Supplemantary Information

Polymorphism of amantadinium niflumate

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Table S1 Selected bond lengths in polymorphs I and II.

Bond	Bond length [Å]	
	polymorph I	polymorph II
O1–C1	1.2632(17)	1.2652(15)
O2–C1	1.2672(19)	1.2562(17)
C1–C2	1.5033(19)	1.5084(17)
C2–C3	1.423(2)	1.4272(17)
C2–C7	1.387(2)	1.3864(18)
C3–N1	1.3748(19)	1.3733(17)
C3–N4	1.3415(19)	1.3408(16)
N4–C5	1.341(2)	1.3401(18)
C5–C6	1.381(2)	1.3800(18)
C6–C7	1.390(2)	1.3871(18)
N1–C8	1.4006(19)	1.3976(17)
C8–C9	1.394(2)	1.3981(18)
C8–C13	1.401(2)	1.4017(19)
C9–C10	1.393(2)	1.3944(18)
C10–C11	1.384(2)	1.389(2)
C10–C14/	1.456(7)	1.4961(18)
C10–Cl41	1.534(6)	
C11–Cl2	1.389(2)	1.3863(19)
C12–Cl3	1.382(2)	1.3793(18)
C14–F1/	1.305(5)	1.3400(16)
C141–F11	1.302(5)	
C14–F2/	1.299(4)	1.3368(16)
C141–F21	1.299(4)	
C14–F3/	1.309(6)	1.3293(18)
C141–F31	1.307(6)	
N3–C1A	1.5124(17)	1.5007(16)
C1A C7A	1.526(2)	1.5280(18)
C1A C2A	1.526(2)	1.5295(17)
C1A C6A	1.5329(18)	1.5314(17)
C2A C3A	1.5413(19)	1.5379(18)
C3A C4A	1.535(2)	1.5359(19)
C3A C9A	1.529(2)	1.533(2)
C4A C5A	1.531(2)	1.5330(19)
C5A C6A	1.540(2)	1.5359(18)
C5A C10A	1.530(2)	1.529(2)
C7A C8A	1.5390(19)	1.5377(18)
C8A C9A	1.535(2)	1.5304(19)

C8A C10A	1.5327(19)	1.5345(19)

Table S2 Selected angles in polymorphs I and II.

Angle	Angle value [°]	Angle value [°]
	polymorph I	polymorph II
O1–C1–O2	123.29(13)	124.49(11)
O1–C1–C2	118.25(13)	116.43(11)
O2–C1–C2	118.43(12)	119.09(10)
N1–C3–C2	119.16(12)	118.69(11)
N1–C3–N4	118.50(13)	118.76(11)
C3–N1–C8	130.39(13)	130.64(11)
C3–N4–C5	117.97(12)	117.66(11)
N1–C8–C9	124.62(14)	124.79(12)
N1–C8–C13	116.41(13)	116.12(11)
N4–C5–C6	124.46(13)	124.61(11)
C2–C7–C6	120.89(13)	120.79(11)
C8–C9–C10	118.90(15)	118.89(12)
C9–C10–C14/ C9–C10–C141	114.2(2) 119.7(3)	120.19(12)
C10–C14–F1/ C10–C141–F11	114.9(4) 112.9(4)	112.44(11)
C10–C14–F2/	112.1(5)	112.39(11)

C10–C141–F21	114.7(4)	
C10–C14–F3/ C10–C141–F31	117.0(5) 109.5(5)	113.92(11)
C11–C12–C13	120.26(16)	120.42(12)
N3–C1A–C2A	109.22(11)	109.02(10)
N3–C1A–C6A	107.98(11)	108.81(10)
N3–C1A–C7A	109.21(11)	109.01(10)
C1A–C2A–C3A	108.59(12)	108.85(10)

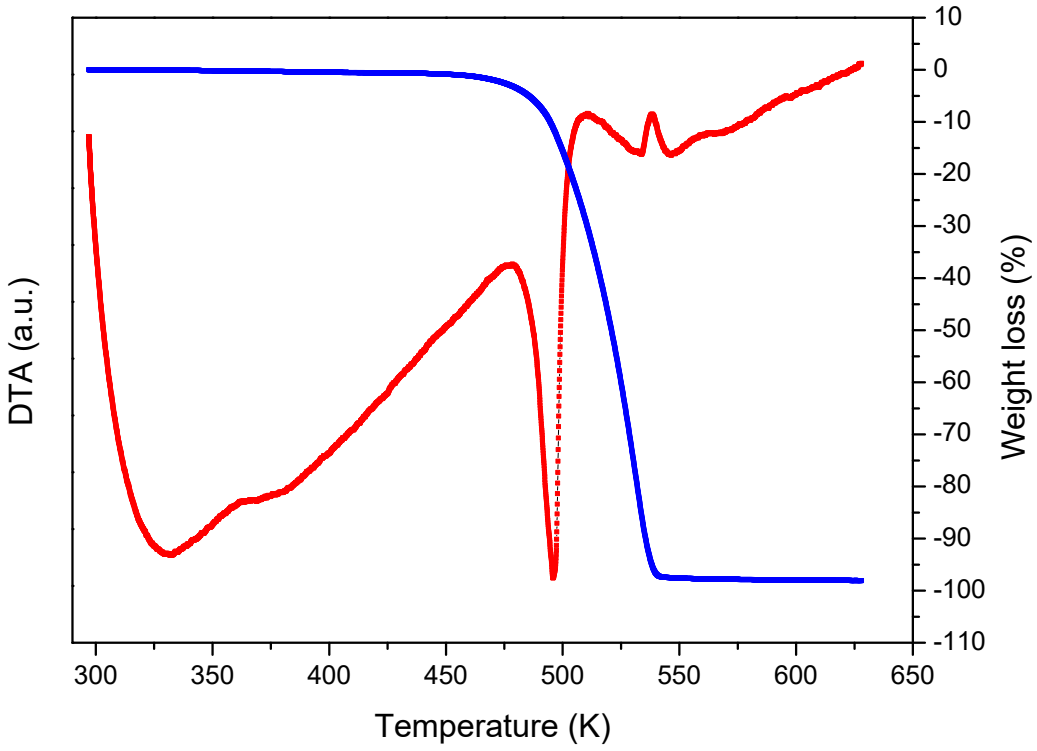

Figure S1. DTA (red) and DTG (blue) curves upon heating run for the polymorph **I**.

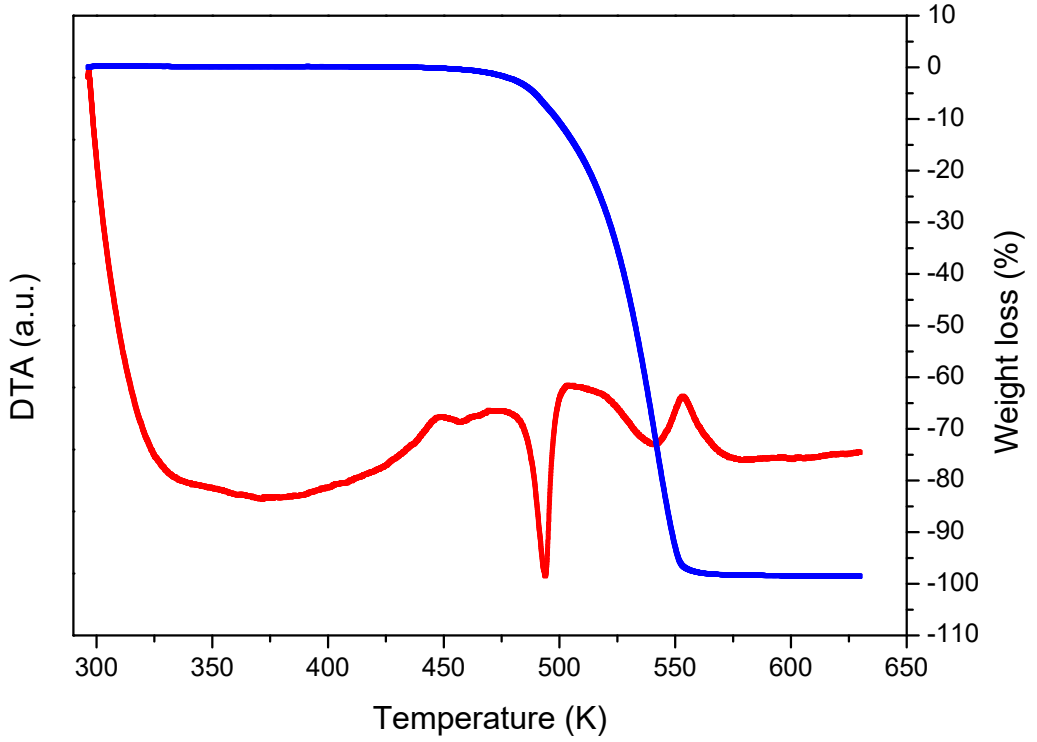

Figure S2. DTA (red) and DTG (blue) curves upon heating run for the polymorph **II**.

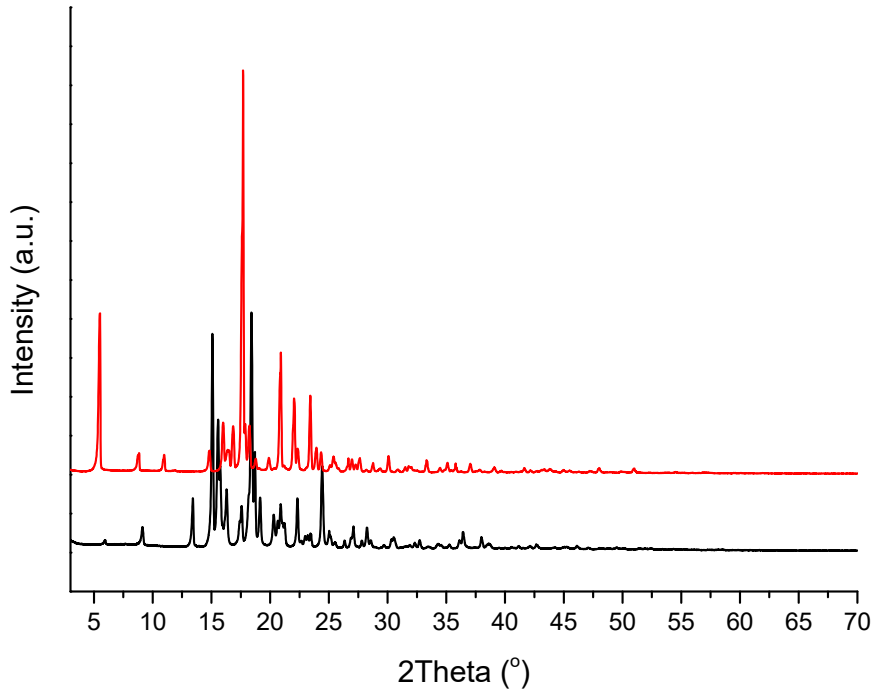

Figure S3. Comparison of diffractograms of polymorphs **I** (red curve) and **II** (black curve).

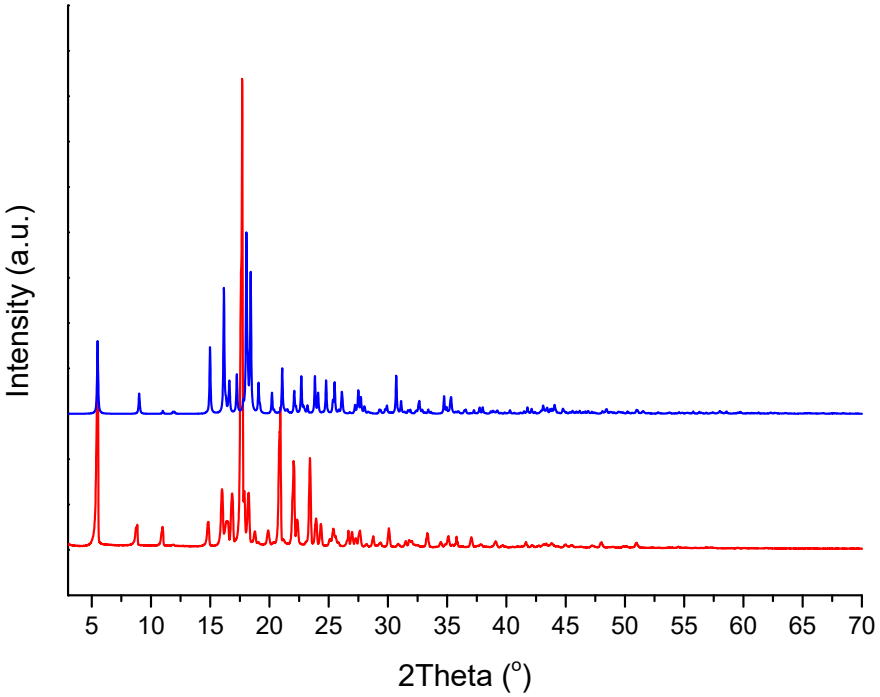

Figure S4. Comparison of diffractograms of polymorph **I**: simulated from single crystal X-ray diffraction (blue curve) and experimental (red curve).

Shifts in the positions (2Theta) of the appropriate reflections in the simulated diffractograms relative to the experimental ones result from different measurement temperatures: XRPD at ambient temperature and single-crystal X-ray measurements at 100 K.

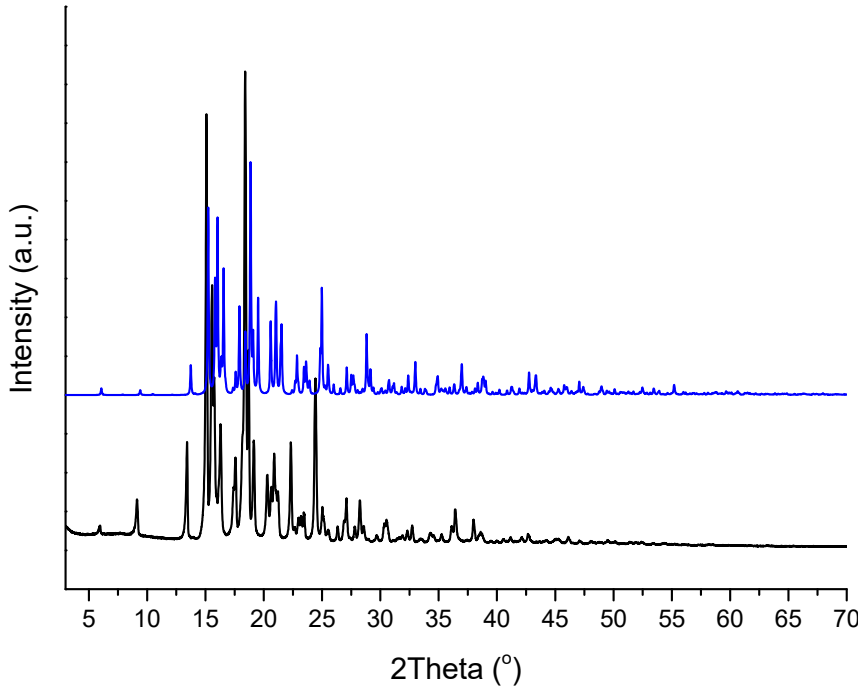

Figure S5. Comparison of diffractograms of polymorph **II**: simulated from single crystal X-ray diffraction (blue curve) and experimental (black curve).

Shifts in the positions (2Theta) of the appropriate reflections in the simulated diffractograms relative to the experimental ones result from different measurement temperatures: XRPD at ambient temperature and single-crystal X-ray measurements at 100 K.

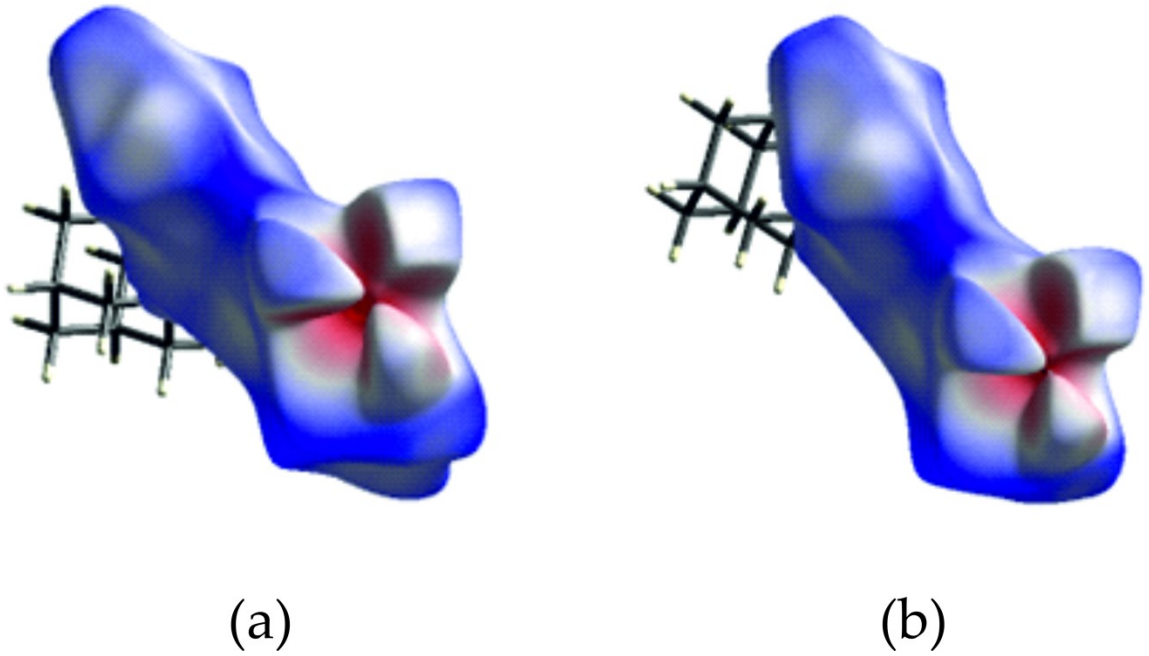

Figure S6. Hirshfeld surface plots of polymorphs **I** (a) and **II** (b) mapped with d_{norm}.

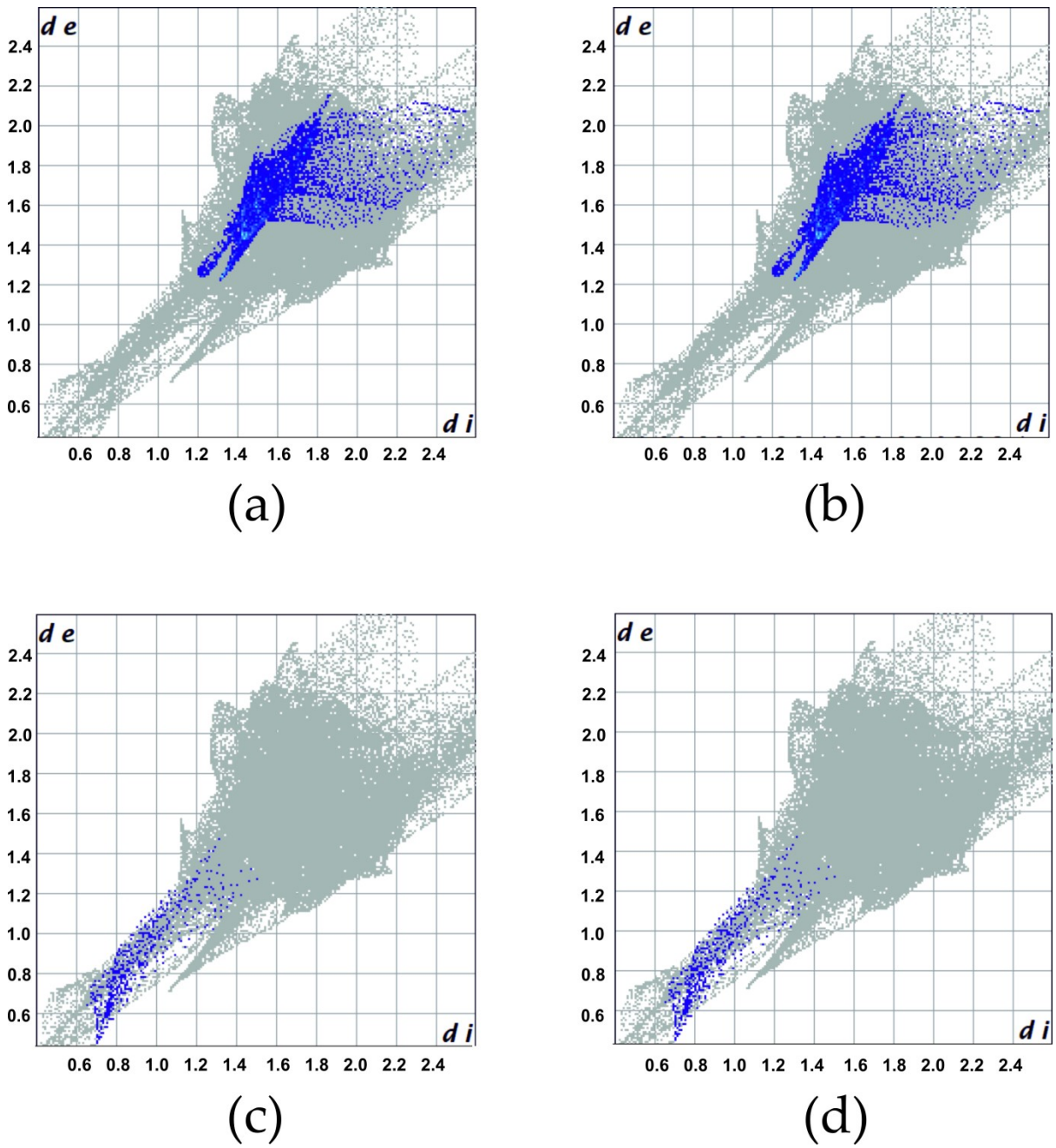

Figure S7. Fingerprint plots of polymorphs: **I** (a,c) and **II** (b,d), showing the contributions from (a, b) H···F interactions, (c, d) C···F interactions.

Hirshfeld surfaces and fingerprint plots (Fig S6, S7) for both polymorphs are prepared using CrystalExplorer software. It revealed that for the studied crystals the differences are very subtle and the program is not sufficient to present them.