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Ruby2020-Based Equations of State for NaCl (B1) and Au: Towards Consistent Pressure Scales Between Multi-Anvil and Diamond-Anvil Cell

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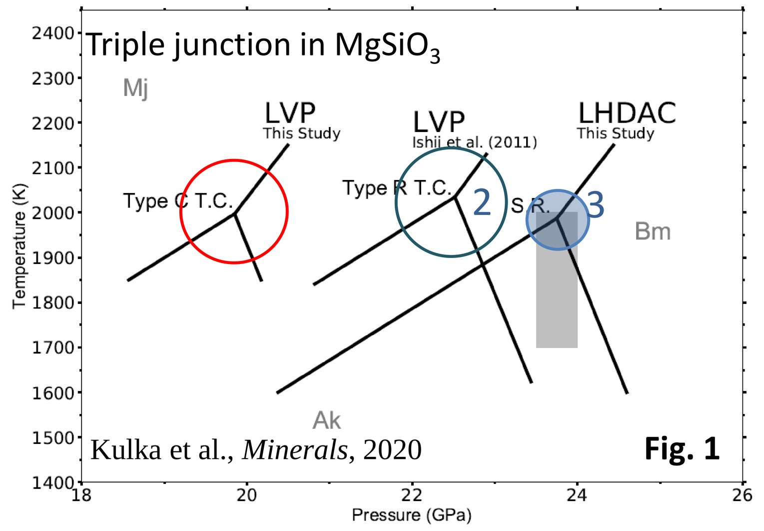
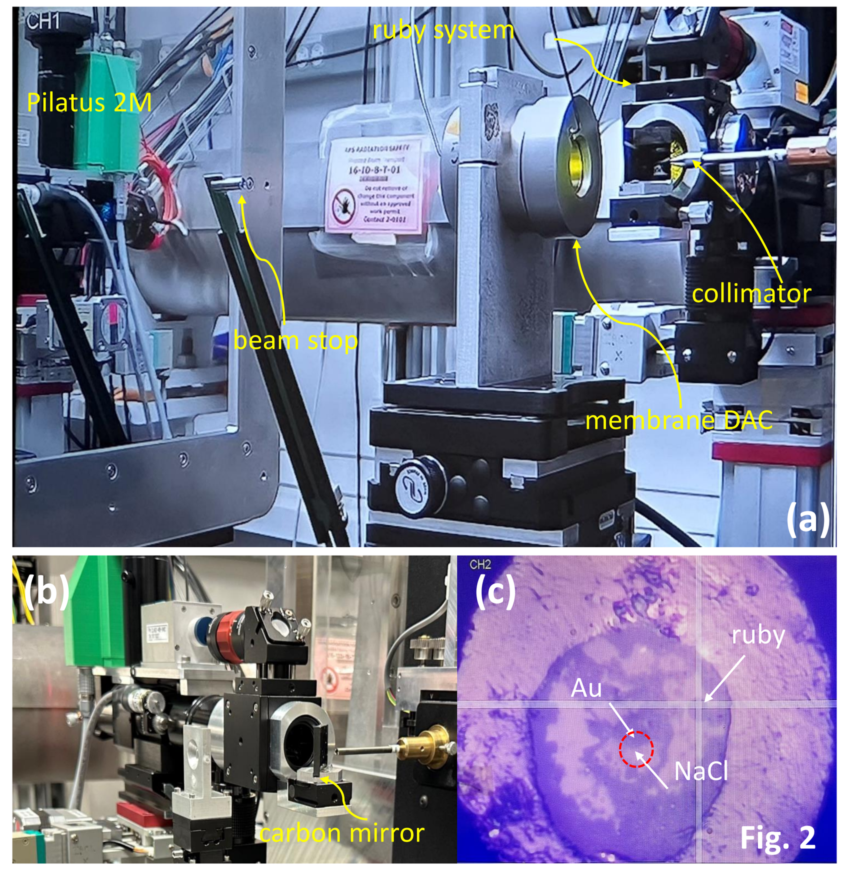
Motivation

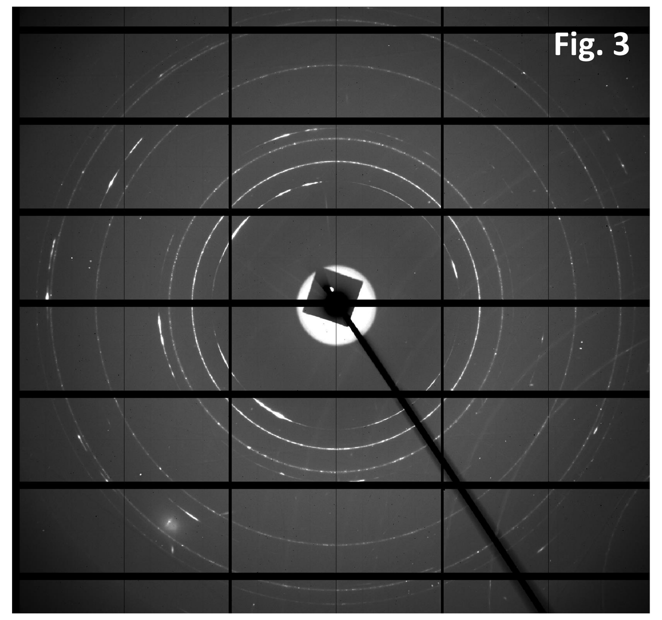


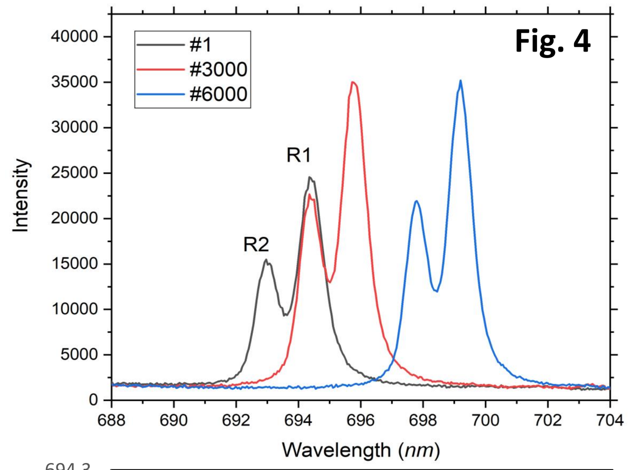
- Fig. 1 (Kulka et al., 2020) compares triple junction positions in $MgSiO_3$ determined in two MAPs (circles 1 and 2) and on in-situ laser heated DAC (circle 3).
- Red circle 1 is based on a pressure calibration in a different MAP and is 4 GPa from lower than the LHDAC data.
- Blue circle 2 is based on a calibration conducted in the MAP used by its authors (Ishii et al., 2011) but only at 1873 K. The result is about 1.5 GPa lower than that of LHDAC.
- Difference between 2 and 3 is due to a combination of different pressure scales, thermal effects in the MAP, and different temperature measurement techniques.

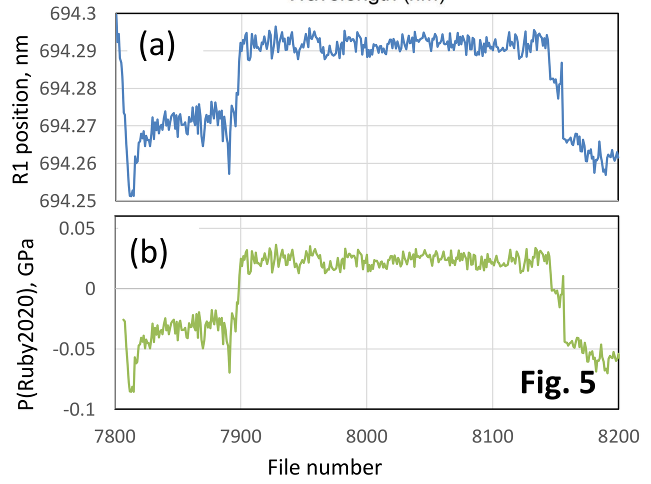
Here we examine consistency of equations of state (EOSs) for NaCl and Au at room T, as a first step towards inter-consistency in pressure measurements between MAP and DAC.

Experimental Method





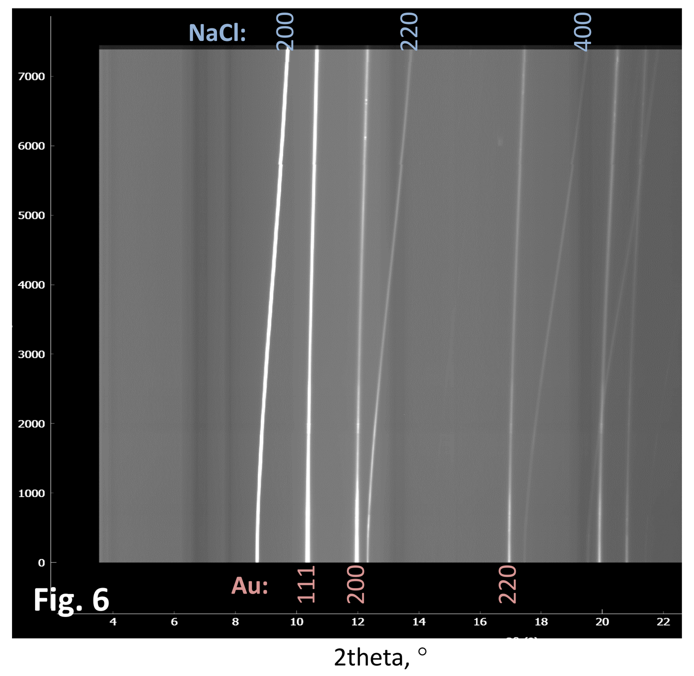




- Fine powders of NaCl and Au were loaded in a DAC with He as pressure medium. A focused X-ray (~5 μm) illuminated both samples. Each XRD pattern contained both NaCl and Au diffraction lines (Figs. 2, 3).
- Pressure was increased automatically using two membranes for compression and decompression (Fig. 2).
- Ruby fluorescence was collected simultaneously with XRD. Ruby2020 scale was used to determine pressure. (Figs. 4).
- XRD and ruby data were collected every 1 s during compression and decompression, yielding a total of 8200 points in one experiment.
- At end of the run, 391 ruby points were measured in the open DAC to define zero-pressure R1 position (Fig. 5).
- 2D XRD patterns were integrated into 1D to determine diffraction line positions.

Results and Discussion

Data



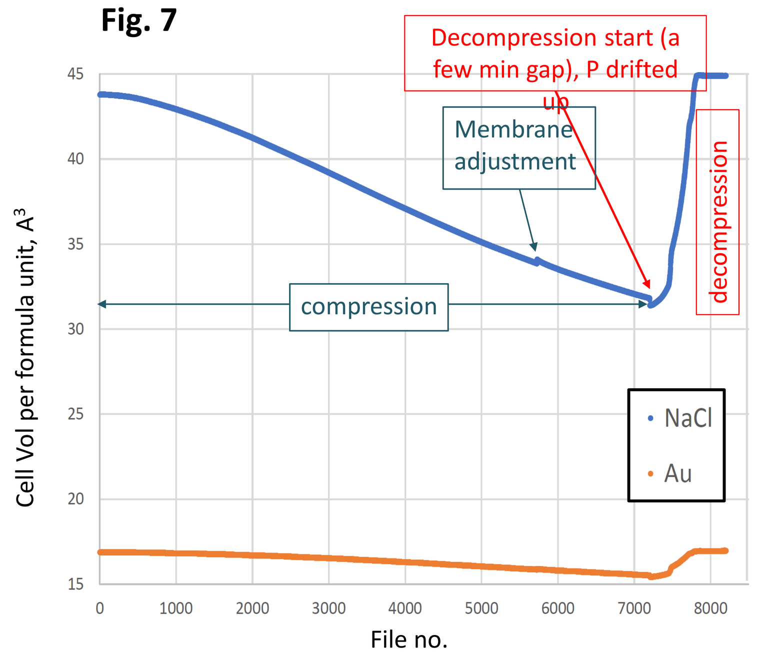
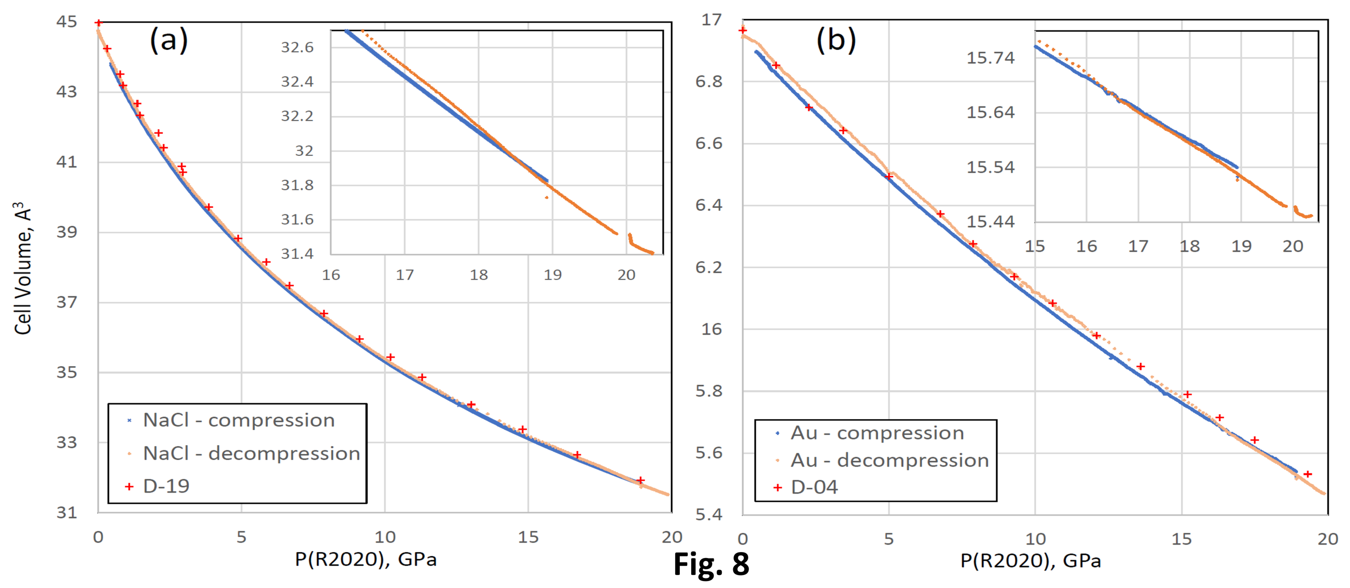


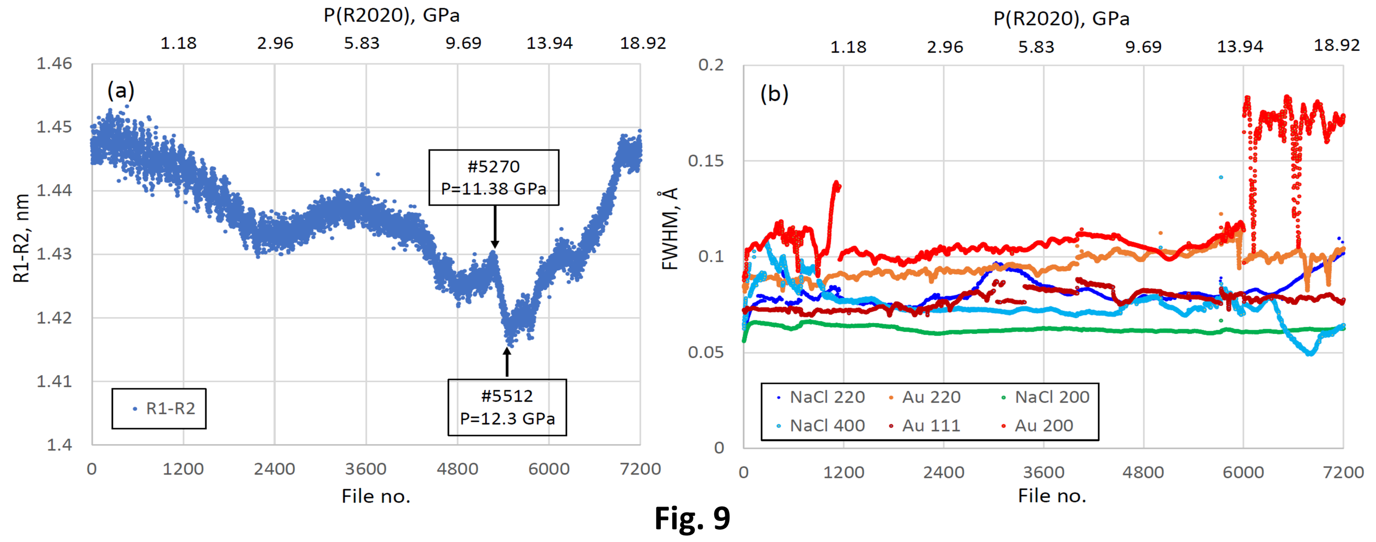
Fig. 6 plots integrated compression 1D XRD data (7200 points). Diffraction lines used to determine unit-cell volumes are labeled. Fig. 7 shows variations of unit-cell volumes during compression and decompression.

P-V relations: compression and decompression



Compression and decompression for NaCl (Fig. 8a) and Au (Fig. 8b). Note inconsistency between compression and decompression data. Results from previous studies are shown for comparison.

Evidence of He solidification around 14 GPa



Ruby R1-R2 distance shows a sharp turnover around 12 GPa, indicating solidification of the helium pressure medium (Fig. 9a). Peak width of Au 220 line shows a sharp jump near 14 GPa (Fig. 9b). Because of this, we only used data below 14 GPa to fit EOS parameters.

EOS fits to hydrostatic data

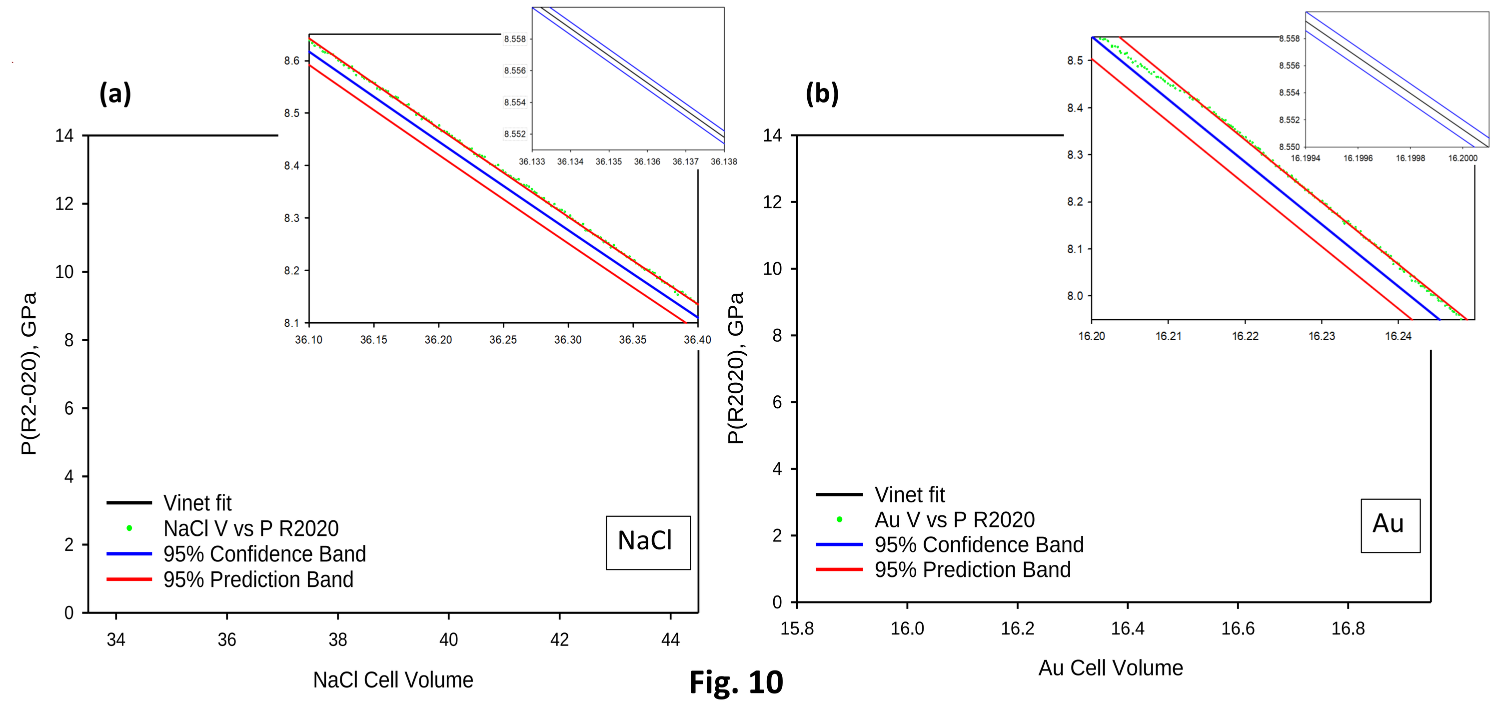


Fig. 10 shows the Rydberg-Vinet (RV) fits to the data below 14 GPa for NaCl (a) and Au (b). Insets display deviations of data (green dots) from the fits (black curves), as well as 95% confidence levels (blue and red curves). Fitting results are summarized in Tables 1 and 2 below.

Table 1. NaCl equation of state: Rydberg-Vinet fits with comparison to the results of D-19. Numbers in bold fonts represent fixed values in the fit.

Data	Ruby scale	V_0 Å^3	K_{T0} GPa	K_0’
This study	Ruby2020	44.6021(8)	23.614(7)	5.303(2)
This study	Ruby2020	44.5936(3)	**23.7**	5.283(1)
D-19	R-DO-07	44.89(6)	23.26(39)	5.3(6)
D-19	Ruby2020	44.89(6)	23.06(39)	5.36(6)
D-19	R-DO-07	44.83(2)	**23.7**	5.278(18)
D-19	Ruby2020	44.80(2)	**23.7**	5.260(19)

Table 2. Au equation of state: Rydberg-Vinet fits with comparison to the results of D-04 and TD-08. Numbers in bold fonts represent fixed values in the fit.

Data	Ruby scale	V_0 Å^3	K_{T0} GPa	K_0’
This study	Ruby2020	16.9407(1)	167.71(6)	5.938(10)
This study	Ruby2020	16.9415(1)	**167**	6.055(3)
D-04	R-D-04	16.962	**167**	6.00(2)
TD-08	R-DO-07	16.962	**167**	5.9(1)

EOS results quoted: NaCl: D-19 - Dewaele, Minerals, 2019; Au: D-04 – Dewaele et al, PRB, 2004; TD-08: Takemura & Dewaele, PRB, 2008.
Ruby scales quoted: Ruby2020, Shen et al, HPR, 2020; R-DO-07: Dorogokupets & Oganov, PRB, 2007.

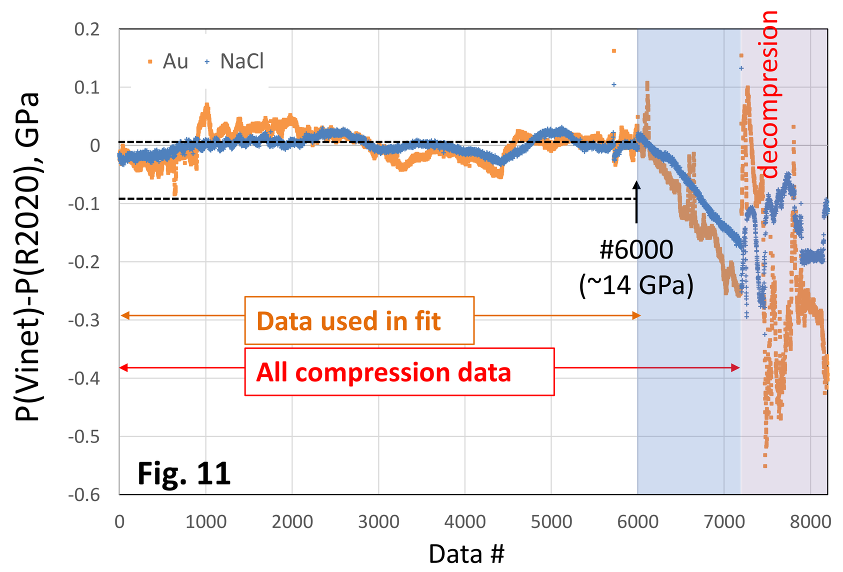


Fig. 11 shows that for compression data up to 14 GPa, pressure difference between Ruby2020 and our RV EOS is within ±0.05 GPa. Compression data above 14 GPa systematically deviate from the Ruby2020 data. This confirms that data above 14 GPa are affected by non-hydrostaticity. The decompression data, on the other hand, exhibit large oscillation.

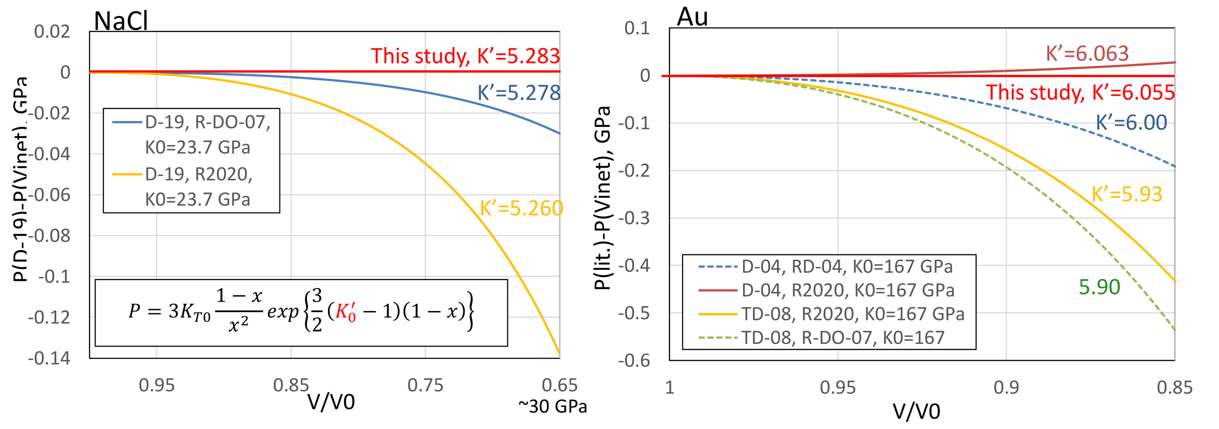
Third-order Birch-Murnaghan EOS (BM3) gives comparable fits, as shown in Table 3 below.

Table 3. BM3 fits to the NaCl and Au data of the present study. Numbers in bold fonts represent fixed values in the fit.

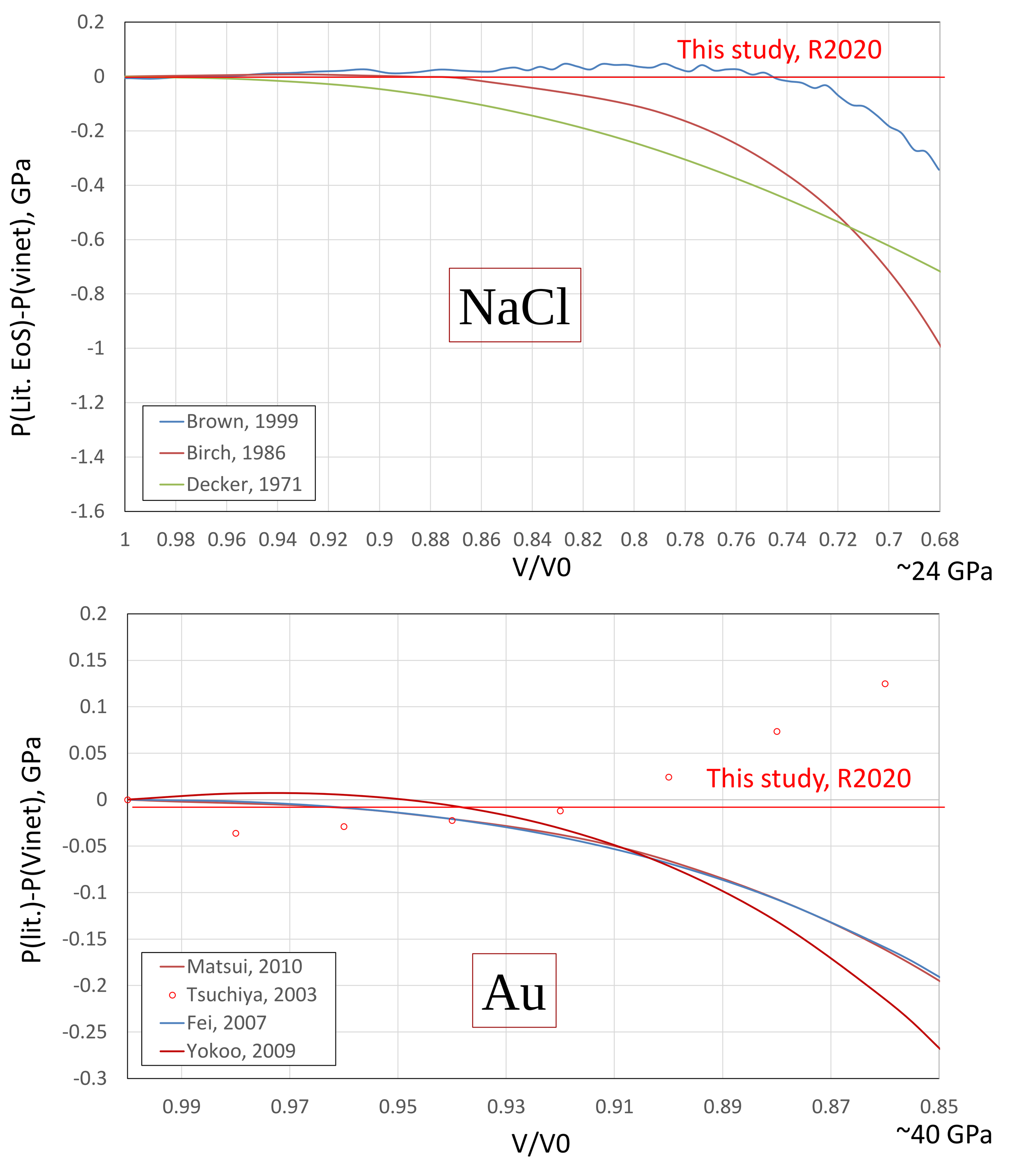
Sample	V_0, Å^3/fu	K_{T0} GPa	K_0’
NaCl	44.572(1)	24.211(9)	4.932(2)
NaCl	44.6226(5)	**23.7**	5.049(1)
Au	16.9406(1)	167.83(6)	5.88(1)
Au	16.9415(1)	**167**	6.022(3)

Comparison with previous work

Comparison with literature EOS studies



Comparison with commonly used pressure scales



References

Birch F.: *Journal of Geophysical Research*, 1986; 91(B5):4949-4954.
Brown J.: *Journal of Applied Physics*, 1999; 86:5801-5808.
Decker DL.: *Journal of Applied Physics*,1971; 42(8):3239-3244.
Dewaele A.: *Minerals*, 2019; 9(11):684.
Dewaele A, Loubeyre P, Mezouar M.: *Physical Review* B, 2004;70:094112.
Fei YW, Ricolleau A, Frank M, et al.: *Proc. Nat. Acad. Sci*., 2007; 104(22):9182-9186.
Ishii T, Kojitani H, Akaogi M.: *Earth and Planetary Science Letters*, 2011; 309(3):185-197.
Kulka BL, Dolinschi JD, Leinenweber KD, et al.: *Minerals*. 2020;10(1):67.
Matsui M.. *Journal of Physics: Conference Series*. 2010; 215(1):012197.
Shen G, Wang Y, Dewaele A, et al.: *High Pressure Research*. 2020:1-16.
Takemura K, Dewaele A.: *Physical Review* B. 2008;78(10):104119.
Tsuchiya T.: *Journal of Geophysical Research*, 2003;108(B10):2462.
Yokoo M, Kawai N, Nakamura KG, et al.: *Physical Review* B. 2009; 80(10):104114.

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