Crystal structure and phase transition of the C–H···F H–bonded supramolecular compound with 4-nitroanilinium based on 18-crown-6

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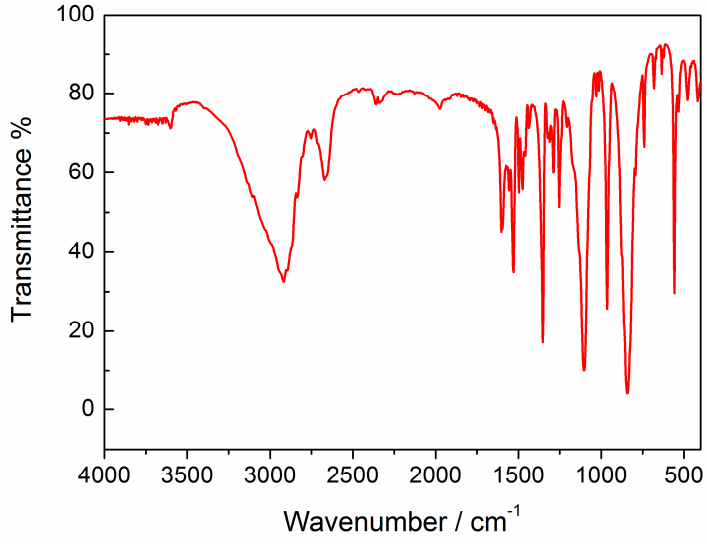

Figure S1. IR spectrum of compound **1**

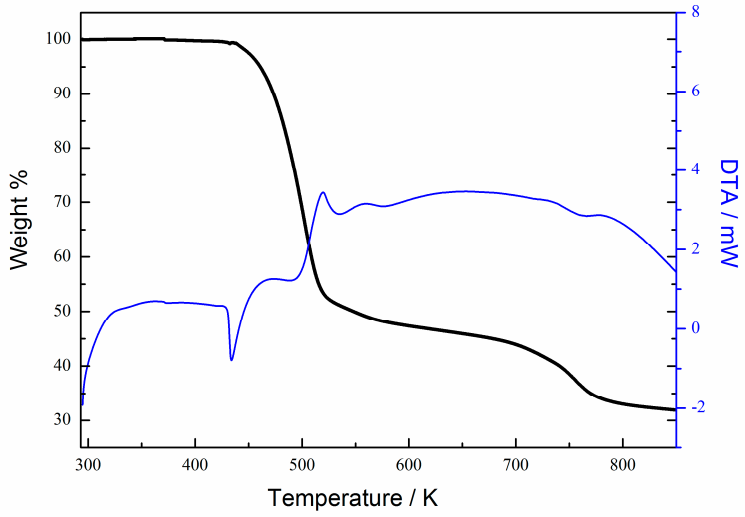

Figure S2. TG and DTA curves for compound **1**

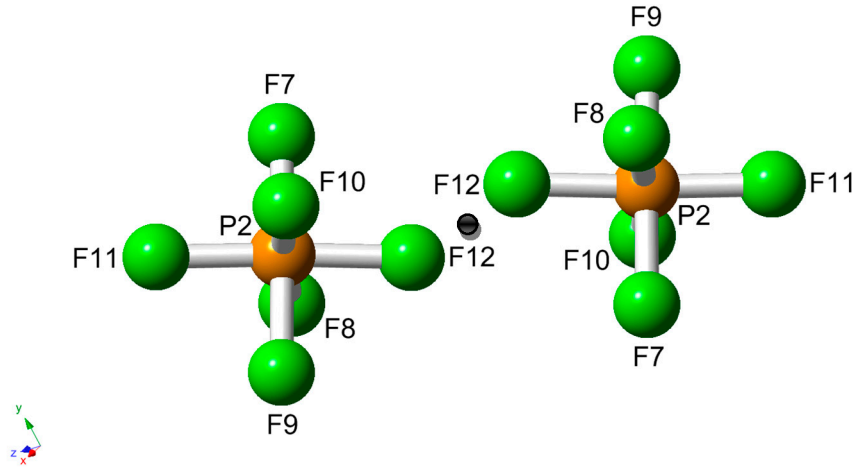

Figure S3. Molecular graph of a model hexafluorophosphate dimer in configuration.

Table S1. Hydrogen-bond C–H···F geometry (Å,°) for complex **1**

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
		100K		
C14–H14A···F6	0.931	2.527	3.345	146.843
C15–H15A···F2	0.930	2.509	3.328	147.013
C17–H17A···F4	0.930	2.885	3.371	113.844
C18–H18A···F4	0.930	2.606	3.228	124.800
C32–H32A···F11	0.930	2.627	3.489	154.352
C33–H33A···F9	0.929	2.819	3.546	135.957
C35–H35A···F12	0.929	2.699	3.400	132.900
C36–H36A···F8	0.931	2.484	3.309	147.931
		296K		
C14–H14A···F6	0.930	2.683	3.490	145.644
C15–H15A···F2	0.929	2.671	3.499	148.682
C17–H17A···F4	0.930	2.685	3.390	123.389
C18–H18A···F4	0.931	2.970	3.433	112.304
C32–H32A···F11	0.931	2.547	3.515	147.470
C33–H33A···F9	0.929	2.755	3.637	132.103
C35–H35A···F12	0.930	2.946	3.447	132.245
C36–H36A···F8	0.929	2.675	3.370	150.746

Table S2. Selected bond distances and angles for compound 1 (Å,°)

			100K		
P1–F4A	1.555(7)	P1–F3	1.561(5)	P1–F2	1.571(5)
P3–F14	1.604(3)	P3–F14	1.604(3)	P3–F13	1.602(3)
P3–F13	1.602(3)	P3–F15	1.602(2)	P3–F15	1.602(2)
P2–F7	1.591(6)	P2–F10	1.570(6)	P2–F8	1.567(6)
P2–F11	1.561(6)	P2–F12	1.523(5)	P2–F9	1.519(6)
P1–F2A	1.605(7)	P1–F1	1.589(5)	P1–F5	1.589(4)
P1–F3A	1.586(6)	P1–F6	1.578(4)	P1–F4	1.576(5)
P1–F1A	1.570(6)				
F3–P1–F2	92.5(4)	F1A–P1–F2	42.3(4)	F3–P1–F4	88.8(4)
F3A–P1–F2A	87.5(5)	F1A–P1–F2A	87.6(5)	F4A–P1–F2A	169.5(4)

F5–P1–F1	85.8(3)	F6–P1–F1	94.2(3)	F4–P1–F1	87.7(4)
F2–P1–F1	90.1(4)	F3–P1–F1	172.8(3)	F6–P1–F5	179.5(3)
F4–P1–F5	88.2(3)	F2–P1–F5	84.4(3)	F3–P1–F5	87.8(3)
F4–P1–F6	92.3(3)	F2–P1–F4	172.4(3)	F3–P1–F6	92.3(3)
F2–P1–F6	95.2(3)				

296K

P1–F5	1.508(5)	P1–F6	1.551(5)	P1–F2A	1.569(12)
P1–F2	1.571(9)	P1–F3A	1.571(11)	P1–F4	1.574(10)
P1–F1A	1.579(11)	P1–F1	1.580(11)	P1–F3	1.582(9)
P1–F4A	1.597(12)	P2–F8	1.500(12)	P2–F11	1.519(14)
P2–F7	1.528(12)	P2–F10	1.535(14)	P2–F9	1.541(13)
P2–F12	1.548(14)	P3–F13	1.598(3)	P3–F15	1.601(3)
P3–F14	1.600(3)	P3–F14	1.600(3)	P3–F15	1.601(3)
F5–P1–F6	179.0(4)	F1–P1–F3	164.6(5)	F3A–P1–F4A	88.4(6)
F5–P1–F2	96.0(4)	F6–P1–F2	84.6(4)	F5–P1–F3A	80.4(4)
F5–P1–F4	102.3(4)	F6–P1–F4	77.1(4)	F2–P1–F4	161.7(4)
F3A–P1–F4	47.4(5)	F5–P1–F1	96.3(4)	F6–P1–F1	82.9(4)
F2–P1–F1	88.1(5)	F4–P1–F1	89.0(6)	F5–P1–F3	98.9(4)
F6–P1–F3	81.9(3)	F2–P1–F3	88.0(5)	F4–P1–F3	90.0(5)
F1A–P1–F4A	86.5(6)				
F8–P2–F11	94.6(8)	F11–P2–F10	91.3(8)	F7–P2–F10	89.9(7)
F8–P2–F7	90.6(7)	F11–P2–F7	91.0(7)	F8–P2–F10	174.0(7)
F8–P2–F9	90.6(7)	F11–P2–F9	88.1(7)	F7–P2–F9	178.6(7)
F10–P2–F9	88.9(7) .	F8–P2–F12	84.8(8)	F11–P2–F12	177.5(8)
F7–P2–F12	91.4(7)	F10–P2–F12	89.2(8)	F9–P2–F12	89.5(7)
F13–P3–F15	90.15(15)	F14–P3–F15	89.69(15)	F14–P3–F15	89.69(15)