Electronic Supplementary Material (ESI) for CrystEngComm

ELECTRONIC SUPPLEMENTARY DATA

for

Temperature-induced chiral Ag(I) coordination polymers with structural variation from 1D to 2D: synthesis, luminescence and SHG response

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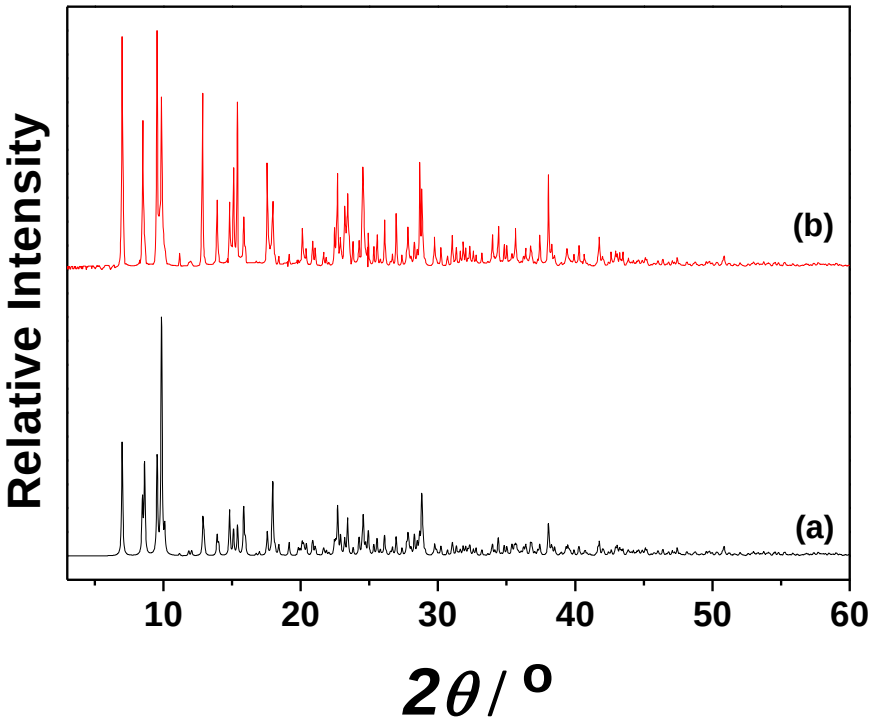

Figure S1. The XRD patterns of **1**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

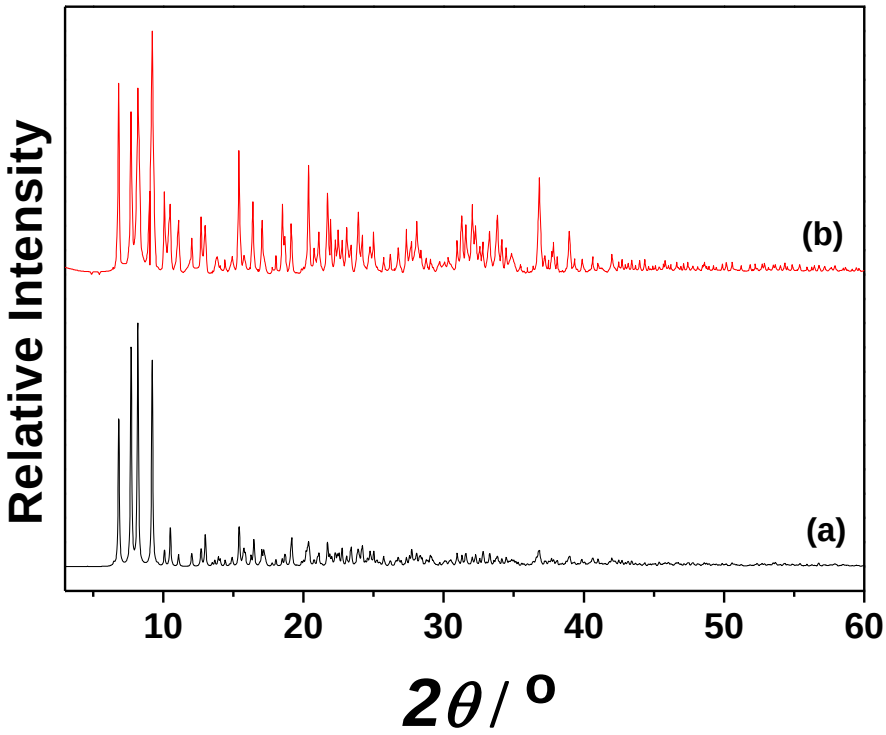

Figure S2. The XRD patterns of **2**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

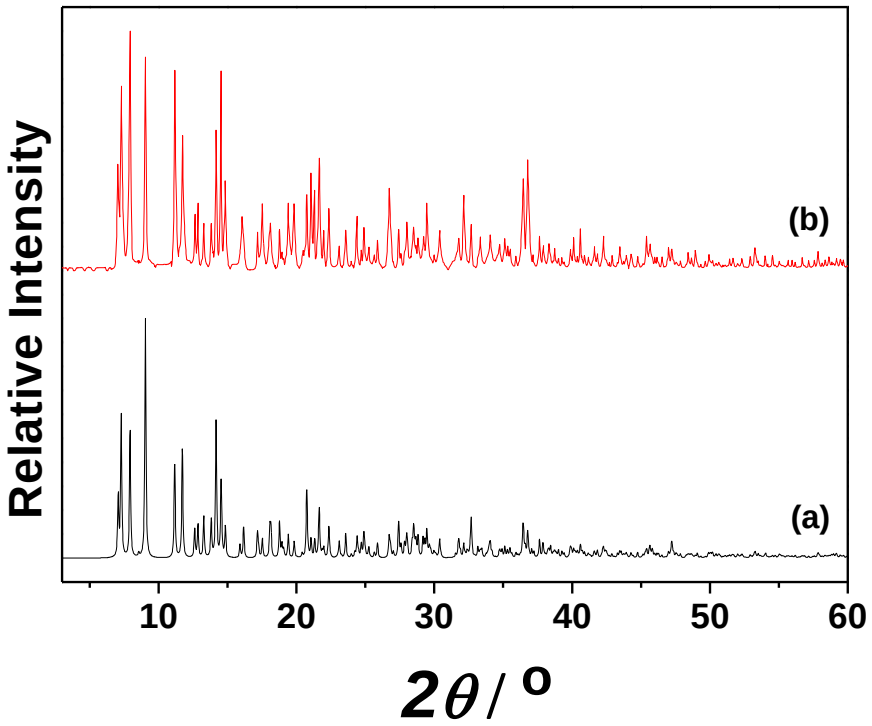

Figure S3. The XRD patterns of **3**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

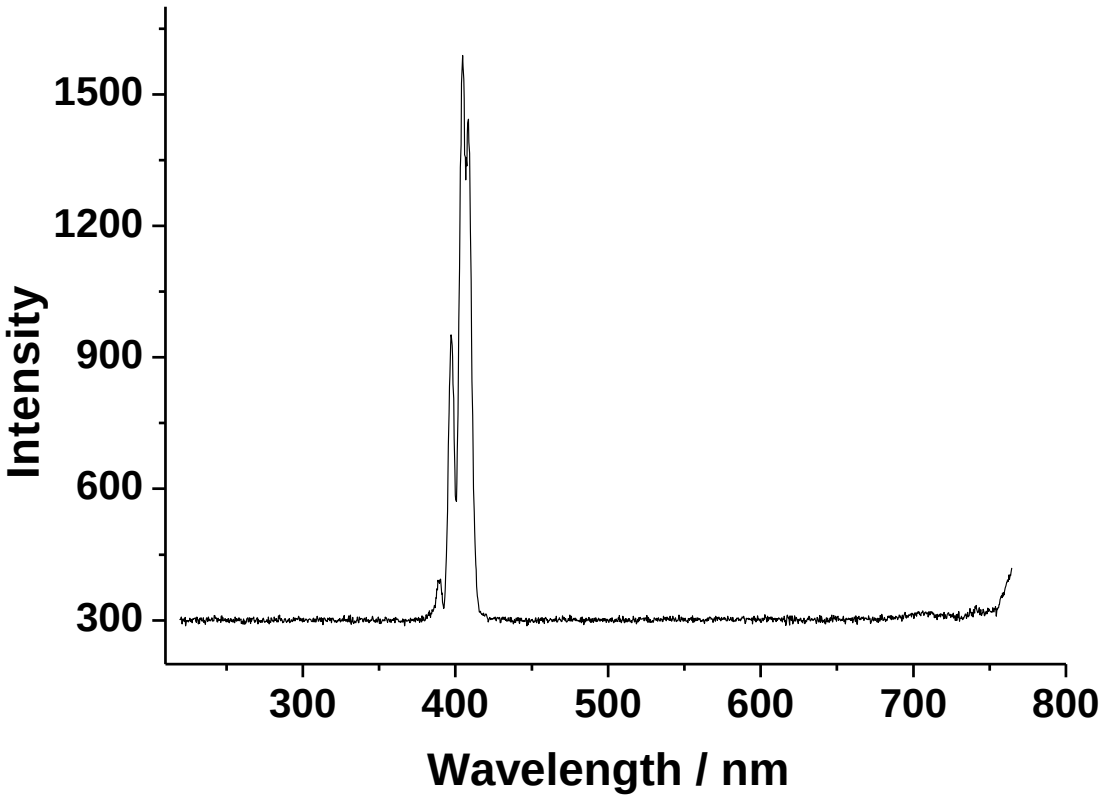

Figure S4. SHG spectrum of KDP.

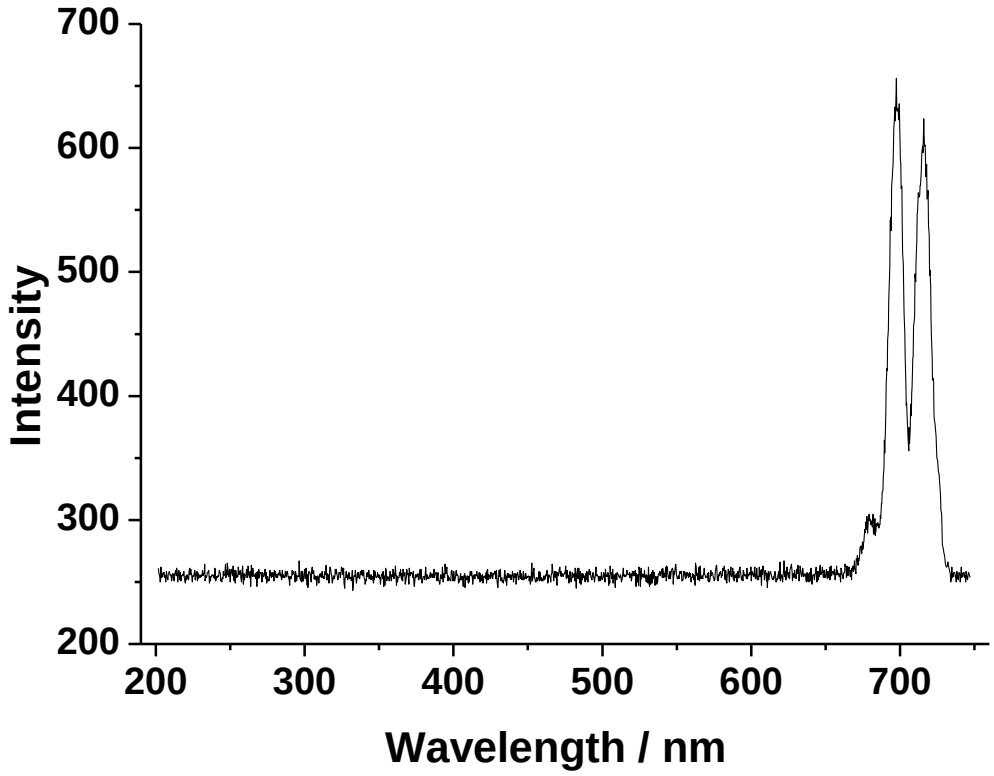

Figure S5. SHG spectrum of **1**.

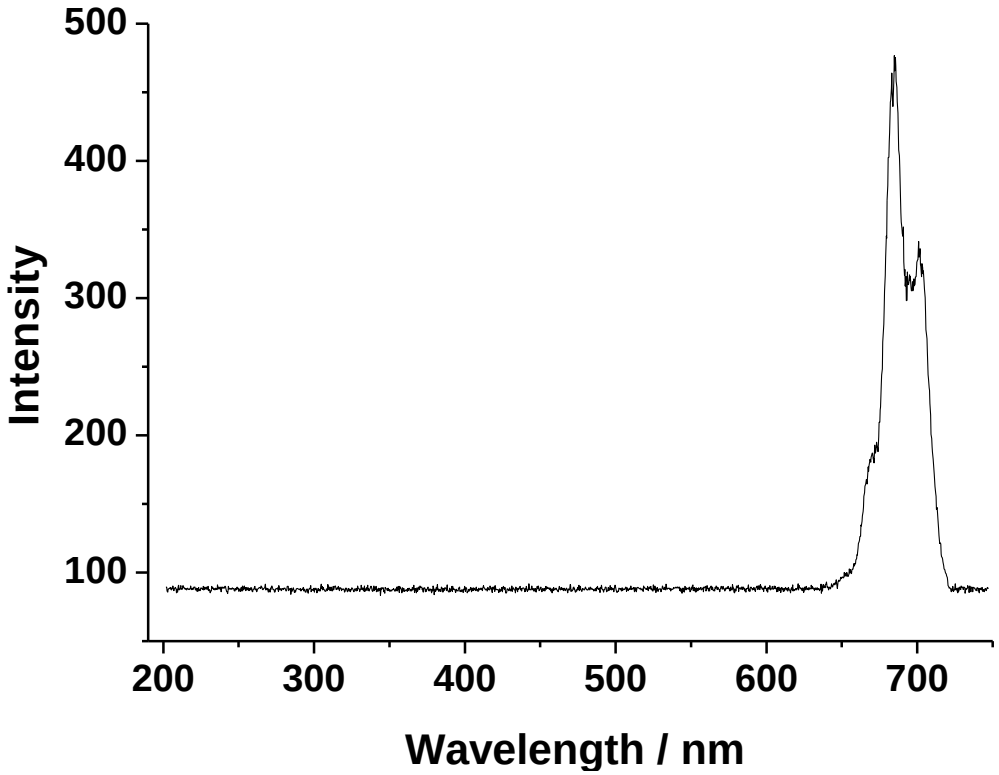

Figure S6. SHG spectrum of **2**.

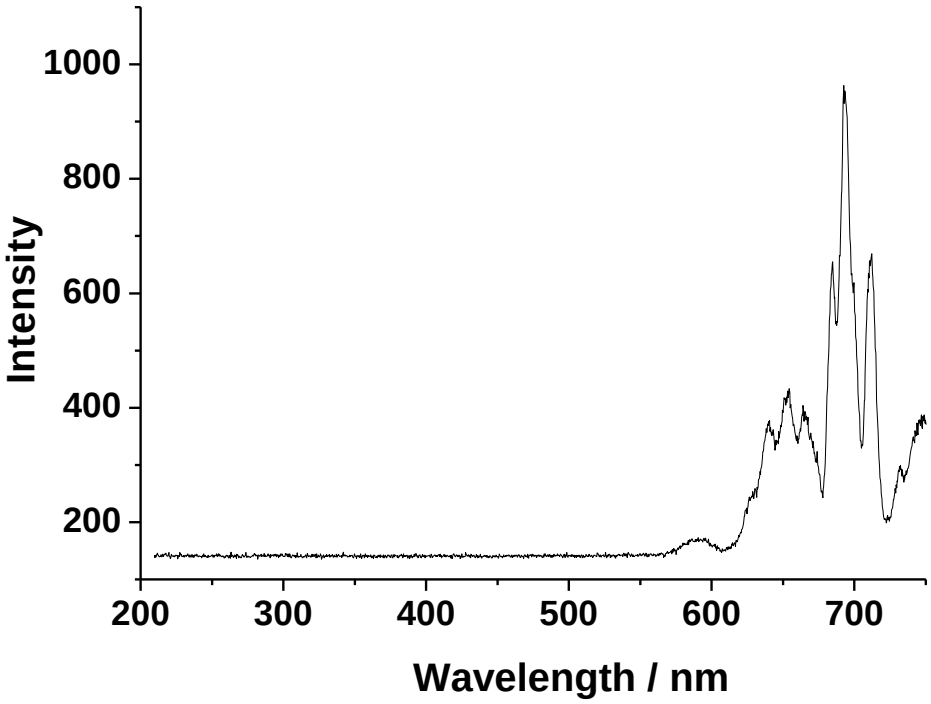

Figure S7. SHG spectrum of **3**.

Table S1. Selected bond lengths (Å) and angles (°) for **1**-**3**.

		1	
Ag1-N2	2.302(8)	Ag2-N7	2.219(8)
Ag1-N3	2.307(8)	Ag3-O1w	2.504(9)
Ag1-N5	2.173(8)	Ag3-N4	2.205(9)
Ag2-N1	2.150(7)	Ag3-N8a	2.154(9)
Ag2-N6	2.366(8)	N2-Ag1-N3	76.2(3)
N2-Ag1-N5	142.3(3)	N6-Ag2-N7	77.2(3)
N3-Ag1-N5	141.5(3)	O1W-Ag3-N4	97.9(3)
N1-Ag2-N6	128.9(3)	O1W-Ag3-N8a	106.0(3)
N1-Ag2-N7	152.6(3)	N4-Ag3-N8a	156.0(4)
		2	
Ag1-N2	2.391(10)	Ag3-N13	2.169(10)
Ag1-N3	2.262(10)	Ag4-N9	2.218(10)
Ag1-N5	2.150(10)	Ag4-N14	2.374(8)
Ag2-N1	2.175(10)	Ag4-N15	2.281(9)
Ag2-N6	2.408(9)	Ag5-N8	2.227(10)
Ag2-N7	2.244(9)	Ag5-N12	2.254(10)
Ag3-N10	2.372(10)	Ag5-N4b	2.197(10)
Ag3-N11	2.265(10)	N2-Ag1-N3	77.3(3)
N2-Ag1-N5	130.5(3)	N9-Ag4-N14	131.1(3)
N3-Ag1-N5	151.8(3)	N9-Ag4-N15	152.0(3)
N1-Ag2-N6	126.9(4)	N14-Ag4-N15	76.9(3)
N1-Ag2-N7	156.8(4)	N8-Ag5-N12	106.4(3)
N6-Ag2-N7	76.3(3)	N4_b-Ag5-N8	129.5(4)
N10-Ag3-N11	77.8(4)	N4_b-Ag5-N12	122.4(4)
N10-Ag3-N13	130.1(3)	N11-Ag3-N13	151.8(4)

		3	
Ag1-N2	2.373(18)	Ag2-N7	2.365(18)
Ag1-N3	2.386(18)	Ag3-N4	2.39(2)
Ag1-N5	2.223(18)	Ag3-N4a	2.39(2)
Ag2-N1	2.214(19)	Ag3-N8b	2.33(2)
Ag2-N6	2.285(19)	Ag3-N8d	2.33(2)
N2-Ag1-N3	74.5(6)	N4-Ag3-N4_a	80.4(7)
N2-Ag1-N5	155.0(6)	N4-Ag3-N8b	113.7(7)
N3-Ag1-N5	130.2(6)	N4-Ag3-N8d	118.3(7)
N1-Ag2-N6	141.5(7)	N4a-Ag3-N8b	118.3(7)
N1-Ag2-N7	140.9(7)	N4a-Ag3-N8d	113.7(7)
N6-Ag2-N7	76.6(6)	N8b-Ag3-N8d	110.1(7)

Symmetry code for **1**: a, x, y, -1+z. for **2**: b, -x, 1/2+y, 2-z. for **3**: a, 1-x,y,3-z; b, -1/2+x, -1/2+y, z; d, 3/2-x, -1/2+y, 3-z.

Table S2. Selected hydrogen bond lengths (Å) and bond angles (º) of **1**-**3** (D, donor atom; A, acceptor atom).

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	D-H···A [º]]
		1		
O1w-H1wa···O4w	0.93	2.26	3.006(17)	137
O1w-H1wb···F1c	0.93	1.99	2.823(11)	148
N2-H2wb··O2w	0.91	2.18	3.050(11)	159
O2w-H2wa···F3c	0.85	2.04	2.887(12)	179
N3-H3b···F6	0.91	2.18	3.070(10)	167
O2w-H2wb···O3w	0.85	1.90	2.745(14)	179
O3w-H3wa···F10	0.85	2.05	2.822(13)	152
O3w-H3wb···F8	0.85	1.98	2.830(13)	179
N6-H6c···F2	0.91	2.33	3.115(11)	144
O4w-H4wa···F8d	0.85	2.24	2.891(16)	133
N7-H7b···F2	0.91	2.20	3.086(11)	164
		2		
O1w-H1wa···O4	0.83	2.19	2.93(6)	150
O1w-H1wb···O3w	0.85	2.45	3.30(7)	179
N2-H2b···O1c	0.93	2.47	3.09(2)	124
N3-H3b···O1	0.90	2.19	2.949(14)	142

O2w-H2wb···O3w	0.85	2.54	3.09(4)	123
O4-H4b···F7	0.85	2.21	3.04(3)	166
N6-H6c···O3	0.91	2.38	3.117(17)	138
N7-H7b···F3	0.90	2.28	2.937(13)	129
N10-H10c···F16	0.90	2.46	3.147(13)	133
N11-H11c···F10	0.90	2.20	3.070(17)	160
N14-H14a···F16d	0.90	2.35	3.130(12)	144
		3		
N2-H2b···F12	0.93	2.33	3.24(3)	164
N2-H2b···F8d	0.93	2.43	3.22(4)	143
N3-H3b···F9e	0.93	2.53	3.12(2)	122
N6-H6c···F3	0.93	2.40	3.10(2)	133
N7-H7b···F10e	0.93	2.28	3.18(2)	161

Symmetry code for **1**: c, -x, 1/2+y, -z; d, -1+x, y, z. for **2**: c, -x, -1/2+y, 2-z; d, 1-x, -1/2+y, 3-z; x, x, y, 1+z. for **3**: d: 3/2-x, -1/2+y, 3-z; e, 3/2-x, 1/2+y, 3-z.

Table S3. Crystal data and structure Refinement for **4**.

Compound	**4**
Formula	$C_{36}H_{48}Ag_{2.5}Cl_{2.5}O_{10}N_8$
FW	1111.13
Crystal system	monoclinic
Space group	*C*2
a / Å	23.966(3)
b / Å	15.116(2)
c / Å	13.0659(18)
β / º	111.746(1)
V / Å^3	4396.5(10)
Z	4
D_c / g cm^{-3}	1.679
T / K	173(2)
F(000)	2240
μ / mm^{-1}	1.321
Flack x	-0.04(13)
R_1 (I > 2σ)	0.0821
wR_2 (all data)	0.1821
GOF	1.078

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, [b] $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S4. Selected bond lengths (Å) and angles (°) for **4**.

		1	
Ag1-N2	2.32(2)	Ag2-N7	2.34(2)
Ag1-N3	2.38(2)	Ag3-N4	2.37(3)
Ag1-N5	2.23(2)	Ag3-N4a	2.37(3)
Ag2-N1	2.20(2)	Ag3-N8b	2.29(2)
Ag2-N6	2.30(2)	Ag3-N8d	2.29(2)
N2-Ag1-N3	75.6(7)	N4-Ag3-N4a	79.8(9)
N2-Ag1-N5	153.9(8)	N4-Ag3-N8b	113.0(9)
N3-Ag1-N5	130.5(8)	N4-Ag3-N8d	119.3(9)
N1-Ag2-N6	141.0(8)	N4a-Ag3-N8b	119.3(9)
N1-Ag2-N7	141.7(8)	N4a-Ag3-N8d	113.0(9)
N6-Ag2-N7	76.2(8)	N8b-Ag3-N8d	110.0(9)

Symmetry code: a, 1-x, y, 1-z; b, -1/2+x, -1/2+y, z; d, -1/2-x, -1/2+y, 1-z.

Table S5. Selected hydrogen bond lengths (Å) and bond angles (º) of **4** (D, donor atom; A, acceptor atom).

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	D-H···A [º]]
		1		
N3-H3b···O9f	0.86	2.45	3.05(4)	127
N6-H6c···O4	0.86	2.41	3.08(3)	134
N7-H7b··O10f	0.86	2.53	3.34(4)	157

Symmetry code: f, -1/2-x, 1/2+y, 1-z.

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