31541	10974	30848
Independent reflections	2503	2162	4751
Observed reflections with [$I > 2\sigma(I)$]	1866	1379	2918
R_{int}	0.0703	0.073	0.1314
θ_{min} (°)	5.164	5.117	5.088
θ_{max} (°)	27.506	27.501	27.495
h	-9 → 9	-17 → 17	-6 → 6
k	-15 → 15	-7 → 7	-16 → 16
l	-16 → 16	-31 → 29	-21 → 21
Refinement			
$R[F^2 > 2\sigma(F^2)]$	0.0561	0.0482	0.0546
$wR(F^2)$	0.1342	0.1111	0.1003
S	1.031	1.013	1.008
No. of reflections	2503	2146	4751
No. of parameters	149	138	290
H-atom treatment		Constrained refinement	

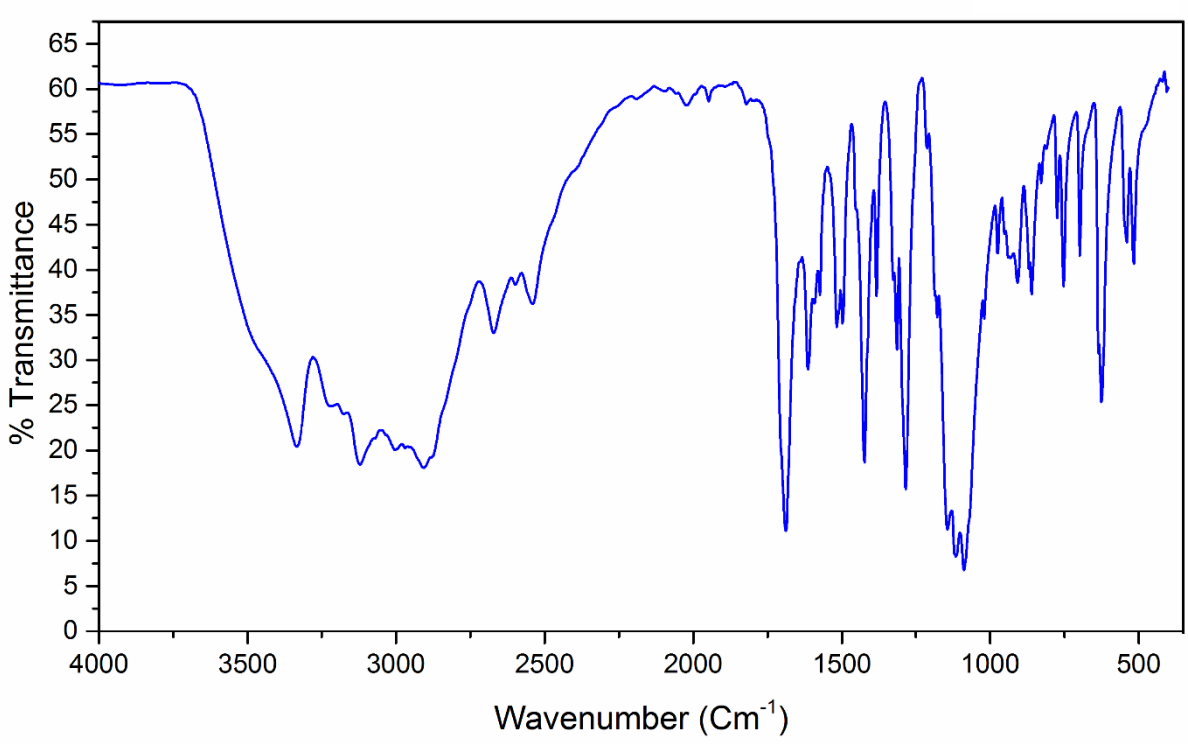
Weighting scheme	$w = 1/[\sigma^2 (F_o^2) + (0.0614P)^2 + 1.0043\ P]$ where $P = (F_o^2 + 2\ F_c^2)/3$	$w = 1/[\sigma^2 (F_o^2) + (0.0623P)^2 + + 0.6027\ P]$ where $P = (F_o^2 + 2\ F_c^2)/3$	$w = 1/[\sigma^2 (F_o^2) + (0.0365P)^2 + 0.7374\ P]$ where $P = (F_o^2 + 2\ F_c^2)/3$
$(\Delta/\sigma)_{max}$		0.000	
ρ_{max} (e Å^{-3})	0.343	0.241	0.322
ρ_{min} (e Å^{-3})	-0.427	-0.230	-0.327



(a)

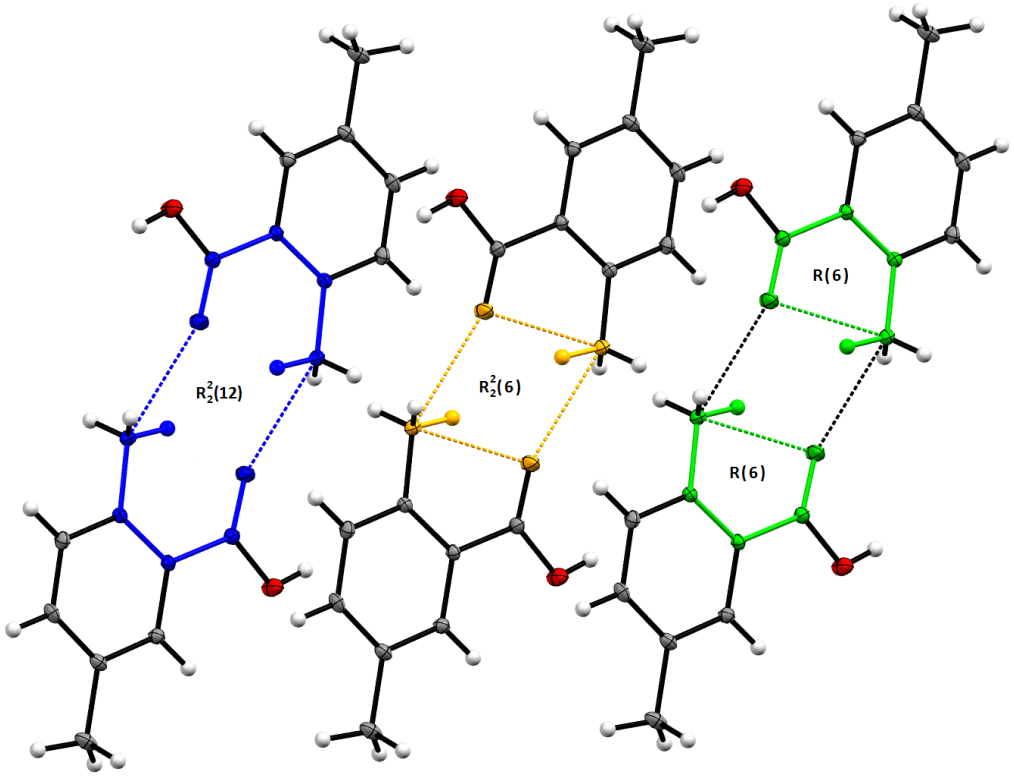


(b)

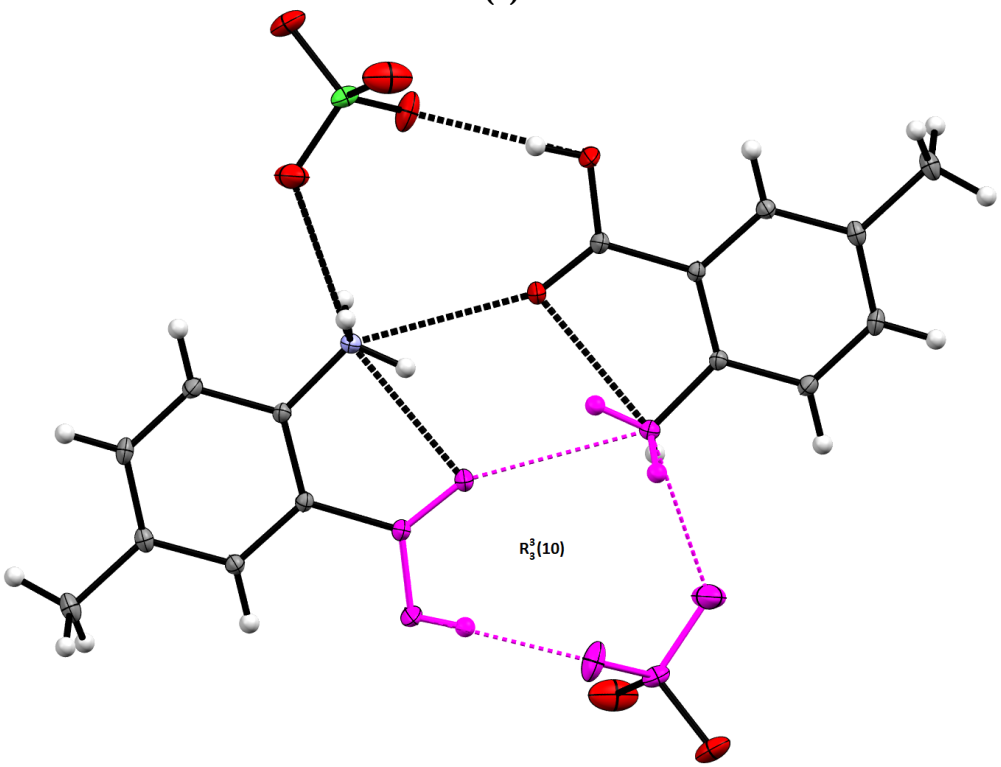


(c)

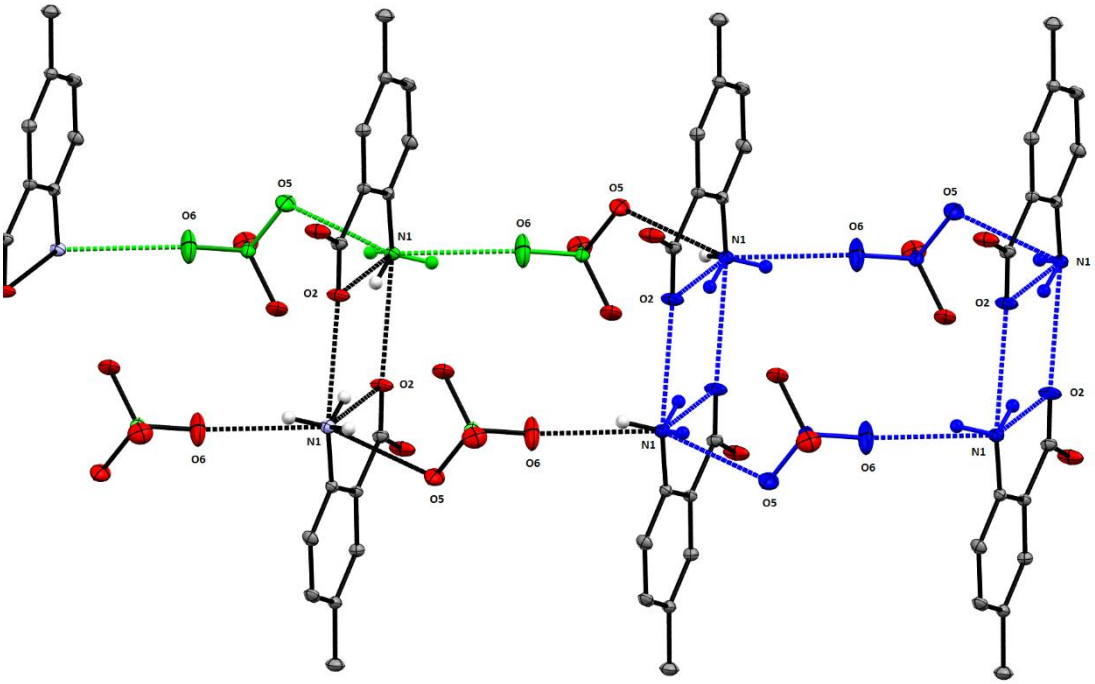
Figure S1. FTIR spectra for a) compound (**1**), b) compound (**2**) and c) compound (**3**).



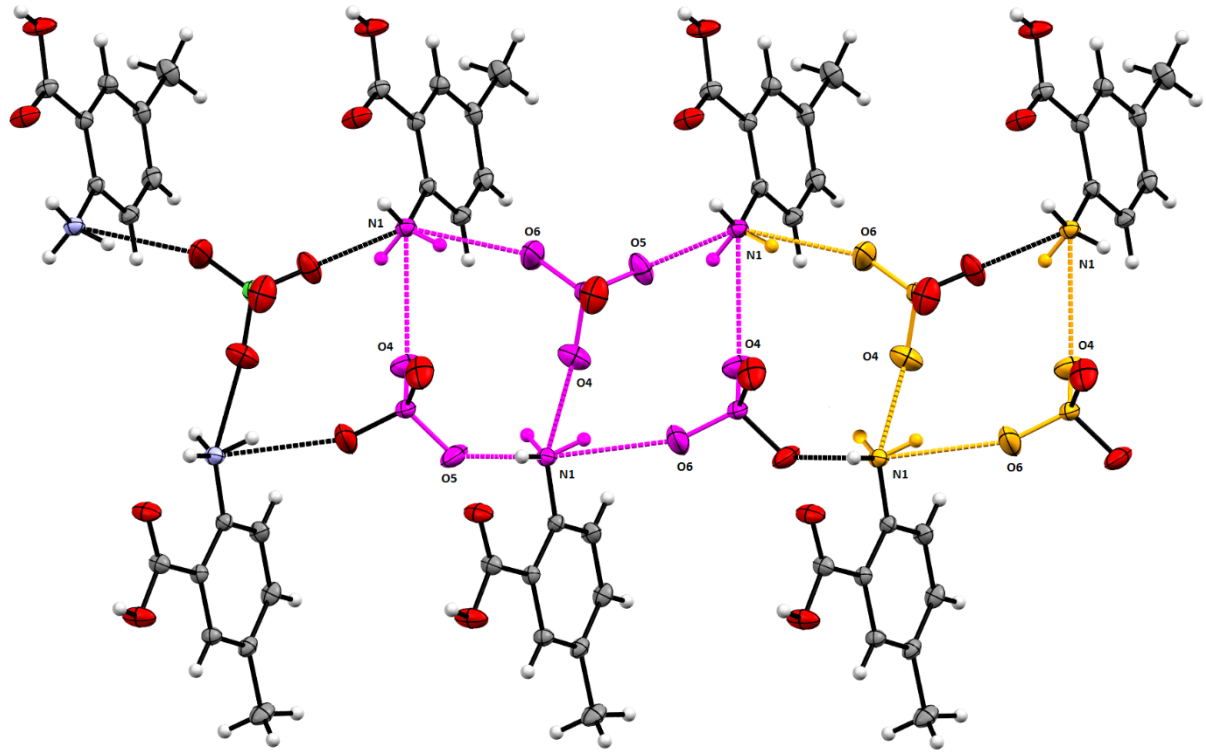
(a)



(b)

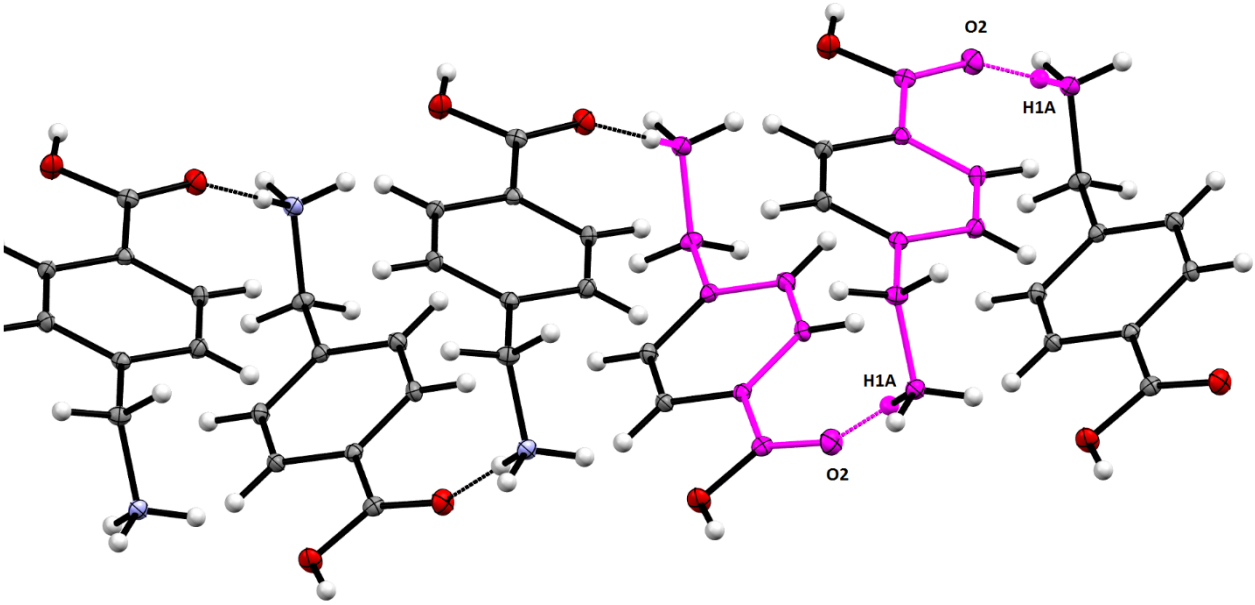


(c)

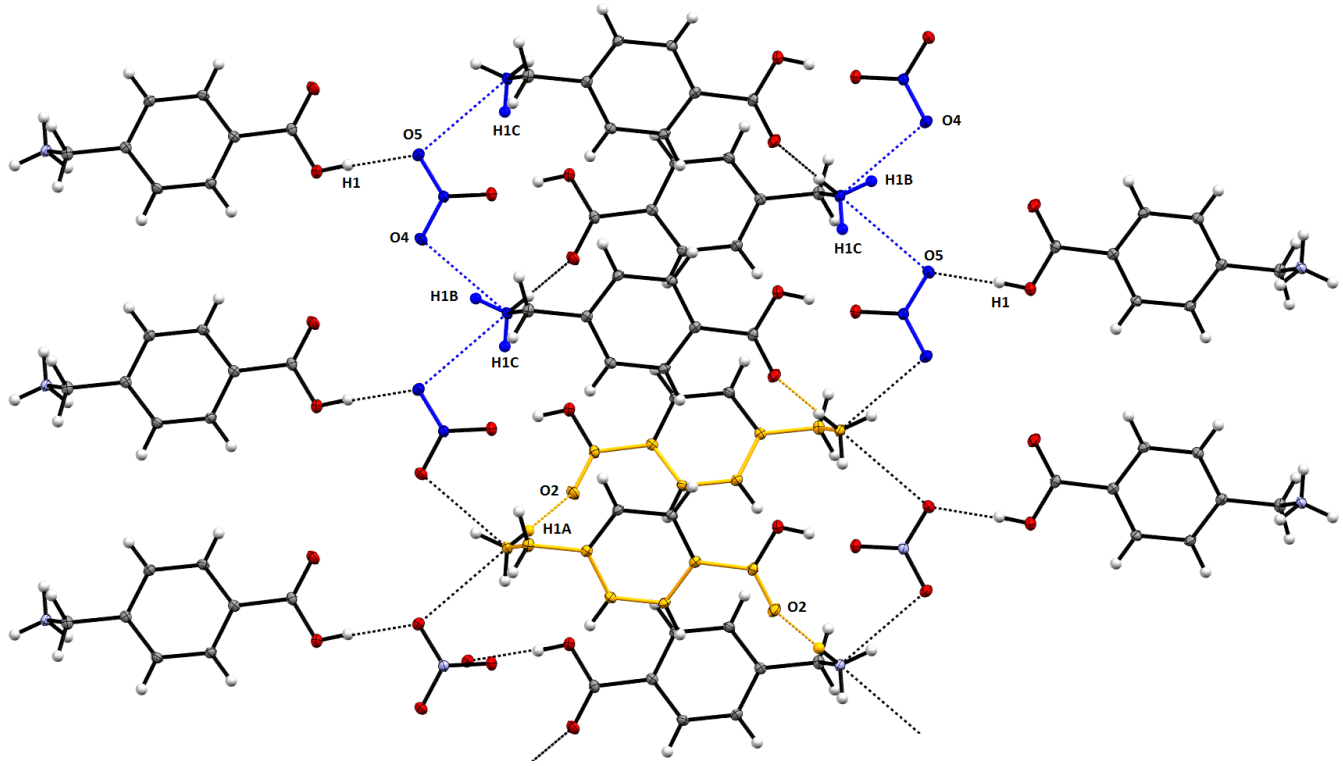


(d)

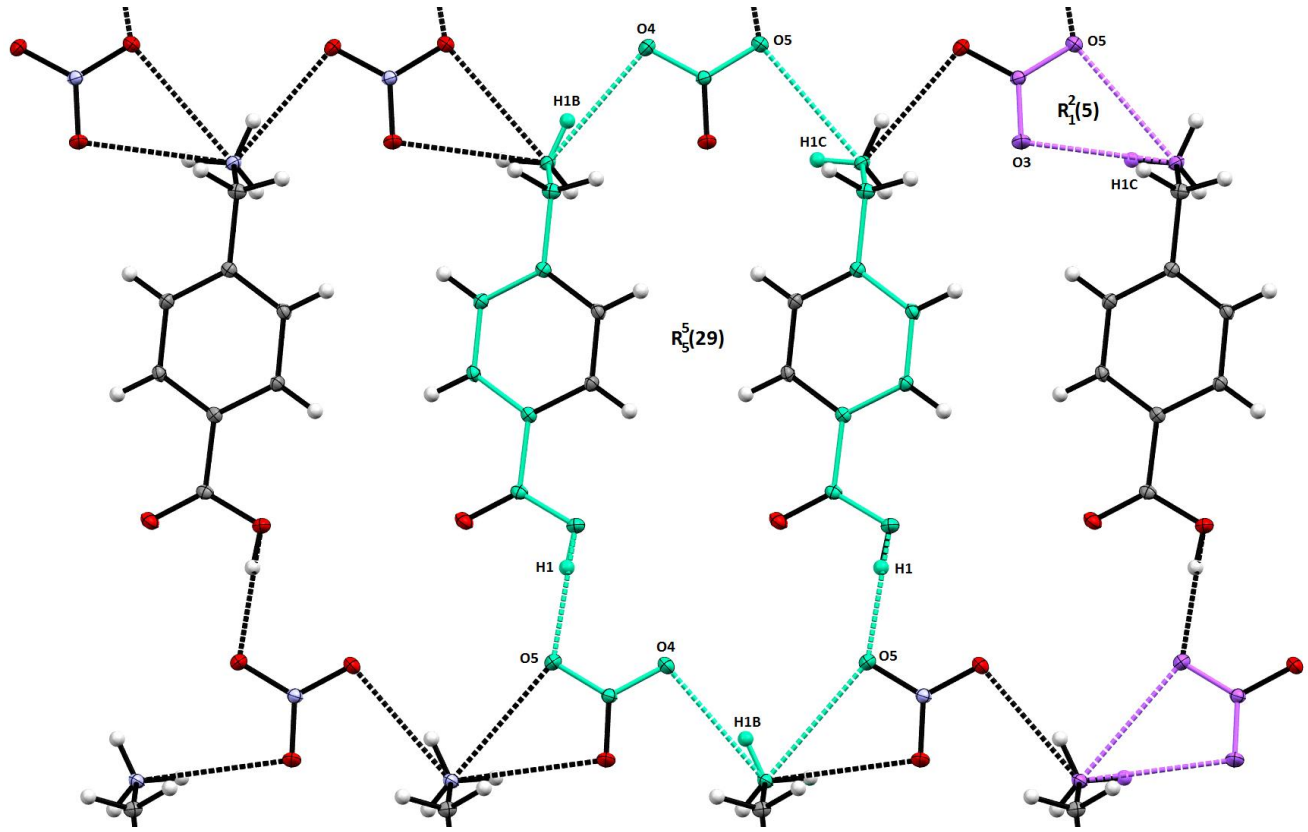
Figure S2. Graph set motifs observed in compound (**1**). a) The $R^2_2(12)$ first-level graph set descriptor of the intermolecular interaction N1–H1A…O2, given in blue and the alternating edge-fused R(6)-R^2_2(6)-R(6) rings resulting from the combination of intermolecular and intramolecular interactions N1–H1A…O2 (R^2_2(6) is drawn in yellow and R(6) in light green). b) The complementary DAD-ADA arrays of hydrogen bonded patterns described as edge-fused R^3_3(10)-R^2_2(12)/R^2_2(6)-R^3_3(10) rings linking two cations and two anions related with an inversion center (the R^3_3(10) rings are given in magenta). c) A crystal structure fragment displaying the edge-fused R^2_2(6)-R^6_4(20)-R^2_2(6) rings and the C^2_2(6) chains drawn in blue and green, respectively. d) C^2_2(6) and R^4_3(11) graph-sets describing the combination of N1–H1B…O4 and N1–H1C…O6 (drawn in yellow), together with N1–H1B…O5 (highlighted in magenta).



(a)

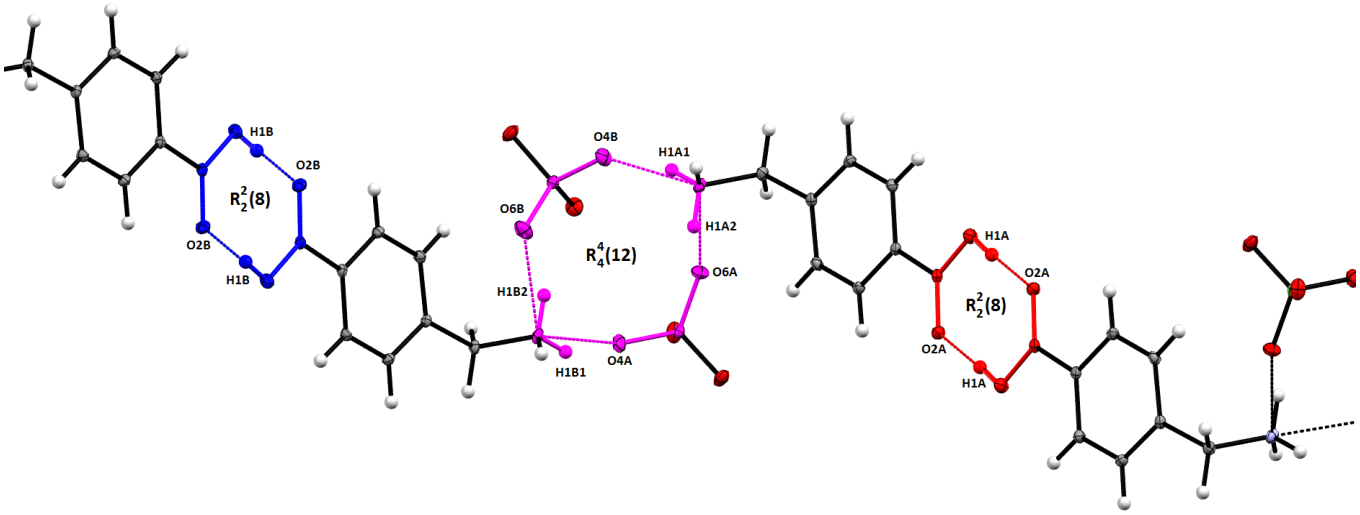


(b)

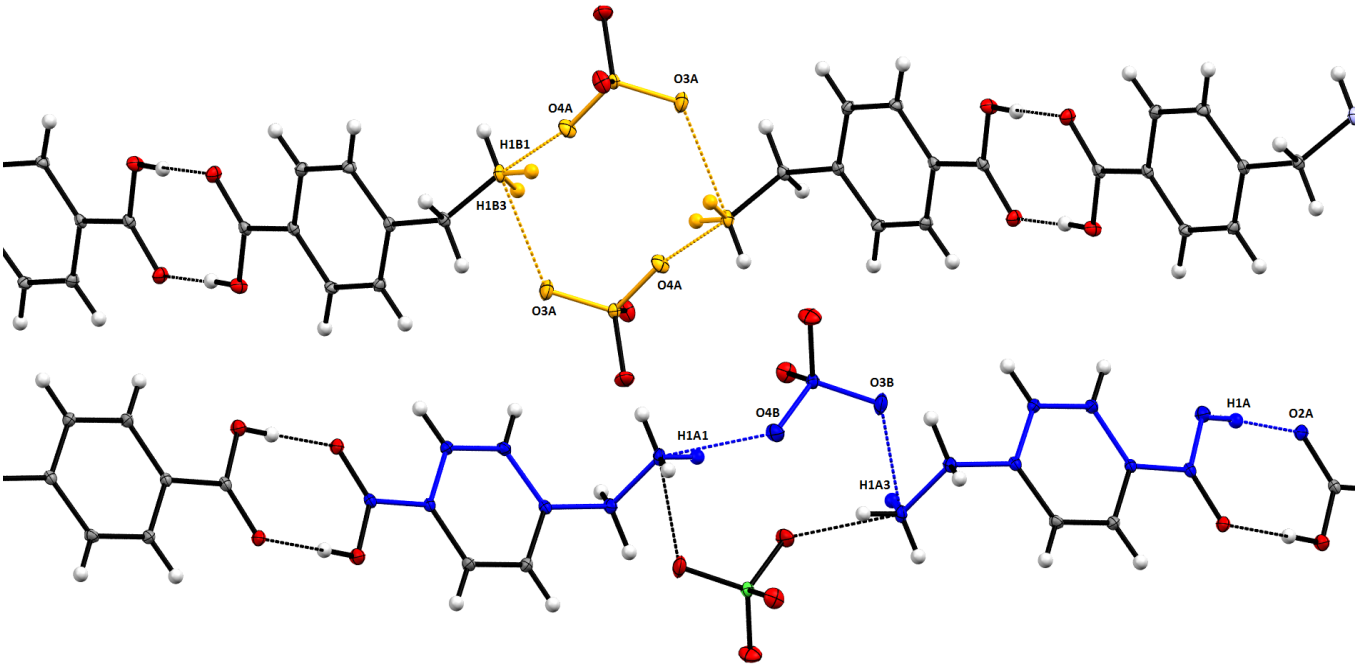


(c)

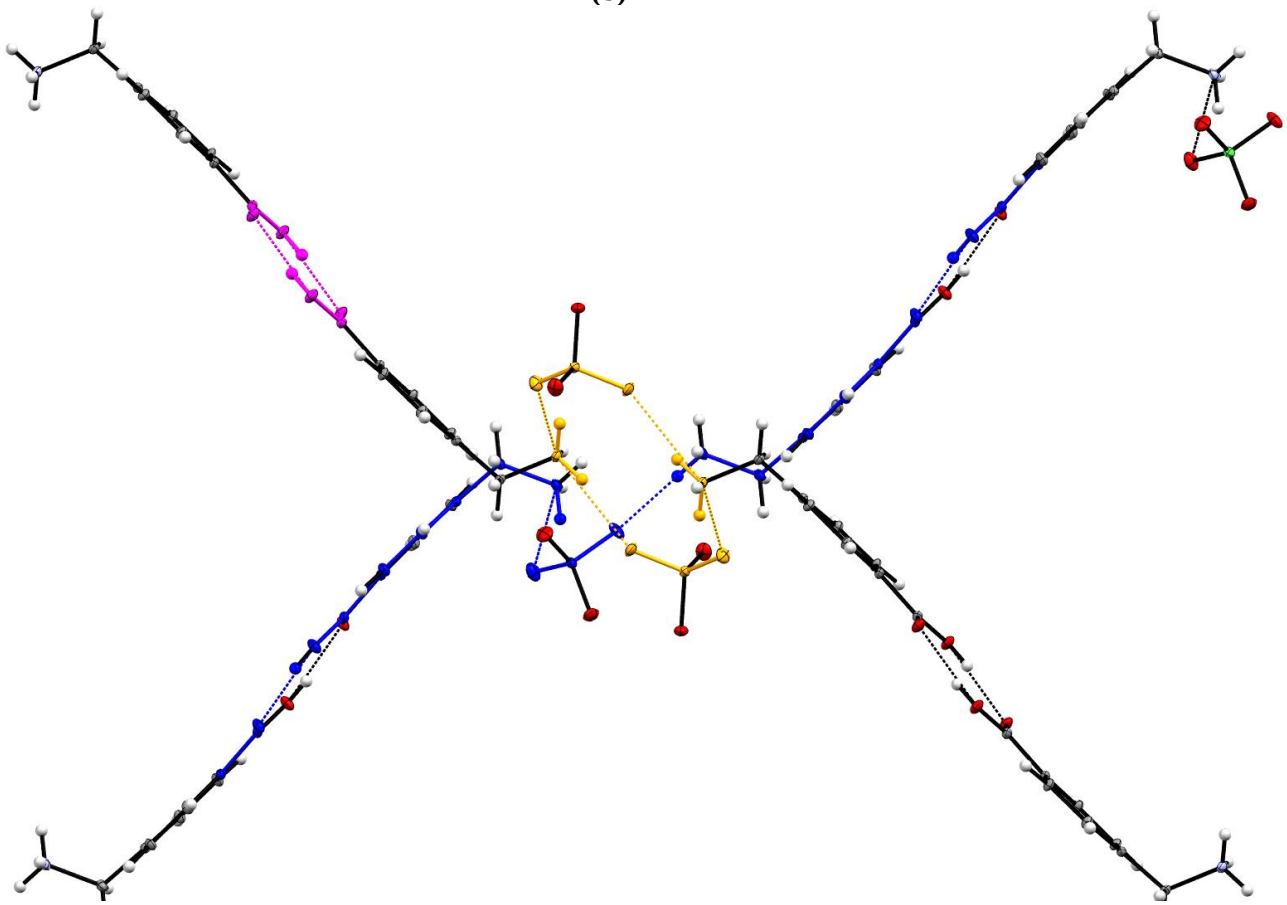
Figure S3. Graph-set motifs describing the hydrogen bonding in (**2**). a) The C(9) first-level graph set descriptor resulting from the interaction N1–H1A…O2 and highlighted in magenta. b) A crystal structure fragment displaying the $C^2_2(6)$ infinite chains drawn in blue linked together through the C(9) chains (given in yellow) and the O1–H1…O5 hydrogen bond to build up zig-zag sheets. c) The infinite edge-fused $R^2_1(5)$-$R^5_5(29)$-$R^2_1(5)$ rings generating layers. The $R^2_1(5)$ rings are drawn in violet, while the $R^5_5(29)$ ones are highlighted in light green.



(a)



(b)



(c)

Figure S4. a) The DA-AD self-assembly forming carboxylic acid dimers described as $R^2_2(8)$ rings (dimers A are drawn in red and the dimers resulting from molecules B are given in blue). The twelve-membered $R^4_4(12)$ rings resulting from the combination of two anions (A and B) and two cations (A and B) is highlighted as a magenta ring. b) Infinite $C^3_3(22)$ chains (drawn in blue) built up from the association of anions and cationic dimers creating $R^4_4(12)$ graph sets (given in yellow). c) Infinite cross-chains resulting from two $C^3_3(22)$ chains belonging to cations A and B. The $C^3_3(22)$, $R^4_4(12)$ and $R^2_2(8)$ descriptors are drawn in blue, yellow and purple, respectively.

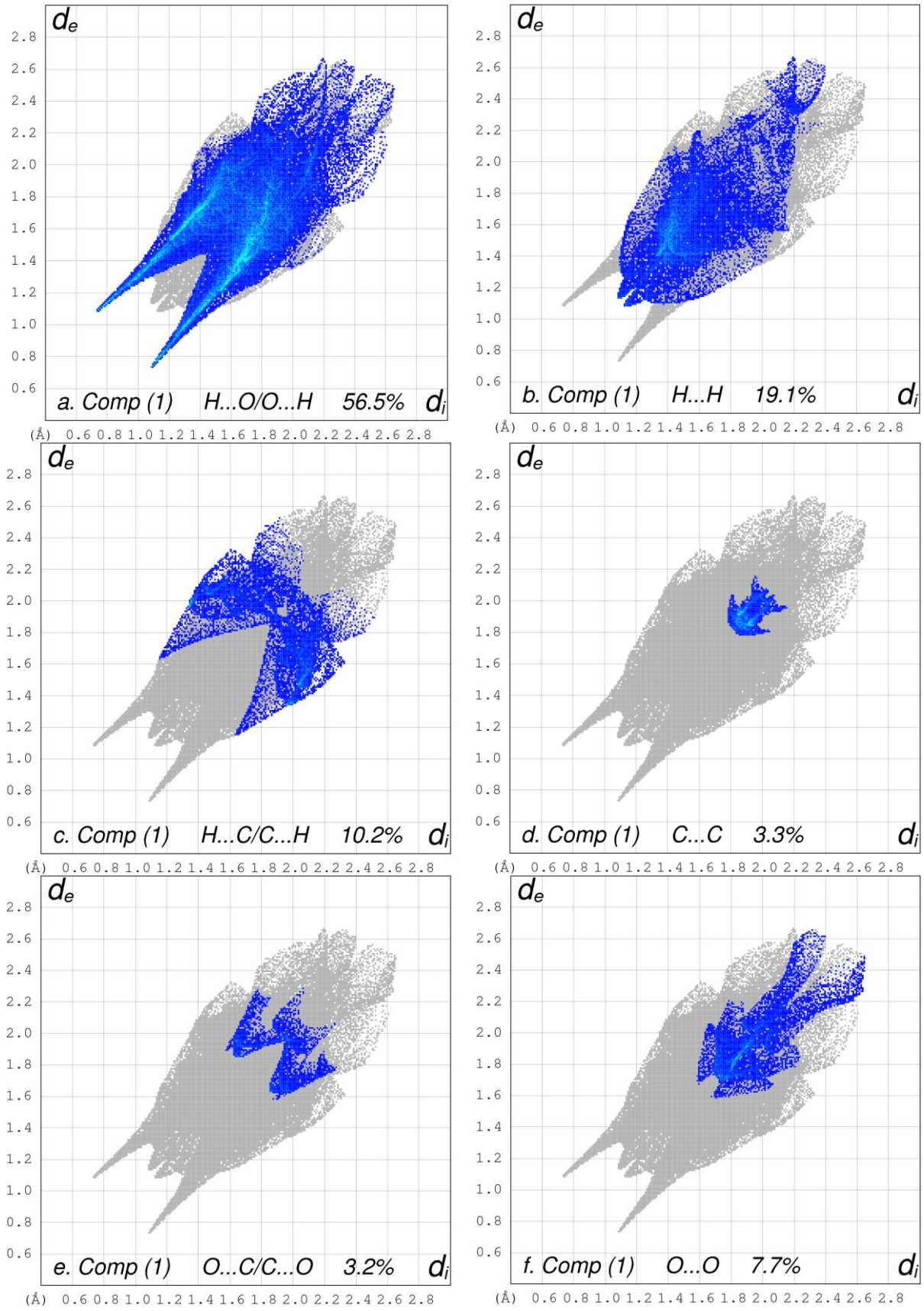
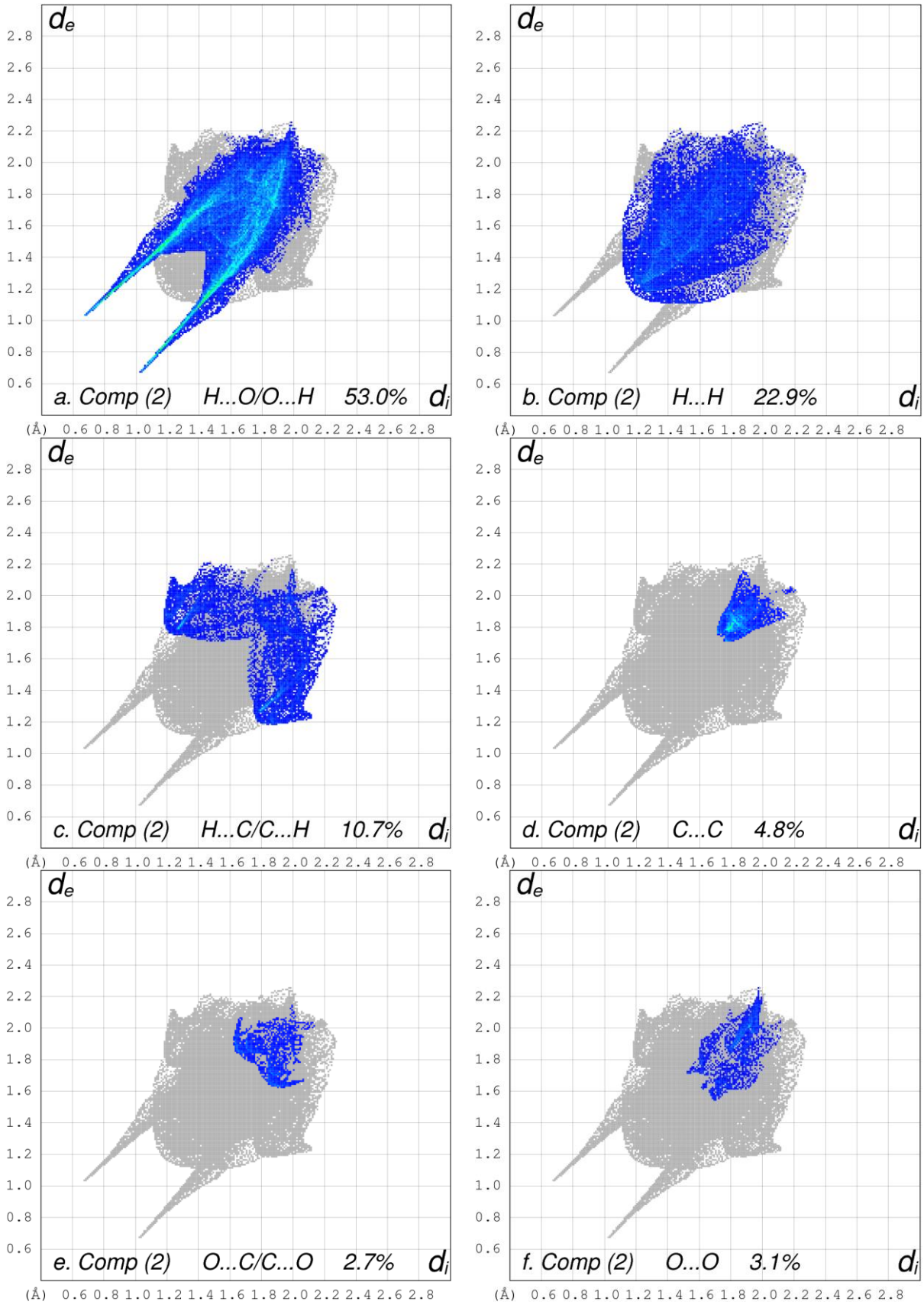


Figure S5. Decomposed fingerprint plots into various intermolecular interactions within compound (**1**). a) H…O/O…H contacts (56.5%). b) H..H contacts (19.1%). c) H…C/C…H contacts (10.2%). d) C…C contacts (3.3%). e) O…C/C…O contacts (3.2%). f) O…O contacts (7.7%).


de
di
a. Comp (2) H...O/O...H 53.0%
b. Comp (2) H...H 22.9%
c. Comp (2) H...C/C...H 10.7%
d. Comp (2) C...C 4.8%
e. Comp (2) O...C/C...O 2.7%
f. Comp (2) O...O 3.1%
(Å) 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

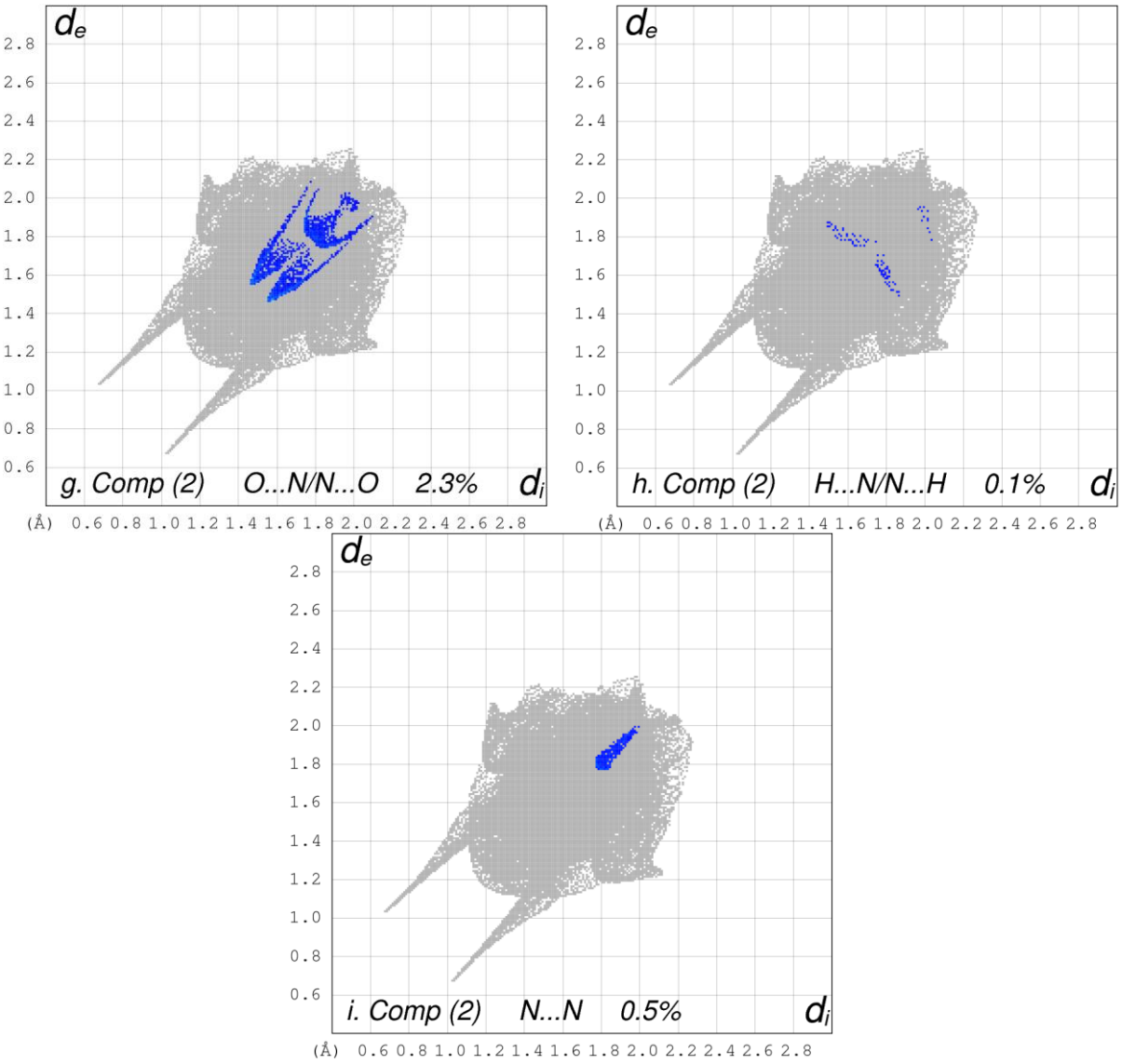


Figure S6. Close contacts to the Hirshfeld surfaces of molecules in (**2**) broken down into different intermolecular interaction types. a) H…O/O…H contacts (53.0%). b) H..H contacts (22.9%). c) H…C/C…H contacts (10.7%). d) C…C contacts (4.8%). e) O…C/C…O contacts (2.7%). f) O…O contacts (3.1%). g) O…N/N…O contacts (2.3%). h) H…N/N…H contacts (0.1%). i) N…N contacts (0.5%).

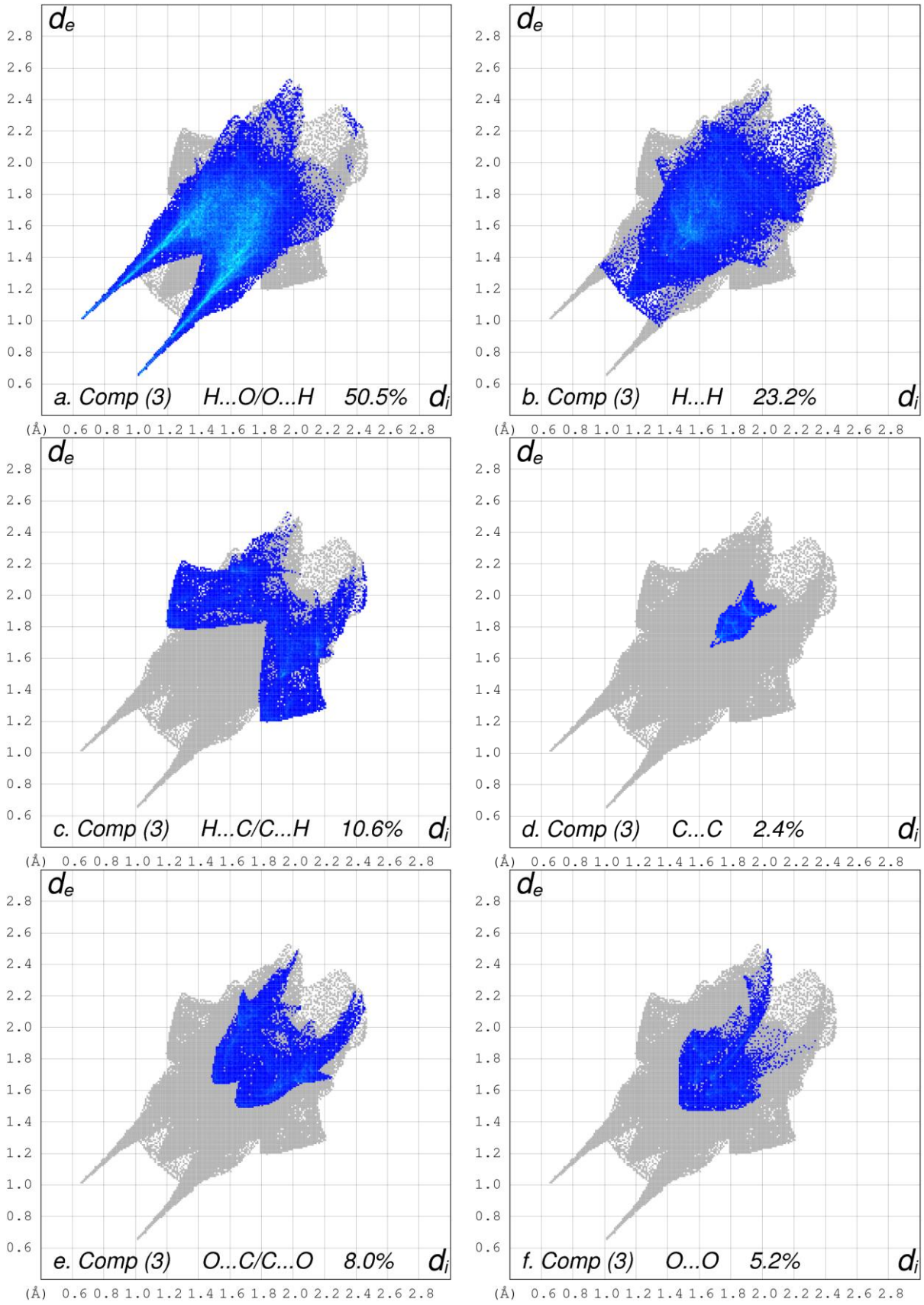


Figure S7. Decomposed fingerprint plots of the intermolecular interactions within (**3**). a) H…O/O…H contacts (50.5%). b) H..H contacts (23.2%). c) H…C/C…H contacts (10.6%). d) C…C contacts (2.4%). e) O…C/C…O contacts (8.0%). f) O…O contacts (5.2%).