Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

In situ IR spectral identification of $NH_4H_2PO_4$ structural evolution during crystallization in water–ethanol mixed solvent

Congting Sun and Dongfeng Xue*

State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry,

Chinese Academy of Sciences, Changchun 130022, China

*Corresponding author. E-mail: dongfeng@ciac.ac.cn

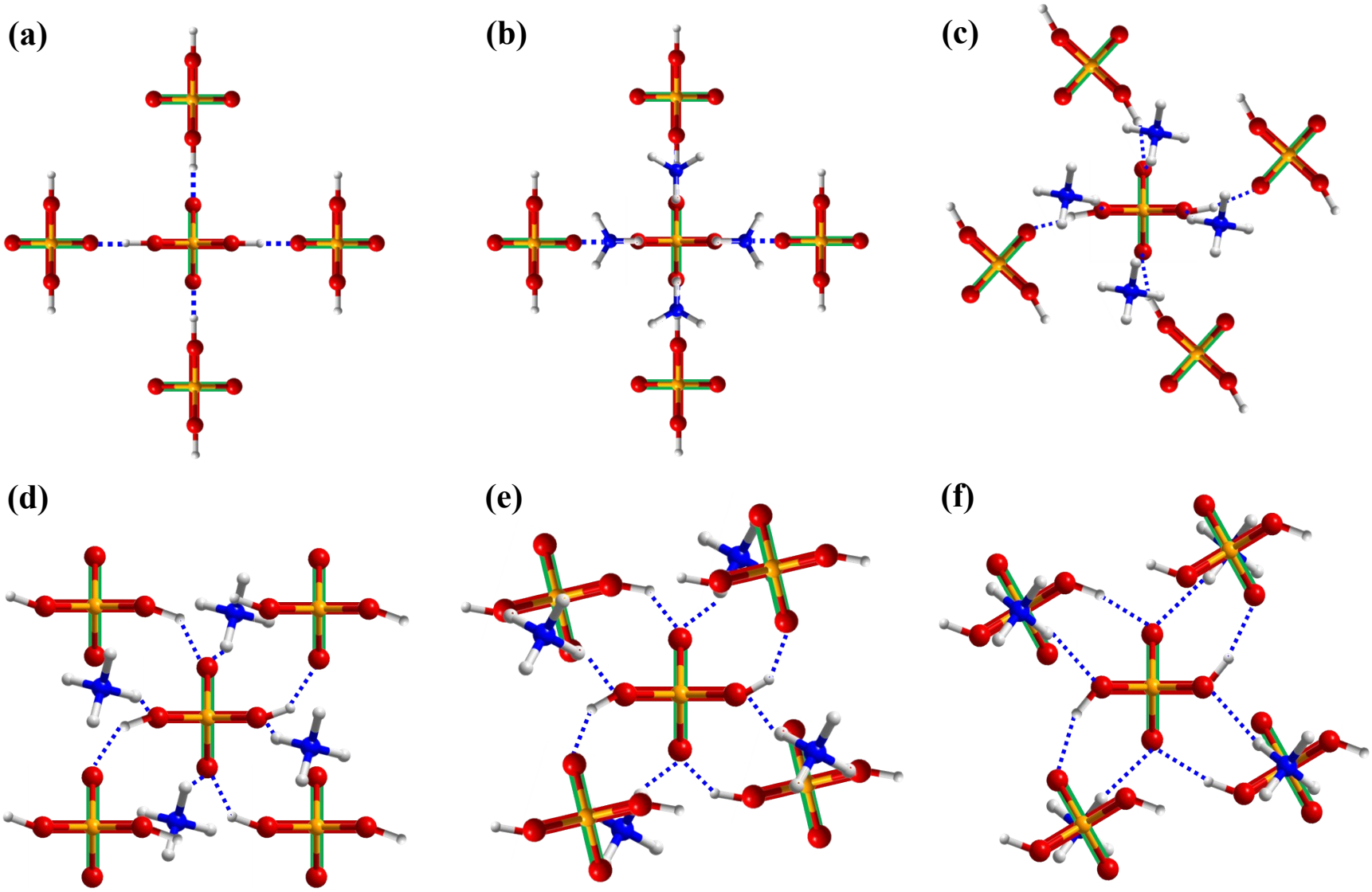

Figure S1 Molecule motion from $(H_2PO_4^-)_n$ framework (a) to amorphous precursor phase $NH_4H_2PO_4$ (b–e) and crystalline state $NH_4H_2PO_4$ (f).

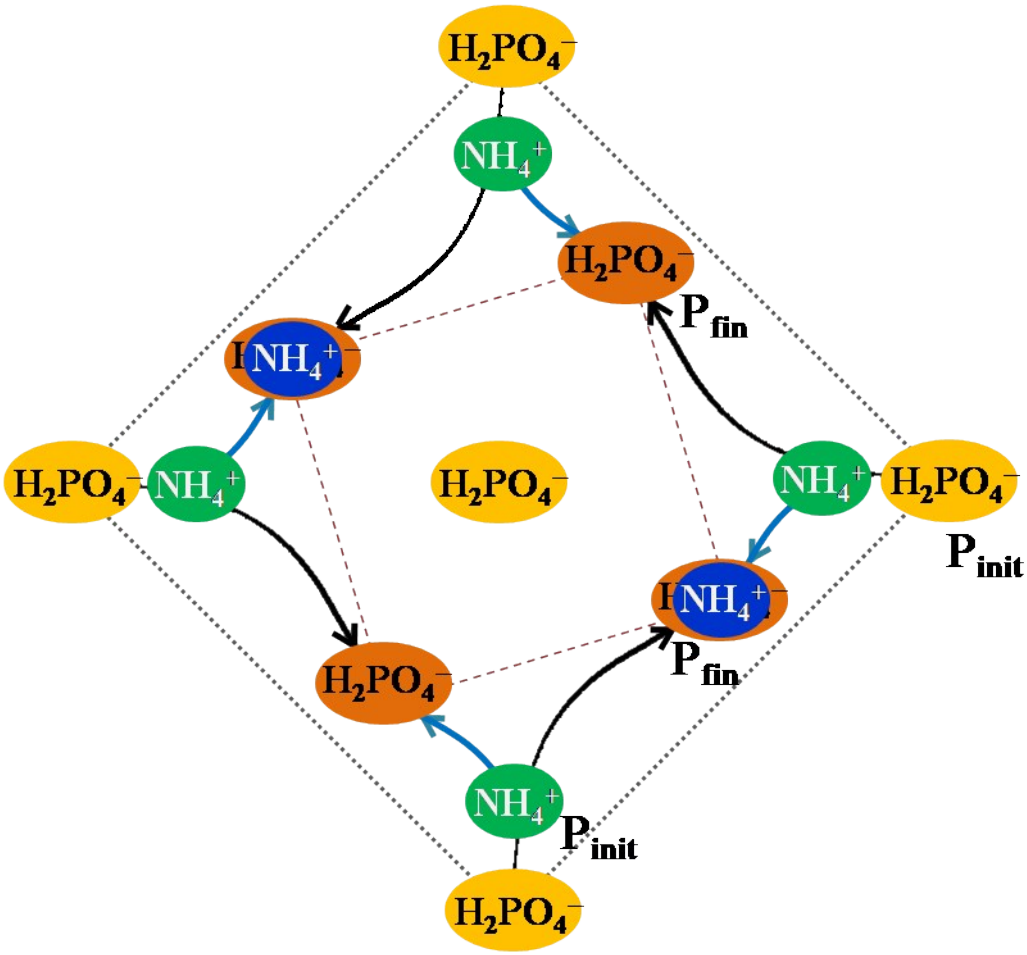

Figure S2 Motion tracks of NH_4^+ and $H_2PO_4^-$ groups in $NH_4H_2PO_4$ molecule in the transition from amorphous precursor phase to crystalline state. $H_2PO_4^-$ groups move along the black line in an anticlockwise direction surrounding the center $H_2PO_4^-$ group with 60.26°. NH_4^+ groups move along the blue line in a clockwise direction surrounding the center $H_2PO_4^-$ group with 29.74°.

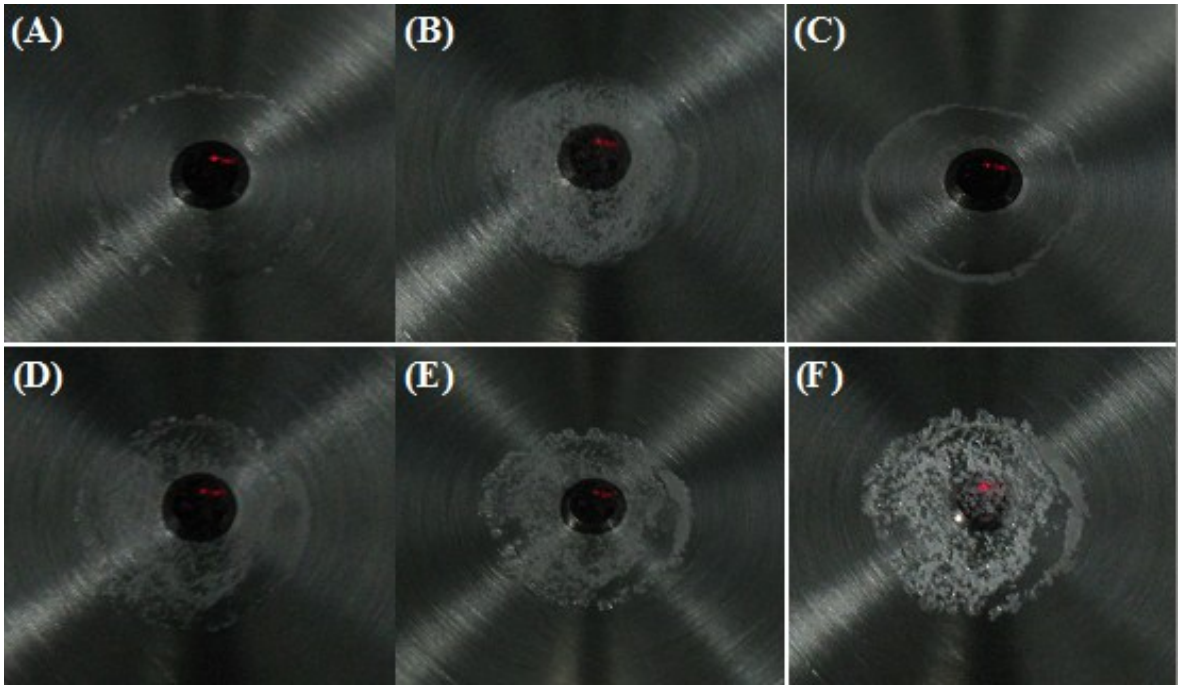

Figure S3 Photographs of $NH_4H_2PO_4$ aqueous crystallization system in IR measurements. (A) 5 μL $NH_4H_2PO_4$ aqueous solution with the concentration of 1.17 mol/L (unsaturated solution) added to diamond wafer. (B–F) $NH_4H_2PO_4$–H_2O–ethanol crystallization process with $V(H_2O)$: V(ethanol) = 1 : 1.

Table S1 The volume of H_2O and mole mass of $NH_4H_2PO_4$ in 1 mL $NH_4H_2PO_4$ aqueous solution

Concentration (mol/L)	Solution volume (mL)	$NH_4H_2PO_4$ mole mass (mol)	Volume of H_2O (mL)
1.17	1	1.17×10^{3}	0.943
1.86	1	1.86×10^{3}	0.926
2.33	1	2.33×10^{3}	0.893