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Supporting information for article:

Temperature-induced first-order displacive phase transition of isonicotinamide-4-methoxybenzoic acid co-crystal

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Table S1 Selected geometry parameters (Å, °) of **1** at different temperatures and reported multi-component crystals of isonicotinamide-substituted benzoic acid in CSD refcode.

Compound	∠(C—N—C)	*d* (N—C)			*d* (O—C)			*d* (O—H) or *d* (N—H$^+$)*
		1	2	average	1	2	1:2 ratio	
Co-crystal								
1_100	117.71 (10)	1.3376 (15)	1.3389 (15)	1.339	1.3256 (14)	1.2286 (14)	1.079	0.99 (2)
1_140	117.53 (10)	1.3356 (15)	1.3373 (15)	1.337	1.3224 (14)	1.2268 (14)	1.077	0.96 (2)
1_142	117.38 (12)	1.3355 (18)	1.3347 (18)	1.335	1.3205 (16)	1.2241 (16)	1.078	0.98 (2)
1_143	117.69 (13)	1.3374 (19)	1.3377 (19)	1.338	1.3241 (17)	1.2230 (17)	1.083	1.01 (2)
1_150	117.66 (11)	1.3383 (16)	1.3359 (16)	1.337	1.3214 (14)	1.2229 (14)	1.080	0.97 (2)
1_200	117.64 (14)	1.336 (2)	1.331 (2)	1.334	1.3222 (18)	1.2218 (17)	1.082	0.96 (2)
1_250	117.43 (14)	1.331 (2)	1.330 (2)	1.331	1.3179 (19)	1.2197 (18)	1.080	0.96 (3)
1_300	117.36 (14)	1.335 (2)	1.327 (2)	1.331	1.3172 (19)	1.2189 (18)	1.080	0.98 (3)
AJAKEB[1]	118.62 (15)	1.338 (2)	1.342 (2)	1.340	1.307 (2)	1.222 (2)	1.070	0.90
ASAXOH[2]	117.29 (18)	1.329 (2)	1.330 (2)	1.330	1.311 (2)	1.214 (2)	1.080	1.11 (2)
ASAXUN[2]	117.0 (2)	1.328 (3)	1.332 (3)	1.330	1.317 (3)	1.223 (3)	1.077	1.04 (3)
ASAXUN01[3]	118.38 (15)	1.339 (2)	1.345 (2)	1.342	1.317 (2)	1.2275 (19)	1.073	1.00 (3)
BUDWEC[4]	117.67 (15)	1.331 (2)	1.338 (2)	1.335	1.313 (2)	1.227 (2)	1.070	1.02
CACGUK[3]	118.19 (12)	1.3365 (18)	1.3419 (18)	1.339	1.3076 (17)	1.2232 (17)	1.069	1.12 (3)
HANHEL[3]	118.49 (11)	1.3352 (17)	1.3385 (16)	1.337	1.3079 (15)	1.2177 (16)	1.074	1.01 (3)
LUNMEM[5]	118.18 (13)	1.3355 (19)	1.3384 (19)	1.337	1.3087 (17)	1.2263 (17)	1.067	0.92
LUNMIQ[5]	117.3 (4)	1.329 (5)	1.337 (5)	1.333	1.314 (4)	1.222 (4)	1.075	1.16
LUNMOW[5]	117.7 (4)	1.336 (5)	1.340 (5)	1.338	1.302 (5)	1.215 (5)	1.072	1.10
PIRPAJ[6]	118.60 (13)	1.335 (2)	1.343 (2)	1.339	1.2942 (19)	1.2221 (19)	1.059	0.84
PIRPEN[6]	118.22 (12)	1.3355 (19)	1.3418 (19)	1.339	1.3036 (17)	1.2219 (17)	1.067	0.95 (3)
PIRPIR[6]	118.30 (13)	1.333 (2)	1.343 (2)	1.338	1.2967 (19)	1.2248 (19)	1.059	0.84
PIRPUD[6]	118.33 (12)	1.3398 (19)	1.3400 (19)	1.340	1.3081 (17)	1.2181 (17)	1.074	0.84
PIRQAK[6]	117.80 (19)	1.332 (3)	1.337 (3)	1.335	1.311 (3)	1.213 (2)	1.081	0.93 (4)
	118.92 (18)	1.334 (3)	1.337 (3)	1.336	1.305 (2)	1.220 (2)	1.070	N/A
PIRQEO[6]	118.73 (10)	1.3325 (16)	1.3445 (16)	1.339	1.2948 (14)	1.2166 (15)	1.064	0.84
PIRQIS[6]	117.94 (18)	1.334 (3)	1.342 (3)	1.338	1.302 (2)	1.217 (2)	1.070	1.06 (4)
PIRQIS01[6]	117.3 (3)	1.327 (5)	1.344 (5)	1.336	1.303 (4)	1.213 (4)	1.074	0.84
	117.8 (4)	1.333 (5)	1.341 (5)	1.337	1.300 (4)	1.213 (4)	1.072	0.84
PIRQUE[6]	118.28 (17)	1.336 (2)	1.336 (2)	1.336	1.304 (2)	1.223 (2)	1.066	1.09 (3)
PIRREP[6]	118.35 (12)	1.336 (3)	1.337 (2)	1.337	1.304 (2)	1.216 (2)	1.072	1.08 (3)
RINHUT[7]	118.52 (12)	1.3337 (18)	1.3373 (18)	1.336	1.3014 (17)	1.2270 (16)	1.061	0.84
XAQQEM[8]	117.86 (19)	1.334 (3)	1.344 (3)	1.339	1.320 (3)	1.233 (3)	1.071	0.94
Salt*								
BIZTOV[9]	121.2 (3)	1.340 (3)	1.340 (4)	1.340	1.285 (3)	1.262 (3)	1.018	1.02 (4)
BIZTOV01[7]	121.4 (4)	1.336 (5)	1.342 (6)	1.339	1.290 (5)	1.263 (5)	1.021	0.88
PICLUK[10]	121.39 (11)	1.3391 (18)	1.3393 (19)	1.339	1.2650 (17)	1.2374 (17)	1.022	1.02 (2)
PICLUK01[9]	121.34 (15)	1.333 (2)	1.340 (2)	1.337	1.261 (2)	1.239 (2)	1.018	0.99 (2)
PIRNUB[6]	120.92 (18)	1.338 (3)	1.345 (3)	1.342	1.273 (2)	1.237 (2)	1.029	0.98 (2)
UQACIZ[11]	122.08 (19)	1.338 (3)	1.346 (3)	1.342	1.259 (3)	1.248 (3)	1.009	0.91 (3)

Table S2 Center of mass distance (Å), molecule-molecule energies (Coulombic, polarization, dispersion, repulsion and total) (kJ mol^{-1}) and energy difference of *A*…*A*, *A*…*B*, *B*…*A* and *B*…*B* contacts calculated from *PIXEL* method.

Symmetry code	T_1 = 142 K						T_2 = 143 K						$\Delta E_{coul.}$	$\Delta E_{pol.}$	$\Delta E_{disp.}$	$\Delta E_{rep.}$	$\Delta E_{tot.}$	
	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$						
A···*A*																		
x, –*y*+1/2, *z*+1/2	13.492	–0.2	0.0	0.0	0.0	–0.2	13.232	–0.5	0.0	0.0	0.0	–0.6	–0.3	0.0	0.0	0.0	–0.4	inter
x, *y*–1, *z*	5.126	–2.9	–3.7	–25.8	17.4	–15.0	5.224	1.8	–1.5	–17.8	6.7	–10.8	4.7	2.2	8.0	–10.7	4.2	intra
x, *y*+1, *z*	5.126	–2.9	–3.7	–25.8	17.4	–15.0	5.224	1.8	–1.5	–17.8	6.7	–10.8	4.7	2.2	8.0	–10.7	4.2	intra
–*x*+3/2, *y*, –*z*+1	9.123	1.6	–0.2	–0.6	0.0	0.9	9.763	2.4	–0.2	–0.5	0.0	1.8	0.8	0.0	0.1	0.0	0.9	intra
–*x*+1, *y*–3/2, –*z*+3/2	10.899	–0.6	0.0	–0.3	0.0	–0.9	10.698	–0.9	0.0	–0.3	0.0	–1.2	–0.3	0.0	0.0	0.0	–0.3	inter
–*x*+1, *y*–1/2, –*z*+3/2	8.138	–5.4	–1.5	–7.9	6.0	–8.8	7.737	–7.7	–2.1	–11.3	9.6	–11.5	–2.3	–0.6	–3.4	3.6	–2.7	inter
–*x*+1, *y*+1/2, –*z*+3/2	8.138	–5.4	–1.5	–7.9	6.0	–8.8	7.737	–7.7	–2.1	–11.3	9.6	–11.5	–2.3	–0.6	–3.4	3.6	–2.7	inter
–*x*+1, *y*+3/2, –*z*+3/2	10.899	–0.6	0.0	–0.3	0.0	–0.9	10.698	–0.9	0.0	–0.3	0.0	–1.2	–0.3	0.0	0.0	0.0	–0.3	inter
–*x*+1, –*y*+1, –*z*+1	12.850	0.4	0.0	0.0	0.0	0.4	12.549	0.5	0.0	0.0	0.0	0.5	0.1	0.0	0.0	0.0	0.1	intra
–*x*+3/2, –*y*–3/2, –*z*+3/2	7.662	0.6	–0.3	–3.7	0.2	–3.2	8.143	–1.2	–0.1	–0.9	0.0	–2.1	–1.8	0.2	2.8	–0.2	1.1	inter
–*x*+3/2, –*y*–1/2, –*z*+3/2	5.645	–5.7	–3.3	–21.3	15.5	–14.9	5.411	–6.2	–2.8	–20.2	13.3	–15.9	–0.5	0.5	1.1	–2.2	–1.0	inter
–*x*+3/2, –*y*+1/2, –*z*+3/2	7.589	0.2	–0.1	–1.2	0.0	–1.0	6.843	1.5	–0.5	–7.1	1.4	–4.7	1.3	–0.4	–5.9	1.4	–3.7	inter
x, –*y*–3/2, *z*–1/2	13.533	–0.5	0.0	0.0	0.0	–0.5	13.949	–0.3	0.0	0.0	0.0	–0.4	0.2	0.0	0.0	0.0	0.1	inter
x, –*y*–3/2, *z*+1/2	13.533	–0.5	0.0	0.0	0.0	–0.5	13.949	–0.3	0.0	0.0	0.0	–0.4	0.2	0.0	0.0	0.0	0.1	inter
x, –*y*–1/2, *z*–1/2	12.503	–0.7	0.0	–0.1	0.0	–0.8	12.551	–0.8	0.0	–0.1	0.0	–0.9	–0.1	0.0	0.0	0.0	–0.1	inter
x, –*y*–1/2, *z*+1/2	12.503	–0.7	0.0	–0.1	0.0	–0.8	12.551	–0.8	0.0	–0.1	0.0	–0.9	–0.1	0.0	0.0	0.0	–0.1	inter
x, –*y*+1/2, *z*–1/2	13.492	–0.2	0.0	0.0	0.0	–0.2	13.232	–0.5	0.0	0.0	0.0	–0.6	–0.3	0.0	0.0	0.0	–0.4	inter
A···*B*																		
x–1/2, –*y*, *z*	6.851	–2.2	–0.8	–8.3	3.1	–8.2	7.114	–1.2	–0.6	–7.4	2.4	–6.9	1.0	0.2	0.9	–0.7	1.3	intra
x, –*y*+1/2, *z*+1/2	10.896	1.2	0.0	–0.1	0.0	1.0	10.678	1.1	0.0	–0.1	0.0	0.9	–0.1	0.0	0.0	0.0	–0.1	inter
x, *y*–3, *z*	10.912	–0.6	0.0	–0.1	0.0	–0.7	11.481	–0.5	0.0	0.0	0.0	–0.5	0.1	0.0	0.1	0.0	0.2	intra
x, *y*–2, *z*	7.072	–1.8	–0.1	–0.7	0.0	–2.6	7.515	–1.4	–0.1	–0.5	0.0	–1.9	0.4	0.0	0.2	0.0	0.7	intra
x, *y*–1, *z*	5.789	–6.8	–2.4	–17.3	11.3	–15.2	5.976	–6.0	–1.9	–13.3	7.3	–13.8	0.8	0.5	4.0	–4.0	1.4	intra
x, *y*+1, *z*	12.577	–0.5	0.0	–0.1	0.0	–0.6	12.568	–0.6	0.0	–0.1	0.0	–0.7	–0.1	0.0	0.0	0.0	–0.1	intra
–*x*+3/2, *y*–2, –*z*+1	6.970	–2.3	–1.4	–5.5	1.4	–7.7	7.415	–0.3	–1.7	–6.5	2.3	–6.2	2.0	–0.3	–1.0	0.9	1.5	intra
–*x*+3/2, *y*–1, –*z*+1	5.664	–40.4	–13.3	–21.1	38.4	–36.5	5.850	–40.0	–13.7	–19.4	36.6	–36.4	0.4	–0.4	1.7	–1.8	0.1	intra
–*x*+3/2, *y*, –*z*+1	8.254	0.2	–0.5	–1.3	0.0	–1.6	8.249	1.2	–0.4	–1.0	0.0	–0.2	1.0	0.1	0.3	0.0	1.4	intra
–*x*+3/2, *y*+1, –*z*+1	12.520	0.6	0.0	0.0	0.0	0.5	12.508	0.6	0.0	0.0	0.0	0.6	0.0	0.0	0.0	0.0	0.1	intra
x–1/2, *y*–3/2, *z*+1/2	11.230	–0.5	0.0	–0.1	0.0	–0.7	11.116	–0.3	0.0	–0.2	0.0	–0.5	0.2	0.0	–0.1	0.0	0.2	inter
x–1/2, *y*–1/2, *z*+1/2	11.657	–0.4	0.0	0.0	0.0	–0.5	11.407	–0.4	0.0	–0.1	0.0	–0.5	0.0	0.0	–0.1	0.0	0.0	inter
–*x*+2, *y*–5/2, –*z*+3/2	13.159	–0.4	0.0	0.0	0.0	–0.5	13.171	–0.3	0.0	0.0	0.0	–0.3	0.1	0.0	0.0	0.0	0.2	inter
–*x*+2, *y*–3/2, –*z*+3/2	11.418	–0.3	0.0	–0.1	0.0	–0.4	11.199	–0.4	0.0	–0.1	0.0	–0.5	–0.1	0.0	0.0	0.0	–0.1	inter
–*x*+2, –*y*+1, –*z*+1	10.705	0.8	0.0	–0.1	0.0	0.6	10.919	0.8	0.0	–0.1	0.0	0.7	0.0	0.0	0.0	0.0	0.1	intra
–*x*+2, –*y*+2, –*z*+1	12.523	0.9	0.0	–0.1	0.0	0.8	12.551	0.9	0.0	–0.1	0.0	0.8	0.0	0.0	0.0	0.0	0.0	intra
–*x*+2, –*y*+3, –*z*+1	15.862	0.5	0.0	0.0	0.0	0.5	15.825	0.5	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	intra
x–1/2, –*y*+1, *z*	6.051	–8.9	–5.0	–14.5	17.0	–11.4	5.860	–8.5	–4.0	–11.9	12.5	–11.9	0.4	1.0	2.6	–4.5	–0.5	intra
x–1/2, –*y*+2, *z*	8.880	2.4	–0.1	–0.5	0.0	1.8	8.524	2.6	–0.2	–0.5	0.0	1.9	0.2	–0.1	0.0	0.0	0.1	intra
–*x*+3/2, –*y*–3/2, –*z*+3/2	13.333	–0.6	0.0	–0.1	0.0	–0.7	13.837	–0.3	0.0	–0.1	0.0	–0.3	0.3	0.0	0.0	0.0	0.4	inter
–*x*+3/2, –*y*–1/2, –*z*+3/2	9.414	–2.1	–1.9	–7.8	8.2	–3.6	9.660	–1.6	–1.4	–6.4	5.0	–4.4	0.5	0.5	1.4	–3.2	–0.8	inter
–*x*+3/2, –*y*+1/2, –*z*+3/2	7.212	–0.8	–0.2	–3.6	0.3	–4.2	7.053	–4.1	–1.6	–10.8	6.6	–9.8	–3.3	–1.4	–7.2	6.3	–5.6	inter

Table S2 *Cont.*

Symmetry code	T_1 = 142 K						T_2 = 143 K						$\Delta E_{coul.}$	$\Delta E_{pol.}$	$\Delta E_{disp.}$	$\Delta E_{rep.}$	$\Delta E_{tot.}$	
	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$						
–*x*+3/2, –*y*+3/2, –*z*+3/2	8.244	0.4	0.0	–0.3	0.0	0.1	7.795	0.0	0.0	–0.5	0.0	–0.5	–0.4	0.0	–0.2	0.0	–0.6	inter
x, –*y*–1/2, *z*+1/2	12.463	0.6	0.0	–0.1	0.0	0.6	12.553	0.2	0.0	–0.1	0.0	0.2	–0.4	0.0	0.0	0.0	–0.4	inter
x, –*y*+3/2, *z*+1/2	11.606	0.4	0.0	–0.1	0.0	0.3	11.182	0.8	0.0	–0.1	0.0	0.7	0.4	0.0	0.0	0.0	0.4	inter
B···*A*																		
x, *y*, *z*	8.340	–99.4	–59.9	–20.6	130.0	–49.9	8.339	–98.5	–62.2	–20.5	133.8	–47.4	0.9	–2.3	0.1	3.8	2.5	intra
x, *y*–1, *z*	12.577	–0.5	0.0	–0.1	0.0	–0.6	12.568	–0.6	0.0	–0.1	0.0	–0.7	–0.1	0.0	0.0	0.0	–0.1	intra
x, *y*+1, *z*	5.789	–6.8	–2.4	–17.3	11.3	–15.2	5.976	–6.0	–1.9	–13.3	7.3	–13.8	0.8	0.5	4.0	–4.0	1.4	intra
x, *y*+2, *z*	7.072	–1.8	–0.1	–0.7	0.0	–2.6	7.515	–1.4	–0.1	–0.5	0.0	–1.9	0.4	0.0	0.2	0.0	0.7	intra
x, *y*+3, *z*	10.912	–0.6	0.0	–0.1	0.0	–0.7	11.481	–0.5	0.0	0.0	0.0	–0.5	0.1	0.0	0.1	0.0	0.2	intra
–*x*+3/2, *y*–1, –*z*+1	12.520	0.6	0.0	0.0	0.0	0.5	12.508	0.6	0.0	0.0	0.0	0.6	0.0	0.0	0.0	0.0	0.1	intra
–*x*+3/2, *y*, –*z*+1	8.254	0.2	–0.5	–1.3	0.0	–1.6	8.249	1.2	–0.4	–1.0	0.0	–0.2	1.0	0.1	0.3	0.0	1.4	intra
–*x*+3/2, *y*+1, –*z*+1	5.664	–40.4	–13.3	–21.1	38.4	–36.5	5.850	–40.0	–13.7	–19.4	36.6	–36.4	0.4	–0.4	1.7	–1.8	0.1	intra
–*x*+3/2, *y*+2, –*z*+1	6.970	–2.3	–1.4	–5.5	1.4	–7.7	7.415	–0.3	–1.7	–6.5	2.3	–6.2	2.0	–0.3	–1.0	0.9	1.5	intra
x+1/2, *y*+1/2, *z*–1/2	11.657	–0.4	0.0	0.0	0.0	–0.5	11.407	–0.4	0.0	–0.1	0.0	–0.5	0.0	0.0	–0.1	0.0	0.0	inter
x+1/2, *y*+3/2, *z*–1/2	11.230	–0.5	0.0	–0.1	0.0	–0.7	11.116	–0.3	0.0	–0.2	0.0	–0.5	0.2	0.0	–0.1	0.0	0.2	inter
–*x*+2, *y*+3/2, –*z*+3/2	11.418	–0.3	0.0	–0.1	0.0	–0.4	11.199	–0.4	0.0	–0.1	0.0	–0.5	–0.1	0.0	0.0	0.0	–0.1	inter
–*x*+2, *y*+5/2, –*z*+3/2	13.159	–0.4	0.0	0.0	0.0	–0.5	13.171	–0.3	0.0	0.0	0.0	–0.3	0.1	0.0	0.0	0.0	0.2	inter
–*x*+2, –*y*+1, –*z*+1	10.705	0.8	0.0	–0.1	0.0	0.6	10.919	0.8	0.0	–0.1	0.0	0.7	0.0	0.0	0.0	0.0	0.1	intra
–*x*+2, –*y*+2, –*z*+1	12.523	0.9	0.0	–0.1	0.0	0.8	12.551	0.9	0.0	–0.1	0.0	0.8	0.0	0.0	0.0	0.0	0.0	intra
–*x*+2, –*y*+3, –*z*+1	15.862	0.5	0.0	0.0	0.0	0.5	15.825	0.5	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	intra
x+1/2, –*y*, *z*	6.851	–2.2	–0.8	–8.3	3.1	–8.2	7.114	–1.2	–0.6	–7.4	2.4	–6.9	1.0	0.2	0.9	–0.7	1.3	intra
x+1/2, –*y*+1, *z*	6.051	–8.9	–5.0	–14.5	17.0	–11.4	5.860	–8.5	–4.0	–11.9	12.5	–11.9	0.4	1.0	2.6	–4.5	–0.5	intra
x+1/2, –*y*+2, *z*	8.880	2.4	–0.1	–0.5	0.0	1.8	8.524	2.6	–0.2	–0.5	0.0	1.9	0.2	–0.1	0.0	0.0	0.1	intra
–*x*+3/2, –*y*–3/2, –*z*+3/2	13.333	–0.6	0.0	–0.1	0.0	–0.7	13.837	–0.3	0.0	–0.1	0.0	–0.3	0.3	0.0	0.0	0.0	0.4	inter
–*x*+3/2, –*y*–1/2, –*z*+3/2	9.414	–2.1	–1.9	–7.8	8.2	–3.6	9.660	–1.6	–1.4	–6.4	5.0	–4.4	0.5	0.5	1.4	–3.2	–0.8	inter
–*x*+3/2, –*y*+1/2, –*z*+3/2	7.212	–0.8	–0.2	–3.6	0.3	–4.2	7.053	–4.1	–1.6	–10.8	6.6	–9.8	–3.3	–1.4	–7.2	6.3	–5.6	inter
–*x*+3/2, –*y*+3/2, –*z*+3/2	8.244	0.4	0.0	–0.3	0.0	0.1	7.795	0.0	0.0	–0.5	0.0	–0.5	–0.4	0.0	–0.2	0.0	–0.6	inter
x, –*y*–1/2, *z*–1/2	12.463	0.6	0.0	–0.1	0.0	0.6	12.553	0.2	0.0	–0.1	0.0	0.2	–0.4	0.0	0.0	0.0	–0.4	inter
x, –*y*+1/2, *z*–1/2	10.896	1.2	0.0	–0.1	0.0	1.0	10.678	1.1	0.0	–0.1	0.0	0.9	–0.1	0.0	0.0	0.0	–0.1	inter
x, –*y*+3/2, *z*–1/2	11.606	0.4	0.0	–0.1	0.0	0.3	11.182	0.8	0.0	–0.1	0.0	0.7	0.4	0.0	0.0	0.0	0.4	inter
B···*B*																		
x, *y*–1, *z*	5.126	0.8	–2.4	–18.6	11.9	–8.3	5.224	0.7	–2.0	–16.4	8.5	–9.1	–0.1	0.4	2.2	–3.4	–0.8	intra
x, *y*+1, *z*	5.126	0.8	–2.4	–18.6	11.9	–8.3	5.224	0.7	–2.0	–16.4	8.5	–9.1	–0.1	0.4	2.2	–3.4	–0.8	intra
–*x*+3/2, *y*–2, –*z*+1	12.224	–0.8	0.0	–0.1	0.0	–0.9	12.336	–0.9	0.0	–0.1	0.0	–1.0	–0.1	0.0	0.0	0.0	–0.1	intra
–*x*+3/2, *y*–1, –*z*+1	8.402	–0.7	–0.4	–1.3	0.0	–2.3	8.384	–1.1	–0.4	–1.3	0.0	–2.8	–0.4	0.0	0.0	0.0	–0.5	intra
–*x*+3/2, *y*, –*z*+1	6.656	1.4	–2.4	–12.6	7.8	–5.8	6.557	1.8	–2.1	–12.8	6.6	–6.6	0.4	0.3	–0.2	–1.2	–0.8	intra
–*x*+3/2, *y*+1, –*z*+1	8.402	–0.7	–0.4	–1.3	0.0	–2.3	8.384	–1.1	–0.4	–1.3	0.0	–2.8	–0.4	0.0	0.0	0.0	–0.5	intra
–*x*+3/2, *y*+2, –*z*+1	12.224	–0.8	0.0	–0.1	0.0	–0.9	12.336	–0.9	0.0	–0.1	0.0	–1.0	–0.1	0.0	0.0	0.0	–0.1	intra
–*x*+2, –*y*+1, –*z*+1	6.662	0.3	–0.1	–0.8	0.0	–0.5	6.877	0.4	0.0	–0.7	0.0	–0.4	0.1	0.1	0.1	0.0	0.1	intra
–*x*+2, –*y*+2, –*z*+1	4.927	–8.6	–4.2	–18.6	14.6	–16.8	4.948	–7.5	–3.8	–19.0	14.0	–16.2	1.1	0.4	–0.4	–0.6	0.6	intra
–*x*+2, –*y*+3, –*z*+1	7.532	–78.7	–25.7	–17.9	62.6	–59.7	7.501	–82.1	–27.6	–18.7	71.6	–56.7	–3.4	–1.9	–0.8	9.0	3.0	intra
–*x*+2, –*y*+4, –*z*+1	11.906	–1.7	0.0	–0.1	0.0	–1.8	11.943	–1.7	0.0	–0.1	0.0	–1.8	0.0	0.0	0.0	0.0	0.0	intra

Table S2 *Cont.*

Symmetry code	T_1 = 142 K						T_2 = 143 K						$\Delta E_{coul.}$	$\Delta E_{pol.}$	$\Delta E_{disp.}$	$\Delta E_{rep.}$	$\Delta E_{tot.}$	
	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$	dist.	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$						
x–1/2, –*y*+2, *z*	10.166	–0.4	–0.1	–0.2	0.0	–0.6	10.053	–0.4	–0.1	–0.2	0.0	–0.6	0.0	0.0	0.0	0.0	0.0	intra
x+1/2, –*y*+2, *z*	10.166	–0.4	–0.1	–0.2	0.0	–0.6	10.053	–0.4	–0.1	–0.2	0.0	–0.6	0.0	0.0	0.0	0.0	0.0	intra
x, –*y*+3/2, *z*–1/2	12.655	–0.4	0.0	0.0	0.0	–0.4	12.705	–0.4	0.0	0.0	0.0	–0.5	0.0	0.0	0.0	0.0	–0.1	inter
x, –*y*+3/2, *z*+1/2	12.655	–0.4	0.0	0.0	0.0	–0.4	12.705	–0.4	0.0	0.0	0.0	–0.5	0.0	0.0	0.0	0.0	–0.1	inter

$\sum E_{tot.}$ (intra, 142) = –397.9 kJ mol^{-1}, $\sum E_{tot.}$ (intra, 143) = –370.8 kJ mol^{-1}, $\sum E_{tot.}$ (inter, 142) = –59.5 kJ mol^{-1} and $\sum E_{tot.}$ (inter, 143) = –82.9 kJ mol^{-1}. $\sum \Delta E_{tot.}$ = 27.1 kJ mol^{-1} and –23.4 kJ mol^{-1} for intra-layer and inter-layer contacts, respectively.

Table S3 Maximum deviations (Å) of 4-methoxybenzoic acid (*A*) and isonicotinamide (*B*) molecules and three selected torsion angles (°).

Temperature (K)	Maximum deviation of molecule *A*		Maximum deviation of molecule *B*		C8—C7—C13—O3	C14—O4—C10—C11	C4—C5—C6—O1
100	−0.152 (1)	at O2	−0.024 (1)	at N2	171.05 (11)	−176.55 (10)	−179.37 (11)
140	−0.151 (1)	at O2	−0.023 (1)	at N2	171.19 (11)	−176.51 (11)	−179.41 (11)
142	−0.151 (1)	at O2	−0.023 (1)	at N2	171.32 (13)	−176.46 (12)	−179.50 (13)
143	0.120 (1)	at O2	0.089 (1)	at O1	−173.82 (15)	−177.43 (15)	172.55 (14)
150	0.121 (1)	at O2	0.090 (1)	at O1	−174.03 (12)	−177.37 (13)	172.57 (12)
200	0.118 (1)	at O2	0.089 (1)	at O1	−174.03 (16)	−177.65 (16)	172.84 (15)
250	0.115 (1)	at O2	0.089 (1)	at O1	−174.12 (17)	−177.76 (18)	172.79 (15)
300	0.115 (1)	at O2	0.088 (1)	at O1	−174.11 (17)	−178.06 (19)	173.08 (15)

Table S4 Dihedral angles of *AB*, *AA* and *BB* molecular pairs.

Temperature (K)	Dihedral angle between *A* and *B* molecules (°)	Dihedral angle between two *A* molecules in *ABBA* array (°)	Dihedral angle between two *B* molecules in *ABBA* array (°)
100	2.92 (5)	0.00 (4)	0.00 (5)
140	2.97 (5)	0.00 (4)	0.00 (5)
142	3.00 (6)	0.00 (5)	0.00 (6)
143	30.77 (5)	0.00 (5)	0.00 (6)
150	30.79 (4)	0.00 (4)	0.00 (5)
200	30.45 (5)	0.00 (6)	0.00 (7)
250	30.11 (6)	0.00 (6)	0.00 (7)
300	29.77 (6)	0.00 (6)	0.00 (7)

Table S5 Molecular overlay root-mean-square deviation (RMSD) and maximum deviation of *AB* dimer of **1** at different temperatures.

	Overlay RMSD (Å)	Overlay maximum deviation (Å)
LTP/LTP		
100/140	0.0099	0.0378
100/142	0.0096	0.0158
HTP/HTP		
143/150	0.0119	0.0519
143/200	0.0168	0.0676
143/250	0.0243	0.0884
143/300	0.0250	0.0674
LTP/HTP		
142/143	0.2738	0.4947

Table S6 Dihedral angle and distance of two *ABBA* arrays and the percentages of inter-array interactions.

Temperature (K)	Dihedral angle between two two-fold-rotation related *ABBA* arrays (°)	Distance between two adjacent parallel *ABBA* arrays (Å)	O…H/ H…O	C…H/ H…C	N…H/ H…N	C…C	C…N/ N…C	C…O/ O…C	H…H
100	79.47	3.283	20.0	19.2	2.3	3.6	2.2	7.8	44.2
140	79.78	3.291	19.9	19.0	2.2	3.6	2.1	7.9	44.5
142	79.78	3.287	19.8	19.1	2.4	3.6	2.1	7.9	44.4
143	87.85	3.624	20.3	18.7	2.1	3.9	2.0	7.8	44.4
150	87.92	3.624	20.3	18.8	2.2	3.9	2.0	7.8	44.3
200	88.15	3.632	20.4	18.7	2.2	3.9	1.9	7.8	44.4
250	88.43	3.639	20.1	18.5	2.3	3.9	1.9	7.8	44.7
300	88.82	3.648	20.0	18.4	2.1	3.9	1.9	7.8	45.1

Table S7 Hirshfeld surface properties of *ABBA* array at different temperatures.

Temperature (K)	Volume ($Å^3$)	Area ($Å^2$)	Globularity	Asphericity	Occupancy per unit cell (%)
100	639.02	50.62	619.54	0.579	24.51
140	640.03	50.58	619.70	0.580	24.52
142	637.70	50.4	618.00	0.580	24.52
143	644.09	48.54	612.31	0.589	24.54
150	643.66	48.56	612.06	0.589	24.54
200	647.56	48.56	614.07	0.589	24.54
250	650.87	48.52	615.45	0.590	24.54
300	656.67	48.62	618.64	0.591	24.55

Occupancy per unit cell = hirshfeld surface volume / cell volume × 100%

Table S8 Coulombic, polarization, dispersion and repulsion energies (kJ mol^{-1}) per molecule in asymmetric unit of **1** from *PIXEL* calculation.

Temperature (K)	$E_{coul.}$	$E_{pol.}$	$E_{disp.}$	$E_{rep.}$	$E_{tot.}$
100	−106.4	−52.9	−99.4	148.4	−110.2
140	−106.0	−52.7	−98.7	145.5	−111.9
142	−107.1	−53.2	−99.3	147.7	−111.8
143	−104.7	−53.1	−95.1	142.4	−110.5
150	−105.1	−53.1	−95.2	142.8	−110.6
200	−103.2	−51.7	−93.3	138.0	−110.3
250	−100.4	−50.3	−92.0	132.4	−110.3
300	−98.7	−49.3	−89.7	127.6	−110.1

Total lattice energy, $E_{lattice}$ (kJ mol^{-1}) = 2 × $E_{tot.}$: $E_{lattice}$ (142) = –223.6 and $E_{lattice}$ (143) = –221.0.

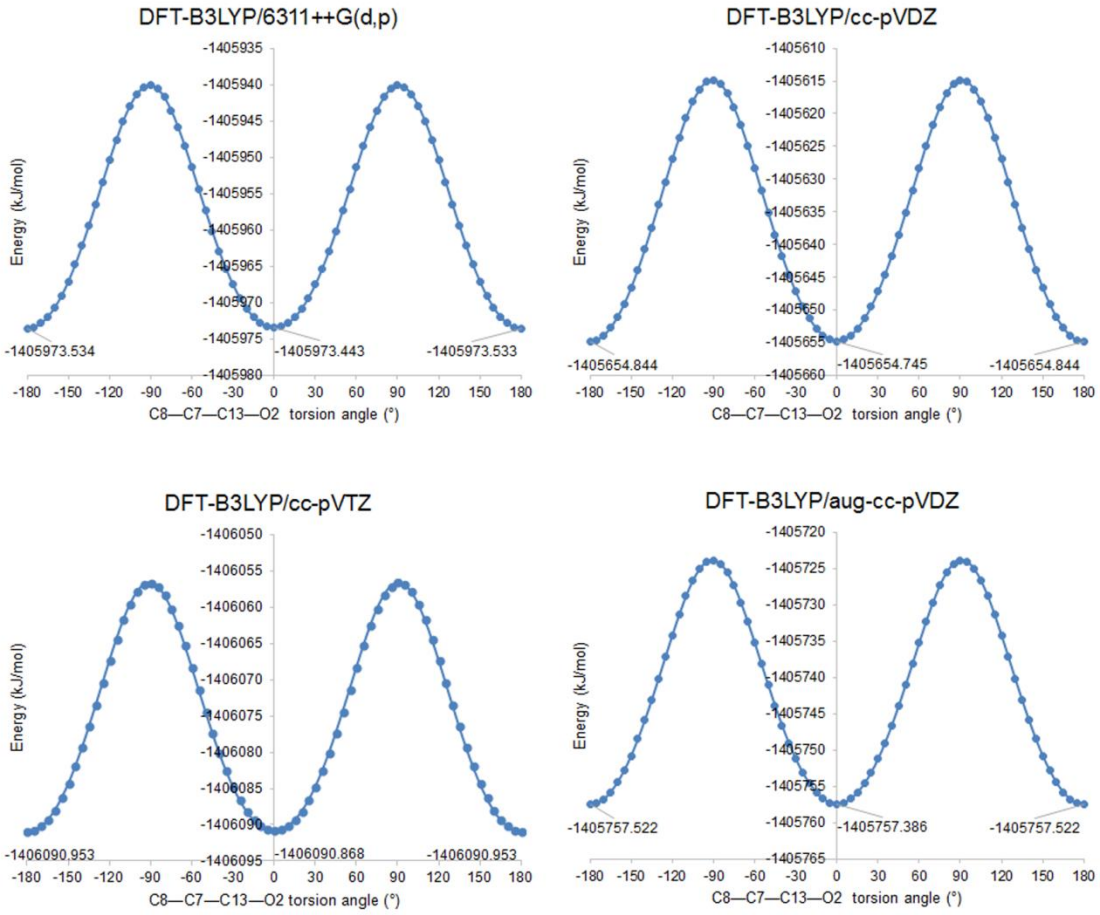

Figure S1 PES scan profiles as a function of C8—C7—C13—O2 torsion angle of molecule *A* at different basis sets.

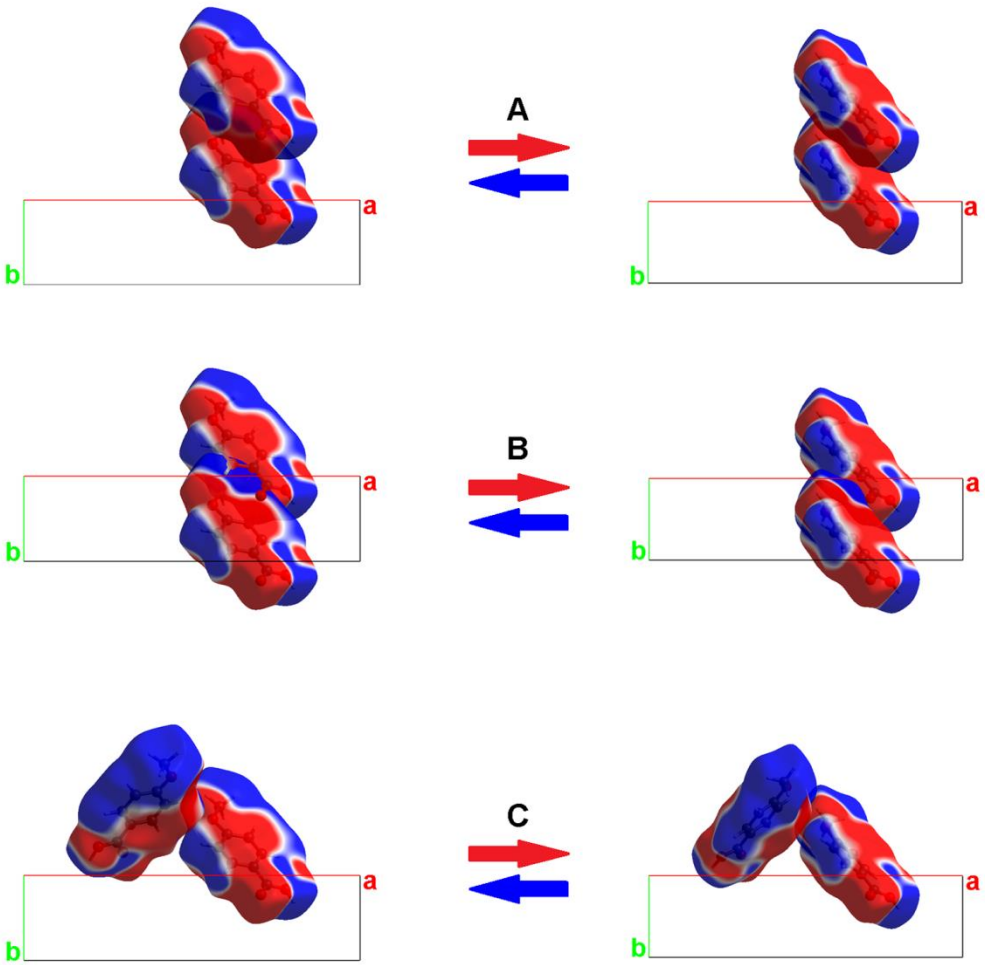

Figure S2 Electrostatic potentials mapped onto Hirshfeld surfaces (HF/cc-pVDZ level of theory, rescaled to ±0.01 a.u.) of contacts **A**−**I** at 142 K (LTP, left column) and 143 K (HTP, right column) with positive and negative regions in blue and red, respectively. The heating and cooling processes near T_c are indicated as red and blue arrows, respectively.

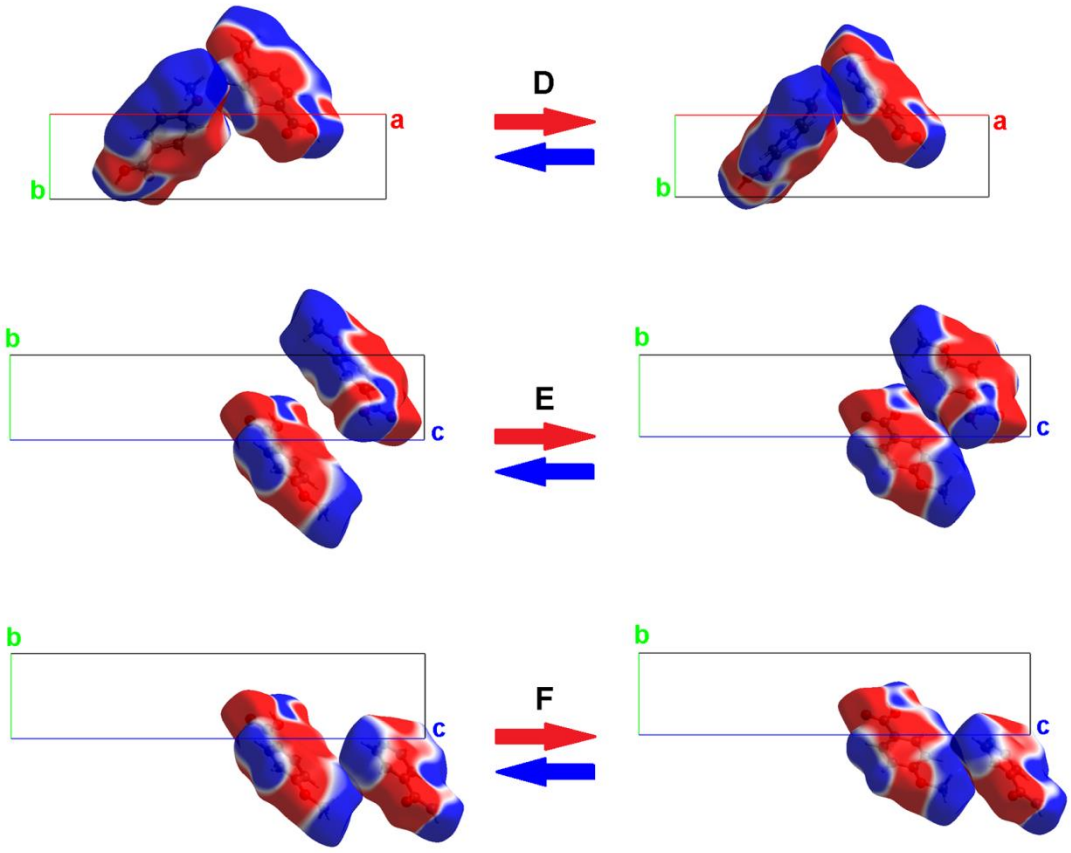

Figure S2 *Cont.*

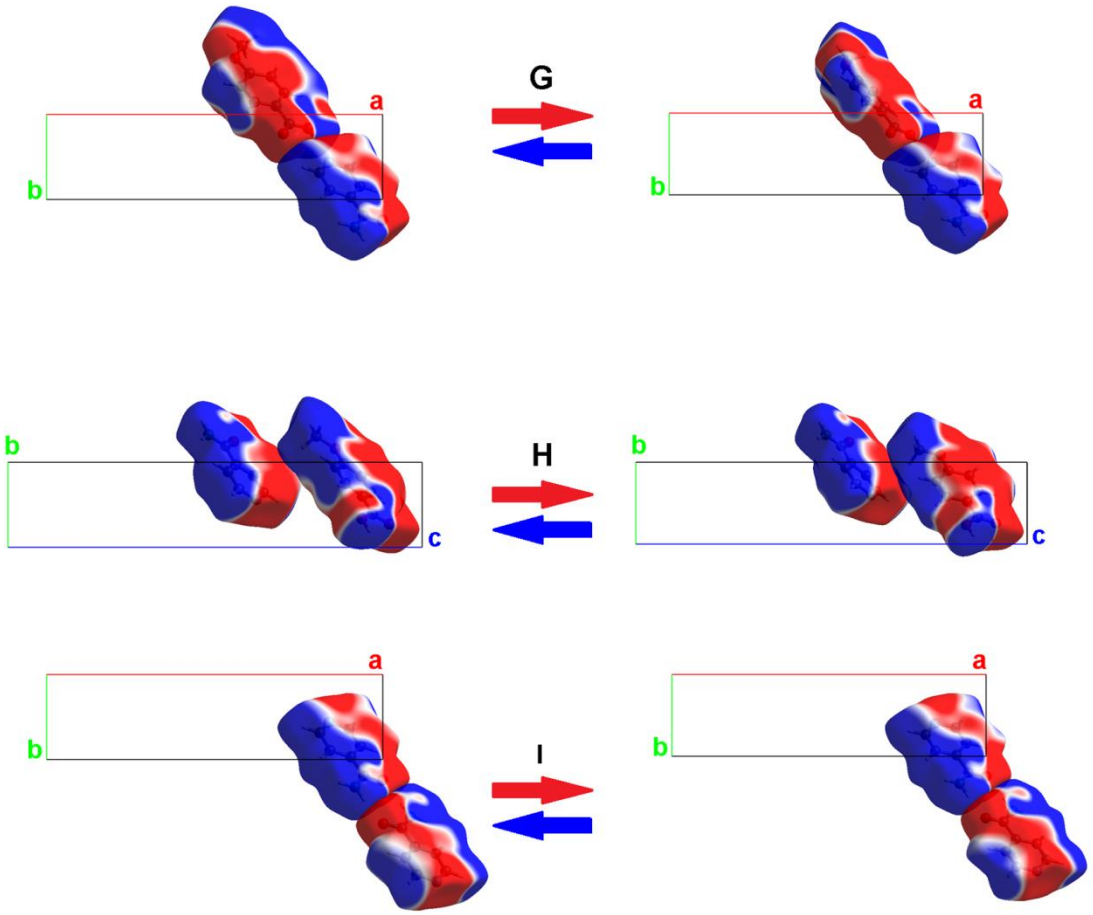

Figure S2 *Cont.*

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