Chirality as a Feature of the Crystal Structure of Lanthanide Ion Complexes—Some Simple Examples

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SUPPLEMENTARY INFORMATION

S1. Crystallography details.

Table S1. Crystal and structure refinement data for the redefined $Er(bipy)_2Cl_2(OH_2)_2]Cl{\cdot}H_2O$ structure described in the in reference [24].

Complex	**5**
Empirical formula	$C_{20}H_{20}Cl_3ErN_4O_2$
Formula weight (g mol^{-1})	622.01
Crystal system	cubic
Space group	*I*23 (No. 197)
Temperature /K	297(2)
a (Å)	25.943(5)
b (Å)	25.943(5)
c (Å)	25.943(5)
α(°)	90
β(°)	90
γ(°)	90
V (Å^3)	17461(10)
Z	24
Calculated density (g cm^{-3})	1.420
Absorption coefficient (mm^{-1})	3.178
F_{000}	7272
Crystal size (mm^3)	0.30 × 0.30 × 0.15
θ range for data collection (°)	2.483 to 24.973
Miller index ranges	-30 ≤ *h* ≤ 1, -30 ≤ *k* ≤ 0, -30 ≤ *l* ≤ 0
Reflections measured	8395
Independent reflections	2916
Reflections with $I > 2\sigma(I)$	2315
R_{int}	0.0764
Data / restraints / parameters	2916 / 87 / 291
Final *R* indices [$I > 2\sigma(I)$]	*R*1 = 0.0475, *wR*2 = 0.1204
R indices (all data)	*R*1 = 0.0664, *wR*2 = 0.1295
Goodness-of-fit on F^2	1.002
$\Delta\rho_{min}$ (e Å^{-3})	-0.502
$\Delta\rho_{max}$ (e Å^{-3})	0.909
Absolute structure parameter	0.31(3)
CCDC	2220101

Table S2. Metal atom environment for $Dy(bipy)_2Cl_2(OH_2)_2]Cl{\cdot}H_2O$, **1**

Bond length (Å)	
Dy1—O1	2.323(15)
Dy1—O2	2.359(19)
Dy1—N11′	2.545(19)
Dy1—N21′	2.56(2)
Dy1—N21	2.561(18)
Dy1—N11	2.565(17)
Dy1—Cl1	2.660(8)
Dy1—Cl2	2.686(8)
Bond angles (°)	
O1—Dy1—O2	81.4(7)
O1—Dy1—N11′	150.4(6)
O2—Dy1—N11′	108.9(6)
O1—Dy1—N21′	73.0(7)
O2—Dy1—N21′	145.5(7)
N11′—Dy1—N21′	84.8(6)
O1—Dy1—N21	112.2(7)
O2—Dy1—N21	149.8(7)
N11′—Dy1—N21	73.0(5)
N21′—Dy1—N21	63.8(7)
O1—Dy1—N11	145.0(7)
O2—Dy1—N11	72.5(6)
N11′—Dy1—N11	62.9(6)
N21′—Dy1—N11	139.4(6)
N21—Dy1—N11	82.7(7)
O1—Dy1—Cl1	81.5(5)
O2—Dy1—Cl1	72.8(5)
N11′—Dy1—Cl1	75.7(4)
N21′—Dy1—Cl1	80.7(5)
N21—Dy1—Cl1	134.0(5)
N11—Dy1—Cl1	111.4(4)
O1—Dy1—Cl2	73.5(5)
O2—Dy1—Cl2	83.9(5)
N11′—Dy1—Cl2	133.9(4)
N21′—Dy1—Cl2	109.7(5)
N21—Dy1—Cl2	75.1(5)
N11—Dy1—Cl2	80.8(5)
Cl1—Dy1—Cl2	148.1(2)
C12′—N11′—Dy1	119.7(13)
C16′—N11′—Dy1	118.4(13)

Table S3. Metal atom environment for $La_2(phen)_2(O_2CCH_3)_4(NO_3)_2$, **2**

Bond length (Å)	
La1—O21	2.428(13)
La1—O31	2.436(15)
La1—O22^{i}	2.481(12)
La1—O11	2.559(13)
La1—O32^{i}	2.570(13)
La1—O12	2.611(13)
La1—N11′	2.681(14)
La1—N11	2.690(14)
La1—O31^{i}	2.758(12)
La1—N1	2.98(2)
La1—C3^{i}	3.00(2)
La1—La1^{i}	4.060(4)
Bond angle (^{o})	
O21—La1—O31	75.3(5)
O21—La1—O22^{i}	134.9(4)
O31—La1—O22^{i}	75.6(5)
O21—La1—O11	130.9(5)
O31—La1—O11	84.0(5)
O22^{i}—La1—O11	78.6(5)
O21—La1—O32^{i}	84.8(5)
O31—La1—O32^{i}	126.1(4)
O22^{i}—La1—O32^{i}	85.3(5)
O11—La1—O32^{i}	140.9(5)
O21—La1—O12	82.9(4)
O31—La1—O12	82.2(5)
O22^{i}—La1—O12	125.8(5)
O11—La1—O12	50.1(4)
O32^{i}—La1—O12	144.7(5)
O21—La1—N11′	78.5(4)
O31—La1—N11′	144.6(4)
O22^{i}—La1—N11′	139.3(4)
O11—La1—N11′	95.8(5)
O32^{i}—La1—N11′	73.9(4)
O12—La1—N11′	71.3(4)
O21—La1—N11	136.3(4)
O31—La1—N11	148.2(4)
O22^{i}—La1—N11	79.8(4)
O11—La1—N11	71.5(5)
O32^{i}—La1—N11	70.7(4)
O12—La1—N11	96.5(5)
N11′—La1—N11	60.5(4)
O21—La1—O31^{i}	69.5(4)
O31—La1—O31^{i}	77.4(5)
O22^{i}—La1—O31^{i}	71.0(4)
O11—La1—O31^{i}	147.4(4)
O32^{i}—La1—O31^{i}	48.7(4)
O12—La1—O31^{i}	149.0(5)
N11′—La1—O31^{i}	114.9(4)
N11—La1—O31^{i}	113.1(5)
O21—La1—N1	106.8(5)
O31—La1—N1	83.2(5)
O22^{i}—La1—N1	103.0(5)

O11—La1—N1	25.5(5)
O32^{i}—La1—N1	150.7(5)
O12—La1—N1	24.6(5)
N11′—La1—N1	82.1(5)
N11—La1—N1	83.1(5)
O31^{i}—La1—N1	160.5(5)
O21—La1—C3^{i}	76.1(5)
O31—La1—C3^{i}	101.6(5)
O22^{i}—La1—C3^{i}	77.0(5)
O11—La1—C3^{i}	152.6(5)
O32^{i}—La1—C3^{i}	24.5(4)
O12—La1—C3^{i}	156.8(5)
O21—La1—O31	75.3(5)
O21—La1—O22^{i}	134.9(4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Table S4. Metal atom environment for Lu(terpy)(O_2CCH_3)$_3$]·$NaNO_3$, **3**

Bond length (Å)	
Lu1—O1	2.291(16)
Lu1—O1"^{i}	2.336(16)
Lu1—O2	2.445(16)
Lu1—N21′	2.474(17)
Lu1—N21	2.492(15)
Lu1—O2"^{i}	2.503(15)
Lu1—N11	2.529(17)
Lu1—C1"^{i}	2.81(2)
Bond angle (°)	
O1′—Lu1—O2′^{i}	82.0(5)
O1′—Lu1—O1	130.4(6)
O2′^{i}—Lu1—O1	84.5(6)
O1′—Lu1—O1"^{i}	81.5(6)
O2′^{i}—Lu1—O1"^{i}	125.4(6)
O1—Lu1—O1"^{i}	141.8(5)
O1′—Lu1—O2	75.9(6)
O2′^{i}—Lu1—O2	76.6(5)
O1—Lu1—O2	54.5(5)
O1"^{i}—Lu1—O2	145.8(5)
O1′—Lu1—N21′	147.8(6)
O2′^{i}—Lu1—N21′	80.8(6)
O1—Lu1—N21′	74.6(6)
O1"^{i}—Lu1—N21′	86.6(6)
O2—Lu1—N21′	125.5(6)
O1′—Lu1—N21	77.5(5)
O2′^{i}—Lu1—N21	145.8(6)
O1′—Lu1—O2′^{i}	82.0(5)
O1′—Lu1—O1	130.4(6)
O2′^{i}—Lu1—O1	84.5(6)
O1′—Lu1—O1"^{i}	81.5(6)
O2′^{i}—Lu1—O1"^{i}	125.4(6)
O1—Lu1—O1"^{i}	141.8(5)
O1′—Lu1—O2	75.9(6)
O2′^{i}—Lu1—O2	76.6(5)
O1—Lu1—O2	54.5(5)
O1"^{i}—Lu1—O2	145.8(5)
O1′—Lu1—N21′	147.8(6)

C12′—N11′—Dy1	119.7(13)
C16′—N11′—Dy1	118.4(13)
O1′—Lu1—O2^{i}	82.0(5)
O1′—Lu1—O1	130.4(6)
O2^{i}—Lu1—O1	84.5(6)
O1′—Lu1—O1"^{i}	81.5(6)
O2^{i}—Lu1—O1"^{i}	125.4(6)
O1—Lu1—O1"^{i}	141.8(5)
O1′—Lu1—O2	75.9(6)
O2^{i}—Lu1—O2	76.6(5)
O1—Lu1—O2	54.5(5)
O1"^{i}—Lu1—O2	145.8(5)
O1′—Lu1—N21′	147.8(6)
O2^{i}—Lu1—N21′	80.8(6)
O1—Lu1—N21′	74.6(6)
O1"^{i}—Lu1—N21′	86.6(6)
O2—Lu1—N21′	125.5(6)
O1′—Lu1—N21	77.5(5)
O2^{i}—Lu1—N21	145.8(6)
O1—Lu1—N21	88.3(6)
O1"^{i}—Lu1—N21	78.2(5)
O2—Lu1—N21	72.1(5)
N21′—Lu1—N21	129.1(5)
O1′—Lu1—O2"^{i}	76.0(5)
O2^{i}—Lu1—O2"^{i}	72.5(6)
O1—Lu1—O2"^{i}	142.6(5)
O1"^{i}—Lu1—O2"^{i}	53.0(5)
O2—Lu1—O2"^{i}	140.5(5)
N21′—Lu1—O2"^{i}	72.9(5)
N21—Lu1—O2"^{i}	127.0(6)
O1′—Lu1—N11	136.2(5)
O2^{i}—Lu1—N11	141.8(5)
O1—Lu1—N11	70.6(6)
O1"^{i}—Lu1—N11	71.4(6)
O2—Lu1—N11	108.7(6)
N21′—Lu1—N11	65.2(5)
N21—Lu1—N11	63.9(5)
O2"^{i}—Lu1—N11	110.7(6)
O1′—Lu1—C1"^{i}	76.2(6)
O2^{i}—Lu1—C1"^{i}	99.4(6)
O1—Lu1—C1"^{i}	153.3(6)
O1"^{i}—Lu1—C1"^{i}	26.1(5)
O2—Lu1—C1"^{i}	152.1(6)
N21′—Lu1—C1"^{i}	80.0(6)
N21—Lu1—C1"^{i}	101.9(6)
O2"^{i}—Lu1—C1"^{i}	27.1(5)
N11—Lu1—C1"^{i}	91.6(6)
O1′—Lu1—C1	103.0(7)
O2^{i}—Lu1—C1	79.0(6)
O1—Lu1—C1	27.4(6)
O1"^{i}—Lu1—C1	155.6(5)
O2—Lu1—C1	27.1(6)
N21′—Lu1—C1	100.2(7)
N21—Lu1—C1	79.4(6)
O2"^{i}—Lu1—C1	151.4(5)
N11—Lu1—C1	90.0(7)
C1"^{i}—Lu1—C1	178.3(7)
O1′—Lu1—Na1^{i}	72.2(4)
O2^{i}—Lu1—Na1^{i}	41.7(5)
O1—Lu1—Na1^{i}	122.2(4)
O1"^{i}—Lu1—Na1^{i}	83.7(4)
O2—Lu1—Na1^{i}	112.6(4)
N21′—Lu1—Na1^{i}	76.8(4)
N21—Lu1—Na1^{i}	146.6(4)

O2"^{i}—Lu1—Na1^{i}	31.2(4)
N11—Lu1—Na1^{i}	135.1(4)
C1"^{i}—Lu1—Na1^{i}	57.7(5)
C1—Lu1—Na1^{i}	120.6(4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Table S5. Metal atom environment for $Lu(phen)(O_2CH)_3(OH_2)]\cdot H_2O$, **4**

Bond length (Å)	
Lu1—O31	2.210(8)
Lu1—O22^{i}	2.299(7)
Lu1—O21	2.311(7)
Lu1—O11	2.314(4)
Lu1—O11^{ii}	2.314(4)
Lu1—O1^{ii}	2.378(8)
Lu1—O1	2.378(8)
Lu1—N1	2.494(7)
Bond angle (°)	
O31—Lu1—O21	87.7(3)
O22^{i}—Lu1—O21	43.8(3)
O31—Lu1—O11	77.1(3)
O22^{i}—Lu1—O11	75.0(2)
O21—Lu1—O11	74.6(2)
O31—Lu1—O11^{ii}	108.3(3)
O22^{i}—Lu1—O11^{ii}	120.3(2)
O21—Lu1—O11^{ii}	142.0(2)
O11—Lu1—O11^{ii}	141.67(19)
O11—Lu1—O1^{ii}	78.9(2)
O11^{ii}—Lu1—O1^{ii}	136.5(2)
O11—Lu1—O1	136.5(2)
O11^{ii}—Lu1—O1	78.9(2)
O1^{ii}—Lu1—O1	58.1(4)
O31—Lu1—N1	76.6(3)
O22^{i}—Lu1—N1	131.3(2)
O21—Lu1—N1	145.7(2)
O11—Lu1—N1	72.3(1)
O11^{ii}—Lu1—N1	72.3(1)
O1^{ii}—Lu1—N1	129.0(2)
O1—Lu1—N1	129.0(2)
O31—Lu1—N1′	139.0(3)
O22^{i}—Lu1—N1′	72.0(2)
O21—Lu1—N1′	114.1(2)
O11—Lu1—N1′	76.30(11)
O11^{ii}—Lu1—N1′	76.30(11)
O1^{ii}—Lu1—N1′	144.1(2)
O1—Lu1—N1′	144.1(2)
N1—Lu1—N1′	66.0(2)

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, -y+1/2, z$.

S2. Details of atom numbering in each complex.

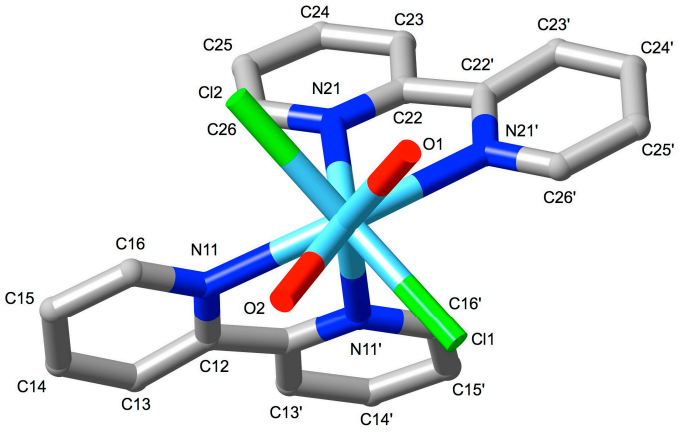

Figure S1. Complex **1**

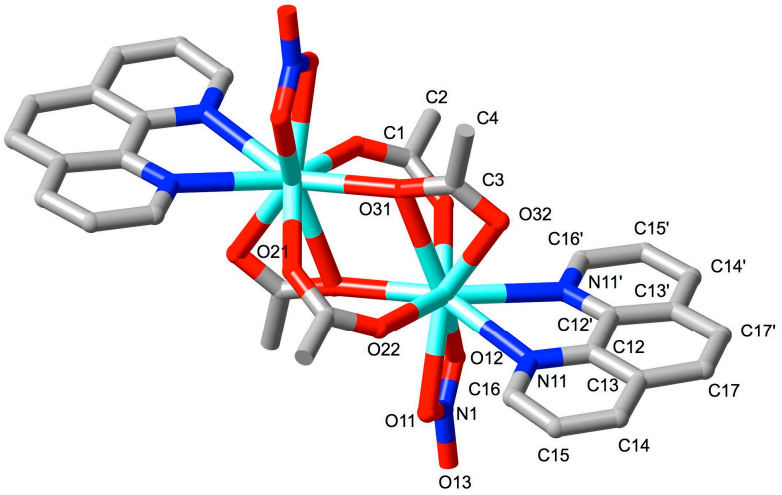

Figure S2. Complex **2** (centrosymmetric dimer)

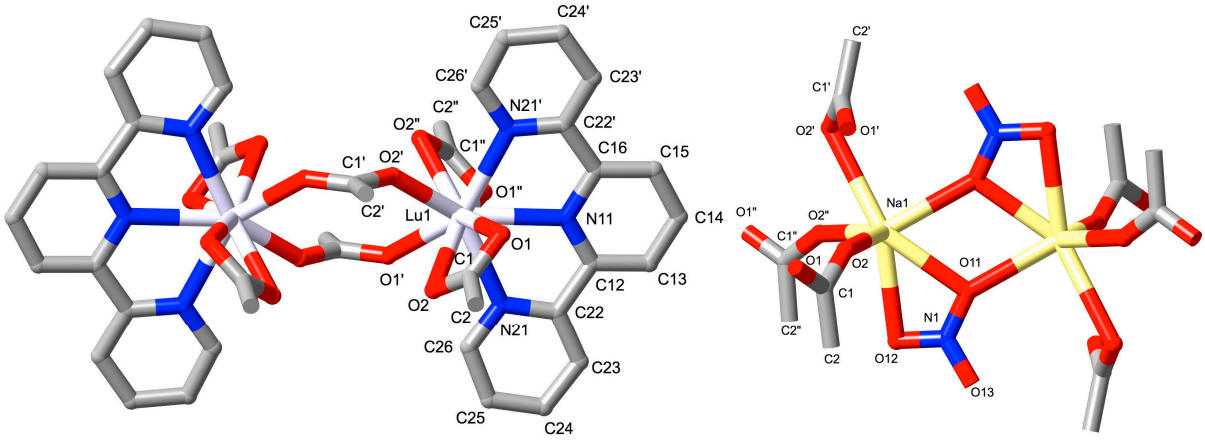

Figure S3. Complex **3** (two centrosymmetric components of a polymer)

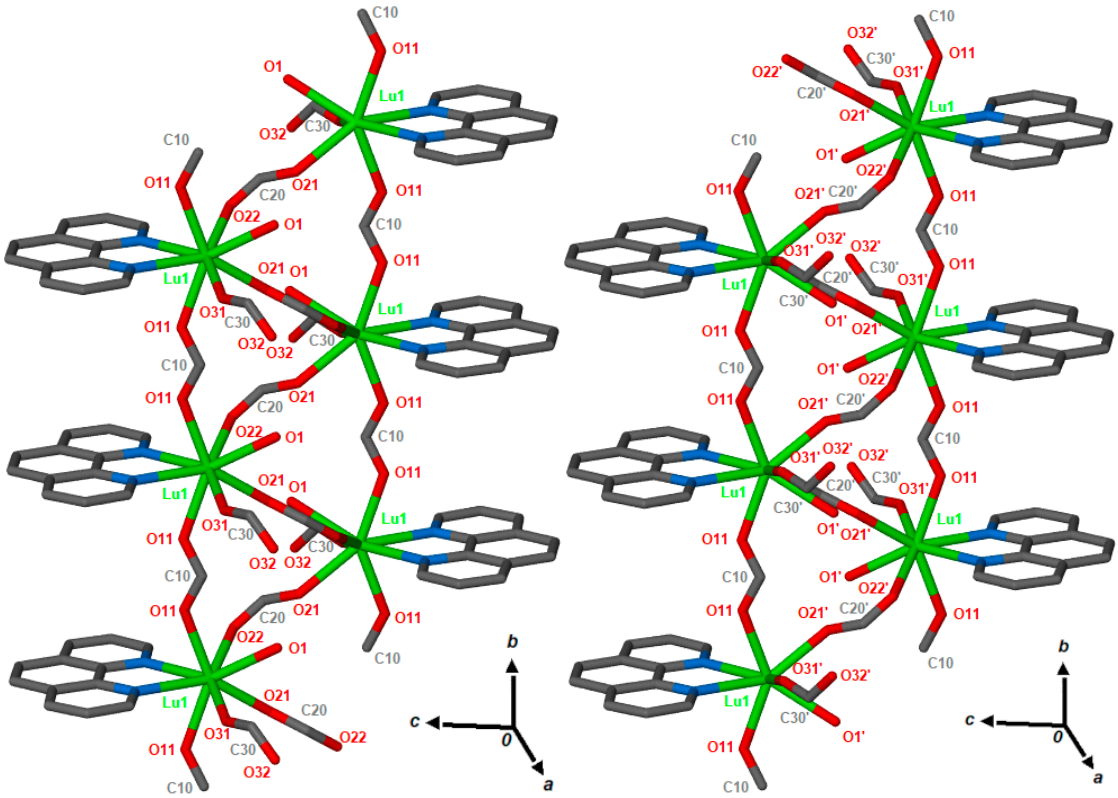

Figure S4. Complex **4** (two mirror-image helical polymer components)

S3. Two-dimensional fingerprint plots generated from the Hirshfeld surfaces, using CrystalExplorer17.

The two-dimensional fingerprint plots for all complexes revealed that the H…H contacts have significant contribution to the total Hirshfeld surfaces and are responsible for the overall stabilization of the crystals, scattered points are reflected homogeneously over a large range of (d_i, d_e) pairs. Significant H···Cl/Cl···H interactions in complex **1** can be seen, indicated by the two symmetrical narrow spikes at the top left and the bottom right in the two-dimensional fingerprint plots. The H…O/O…H and H…C/C…H contacts constitute important interactions in both complexes **2** and **3** with the scattered points distributed evenly in the two-dimensional fingerprint plots. The presence of stacking interactions in the crystal packing for all complexes was found in smaller percentages contributing to the total interaction surface.

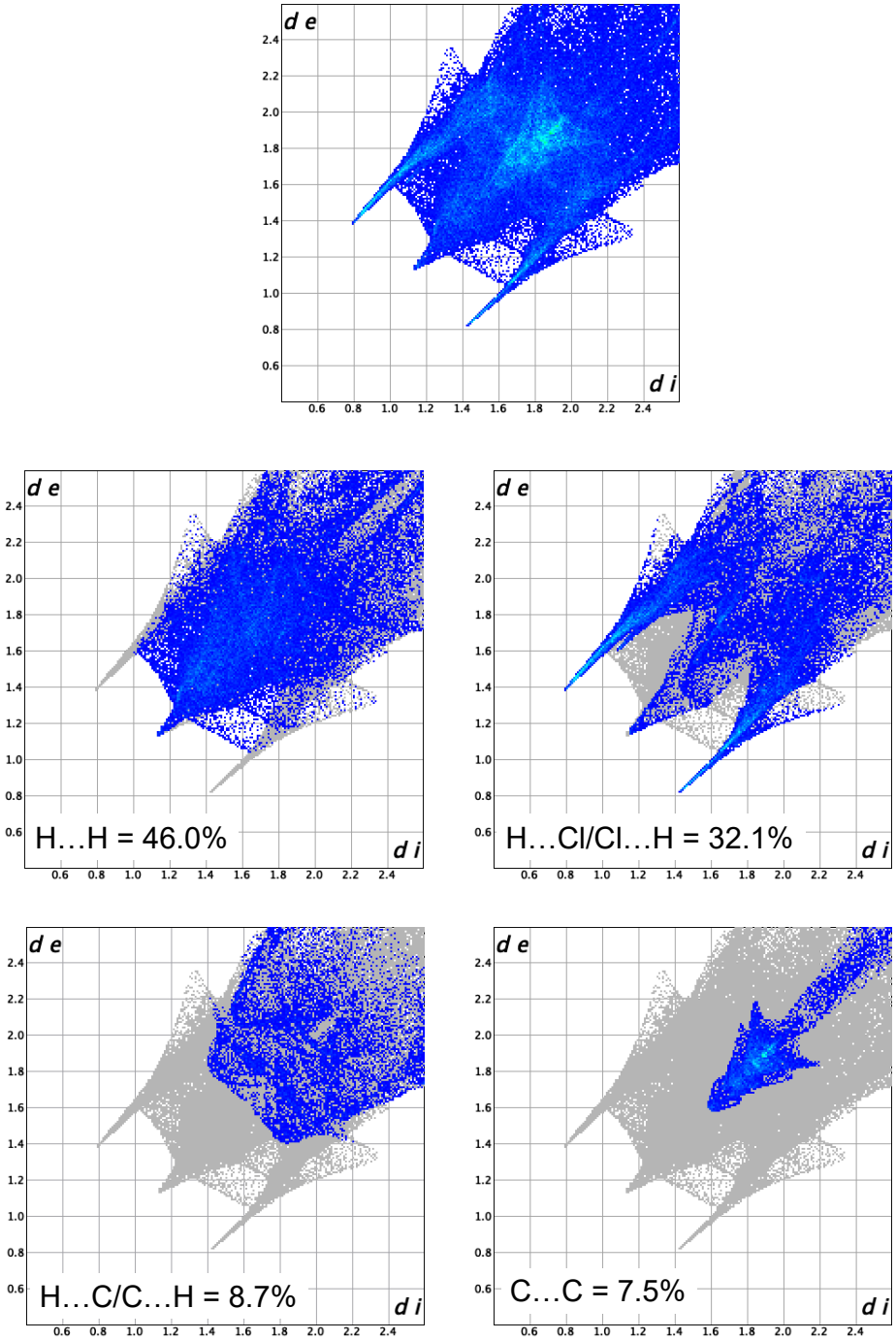

Figure S5. Two-dimensional fingerprint plots for complex **1** showing total interactions (top) and the selected key individual interatomic contacts with the percentages of contribution to the total interaction.

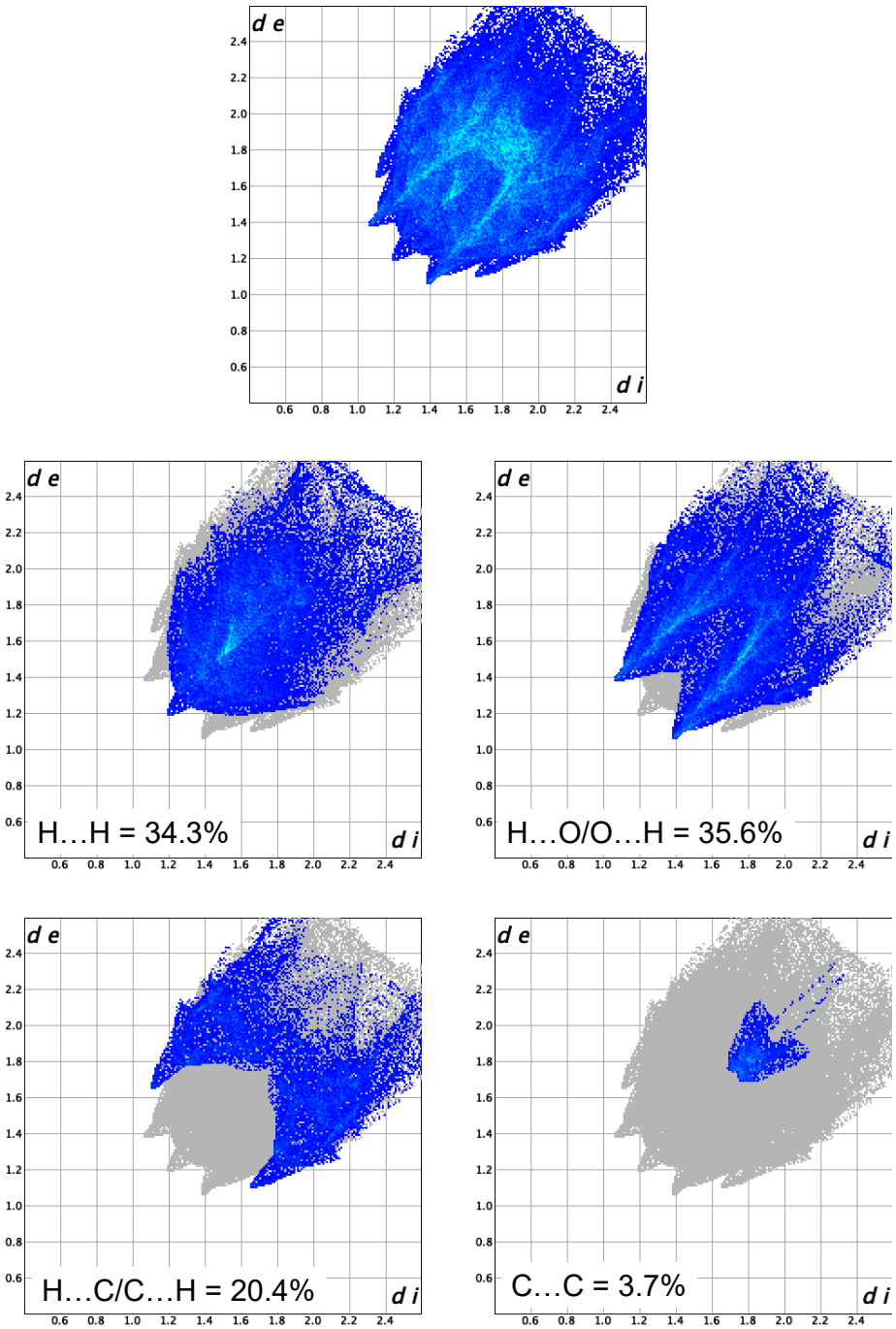

Figure S6. Two-dimensional fingerprint plots for complex **2** showing total interactions (top) and the selected key individual interatomic contacts with the percentages of contribution to the total interaction.

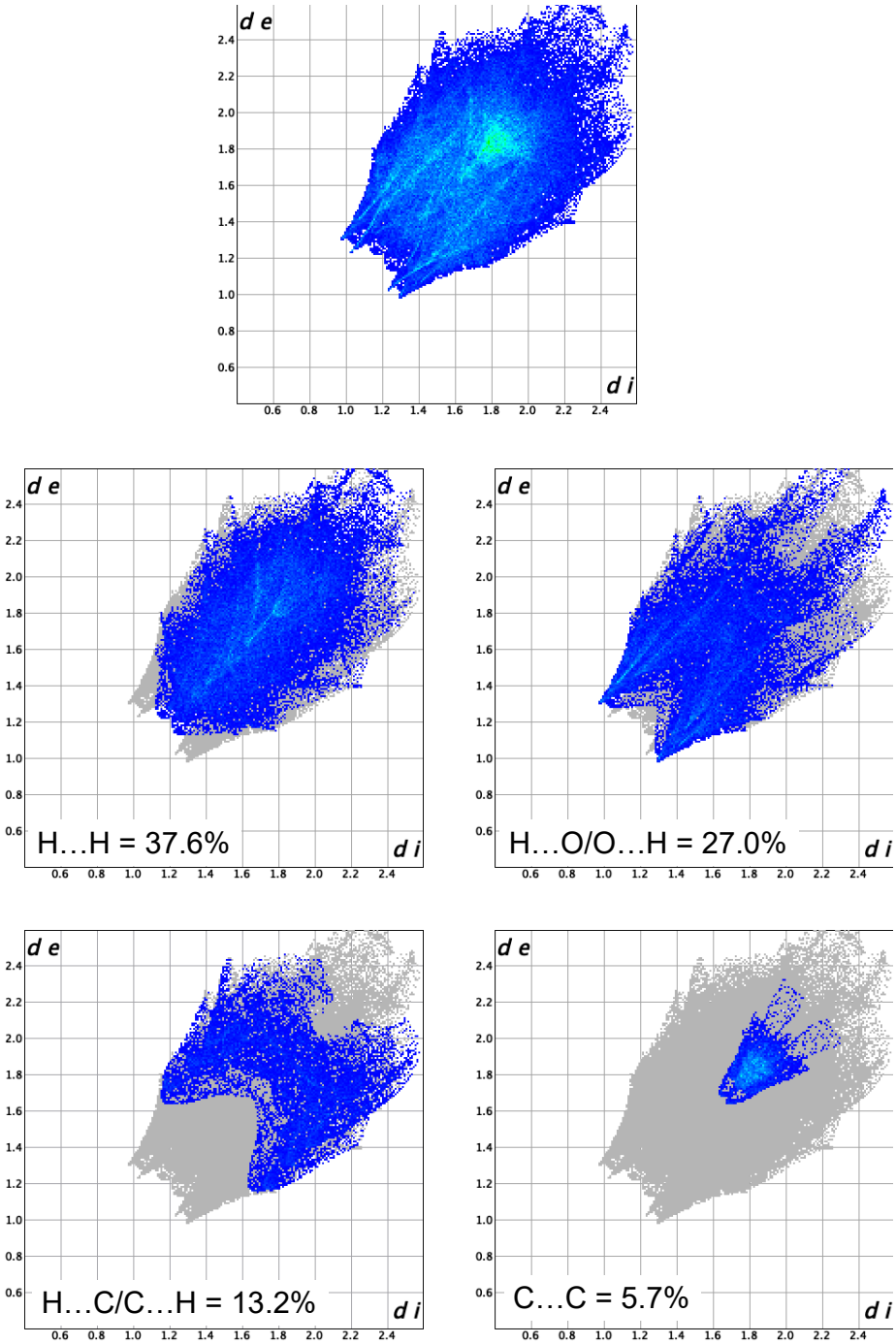

Figure S7. Two-dimensional fingerprint plots for complex **3** showing total interactions (top) and the selected key individual interatomic contacts with the percentages of contribution to the total interaction.

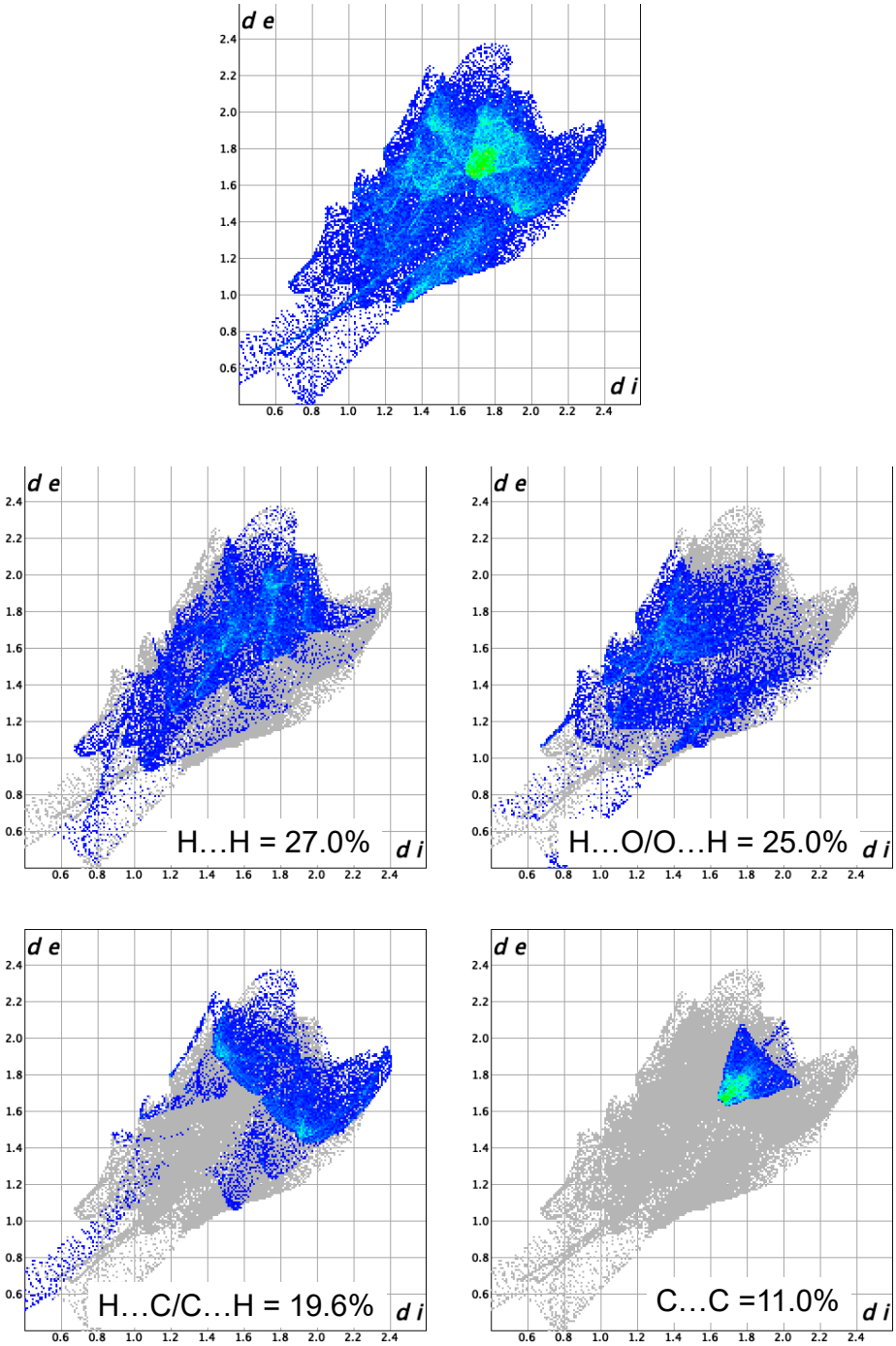

Figure S8. Two-dimensional fingerprint plots for complex **4** showing total interactions (top) and the selected key individual interatomic contacts with the percentages of contribution to the total interaction.