Intermolecular interactions and unexpected isostructurality in the crystal structures of the dichlorobenzaldehyde isomers

Katarzyna A. Solanko[a] and Andrew D. Bond[a]*

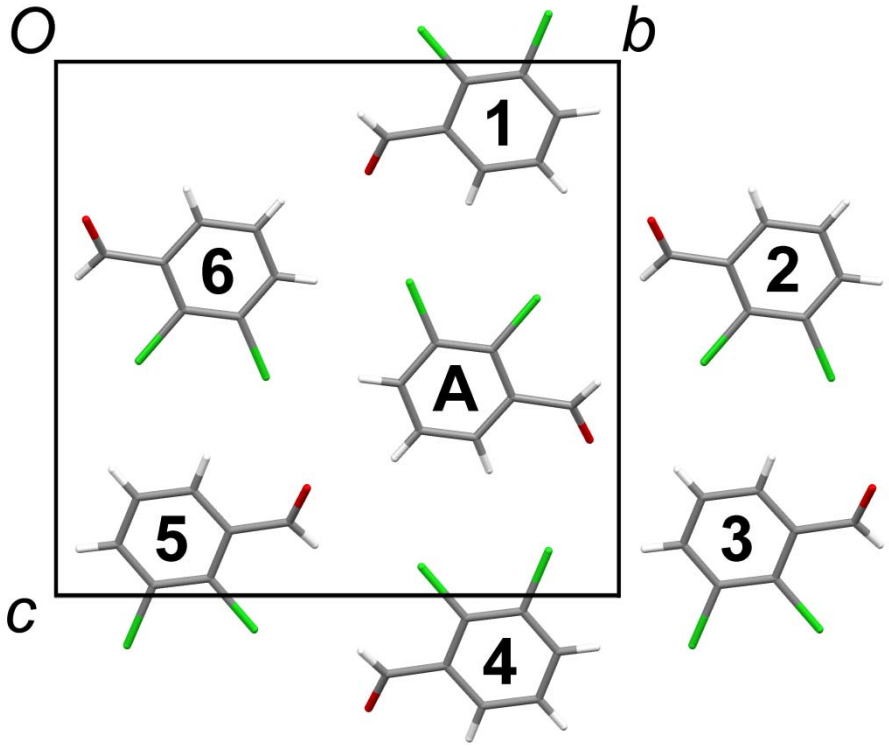
Supporting Information

Tables of intermolecular interaction energies calculated using the PIXEL method

All structures on which the calculations are based, with normalised H-atom positions, are included as the file **optH.cif**

NOTE: all H atom positions are re-calculated in OPIX prior to the calculation.

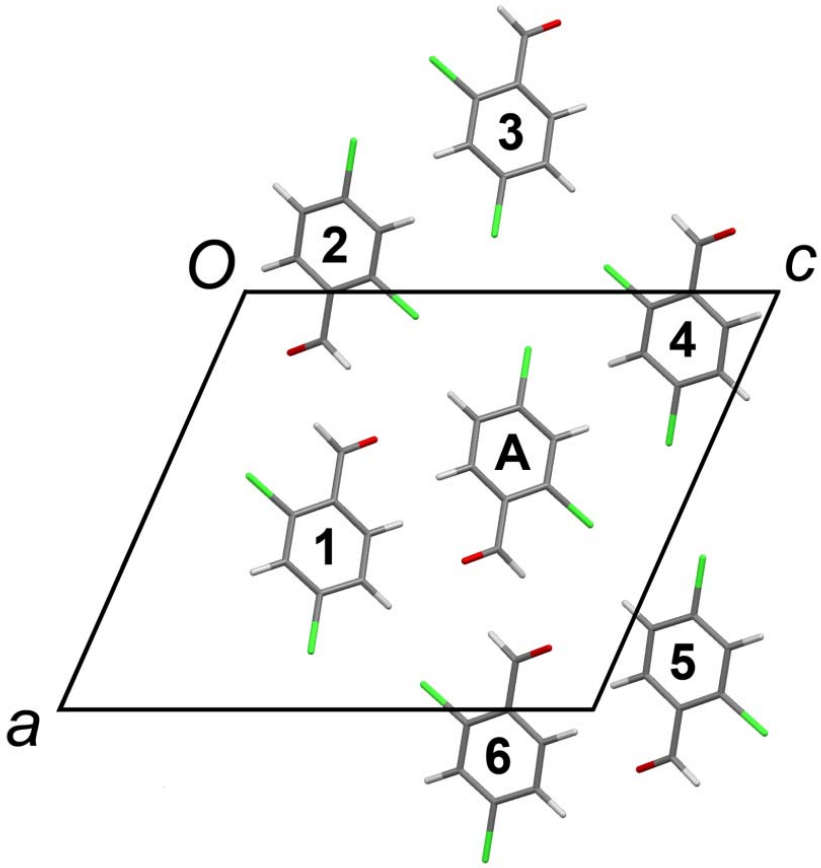
S1. 2,3-Dichlorobenzaldehyde (1)



Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A↔A	–1+x,y,z 1+x,y,z	3.789	–10.8	–4.4	–43.2	37.2	–21.2
A→6	2–x,1–y,1–z	7.409	–5.9	–2.9	–15.9	11.1	–13.7
A→1 **A→4**	–1+x,1.5–y,–0.5+z 1+x,1.5–y,0.5+z	7.484	–8.0	–4.1	–15.3	15.3	–12.1
A→6	1–x,1–y,1–z	8.223	–5.3	–2.2	–11.8	8.3	–10.9
A→1 **A→4**	x,1.5–y, –0.5+z x,1.5–y,0.5+z	6.519	–2.2	–1.1	–13.1	6.7	–9.7
A→2	2–x,2–y,1–z	7.564	–7.0	–3.1	–15.2	15.9	–9.4
A→3 **A→5**	2–x,0.5+y,1.5–z 2–x,–0.5+y,1.5–z	7.772	–2.4	–1.4	–6.6	3.8	–6.7
A→3 **A→5**	3–x,0.5+y,1.5–z 3–x,–0.5+y,1.5–z	8.691	–3.8	–0.6	–2.1	0.5	–6.1
A→2	1–x,2–y,1–z	8.364	0.3	–0.1	–4.3	0.7	–3.4

S2. 2,4-Dichlorobenzaldehyde (2)

[HUGQOQ: R. Cabello, M. Chruszcz, & W. Minor, *Acta Cryst.* (2010) E**66**, o243]



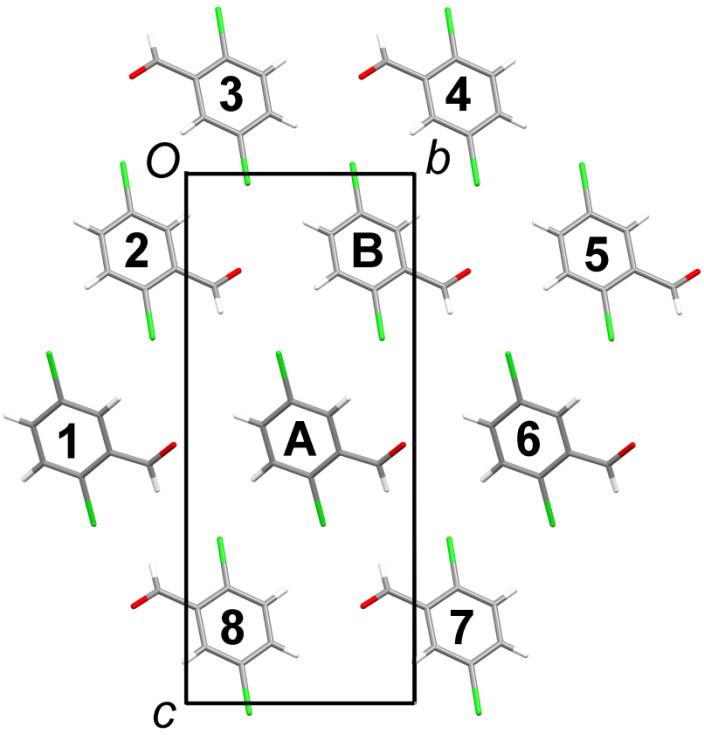
Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A→1	1–x, –1–y,1–z	6.476	–20.7	–6.4	–15.6	17.5	–25.3
A↔A	x, –1+y,z x,1+y,z	3.772	–8.0	–3.4	–41.0	33.6	–18.8
A→4 **A→4**	0.5–x,-0.5+y,1.5–z 0.5–x,0.5+y,1.5–z	6.857	–4.6	–2.8	–19.7	14.2	–12.8
A→1	1–x,-y,1–z	5.560	–1.3	–1.3	–11.9	3.5	–10.9
A→6 **A→6**	1.5–x,-0.5+y,1.5–z 1.5–x,0.5+y,1.5–z	7.980	–6.5	–2.5	–8.2	9.8	–7.4
A→2 **A→5**	–0.5+x, –0.5–y, –0.5+z 0.5+x, –0.5-y,0.5+z	7.955	–0.1	–0.6	–5.5	1.8	–4.4
A→2 **A→5**	0.5+x,0.5–y,0.5+z –0.5+x,0.5–y, –0.5+z	8.154	–3.3	–1.9	–10.1	11.4	–3.8
A→3	–x, –y,1–z	10.238	–1.0	–0.3	–4.4	3.4	–2.3

S3. 2,5-Dichlorobenzaldehyde (3)

A = disordered molecule, **B** = ordered molecule

Stacks **1** and **6** are derived from molecule **A**. Stacks **2**, **3**, **4**, **5**, **7** and **8** are derived from molecule **B.**

[Molecule **A** is taken in one of its orientations so that its centroid is not at the centre of inversion]

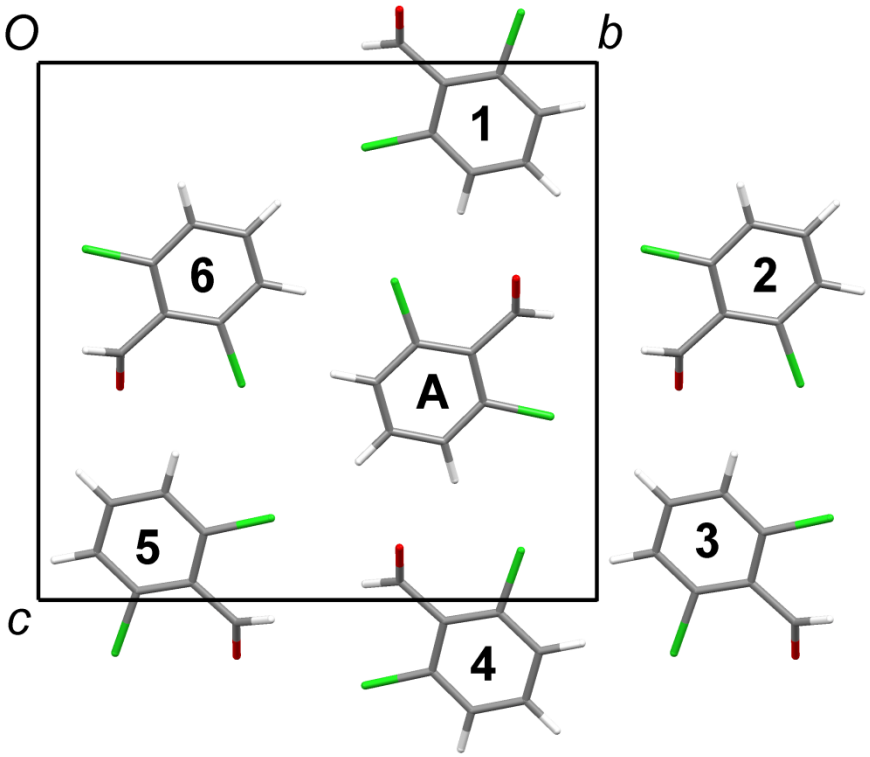


Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A↔A	A(−1+x,y,z) A(1+x,y,z)	3.815	−7.0	−3.9	−42.9	32.0	−21.8
B↔B	B(−1+x,y,z) B(1+x,y,z)	3.815	−8.9	−3.5	−41.2	34.4	−19.3
B→4	B(1−x,2−y,−z)	7.028	−10.9	−4.6	−18.1	17.8	−15.8
A→1 **A→6**	A(1+x,−1+y,z) A(−1+x,1+y,z)	8.162	−9.2	−2.2	−6.2	4.5	−13.0
B→3	B(−x,1−y,−z)	8.024	−6.2	−2.8	−11.9	8.9	−11.9
B→4	B(−x,2−y,−z)	6.104	−4.2	−1.7	−18.8	13.5	−11.1
A↔B		6.843	−4.2	−1.9	−13.5	8.6	−11.0
A→B	B(1+x,y,z)	6.946	−4.2	−1.8	−13.9	9.0	−10.8
A→8	B(1−x,1−y,1−z)	7.002	−4.0	−2.1	−12.7	8.7	−10.1
A→8	B(−x,1−y,1−z)	7.007	−3.7	−1.9	−13.1	9.1	−9.6
B→2 **B→5**	B(x,−1+y,z) B(x,1+y,z)	7.829	−4.4	−1.6	−6.5	3.7	−8.7
B→3	B(1−x,1−y,−z)	8.203	−5.0	−2.2	−13.8	12.7	−8.3
A→7	B(−x,2−y,1−z)	7.525	−6.1	−4.3	−15.8	18.3	−7.9
A→7	B(1−x,2−y,1−z)	8.111	−4.0	−1.3	−7.4	6.9	−5.7
A→2	B(1+x,−1+y,z)	8.373	−1.7	−1.1	−7.4	4.7	−5.5
A→2	B(x,−1+y,z)	8.827	−3.3	−1.3	−6.8	6.9	−4.5
B→2 **B→5**	B(−1+x,−1+y,z) B(1+x,1+y,z)	9.224	−2.8	−0.3	−1.0	0.0	−4.0
A→1 **A→6**	A(x,−1+y,z) A(x,1+y,z)	7.829	0.3	−0.4	−3.0	0.2	−2.9
A→7	B(−1−x,2−y,1−z)	8.750	−0.6	−0.1	−1.5	0.0	−2.2

S4: 2,6-Dichlorobenzaldehyde (4)

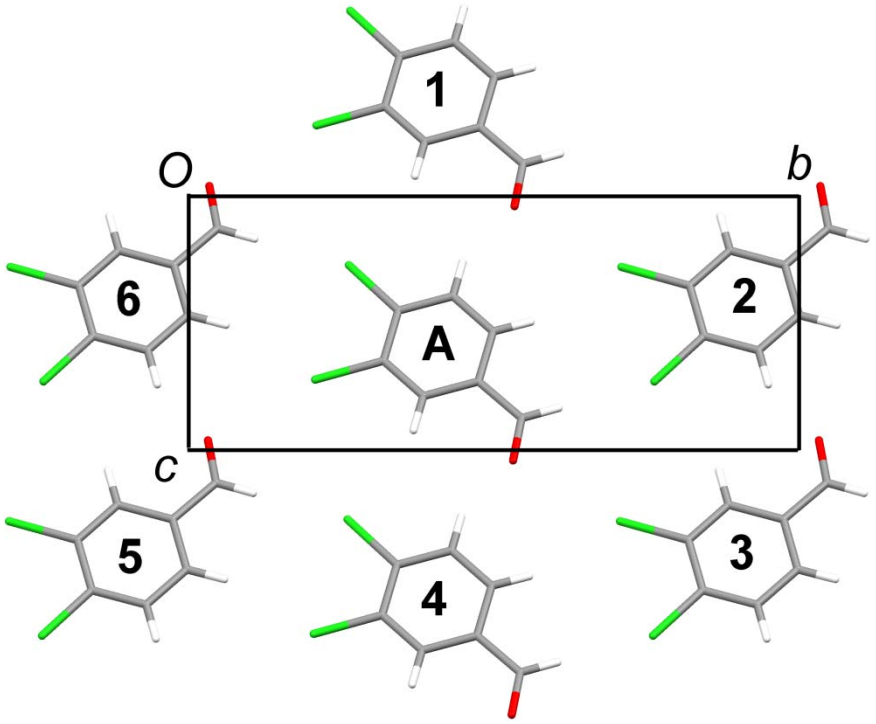
[QEWXIA: A. Gawlicka-Chruszcz, H. Zheng, M. Hyacinth, M. Cymborowski, M. Sabat & W. Minor, *Z. Kristallogr. NCS*, 2006, **221**, 545–546]

For direct comparison with (1), the centroid of the molecule in the asymmetric unit is taken to be at 0.9802, 0.7304, 0.5815 (moved from the published CIF using the symmetry operator 1–*x*,1–*y*,1–*z*).



Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A⟷A	–1+x,y,z 1+x,y,z	3.837	–10.8	–5.2	–42.2	37.0	–21.2
A→1 **A→4**	–1+x,1.5–y,–0.5+z 1+x,1.5–y,0.5+z	7.546	–15.9	–5.6	–16.3	17.8	–20.1
A→6	2–x,1–y,1–z	6.639	–7.5	–3.3	–18.8	13.5	–16.0
A→6	1–x,1–y,1–z	7.569	–7.3	–2.1	–10.6	6.6	–13.5
A→2	2–x,2–y,1–z	7.658	–9.2	–3.5	–16.6	19.1	–10.2
A→1 **A→4**	x,1.5–y,–0.5+z x,1.5–y,0.5+z	6.580	0.0	–1.5	–12.3	5.2	–8.6
A→3 **A→5**	2–x,0.5+y,1.5–z 2–x,–0.5+y,1.5–z	8.124	–2.3	–1.1	–6.1	3.6	–5.9
A→2	3–x,2–y,1–z	8.651	–0.6	0.0	–2.2	0.1	–2.7
A→2	1–x,2–y,1–z	8.476	–0.3	–0.3	–1.8	0.0	–2.4
A→1 **A→4**	–2+x,1.5–y,–0.5+z 2+x,1.5–y,0.5+z	10.001	–1.6	–0.1	–0.4	0.0	–2.1

S5: 3,4-Dichlorobenzaldehyde (5)

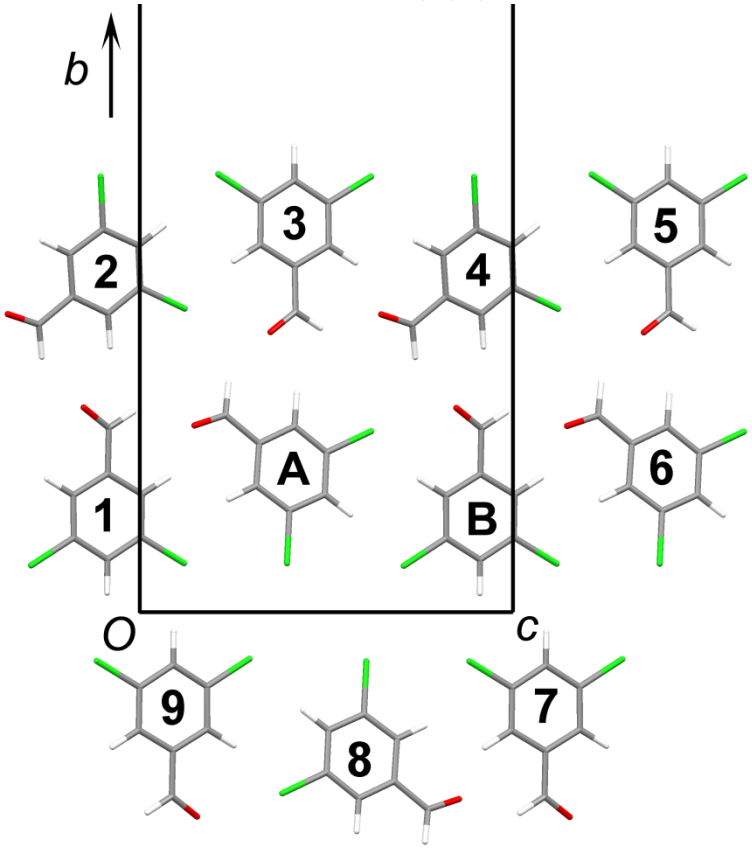


Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A↔A	–1+x,y,z 1+x,y,z	3.809	–4.4	–3.9	–39.4	30.5	–17.2
A→1 **A→4**	1+x,y,–1+z –1+x,y,1+z	7.382	–13.0	–3.6	–11.1	12.5	–15.2
A→1 **A→4**	x,y,–1+z x,y,1+z	6.201	–3.6	–2.3	–17.7	11.9	–11.7
A→2 **A→6**	1–x,0.5+y,1–z 1–x,–0.5+y,1–z	7.967	–4.2	–2.2	–10.8	7.0	–10.2
A→2 **A→6**	–x,0.5+y,1–z –x,–0.5+y,1–z	7.795	–4.4	–1.5	–9.4	5.2	–10.1
A→3 **A→5**	–x,0.5+y,2–z –x,–0.5+y,2–z	8.863	–6.1	–2.1	–7.1	12.3	–3.0

S6: 3,5-Dichlorobenzaldehyde (6)

Two crystallographically distinct molecules labelled **A** and **B**

Stacks **2**, **4**, **6** and **8** are derived from molecule **A**. Stacks **1**, **3**, **5**, **7** and **9** are derived from molecule **B.**



Stack No.	Symmetry Operator	Centroid-Centroid	Coulomb	Pol	Disp	Rep	Total
A→1 **B→6**	B(–1+x,y,–1+z) A(1+x,y,1+z)	6.699	–16.8	–5.2	–17.5	19.3	–20.2
B↔B	B(–1+x,y,z) B(1+x,y,z)	3.779	–6.8	–4.0	–39.4	31.2	–19.1
A↔A	A(–1+x,y,z) A(1+x,y,z)	3.779	–6.8	–4.0	–39.9	32.5	–18.1
B→7	B(1–x,–y,2–z)	7.476	–6.6	–3.6	–20.6	16.3	–14.5
A→3 **B→4**	B(0.5+x,0.5–y,–0.5+z) A(–0.5+x,0.5–y,0.5+z)	7.481	–13.2	–3.8	–9.3	12.5	–13.7
A→B **B→A**	B(1+x,y,z) A(–1+x,y,z)	7.618	–8.2	–3.4	–14.0	12.7	–12.9
A→B		6.594	–3.7	–2.1	–18.7	12.6	–12.0
A→1 **B→6**	B(x,y,–1+z) A(x,y,1+z)	5.774	–2.7	–2.0	–16.6	9.5	–11.9
B→7	B(2–x, –y, –z)	8.131	–4.5	–1.7	–11.8	6.9	–11.1
A→4 **A→2**	A(0.5+x,0.5–y,0.5+z) A(–0.5+x,0.5–y, –0.5+z)	8.551	–3.8	–1.8	–6.5	6.3	–5.8
A→3 **B→4**	B(–0.5+x,0.5–y,–0.5+z) A(0.5+x,0.5–y,0.5+z)	7.379	–0.1	–0.9	–5.2	1.6	–4.5
A→9 **B→8**	B(1–x,–y,1–z) A(1–x,–y,1–z)	9.193	–2.0	–0.8	–5.9	6.3	–2.4
A→8	A(1–x,–y,1–z)	10.300	–0.2	0.0	–2.4	0.6	–2.0