Electronic Supplementary Information

Proflavine and zinc chloride "team chemistry": Combining antibacterial agents via solid-state interaction

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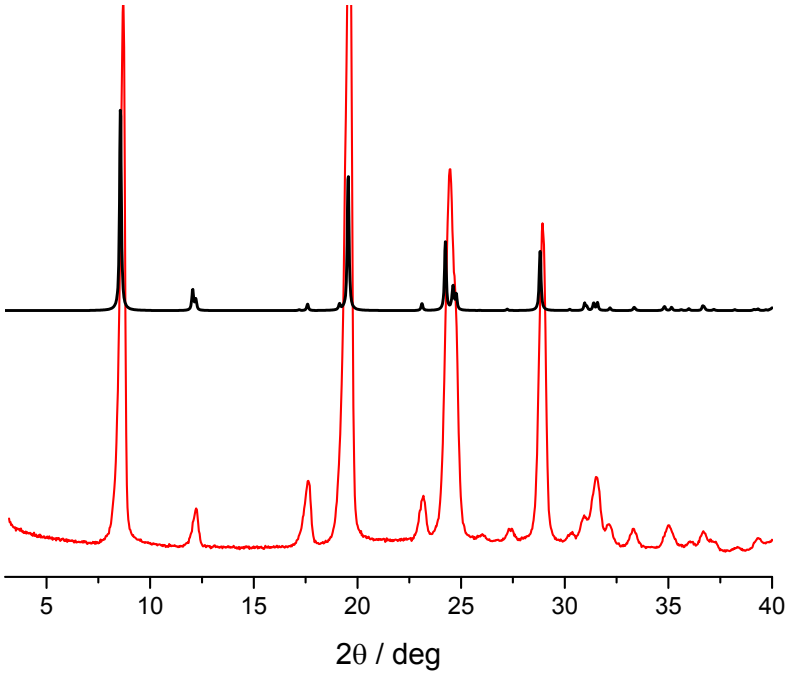

Fig. ESI-1. Comparison between the experimental XRPD pattern for PF·H_2O (red line) and the pattern calculated on the basis of single crystal data from the CSD (PROFLV) (black line).

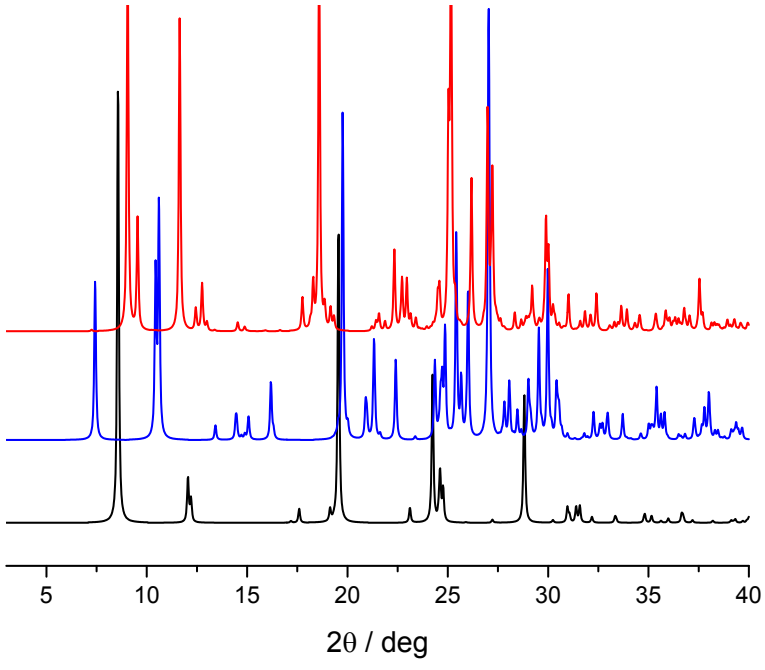

Fig. ESI-2. Comparison between the experimental pattern for [HPF]Cl·$2H_2O$ (red line) and the patterns calculated on the basis of single crystal data for [H_2PF]Cl_2·$2H_2O$ (PROFLC) (blue line) and PF·H_2O (PROFLV) (black line) as a reference.

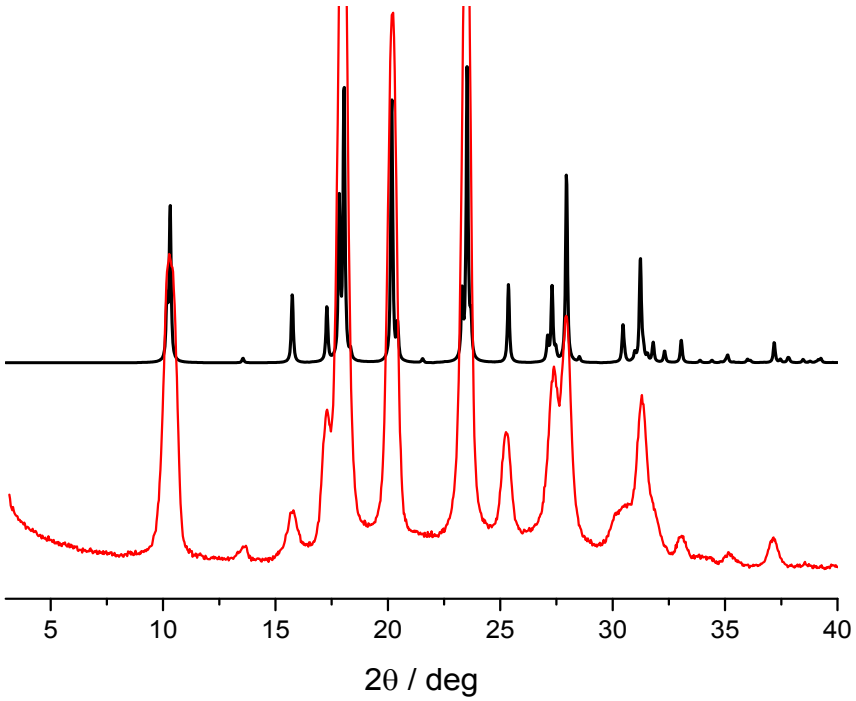

Fig. ESI-3. Comparison between calculated (black line) and experimental (red line) patterns for anhydrous PF.

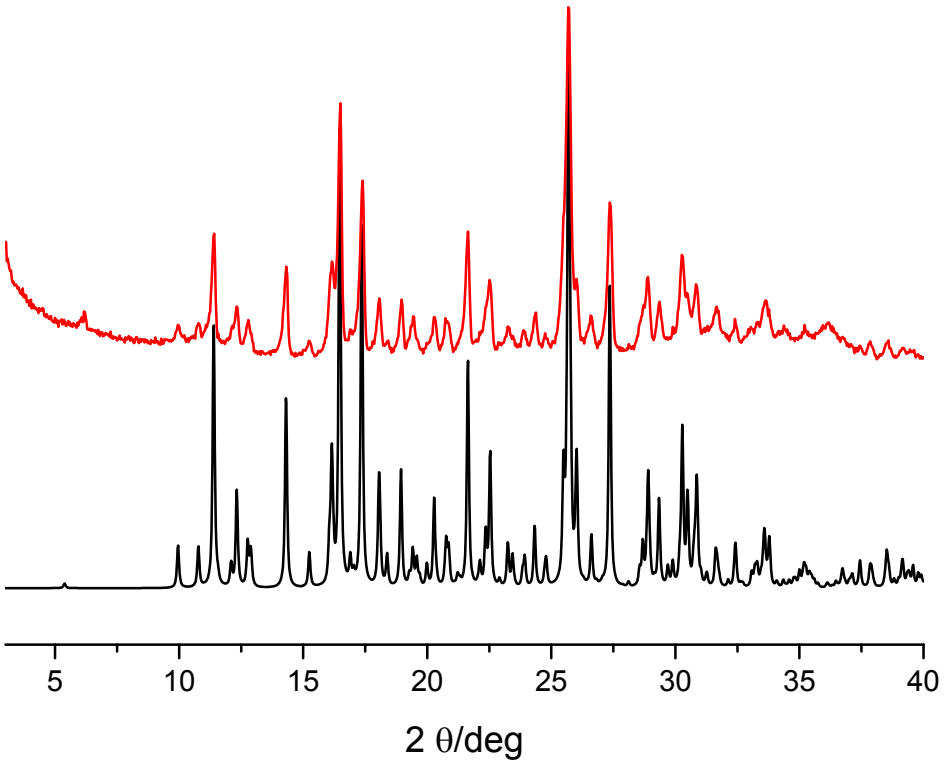

Fig. ESI-4. Comparison between the calculated pattern for $[HPF]_2[ZnCl_4]\cdot H_2O$ **(2)** (black line) and the experimental XRPD pattern of $[HPF]_2[ZnCl_4]\cdot H_2O$ as obtained from solution (red line).

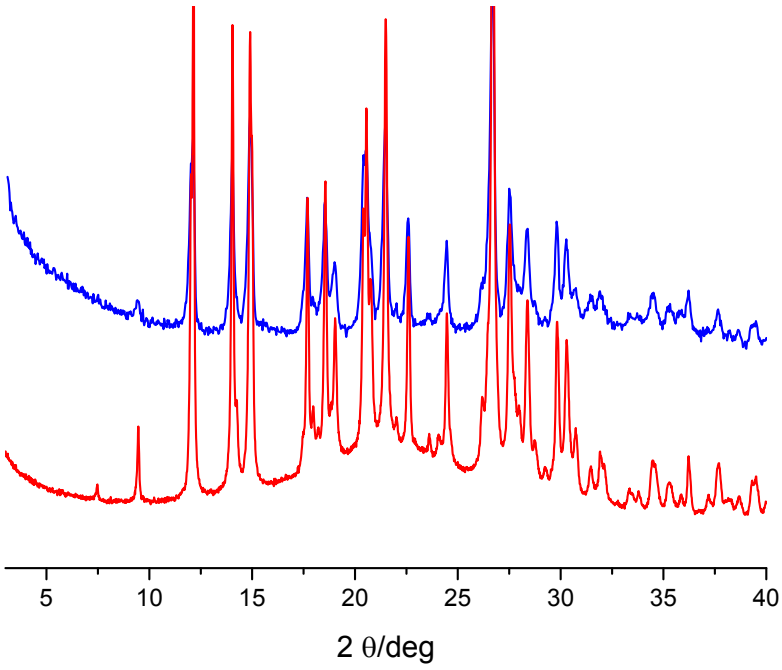

Fig. ESI-5. Comparison between the experimental XRPD pattern of $ZnCl_3$(HPF) **(1)** obtained from solution (red line) and the XRPD pattern of $ZnCl_3$(HPF) obtained from ball milling (blue line).

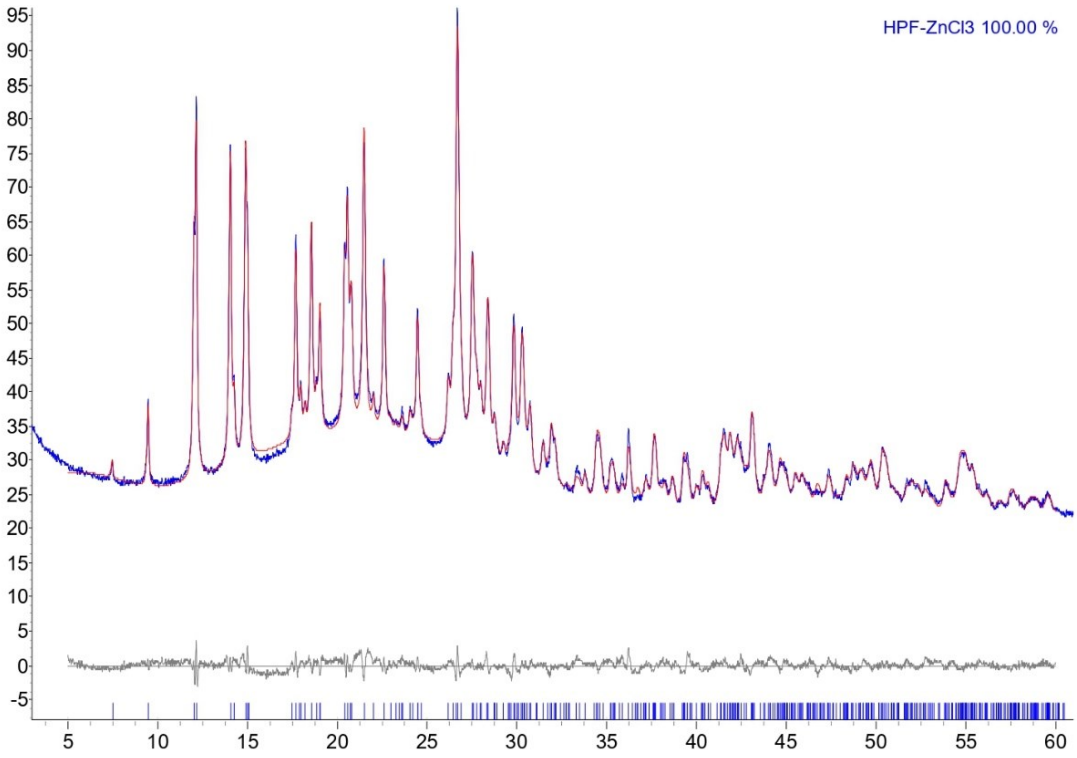

Fig. ESI-6. Rietveld analysis plot of $ZnCl_3$(HPF) **(1)**: In red the calculated pattern, in blue the experimental one, and in grey the difference plot.

Table ESI-1. Crystal data and details of measurements (T = 298 K) for PF anhydrous, [HPF]Cl·2H_2O, $ZnCl_3$(HPF) (**1**) and $[HPF]_2$·$[ZnCl_4]$·H_2O (**2**).

	PF anhydrous	**[HPF]Cl·2H_2O**	**$ZnCl_3$(HPF) (1)[a]**	**$[HPF]_2$·$[ZnCl_4]$·H_2O (2)**
Chemical formula	$C_{13}H_{11}N_3$	$(C_{13}H_{12}N_3^+)$, Cl^-, $2H_2O$	$ZnCl_3(C_{13}H_{12}N_3^+)$	$2(C_{13}H_{12}N_3^+)$, $(ZnCl_4^{2-})$, H_2O
M_r /g mol^{-1}	209.25	281.74	382.00	603.71
Crystal system	Orthorhombic	Triclinic	Triclinic	Triclinic
Space group	$P2_12_12_1$	*P*-1	*P*-1	*P*-1
a / Å	5.9524 (6)	7.5170 (5)	12.1724 (1)	8.7727 (4)
b / Å	10.0773 (9)	12.5737 (10)	9.6326 (3)	10.1439 (5)
c / Å	17.1337 (14)	15.5867 (10)	6.7045 (1)	16.8688 (9)
α / °	90	89.941 (6)	104.8578 (3)	100.796 (4)
β / °	90	77.478 (5)	104.4355 (1)	93.143 (4)
γ / °	90	75.976 (6)	85.7581 (1)	112.422 (4)
V / Å^3	1027.75 (16)	1393.23 (18)	735.81 (3)	1349.85 (12)
Z, Z'	4, 1	4, 2	2, 1	2, 1
d / mg cm^{-3}	1.352	1.343	-	1.589
μ / mm^{-1}	0.08	0.28	-	1.34
Measd reflns	3178	9921	-	9389
Indep reflns	2005	4882	-	4754
Reflns with $I > 2\sigma(I)$	893	2209	-	3296
R_{int}	0.046	0.046	-	0.037
***R1* [$F^2 > 2\sigma(F^2)$]**	0.071	0.062	-	0.064
***wR*(F^2)**	0.223	0.128	-	0.103
R_wp	-	-	0.0389	-
R_p	-	-	0.0308	-
R_exp	-	-	0.0302	-
χ^2	-	-	1.2921	-

[a] powder data.

Crystal data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk and have been allocated the accession numbers CCDC 2081498-2081501.

DSC and TGA

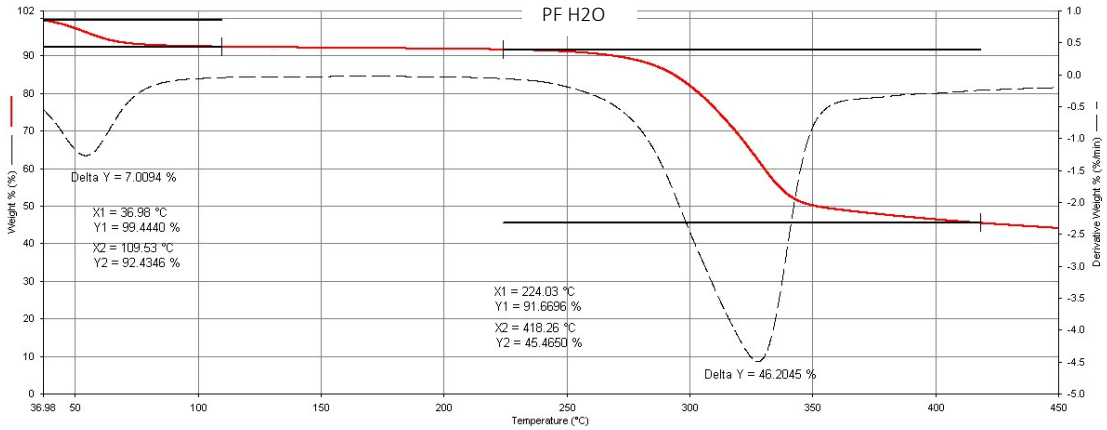

Fig. ESI-7. TGA trace for PF·H_2O.

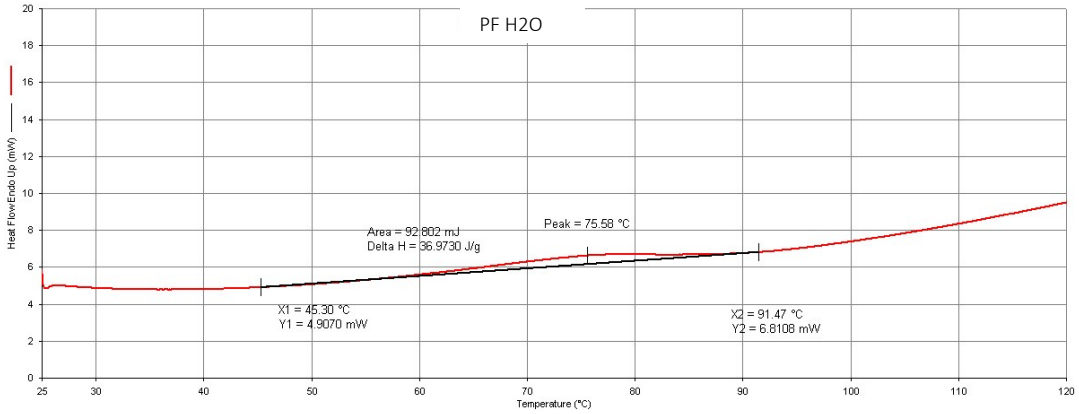

Fig. ESI-8. DSC trace for PF·H_2O from 25°C to 120°C.

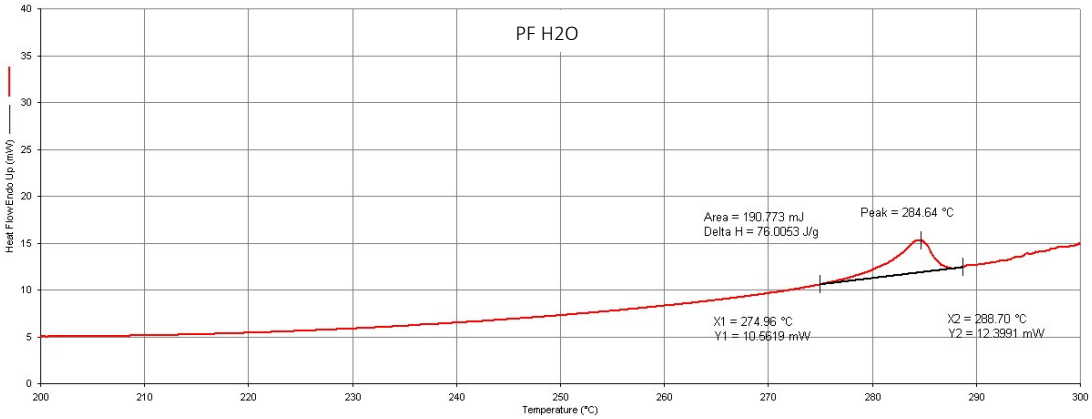

Fig. ESI-9. DSC trace for PF·H_2O from 200°C to 300°C.

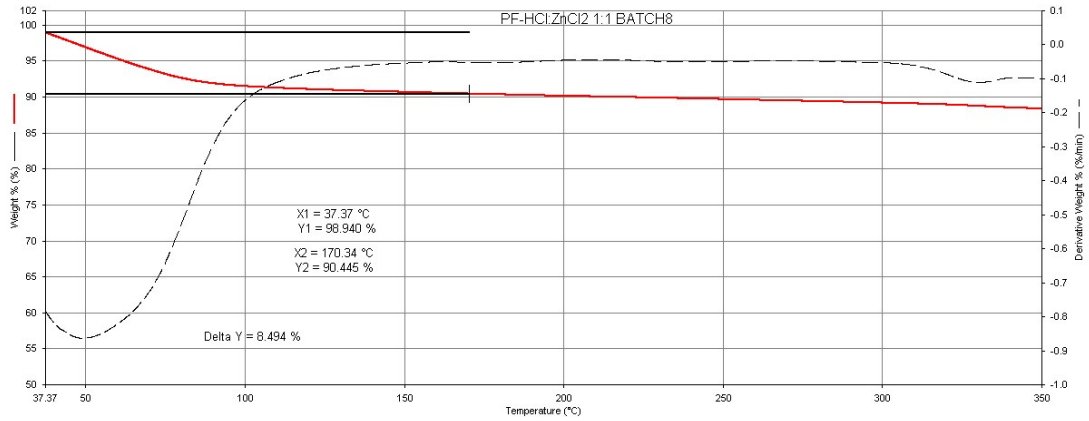

Fig. ESI-10. TGA trace for $ZnCl_3(HPF)$ (**1**).

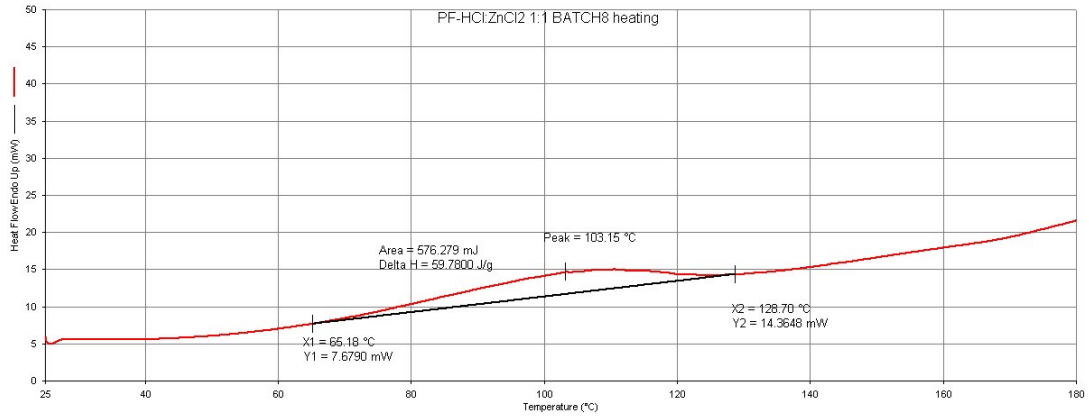

Fig. ESI-11. DSC trace for $ZnCl_3(HPF)$ (**1**).

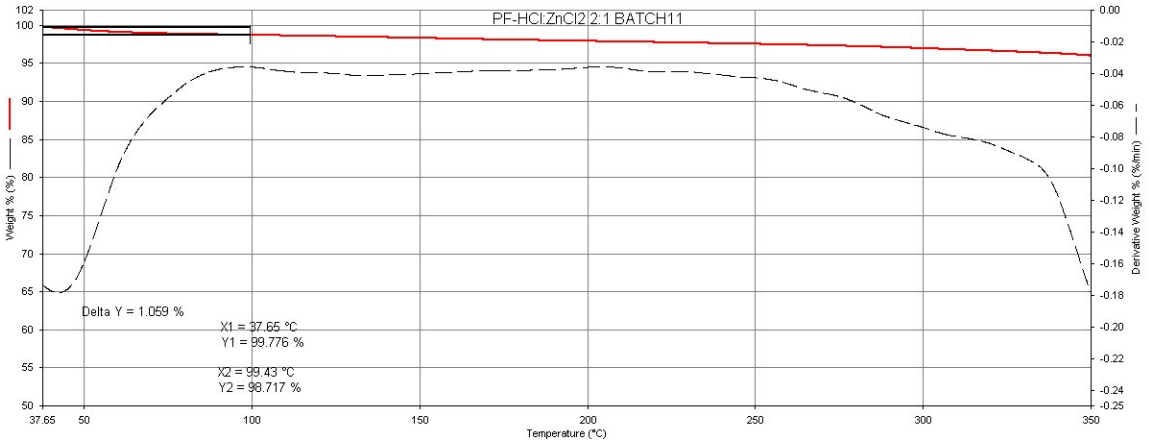

Fig. ESI-12. TGA trace for $[HPF]_2[ZnCl_4]\cdot H_2O$ (**2**).

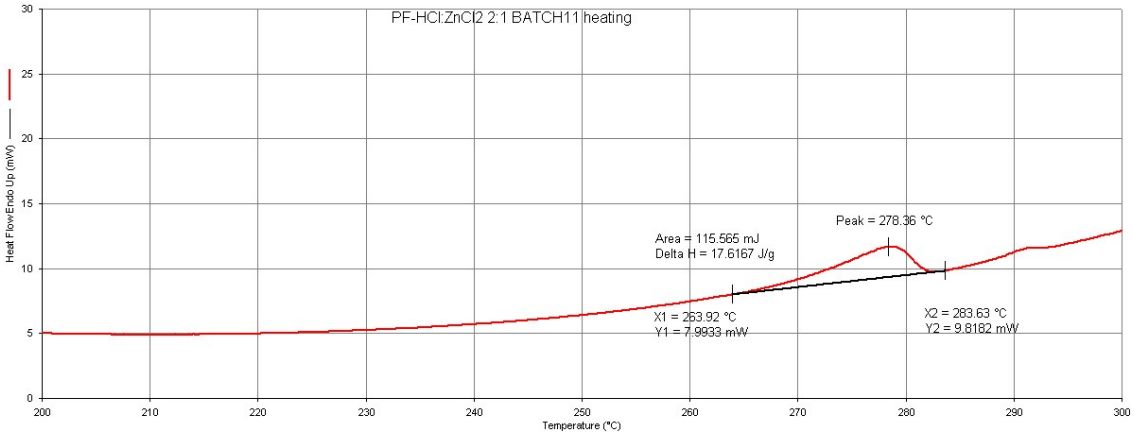

Fig. ESI-13. DSC trace for $[HPF]_2[ZnCl_4]\cdot H_2O$ (**2**).