Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

for

High-Pressure and High-Temperature Transformation of Pb(II)-Natrolite to Pb(II)-Lawsonite

Junhyuck Im[a], Yongmoon Lee[a], Douglas A. Blom[b], Thomas Vogt[b], and Yongjae Lee[a,*]

[a] Department of Earth System Sciences, Yonsei University, Seoul 120749, Korea

[b] NanoCenter, Department of Chemistry & Biochemistry, University of South Carolina, Columbia, SC 29208, USA

*Corresponding author (Email: yongjaelee@yonsei.ac.kr)

Supporting Figures

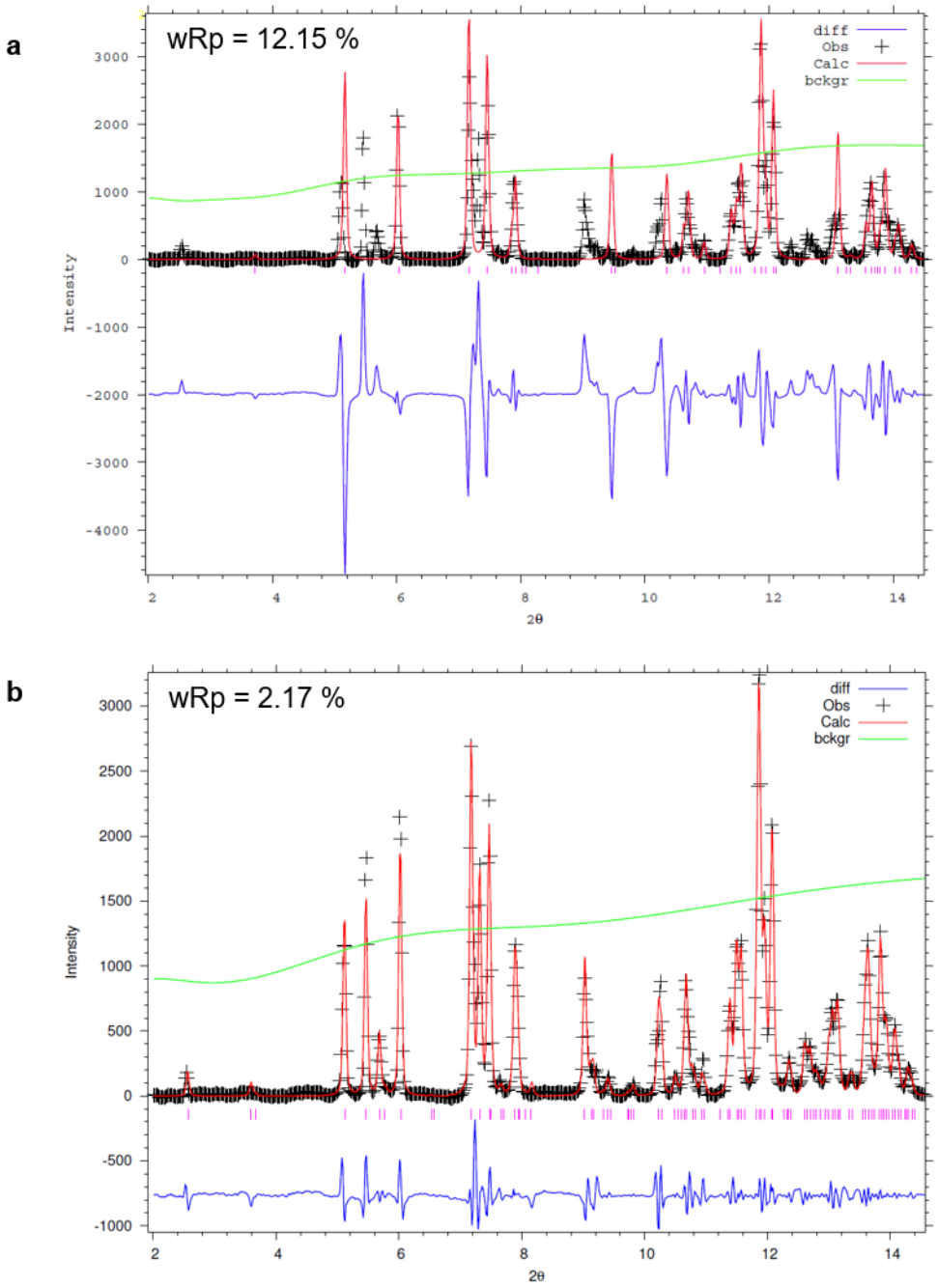


Fig. S1. Lebail fits for Pb-NAT-II' in a water pressure medium at 1.5 GPa. a) Several Bragg reflections are not indexed using a mococlinic **C***c* space group, b) fitting with triclinic **C***1* space group where positions of most Bragg reflections are well matched and difference between data and model significantly improves.

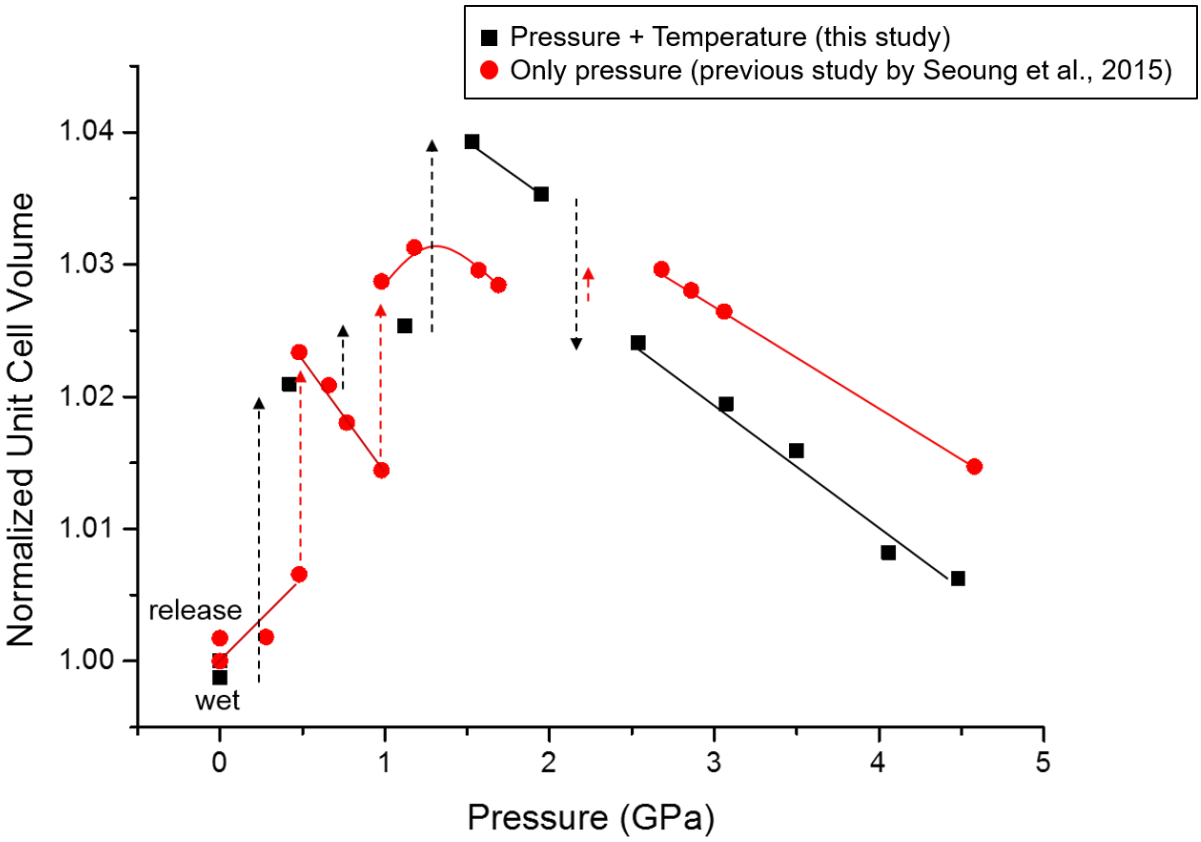
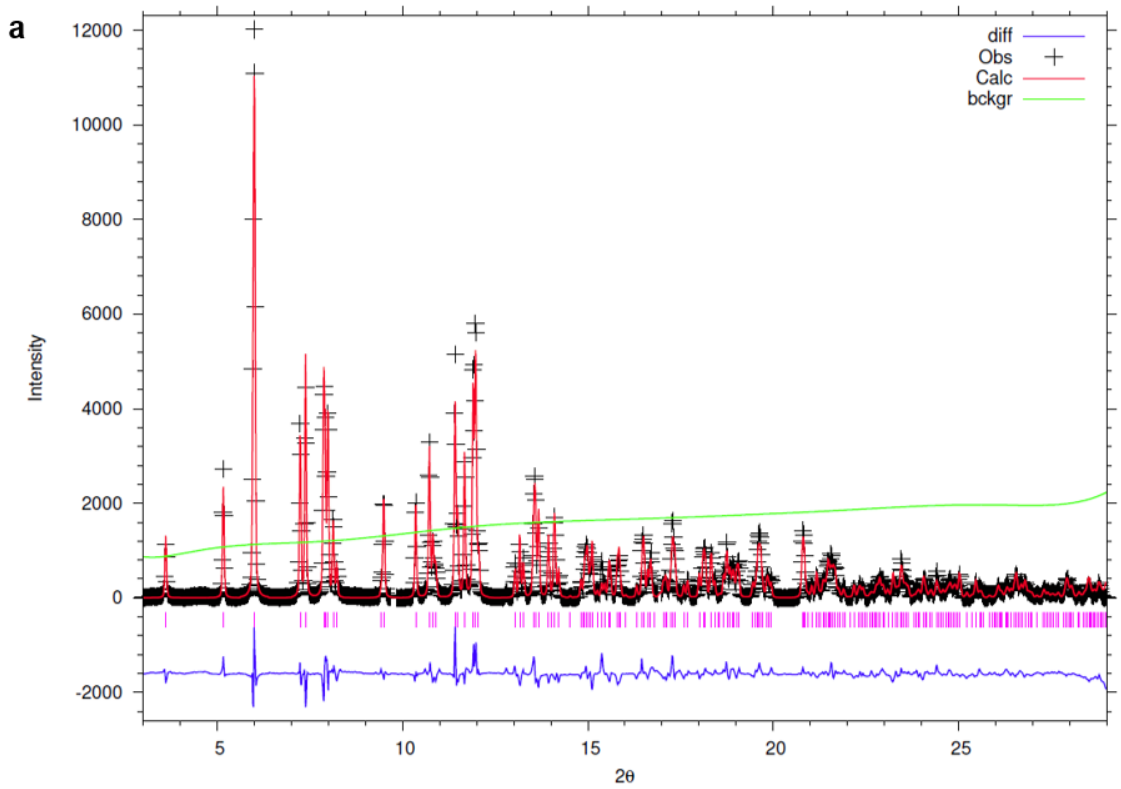
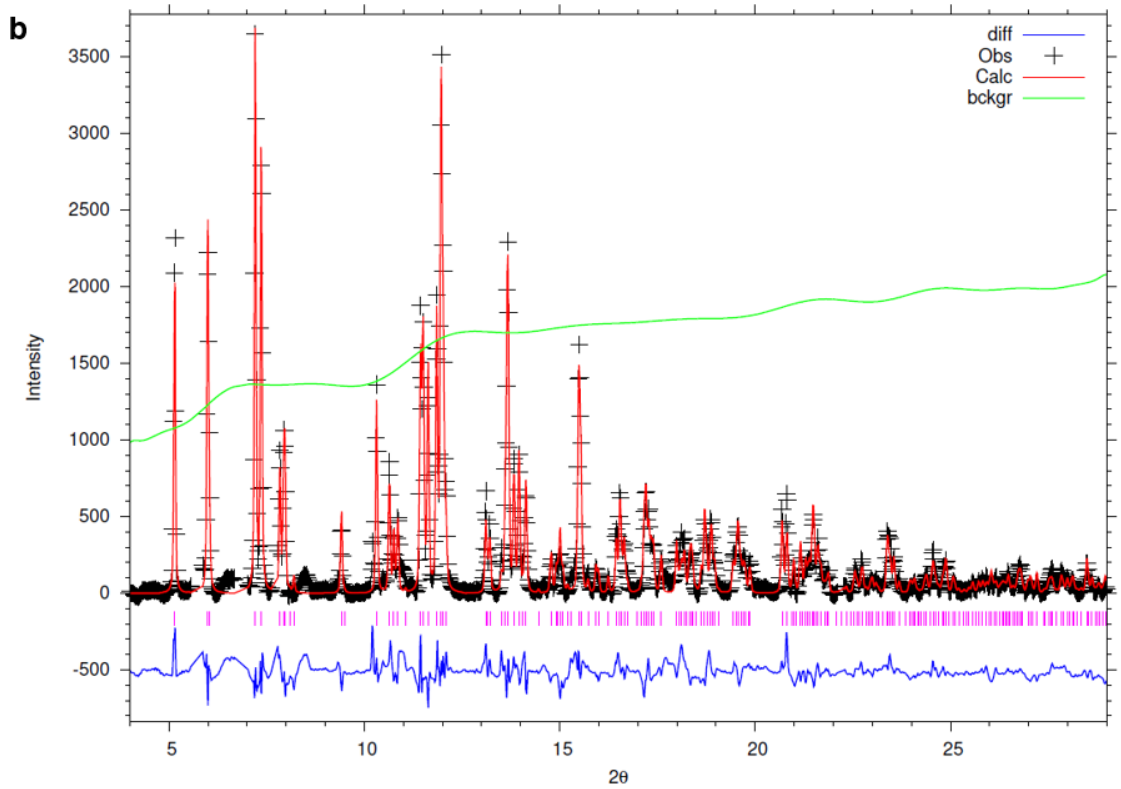


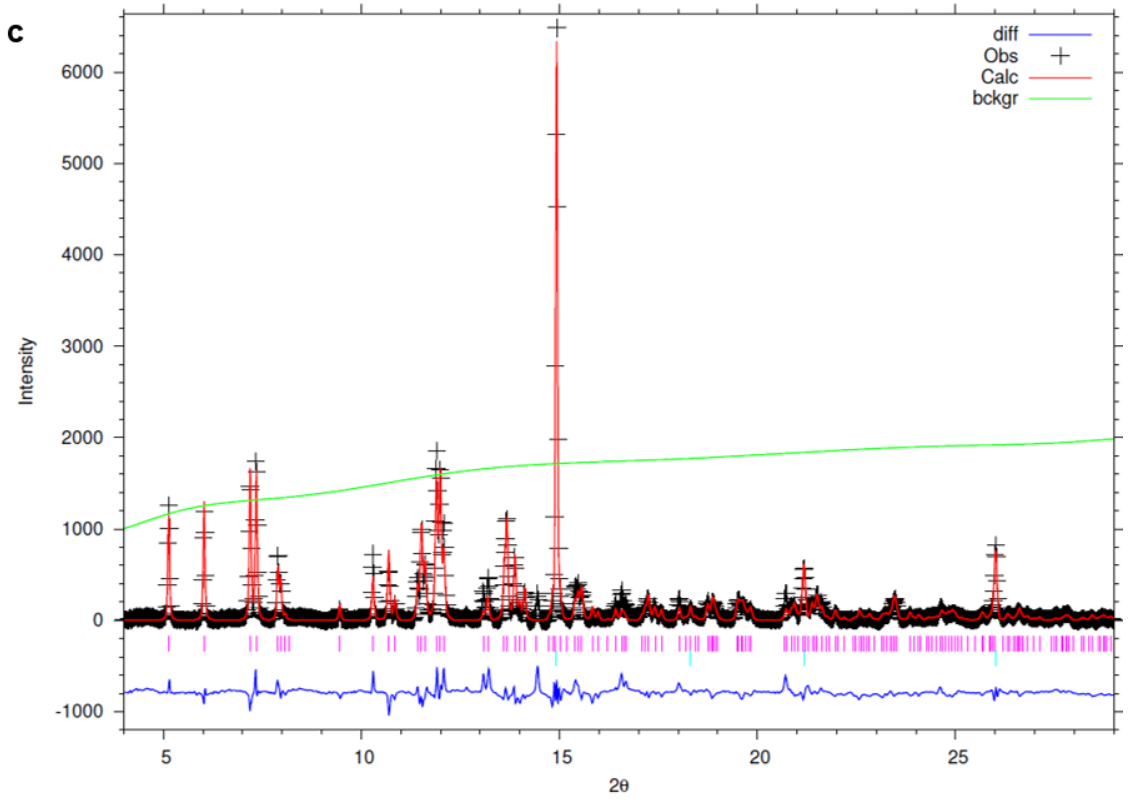
Fig. S2. Changes of the normalized unit-cell volumes as a function of pressure for Pb-NAT in water pressure medium in our earlier high-pressure and recent high-pressure / high-temperature experiments. Black line and symbol: pressure and temperature experiments, red line and symbols: pressure only experiments.



Pb-NAT-I at 0.42 GPa ($_wR_p$(%)=3.65, χ^2=2.951)



Pb-NAT-II at 1.12 GPa ($_wR_p$(%)=2.69, χ^2=3.716)



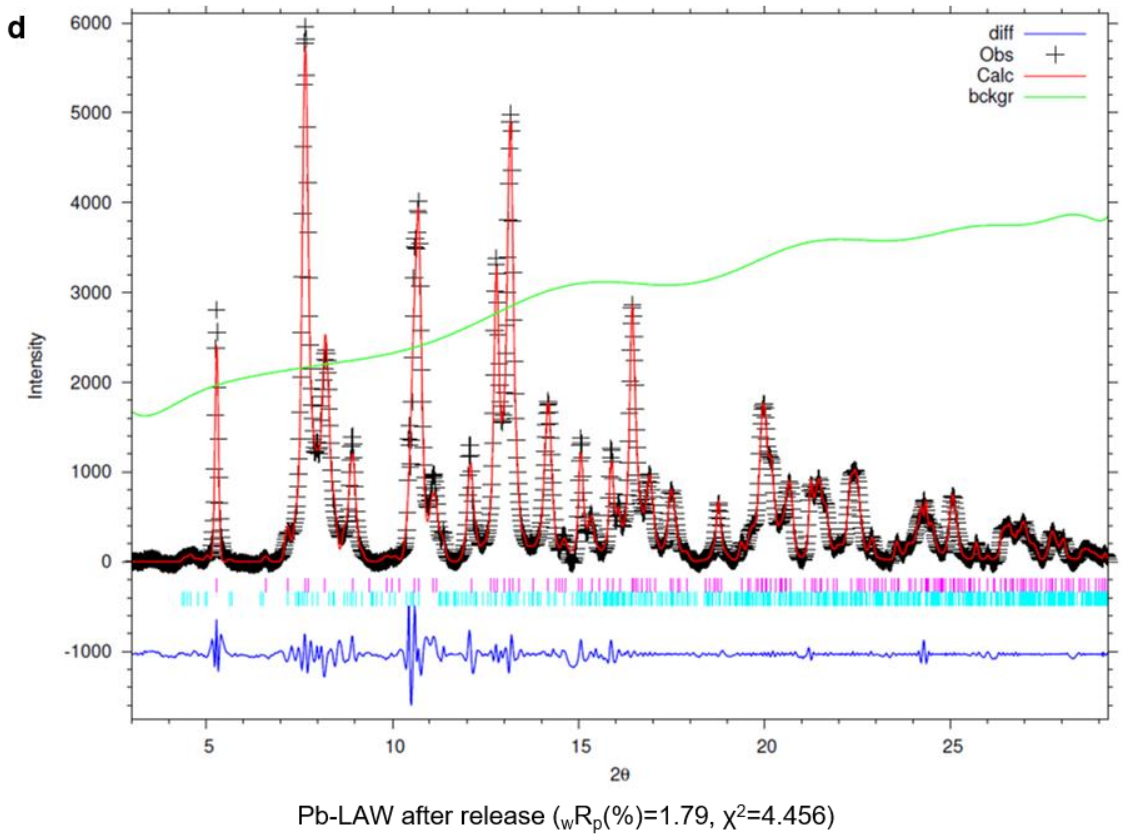


Fig. S3. Final Rietveld refinement fits for Pb-NAT in water pressure medium. a) Pb-NAT-I at 0.4 GPa, b) Pb-NAT-II at 1.1 GPa, c) Pb-NAT-III at 2.5 GPa and d) recovered Pb-LAW.