

Recurrent supramolecular scenarios within complex 3-D hydrogen bond networks derived from organic ammonium salts of (4-amino-1-hydroxybutylidene)-1,1-bisphosphonic acid.

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Supplementary Information

S1. Powder X-ray Diffraction Data.

[enH₂][LH₃].2(H₂O) (Coupled TwoTheta/Theta)

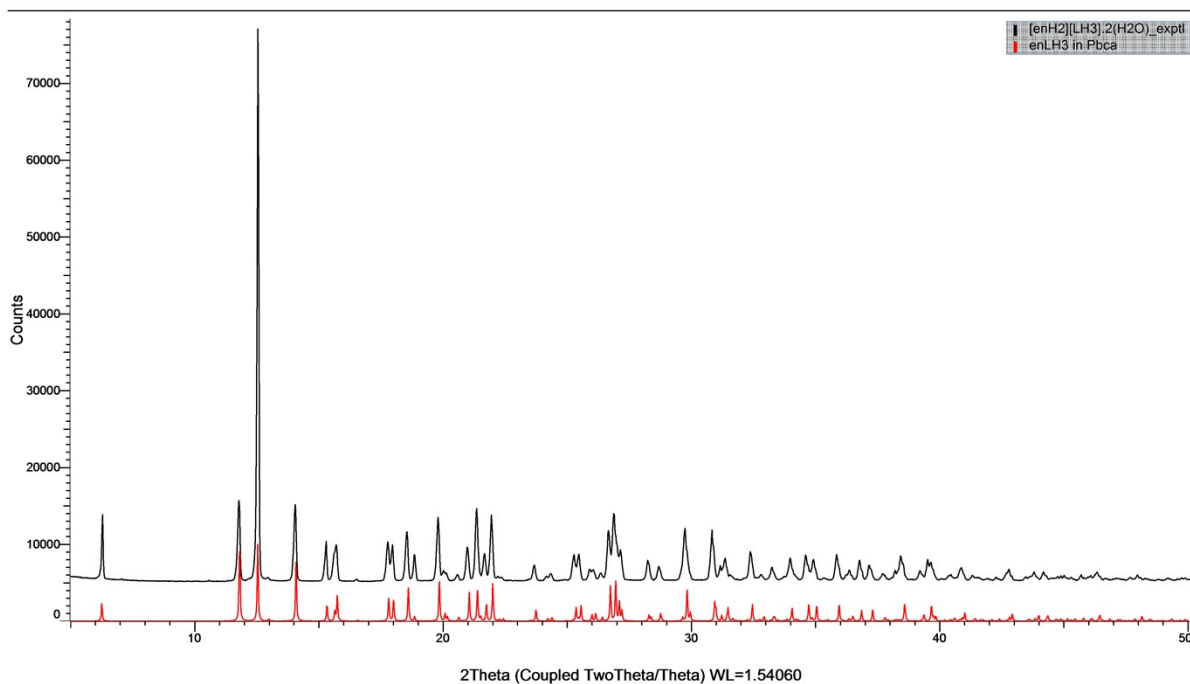


Figure S1.1. Experimental (black) and calculated (red) PXRD patterns for [enH₂][LH₃].2(H₂O) **1**.

MeenLH3_recrist (Coupled TwoTheta/Theta)

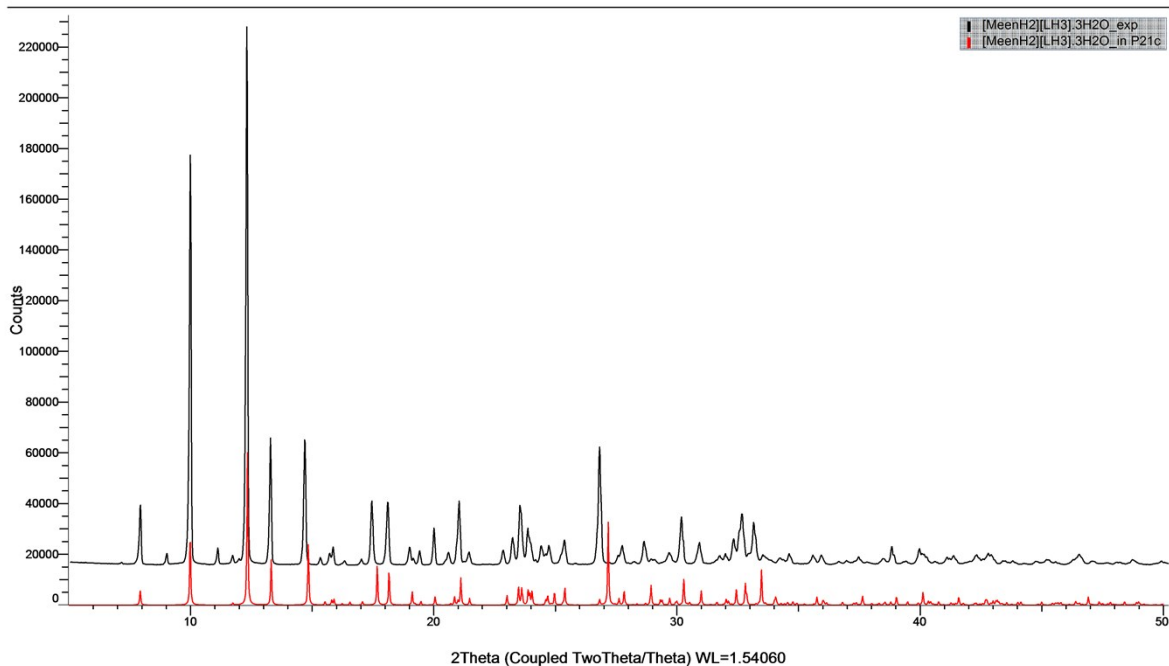


Figure S1.2. Experimental (black) and calculated (red) PXR D pattern for [MeenH₂].[LH₃].3(H₂O) **2**.

[N,N'-Me2enH2].[LH3] (Coupled TwoTheta/Theta)

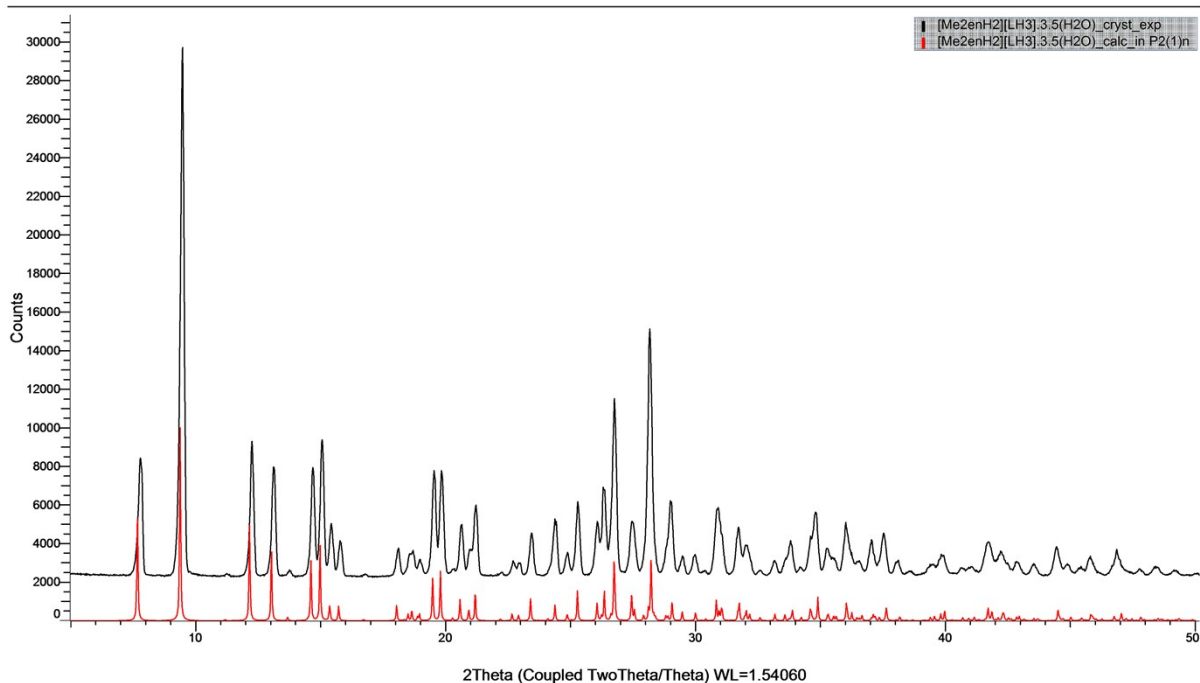


Figure S1.3. Experimental (black) and calculated (red) PXR D pattern for [Me₂enH₂].[LH₃].3.5(H₂O) **3**.

[Et₂enH₂][LH₃].2(H₂O)_crude (Coupled TwoTheta/Theta)

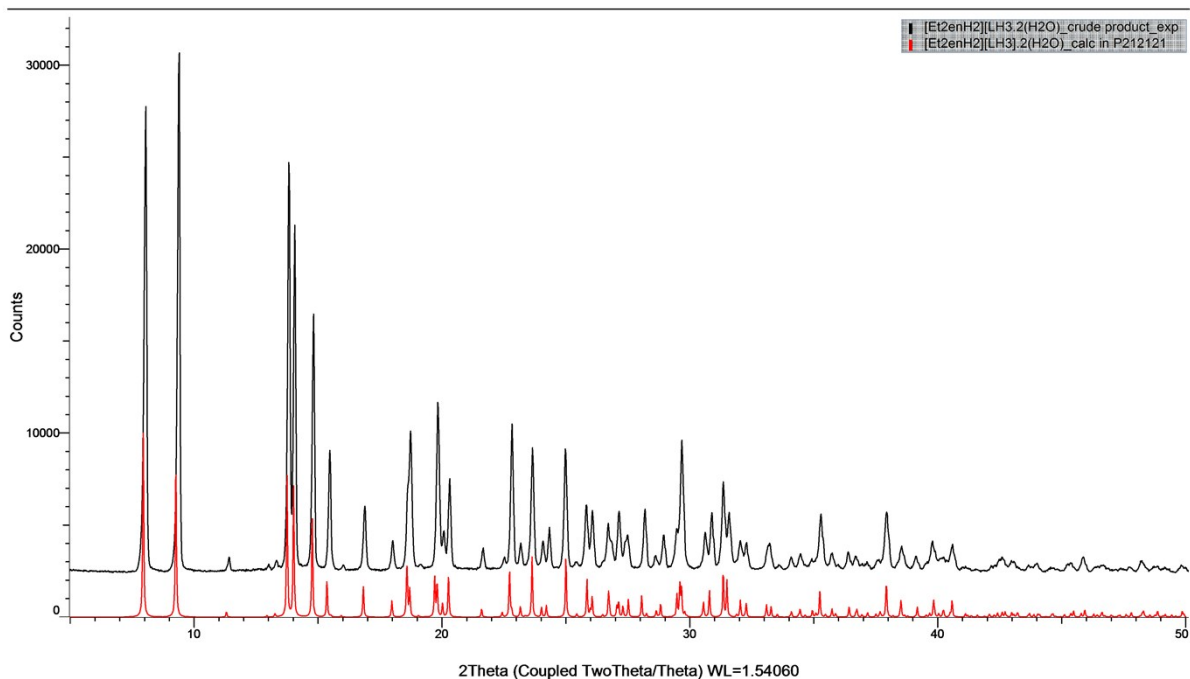


Figure S1.4. Experimental (black) and calculated (red) PXR D patterns for [Et₂enH₂][LH₃].2(H₂O) **4**.

[cy(NH₃)₂][LH₃] (Coupled TwoTheta/Theta)

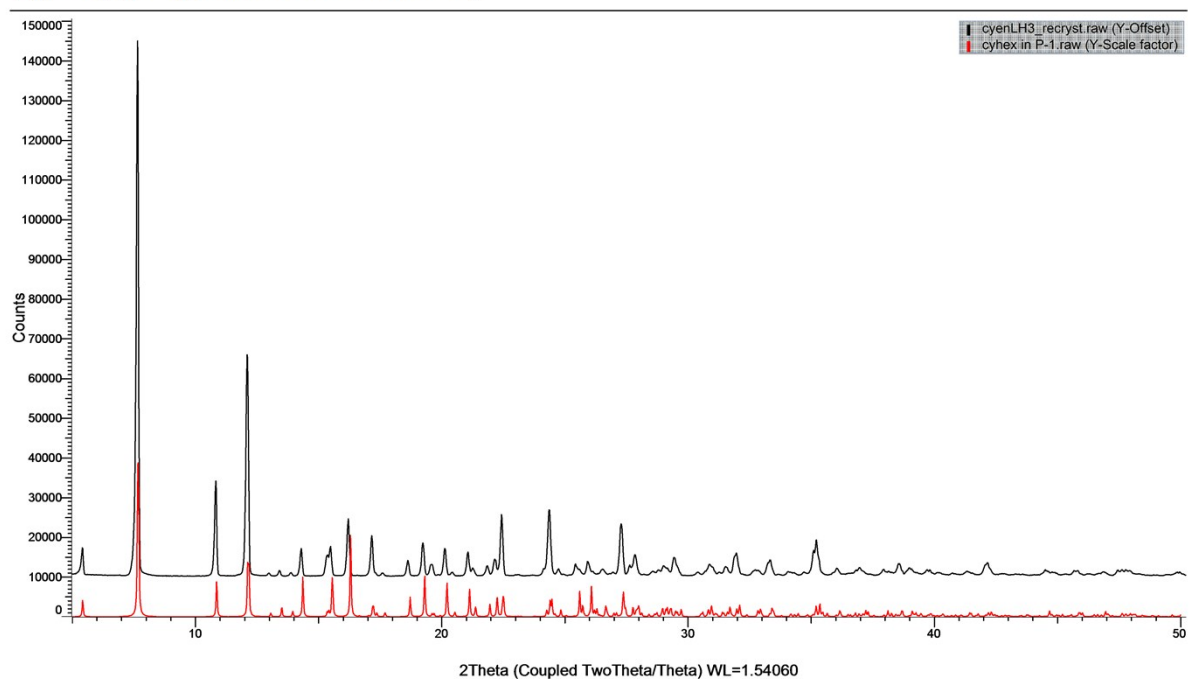


Figure S1.5. Experimental (black) and calculated (red) PXR D patterns for [cdaH₂][LH₃].3(H₂O) **5**.

[xyl(NH3)2][LH3].4H2O_recrist (Coupled TwoTheta/Theta)

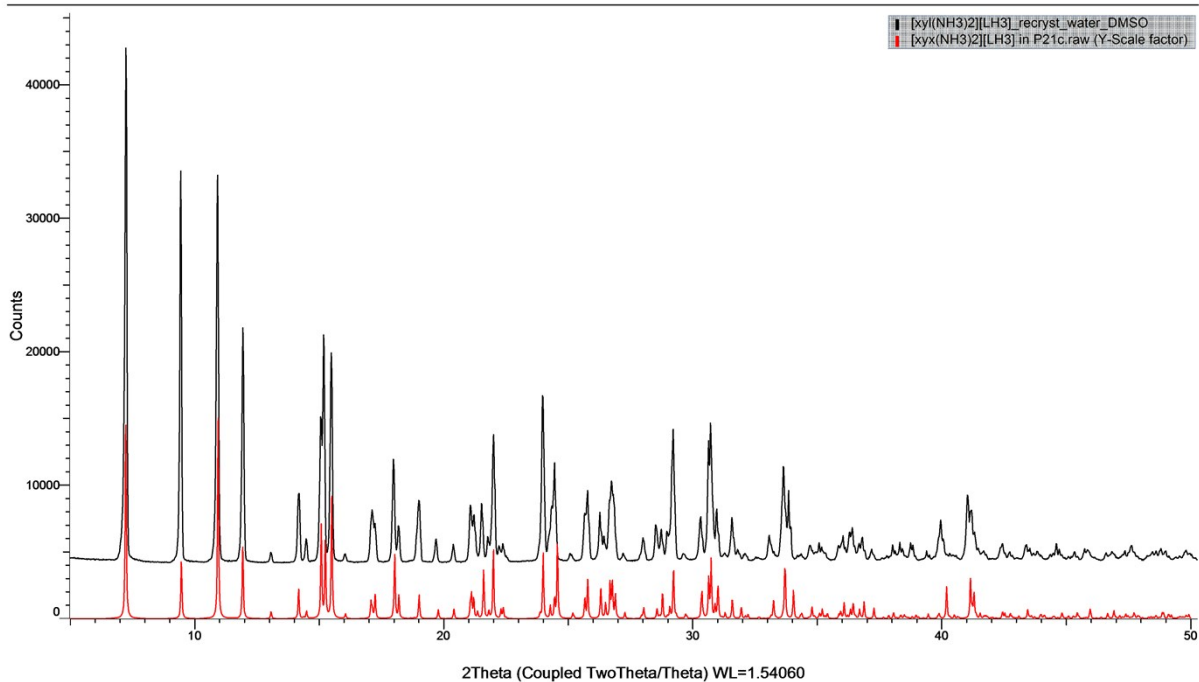


Figure S1.6. Experimental (black) and calculated (red) PXR D patterns for [xdaH₂][LH₃].4(H₂O) **6**.

[onH2][LH3] (Coupled TwoTheta/Theta)

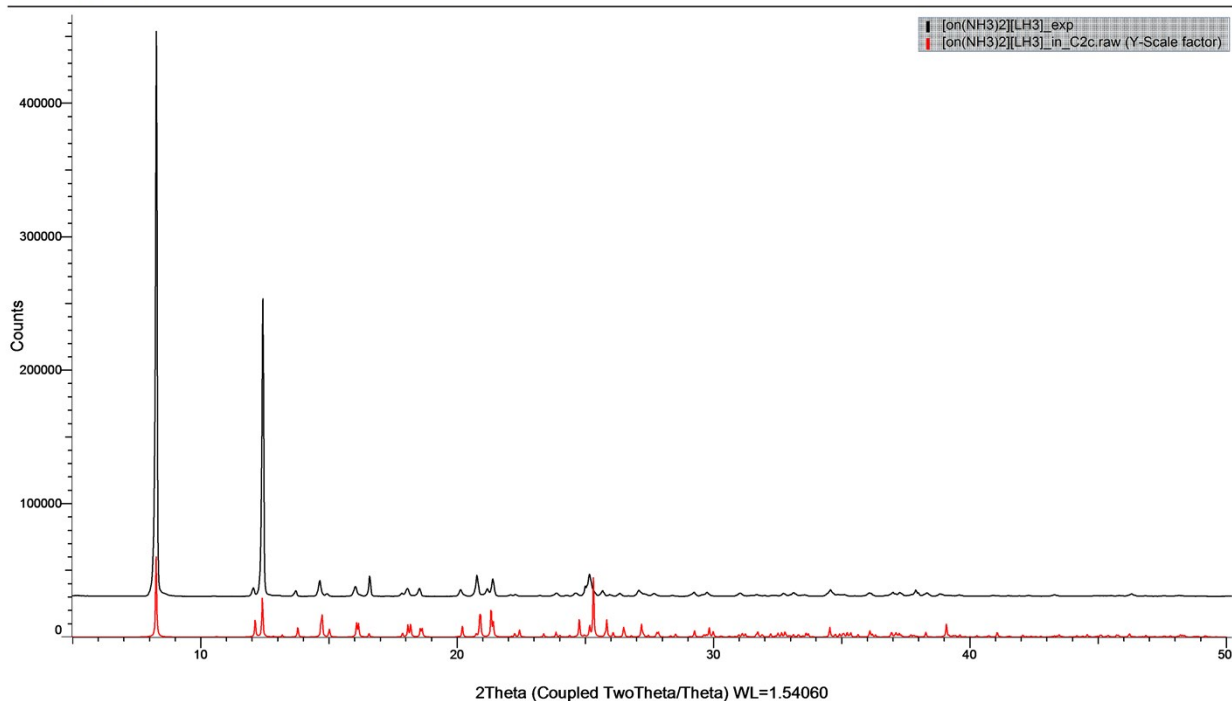


Figure S1.7. Experimental (black) and calculated (red) PXR D patterns for [odaH₂][LH₃].2(H₂O).0.5EtOH **7**.

[PheNH₃]₂[LH₃]₂·CF_01_16 (Coupled TwoTheta/Theta)

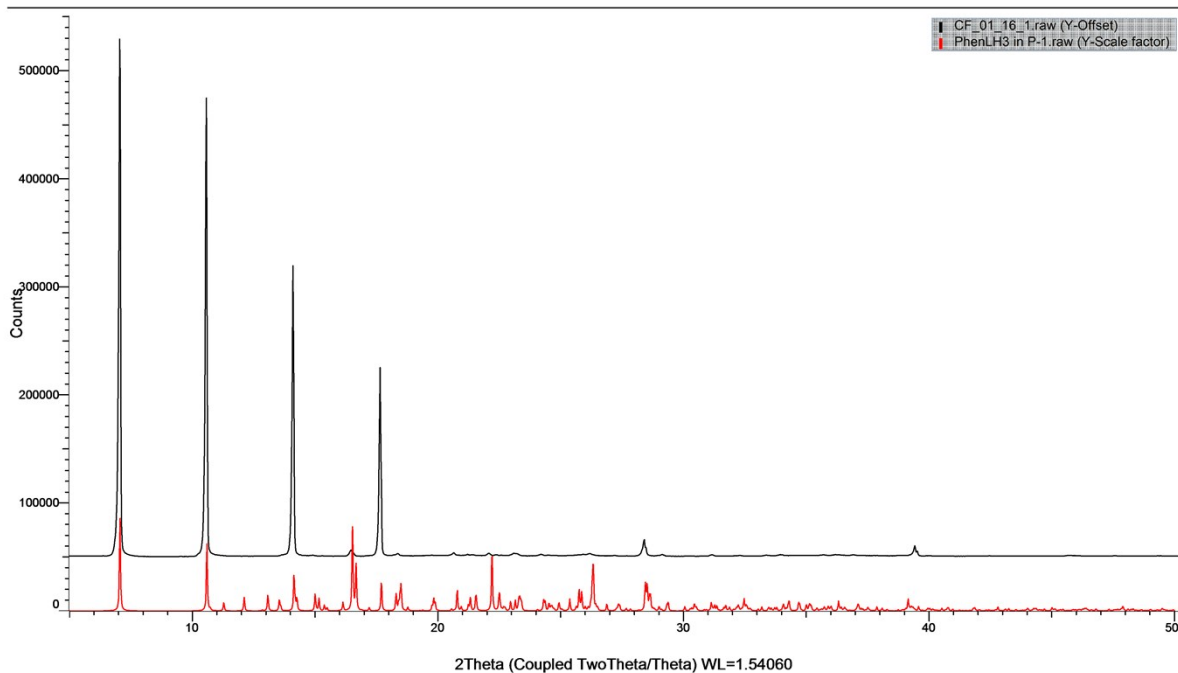


Figure S1.8. Experimental (black) and calculated (red) PXRD pattern for [PheH]₂[LH₃]₂·2(H₂O) **8**. The experimental PXRD appeared to exhibit severe preferred orientation effects, consistent with the plate-like habit and waxy nature of the crystals.

[mel][LH₃]₂·7H₂O_bulk (Coupled TwoTheta/Theta)

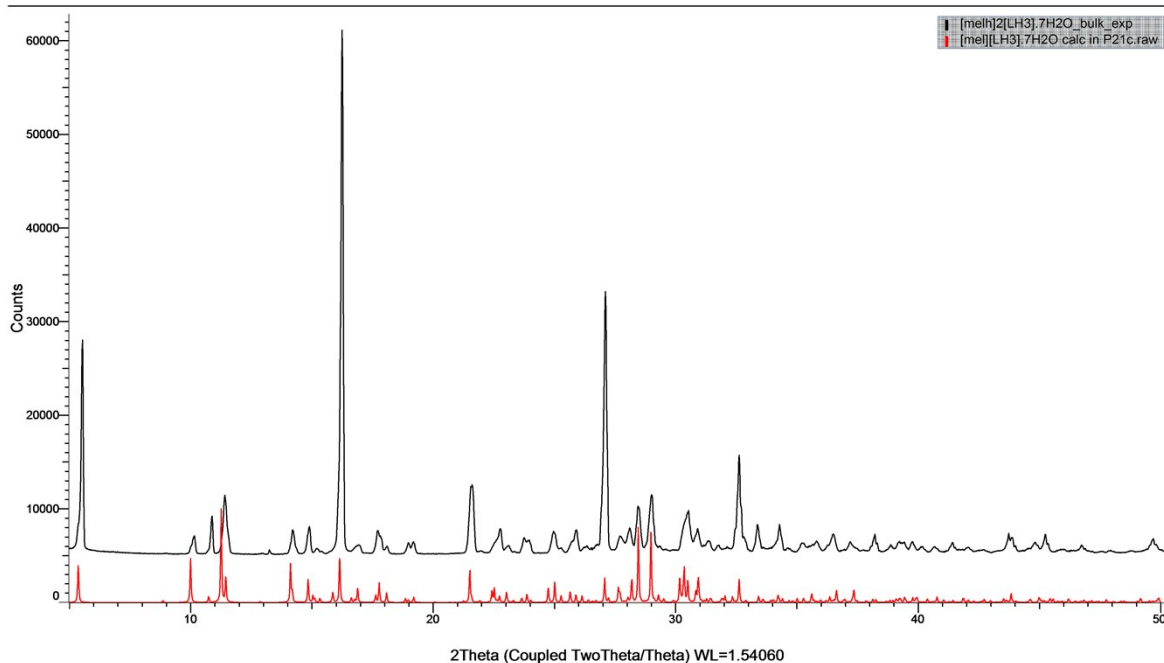


Figure S1.9. Experimental (black) PXRD and calculated (red) PXRD pattern for [melH]₂[LH₃]₂·7(H₂O) **9**.

S2. Crystal Structure Diagrams.

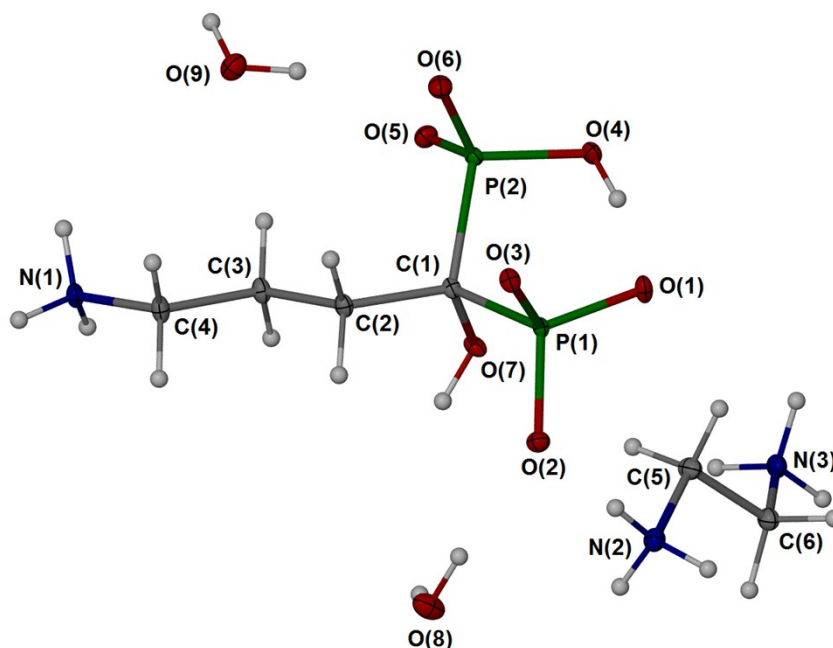


Figure S2.1 Diagram of $[\text{enH}_2][\text{LH}_3] \cdot 2(\text{H}_2\text{O})$ **1** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.

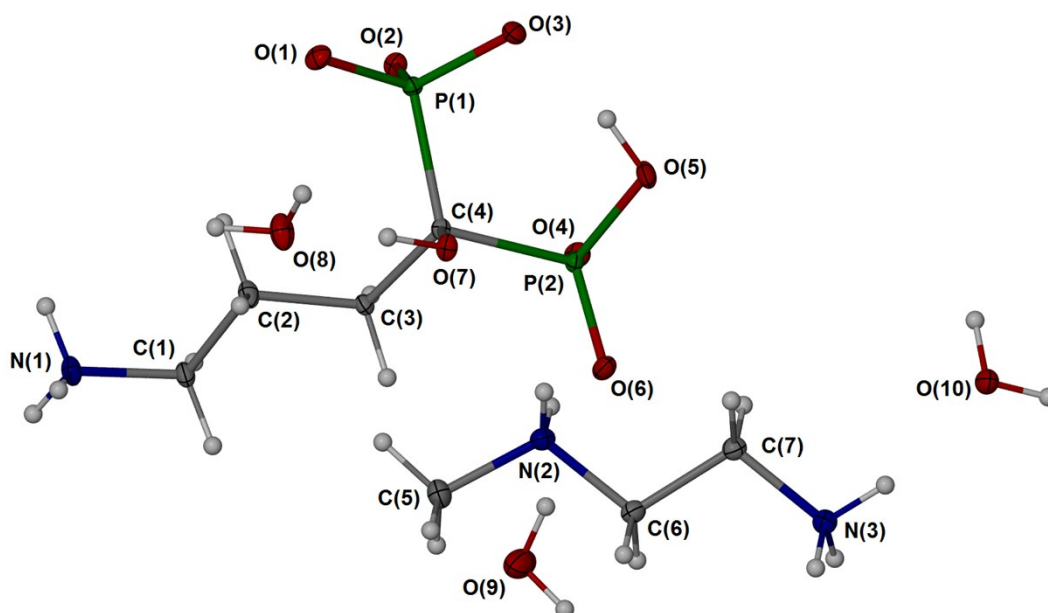


Figure S2.2 Diagram of $[\text{MeenH}_2][\text{LH}_3] \cdot 3(\text{H}_2\text{O})$ **2** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.

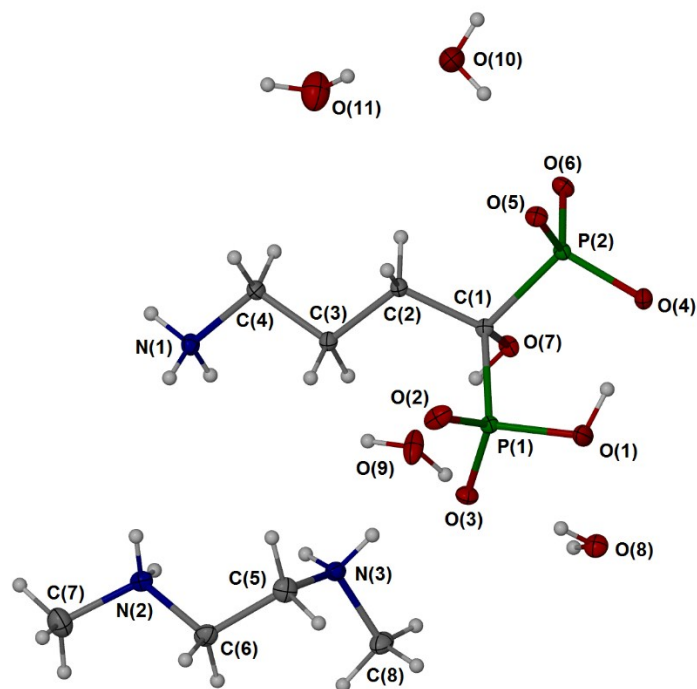


Figure S2.3 Diagram of $[\text{Me}_2\text{enH}_2][\text{LH}_3]\cdot 3.5(\text{H}_2\text{O})$ **3** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.

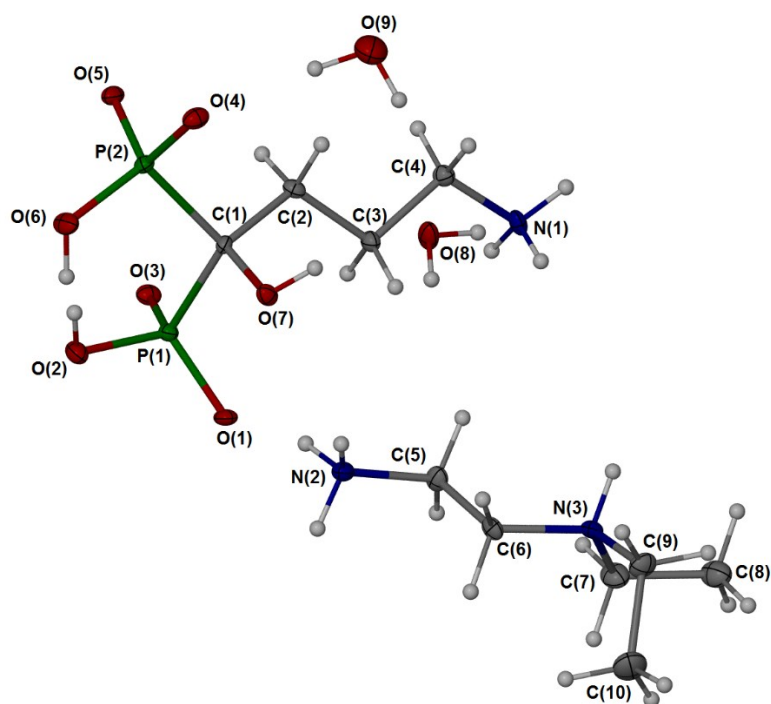


Figure S2.4 Diagram of $[\text{Et}_2\text{enH}_2][\text{LH}_3]\cdot 2(\text{H}_2\text{O})$ **4** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size. The hydrogen atoms attached to O(2) and O(6) represent two components of a single disordered hydrogen position.

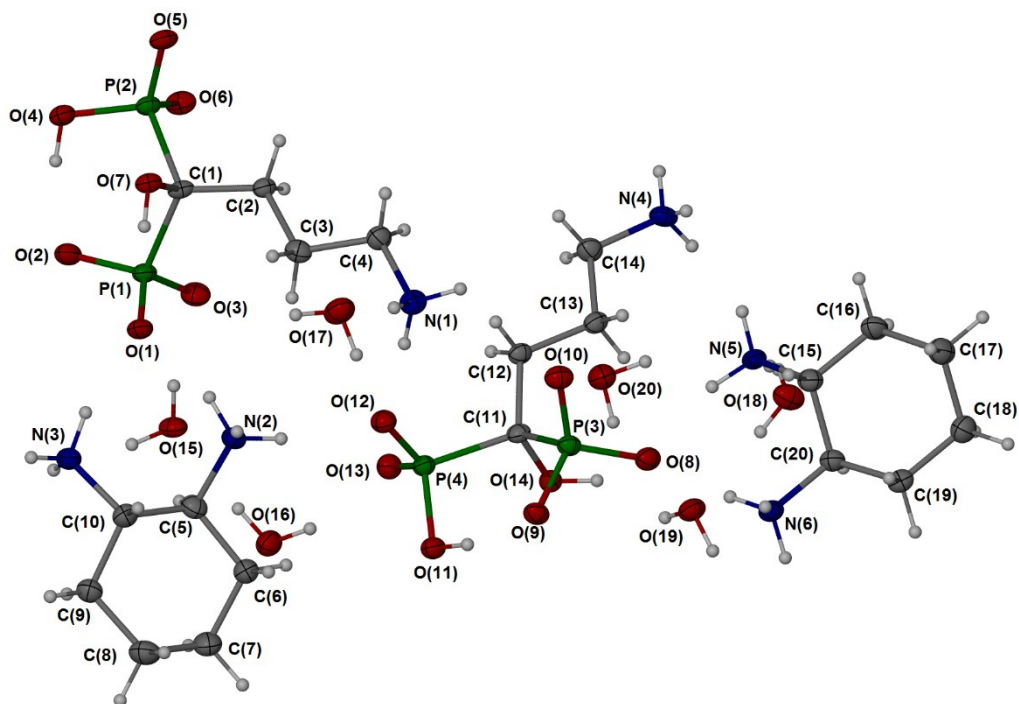


Figure S2.5 Diagram of $[cdaH_2][LH_3] \cdot 3(H_2O)$ **5** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.

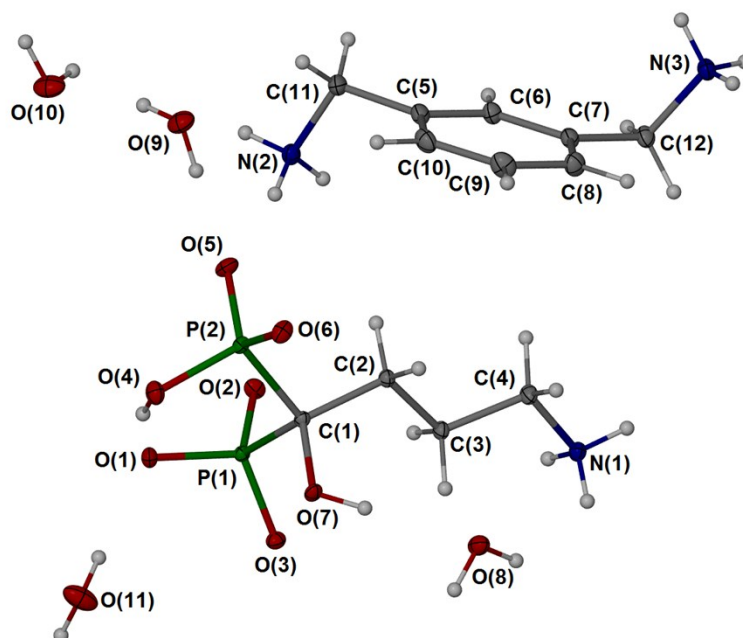


Figure S2.6 Diagram of $[xdaH_2][LH_3] \cdot 4(H_2O)$ **6** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.

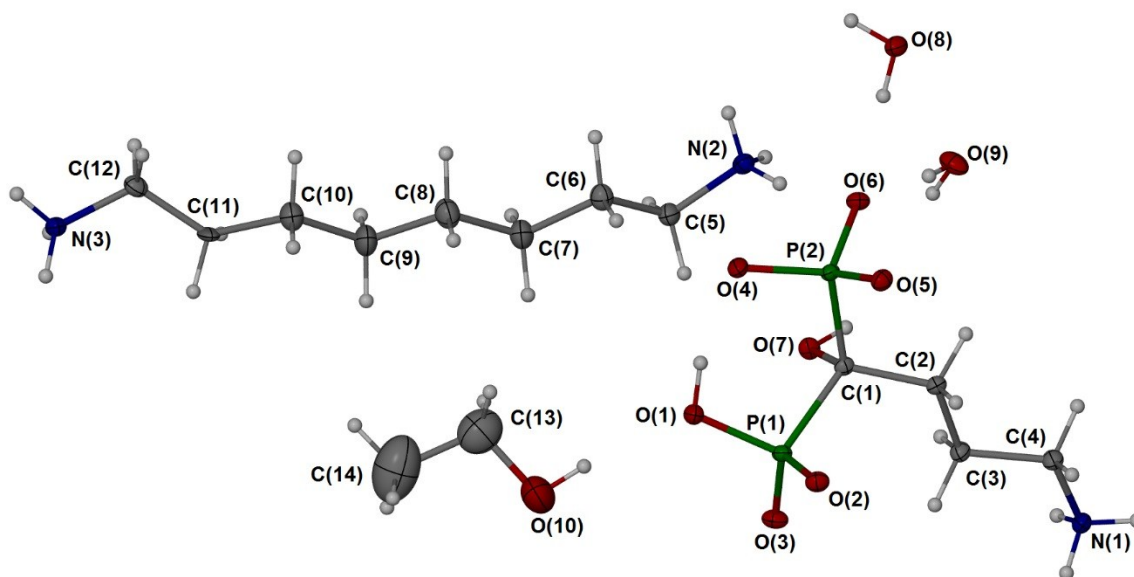


Figure S2.7 Diagram of $[\text{odaH}_2][\text{LH}_3] \cdot 2(\text{H}_2\text{O}) \cdot 0.5\text{EtOH}$ **7** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size. The carbon atoms of the octyl chain C(5)-C(11) were modelled as disordered over two positions, only one component is shown.

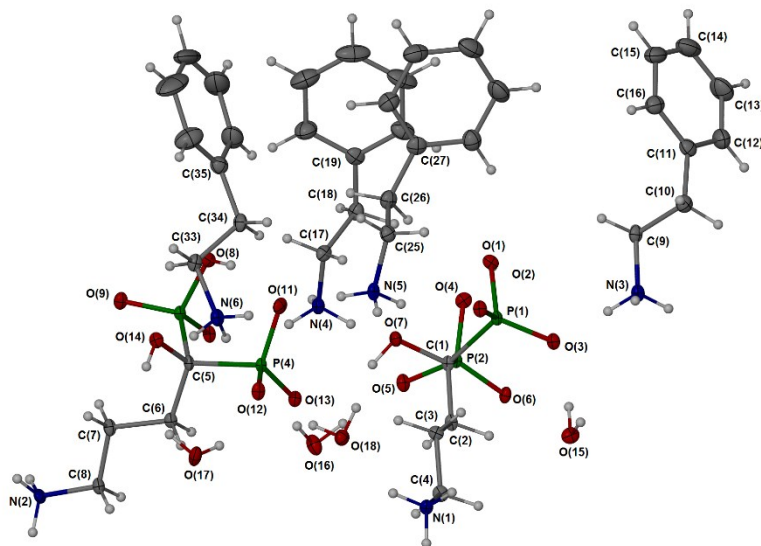


Figure S2.8 Diagram of $[\text{PheaH}]_2[\text{LH}_3] \cdot 2(\text{H}_2\text{O})$ **8** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size. Unlabelled Ph rings are numbered sequentially and anti-clockwise from the *ipso* carbon atom.

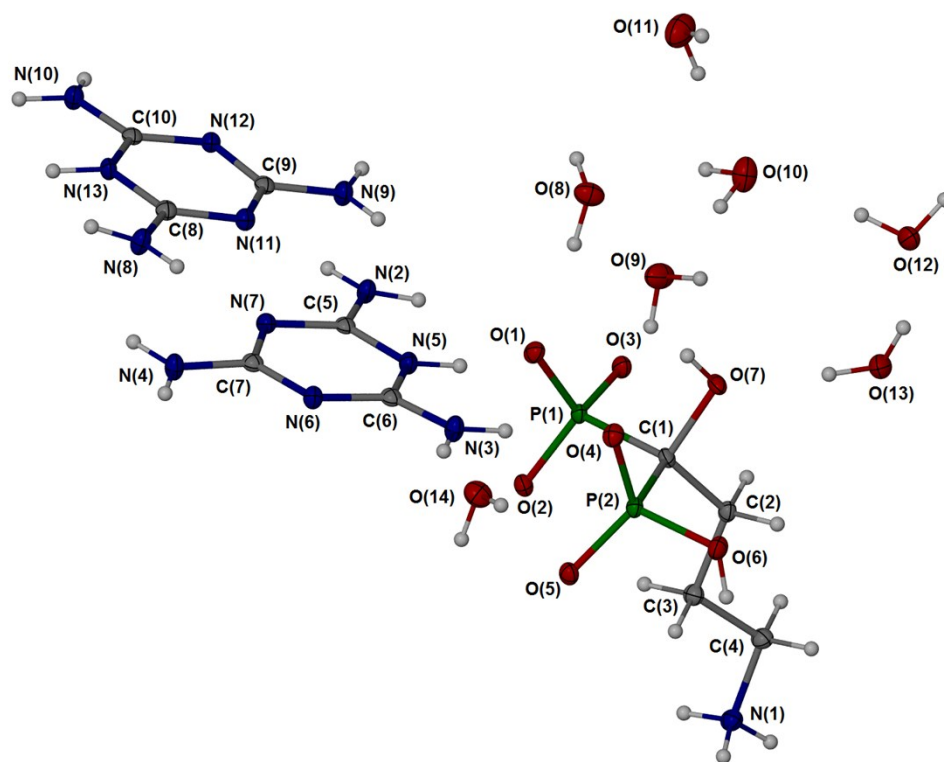


Figure S2.9 Diagram of $[\text{melH}]_2[\text{LH}_3] \cdot 7(\text{H}_2\text{O})$ **9** showing the asymmetric unit and atom labelling scheme. Non-hydrogen atoms are represented by 50% displacement ellipsoids and hydrogen atoms are as spheres of arbitrary size.