

**Open-framework beryllium phosphates with a zeolitic CrB₄
topology and their structural analogue containing 12-ring
channels**

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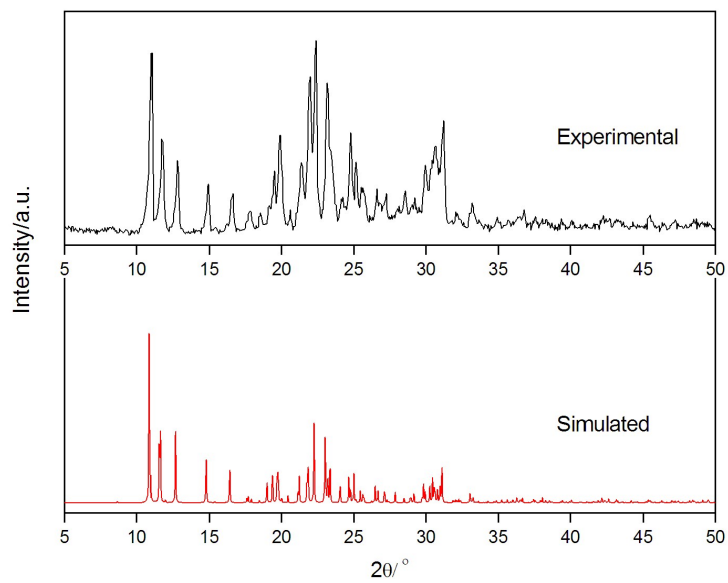


Fig. S1. Simulated and experimental powder XRD patterns of compound 1.

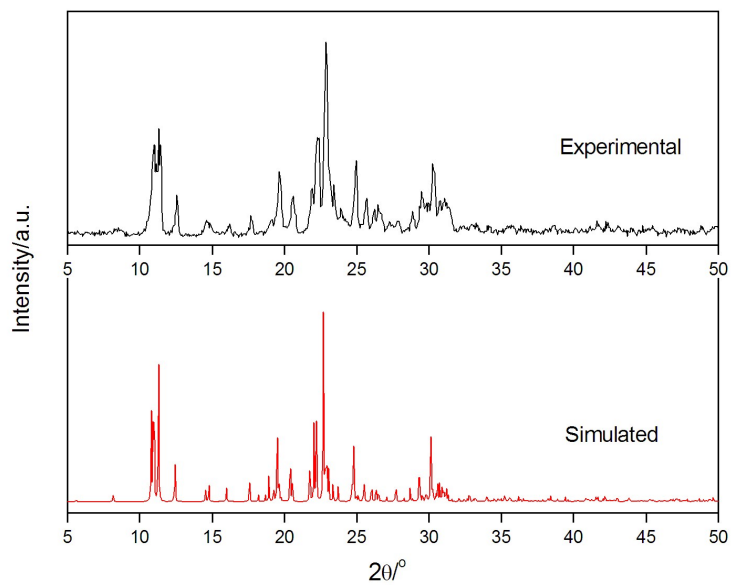


Fig. S2. Simulated and experimental powder XRD patterns of compound 2.

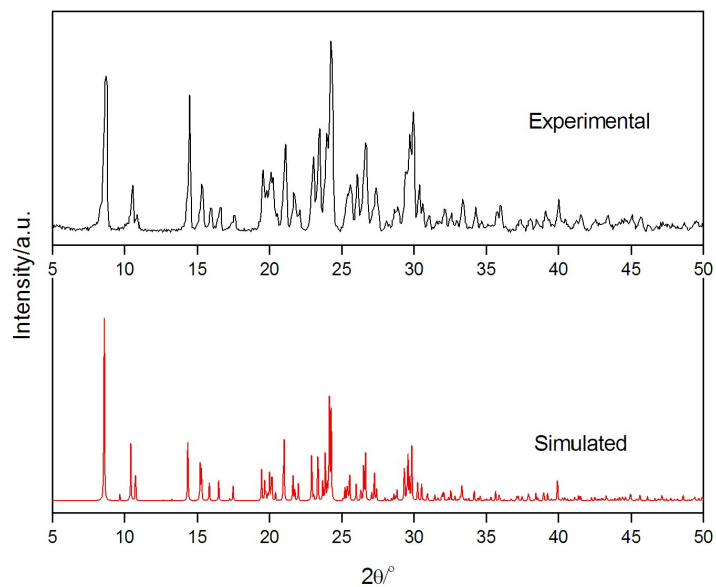


Fig. S3. Simulated and experimental powder XRD patterns of compound 3.

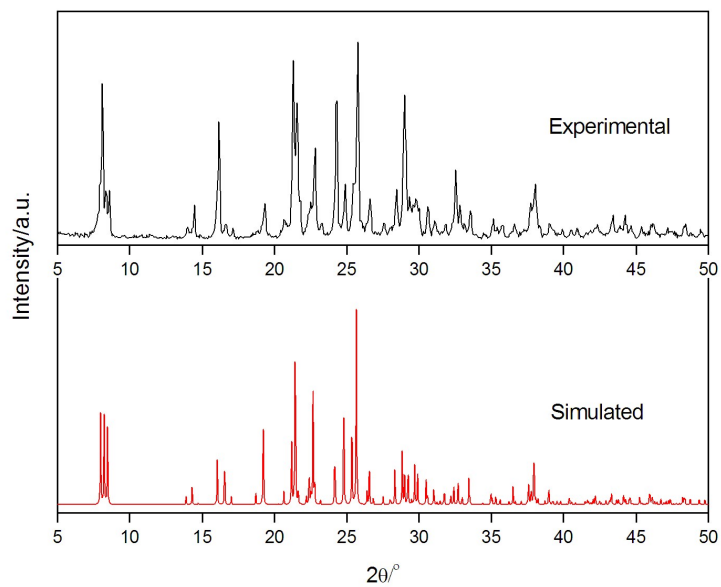


Fig. S4. Simulated and experimental powder XRD patterns of compound 4.

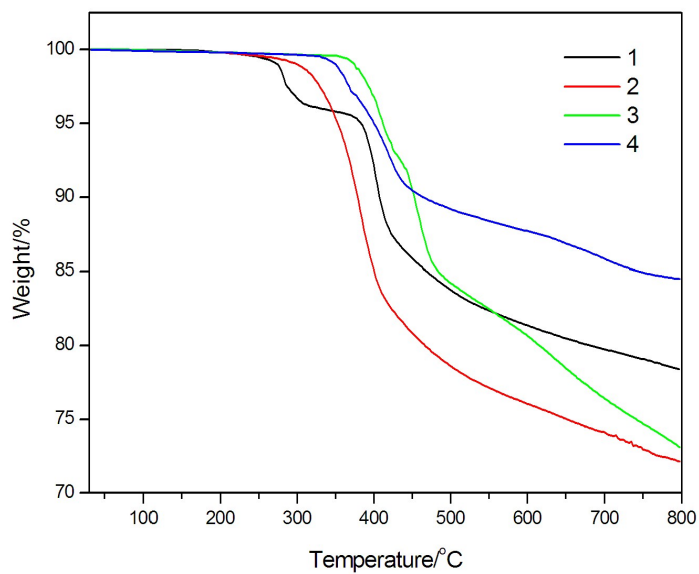


Fig. S5. TGA curve of compounds **1-4**.

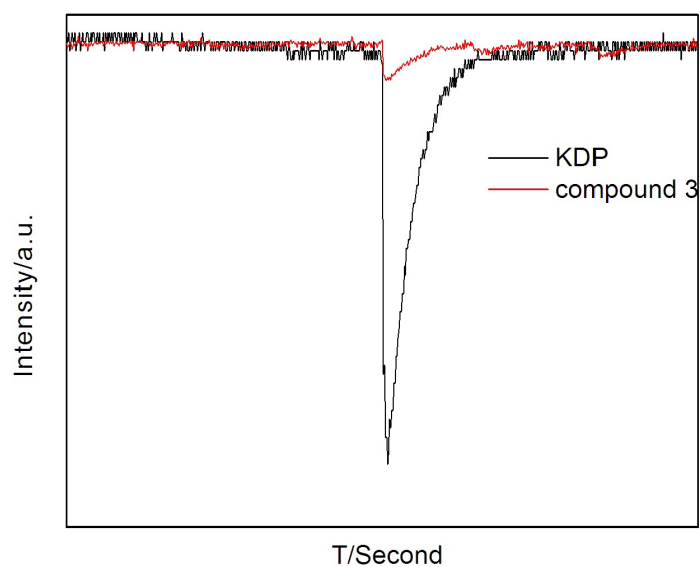


Figure S6. Comparison of the measured SHG response of **3** with that of KDP.

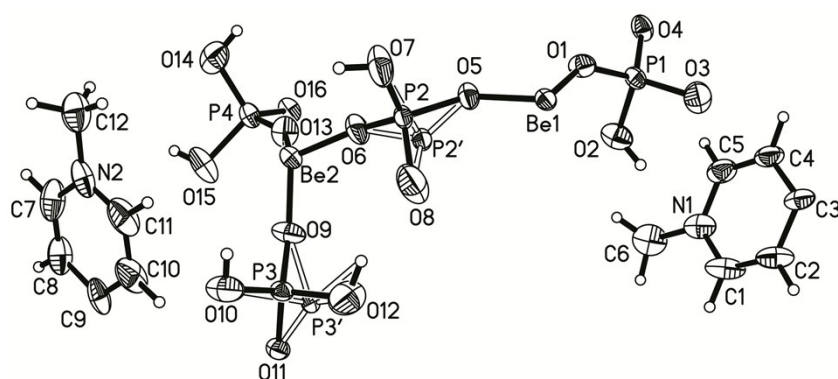


Figure S7. ORTEP plot of the asymmetric unit of compound **1**, showing the labeling scheme and the 30% probability displacement ellipsoid.

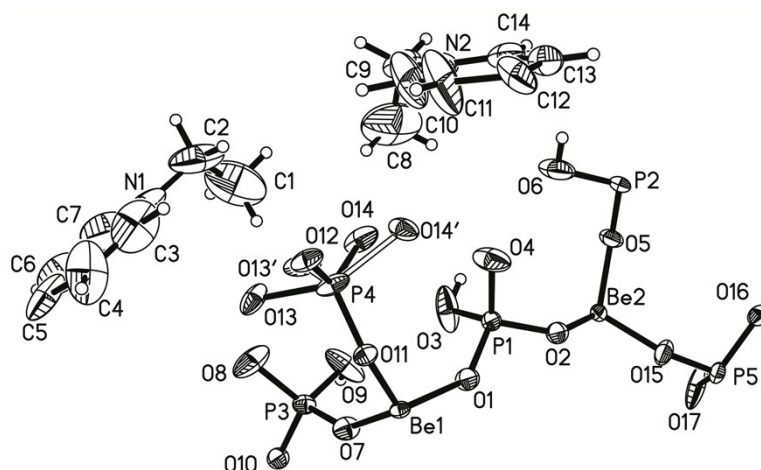


Figure S8. ORTEP plot of the asymmetric unit of compound **2**, showing the labeling scheme and the 30% probability displacement ellipsoid.

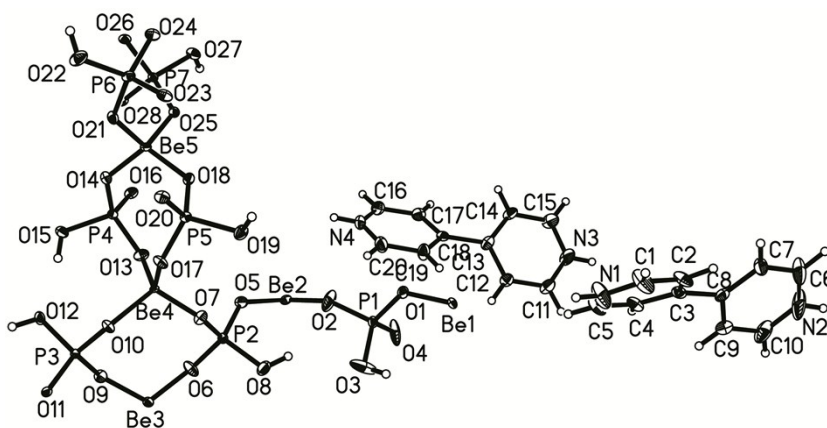


Figure S9. ORTEP plot of the asymmetric unit of compound **3**, showing the labeling scheme and the 30% probability displacement ellipsoid.

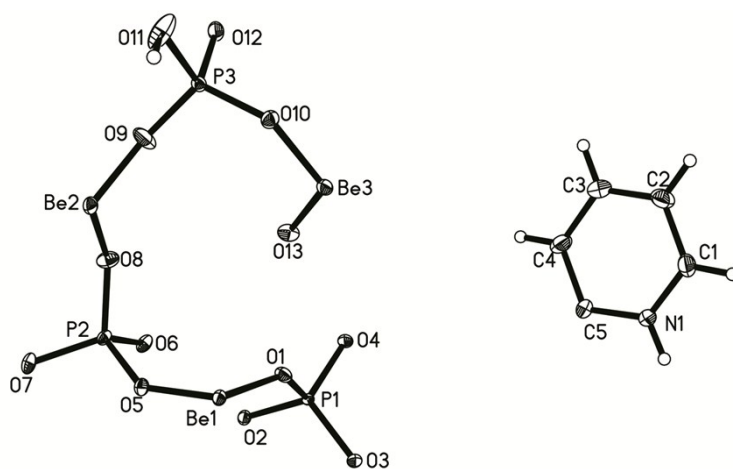


Figure S10. ORTEP plot of the asymmetric unit of compound **4**, showing the labeling scheme and the 30% probability displacement ellipsoid.

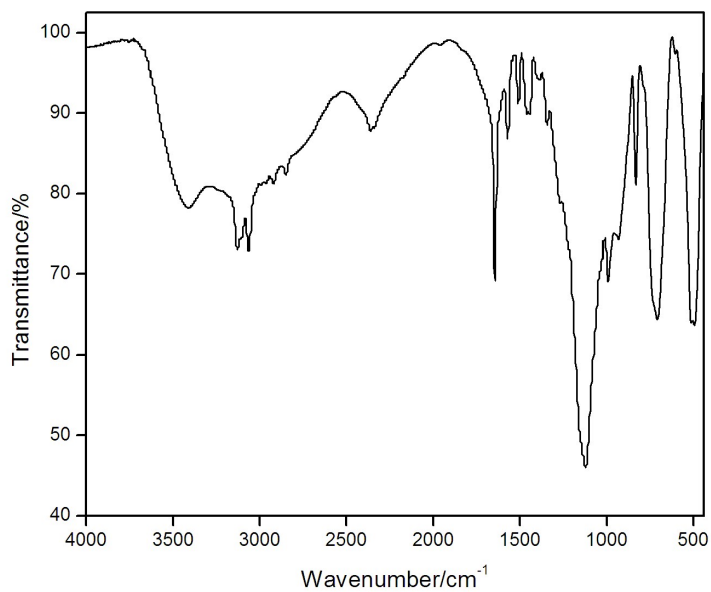


Fig. S11. IR spectrum of compound **1**.

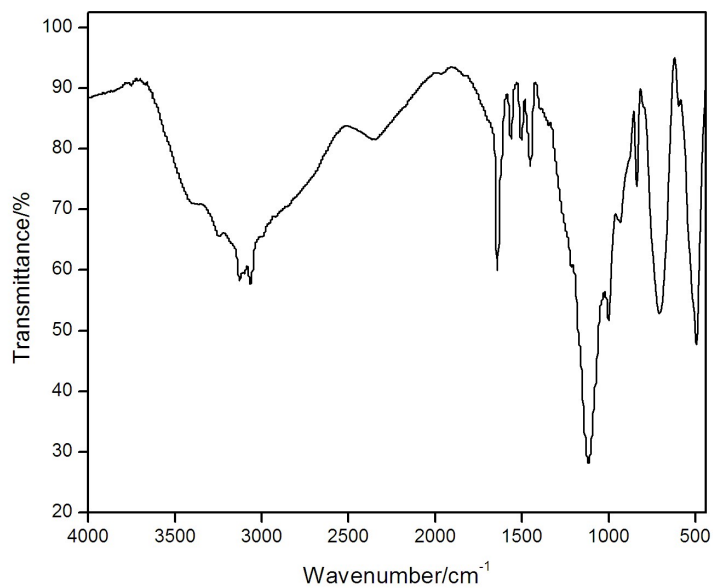


Fig. S12. IR spectrum of compound 2.

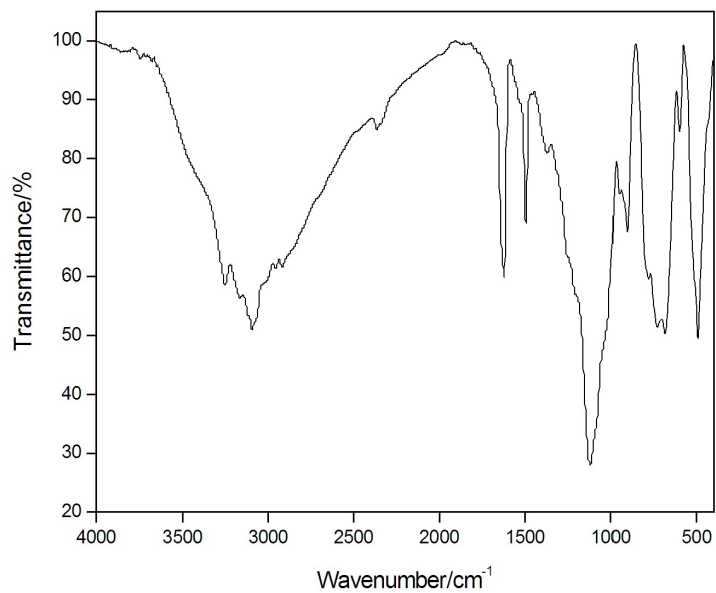


Fig. S13. IR spectrum of compound 3.

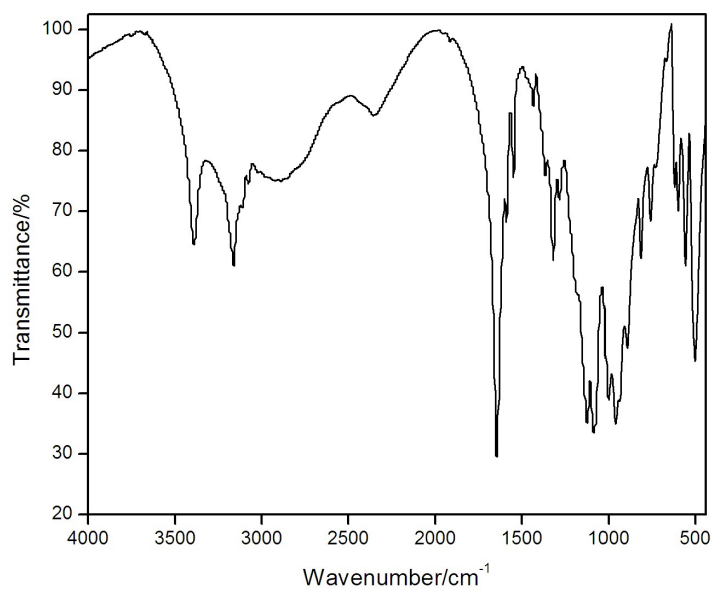


Fig. S14. IR spectrum of compound **4**.

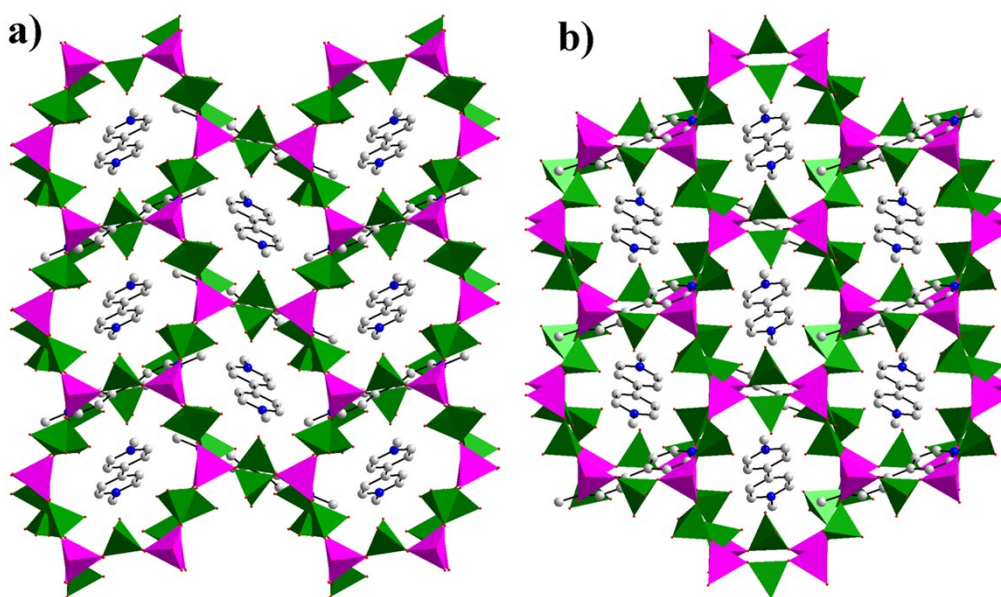


Fig. S15. A view of the structure of **1** along (a) the [100] and (b) [001] directions, showing the 12 MR channels accommodating MV cations.

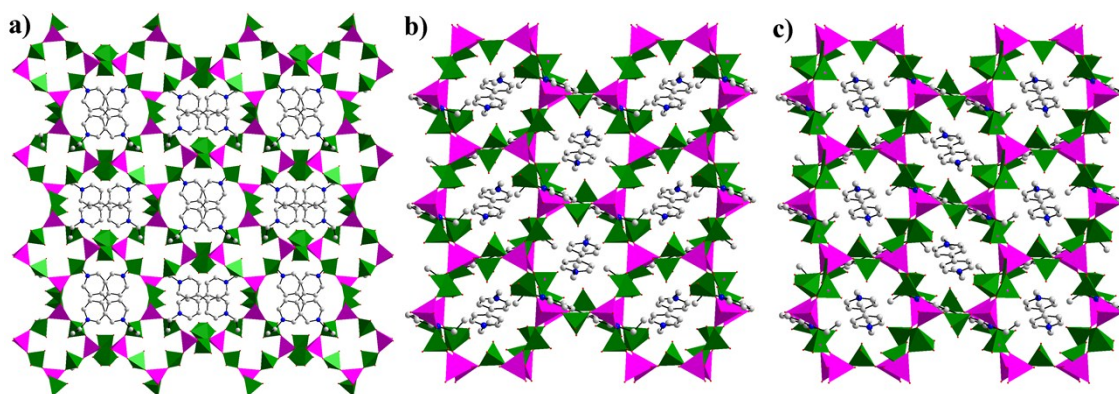


Fig. S16. A view of the structure of **2** along (a) the [100], (b) [110], and (c) [1-10] directions, showing the intersecting 16 MR, 12 MR, and 12 MR channels accommodating EV cations.