

Electronic Supplementary Material for CrystEngComm
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Table S1 - Geometrical parameters for the weak C-H...O interactions.

<i>D-H...A</i>	<i>D-H</i> (Å)	<i>H...A</i> (Å)	<i>D-A</i> (Å)	<i>D-H-A</i> (°)
200 K				
C2-H2A...O3 ¹	0.95	2.78	3.714(2)	167.2
C9-H9...O3 ¹	0.95	2.55	3.466(2)	161.1
C12-H12...O1 ²	0.95	2.79	3.720(2)	166.7
C19-H19...O1 ²	0.95	2.64	3.561(2)	164.6
145 K				
C2-H2A...O3 ¹	0.95	2.76	3.697(2)	167.8
C9-H9...O3 ¹	0.95	2.55	3.465(2)	162.4
C12-H12...O1 ²	0.95	2.77	3.699(2)	166.9
C19-H19...O1 ²	0.95	2.63	3.549(2)	163.4
120 K				
C2-H2A...O3 ³	0.95	2.74	3.670(4)	166.5
C9-H9...O3 ³	0.95	2.65	3.559(4)	161.2
C12-H12A...O1 ⁴	0.95	2.75	3.688(4)	167.4
C15-H15...O1 ⁴	0.95	2.55	3.479(4)	165.0
C22-H22...O7 ³	0.95	2.76	3.702(4)	170.3
C29-H29...O7 ³	0.95	2.56	3.499(4)	169.8
C32-H32...O5 ⁴	0.95	2.76	3.694(4)	168.1
C35-H35...O5 ⁴	0.95	2.68	3.589(4)	160.4
C42-H42...O11 ³	0.95	2.72	3.662(4)	174.3
C49-H49...O11 ³	0.95	2.62	3.564(4)	172.9
C52-H52...O9 ⁴	0.95	2.72	3.651(4)	168.1
C55-H55...O9 ⁴	0.95	2.57	3.487(4)	161.4
C62-H62...O15 ⁵	0.95	2.74	3.684(4)	174.3
C65-H65...O15 ⁵	0.95	2.65	3.600(4)	176.4
C72-H72...O13 ⁶	0.95	2.73	3.663(4)	167.2
C79-H79...O13 ⁶	0.95	2.55	3.473(4)	163.4

¹= x-1,y,z-1, ²= x+1,y,z+1, ³= x,y+1,z, ⁴= x,y-1,z, ⁵= x,y-1,z+1, ⁶= x,y+1,z-1

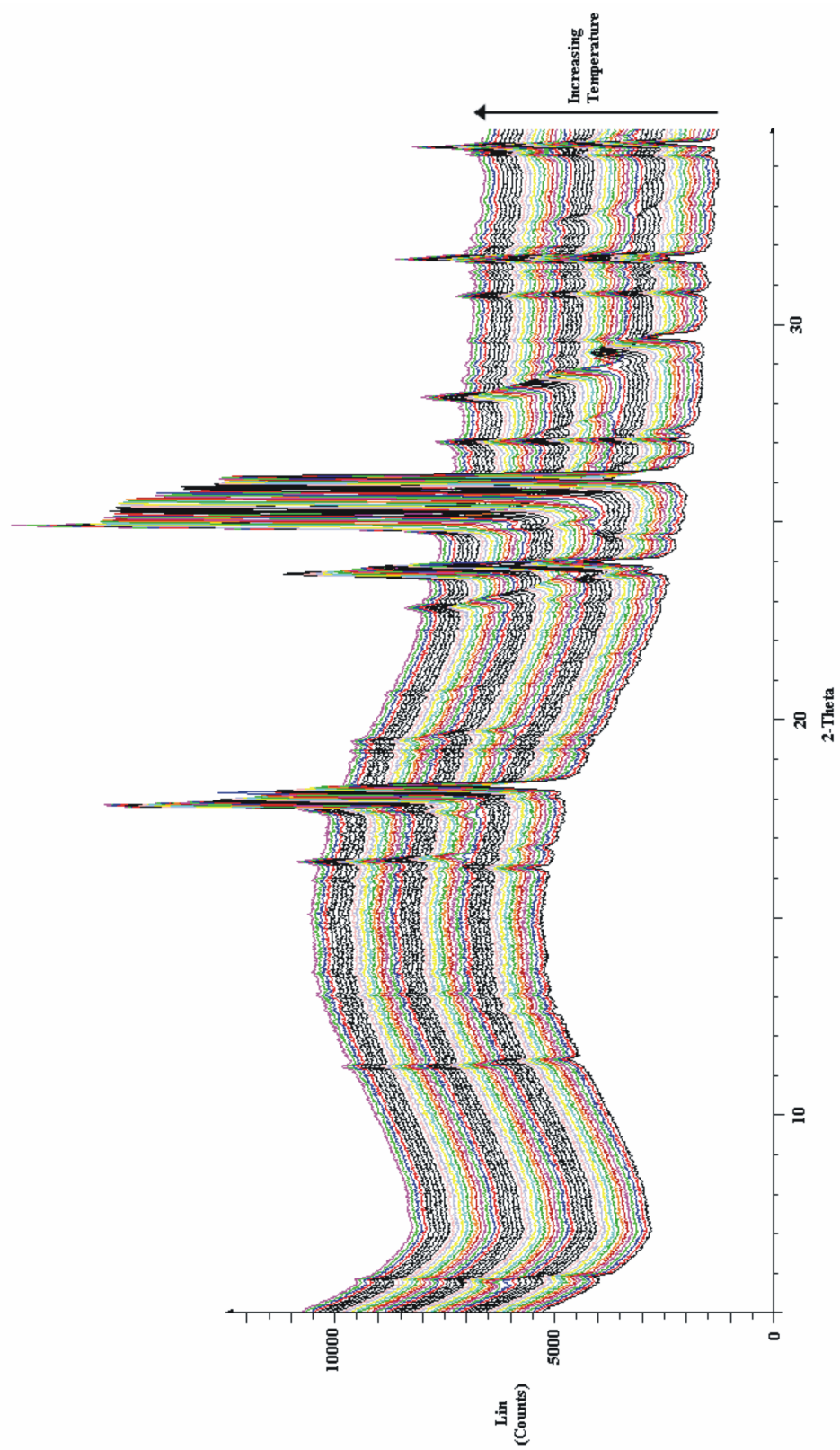


Figure S1 - Variable temperature powder X-ray diffraction scans 6 -300 K.

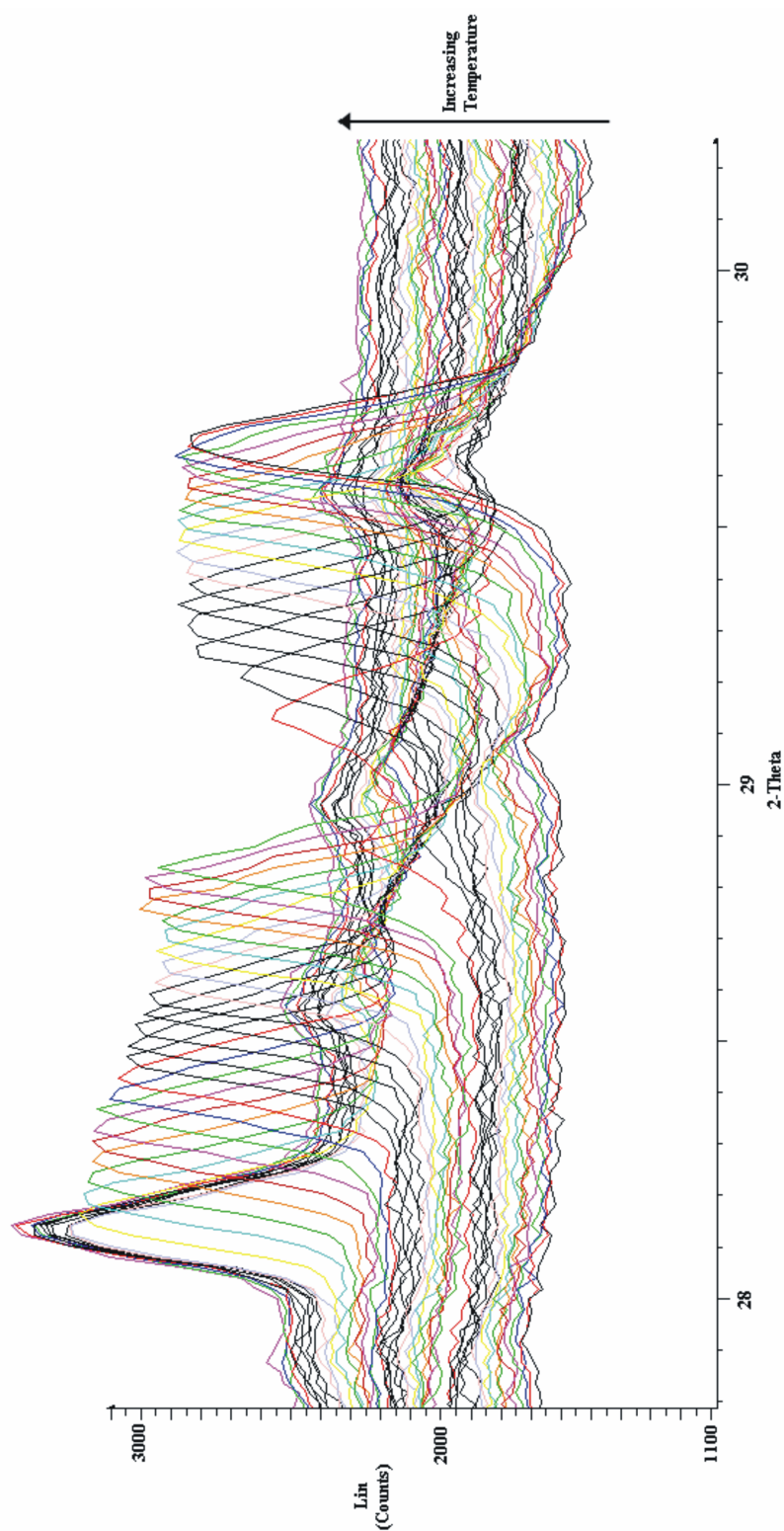


Figure S2 - Variable temperature powder X-ray diffraction data $2\theta = 28\text{-}30^\circ$ recorded over the temperature range 16-300 K. The transition is clearly evident.