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B. A. Chidester, E. C. Thompson, R. A. Fischer, D. L. Heinz, V. B. Prakapenka, Y. Meng, and A. J. Campbell

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An experimental thermal equation of state of B2-KCl

B. A. Chidester[1,*], E. C. Thompson[2], R. A. Fischer[3], D. L. Heinz[1], V. B. Prakapenka[4], Y. Meng[5] and A. J. Campbell[1]

[1]*Department of Geophysical Sciences, University of Chicago, Chicago, IL 60637*

[2]*Department of Earth and Environmental Systems, Sewanee: The University of the South, Sewanee, TN 37375*

[3]*Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA 02138*

[4]*Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60439*

[5]*HPCAT, X-ray Science Division, Argonne National Laboratory, Lemont IL 60439 and*

[*]*Present address: Los Alamos National Laboratory, bchides@lanl.gov*

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Abstract

The alkali halides are often used as optically-transparent pressure-transmitting media and thermal insulators in laser-heated diamond anvil cell experiments. High P–T equations of state for these materials would allow them to be used simultaneously as sensitive *in situ* pressure markers, making sample preparation and data analysis simpler. KCl is especially useful for this application because its high melting point, crystallographic simplicity, and low electron density are ideal for use in high-temperature X-ray diffraction experiments. However, the high-temperature static equation of state data for this material is limited in pressure to 8 GPa. As experiments routinely exceed 100 GPa in pressure and thousands of Kelvin, it is necessary for the equation of state of KCl to be determined experimentally at these conditions if it is to be used as an equation of state calibrant in the future. This work combines new high-pressure, high-temperature data of the B2 phase of KCl (up to 167 GPa and 2400 K) with the previously published room-temperature data of Dewaele et al. (2012) to produce a Mie-Grüneisen-Debye thermal equation of state for this material. The room temperature equation of state parameters are similar to those reported previously: $V_0 =$ 32.0(3) cm^3/mole, $K_0 = 24(1)$ GPa and $K_0' = 4.56(5)$. The thermal parameters, γ_0 and q, are 2.9(4) and 1.0(1), respectively. While a q of 1 is expected, the γ_0 is higher than expected from previous calculations, lower pressure experimental data, and the available shockwave data. Thus, previously-reported equations of state underestimate the pressure of KCl at high temperatures.

I. INTRODUCTION

Alkali halides are simple ionic solids that have been studied under a wide variety of conditions, making them useful benchmark materials to compare between dynamic and static compressional environments. Additionally, their crystallographic simplicity and relatively high compressibilities (K_0 = ~10–30 GPa) make them useful as pressure-transmitting media and potentially sensitive pressure markers in high-pressure X-ray diffraction (XRD) experiments.[1] Furthermore, they are chemically inert and are transparent to near-infrared light, which facilitates their use in high-temperature experiments, such as laser heating in a diamond anvil cell (LH-DAC). Potassium chloride (KCl) has a higher melting point at high pressures than NaCl or LiF,[2] but is less electronically dense than KBr or CsI, making it optimal among alkali halides as a pressure medium, pressure standard, and thermal insulator for this type of high pressure-temperature (P–T) XRD experiment.

The room temperature phase behavior and equations of state of KCl have been investigated up to 165 GPa.[3–6] Early studies of KCl in the diamond anvil cell at room temperature were conducted without the benefit of a (quasi)-hydrostatic pressure medium,[3–5] and the only high-temperature study of this material was limited to 8 GPa and 873 K.[7] More recently, Dewaele et al. (2012)[6] has extended the room temperature data to 165 GPa under hydrostatic conditions using He as the pressure medium and ruby as the pressure standard. Similar to other alkali halides, KCl exhibits the NaCl (B1, $Fm\bar{3}m$) crystal structure at ambient conditions, and transforms to the CsCl (B2, $Pm\bar{3}m$) structure around 2 GPa at room temperature.[7] No other solid phase transitions of this material have been observed up to 165 GPa at room temperature, nor is one expected at high temperatures in this pressure range.[6]

As high P–T experiments in the laser-heated diamond anvil cell routinely push conditions to pressures above 100 GPa and temperatures of several thousand K, a high-temperature, high-pressure equation of state of KCl is necessary to use this material as a pressure standard for this type of experiment. In addition to high-pressure, room-temperature experiments, Dewaele et al.[6] performed molecular dynamics simulations to generate a constant thermal pressure coefficient, αK_T = 0.00224 GPa/K. This value is similar to the thermal pressure coefficient experimentally measured between room temperature and 873 K by Ref. 7, 0.00275 GPa/K, while both of these coefficients are slightly lower than the constant αK_T = 0.0036

GPa/K that can be calculated assuming a constant $C_V = 3nR$ (where n is the number of elements per mole of KCl and R is the ideal gas constant) from the Grüneisen parameter, $\gamma = 2.30$, derived from acoustic wave velocity measurements.[8] A more accurate equation of state requires experimental data to be obtained over a greater range of simultaneous high-temperature, high-pressure conditions. This study combines new high pressure-volume-temperature P–V–T synchrotron XRD data for KCl up to 167 GPa and 2400 K with previous high-pressure, room-temperature data[6] toward the aim of making KCl a useful and reliable pressure standard for future high-pressure experiments.

II. METHODS

KCl (reagent grade) and Pt (99.9+%, 325 mesh) were purchased from Alfa Aesar. To remove adsorbed moisture, the KCl was baked at ∼100 °C for 12–24 hours prior to sample preparation. Generally, LH-DAC samples consist of a thin foil of opaque sample material encased between layers of a soft, transparent material that acts as both the thermal insulator and as the quasi-hydrostatic pressure medium for the experiment. It is possible to use the pressure medium/thermal insulator as an internal pressure calibrant as well (see Campbell et al. (2009)[9], for example). Thus, the samples in this study were configured to produce an equation of state of KCl specifically for use as a pressure standard in this type of sample geometry. Here, platinum (Pt) metal was used as the pressure calibrant and laser-absorbing foil. Pt foils of ∼5 μm thickness were secured between two layers of dried KCl of ∼10 μm thickness. Samples were loaded into diamond anvil cells using Re as the gasket material and diamond culets of 300, 150 or 100 μm in diameter. The entire cell assembly was then dried at 100 °C for ≥30 minutes to ensure total removal of moisture immediately prior to closing and pressurizing the cell. (P–V–T) data were collected by compressing to a target pressure and collecting powder XRD patterns at increasing (and/or decreasing) temperatures during laser heating.

Angle-dispersive synchrotron X-ray diffraction (Fig. 1) was conducted at beamlines 13-ID-D (GSE-CARS) and 16-ID-B (HP-CAT) of the Advanced Photon Source, Argonne National Laboratory. Laser-heating experiments at beamline 13-ID-D were done with monochromatic incident radiation ($\lambda = 0.3344$ or 0.2952 Å) measuring 2.2 by 4 μm.[10] Laser-heating experiments at beamline 16-ID-B were done with monochromatic incident radiation ($\lambda = 0.4066$

Å) measuring 6 by 7.5 μm.[11] Sample-to-detector distances and tilt were calibrated using LaB_6 or CeO_2. The laser was co-aligned with the incident X-rays using the X-ray-induced fluorescence of KCl. Double-sided laser-heating of the samples was performed using 1 μm Yb-doped fiber lasers, adjusting upstream and downstream laser powers to balance temperatures. The highest pressure measurements (sample B86) were conducted using "burst" mode, where the lasers were enabled at the desired laser power only during XRD collection to minimize accumulated heating of the DAC. This allowed the DAC to stay cool enough that the laser-to-X-ray alignment was maintained throughout the entire heating cycle. Surface temperatures were determined spectroradiometrically on both sides using the greybody approximation,[10,11] which were then corrected by -3% for a small axial temperature gradient across the metal to determine the average temperature of the Pt foil.[9,12] The average KCl temperature was taken as the temperature at the midpoint between the surface of the sample and the surface of the diamond anvils; thus, the estimated average temperature of the KCl pressure medium is T_{KCl} = (3*$T_{surface}$ + 295) / 4 ± ($T_{surface}$ - 295) / 4.[9] Although this geometry places a large uncertainty on the KCl temperature, this material remains an effective pressure calibrant because the compressibility of alkali halides far outweighs their thermal expansion over typical P–T conditions.[9]

Powder X-ray diffraction patterns were collected on a CCD image plate and integrated azimuthally to intensity vs. 2θ plots (e.g. Fig. 1) using DIOPTAS.[13] Reflection positions were fit to determine lattice parameters as a function of pressure and temperature using PeakFit (Systat Software). 2 to 7 reflections (110, 200, 211, 220, 310, 321, 222) were averaged to determine the lattice parameters of KCl. Above 45 GPa, the KCl 200 reflection broadened and yielded systematically-higher lattice parameters than all other lines (Fig. 2), so it was not used in the volume calculation in that pressure range. Indeed, the 200 peak broadened so significantly that it was lost in the background above 130 GPa. This phenomenon has been observed previously in KCl[6] and gold[14], and was attributed to sensitivity of the 200 peak to non-hydrostatic strain. Pressure in these experiments was measured using the high P–T equation of state of Pt[15] and 3-8 observed reflections (111, 200, 220, 311, 222, 400, 331, and 420). Note the non-hydrostatic behavior of the 200 reflection was not observed in the Pt. The Pt equation of state[15] is well-calibrated against the same pressure standards used for the room-temperature KCl data.[6]

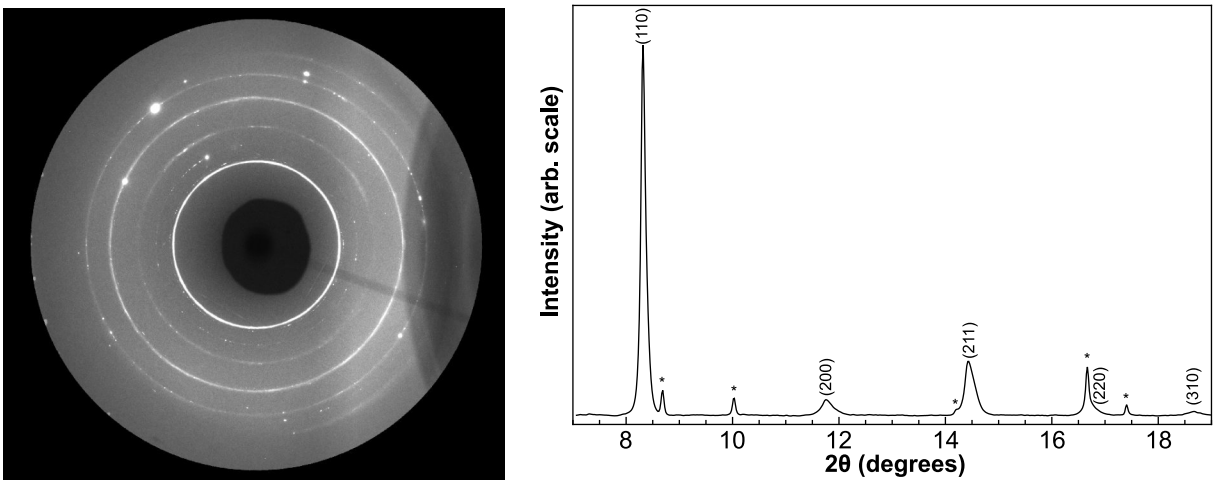

FIG. 1. Left: A typical XRD pattern from this study collected with X-ray wavelength λ = 0.3344 Å. Right: The integration of intensity vs. 2θ of the pattern on the left. The asterisks indicate reflections from the Pt pressure standard, while the KCl reflections are noted with their respective Miller indices (hkl). This pattern was collected at 31.8 ± 0.9 GPa and 1200 ± 100 K (Pt temperature).

III. THERMAL EQUATION OF STATE

The thermal equation of state (EOS) of B2-KCl was determined at high pressures and temperatures for use as a pressure standard in high P–T XRD experiments in the diamond anvil cell. The measured P–V–T data from four experiments are listed in Table A1.[16] Fig. 1 shows a sample diffraction pattern from this study at 31.6 GPa and 1194 K. As expected, the powder diffraction patterns became more "spotty," as opposed to uniformly-defined rings, as temperatures increased. This is due to recrystallization and grain growth at high temperature and was more apparent in Pt than in KCl. The KCl peaks tended to be broad because the X-rays are sampling KCl at a range of temperatures between the Pt surface and the diamond culet. In most cases, data were obtained during cooling because the peak temperatures in each heating cycle significantly relaxed the sample and reduced lattice strain within the KCl. Recent observations of KBr in similar LH-DAC experiments suggest that this material will become opaque near its melting point, resulting in runaway heating and a miscalculation of its temperature.[17] It is unclear whether this behavior occurs in other alkali halides; however, when runaway heating did occur at any point in an experiment, we only used data prior to that event to avoid inaccurate temperatures in our data. All experiments

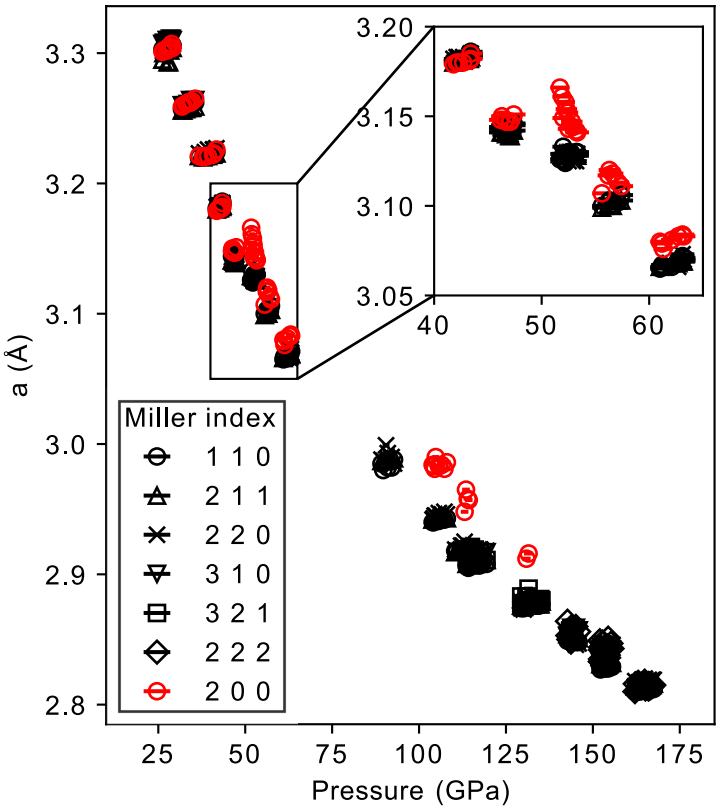

FIG. 2. Lattice parameter (a) for KCl from different XRD reflections. Above 50 GPa, the 200 reflection yields higher lattice parameters than all other reflections, so it was not used in the volume calculation in this pressure range. Above 130 GPa, the 200 peak cannot be distinguished from the background. Inset shows a blow-up of the 40-65 GPa range.

in this study were conducted above 15 GPa to stabilize and protect the diamonds during laser heating. This is well above the B1-to-B2 phase transition in KCl, reported at ∼2 GPa.[7] No other phase transitions were observed up to 167 GPa and 2400 K in this study. Sample #2 was measured at both sector 13-ID-D and sector 16-ID-B. There was no distinguishable difference between these data.

We fit the high temperature data of B2 KCl, along with the room temperature data reported by Dewaele et al.,[6] to a Mie-Grüneisen-Debye (M-G-D) thermal equation of state, defined as:

$$P = P_{300} + P_{thermal}, \tag{1}$$

where the room temperature data are described by:

$$P_{300,BM} = 3K_0 f(1+2f)^{\frac{5}{2}}(1+\frac{3}{2}(K_0'-4)f). \quad (2)$$

Here, $P_{300,BM}$ is the Birch-Murnaghan[18] isothermal equation of state at 300 K, f is the Eulerian strain ($\frac{1}{2}((\frac{V}{V_0})^{\frac{-2}{3}}-1)$), V_0 is the inferred zero-pressure volume of the B2 phase, K_0 and K_0' are the isothermal zero-pressure bulk modulus and its pressure derivative, respectively.

Interestingly, while Dewaele et al.[6] chose the Rydberg-Vinet (R-V) functional form for their isothermal equation of state, we found that a Birch-Murnaghan (B-M) EOS better describes their room temperature data, particularly at low pressures near the B1–B2 transition. With the R-V fit, the lower-pressure, room-temperature residuals exhibit a monotonic trend with pressure, which the authors attributed to the B1–B2 phase transition affecting the bulk modulus of the B2 phase. This led them to fit only their lowest pressure data (2–6 GPa) to determine V_0. We find that when we fit the data to the B-M EOS, the residuals do not show such a trend with pressure and a reasonable, albeit slightly higher, V_0 can be inferred by fitting all of the B2-KCl data simultaneously. The resulting parameters for the calculated equations of state are given in Table 1, along with the thermal EOS parameters available in the literature. In terms of the room temperature B-M EOS, our fit agrees well with the literature data. The inferred zero-pressure volume, $V_0 = 32.0(3)$ cm^3/mole, is the same as reported by both Refs. 5 and 7, within uncertainty. The bulk modulus, $K_0 = 24(1)$ GPa, is very similar to that reported by Ref. 7, but lower than the 28.7 GPa reported by Ref. 5. This discrepancy is likely due to the fact that those authors chose to fix the pressure derivative of the bulk modulus, K_0', to 4. The larger pressure range sampled in Ref. 6 allowed us to fit this parameter to 4.56(5). There is a trade-off between the fitted V_0 and K_0' with K_0, which is especially pronounced when comparing B-M and R-V-type fits; higher fitted V_0 values correspond to higher compressibility and a high change in compressibility with pressure. The room temperature equation of state fitting is demonstrated in Fig. 3, along with the data from Ref. 6 for reference.

The thermal contribution to pressure, $P_{thermal}$, is described by:

$$P_{thermal} = \frac{\gamma}{V} \times (E_{harmonic,\ T} - E_{harmonic,\ 300\ \mathrm{K}}), \quad (3)$$

and

TABLE I. Fitted equation of state parameters. Asterisks indicate parameters that were held constant during fitting. The γ_0 from Refs. 6 and 7 were calculated from the provided αK_T by assuming $\frac{V}{C_V}$ was constant. Values in parentheses are errors on the last digit. B-M is Burch-Murnaghan, R-V is Rydberg-Vinet.

V_0 (cm^3/mole)	K_0 (GPa)	K_0'	γ_0	q	Reference (type of fit)
32.0(3)	24(1)	4.56(5)	2.9(4)	1.0(1)	This study (B-M reference EOS)
34.3(5)	13(1)	6.2(1)	3.4(4)	1.0(1)	This study (R-V reference EOS)
32.8*	17.2	5.89	1.47	1*	Ref. 6 (R-V)
32.25	23.7	4.4	1.78	1*	Ref. 7 (B-M)
31.83	28.7	4*	2.3	1*	Ref. 5 (B-M) + Ref. 8 (acoustic)

$$E_{harmonic} = 9nRT(\frac{T}{\theta_D})^3 \int_0^{\theta_D/T} \frac{x^3}{e^x - 1}\, dx. \quad (4)$$

$\gamma = \gamma_0(\frac{V}{V_0})^q$ is the Grüneisen parameter, q is a constant, V is the volume, $E_{harmonic}$ is the harmonic contribution to thermal pressure at temperature, T, n is the number of atoms per mole of KCl (2), R is the ideal gas constant and θ_D is the ambient-pressure Debye temperature, 235 K.[8]

Instead of fitting a constant thermal pressure term (αK_T), we fit our data to the Debye energy (Eq. 4), because at high pressures the Debye temperature is expected to exceed its value at room temperature, such that the product αK_T is unlikely to be well approximated as a constant.[5] The thermal parameters, γ_0 and q, that describe our data are 2.9(4) and 1.0(1), respectively. The high-temperature data are also presented in Fig. 3, color-coded by median temperature and plotted with their corresponding isotherms. The root-mean-square misfit to the data over the whole pressure and temperature range is $\pm$1.6 GPa. The region of largest error falls between 40 and 100 GPa, as shown in the residuals plot in Fig. 3. In this pressure range, the two largest XRD peaks in the high-temperature data, the 110 of KCl and the 111 of Pt, cross in 2θ space. We attribute the misfit in pressure to the high-temperature data in this range to variations in calculated volume as a result of slight overlaps of these two peaks.

Our fitted q value of 1.0(1) is typical and means that the Grüneisen parameter varies proportional to volume. The fitted value of γ_0 is higher than expected based on both previous

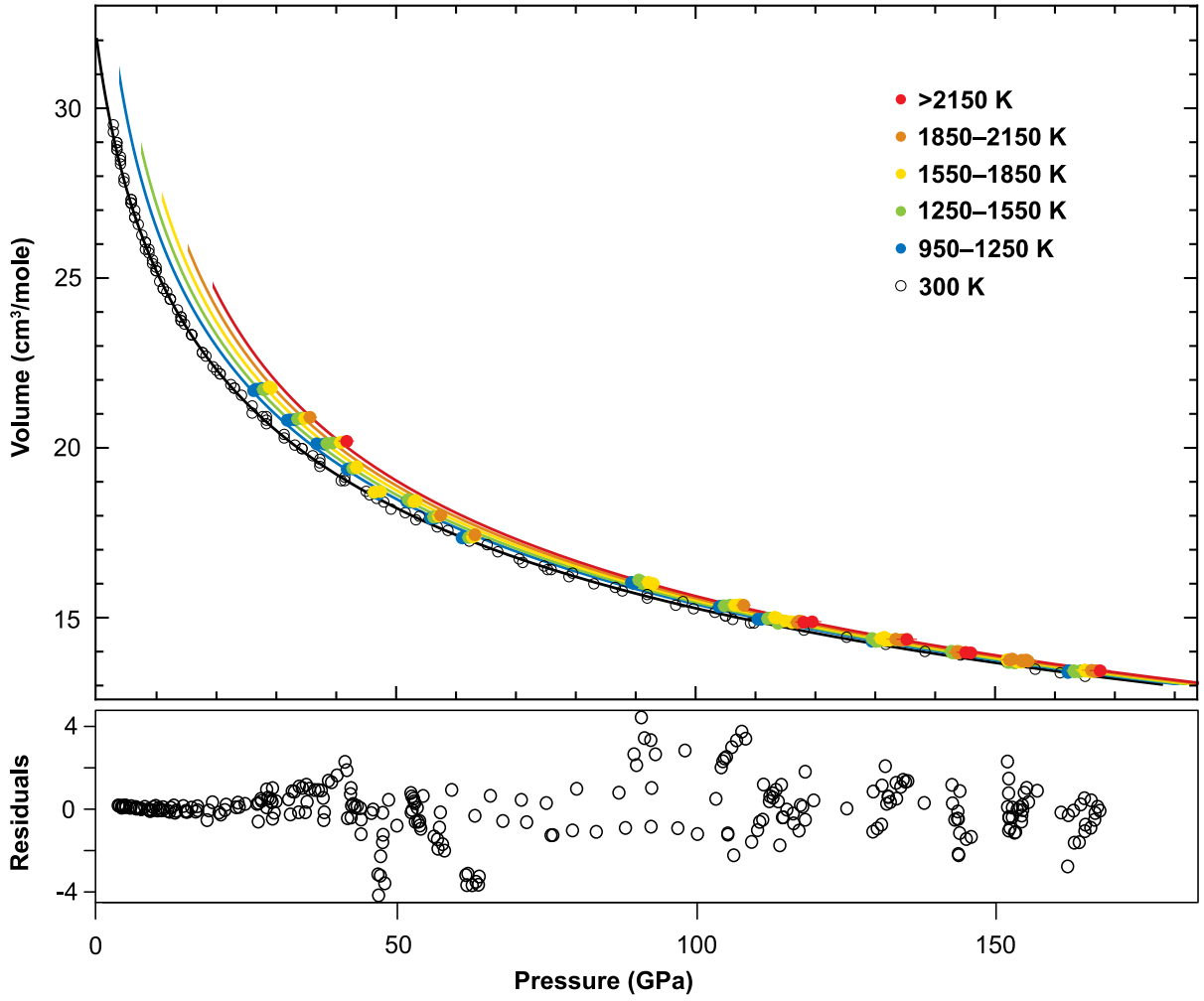

FIG. 3. Top: High P–T KCl data. Open black circles are room temperature data from Dewaele et al. (2012).[6] High temperature data are color-coded by median temperature. Solid curves are isotherms calculated from the B-M equation of state parameters in Table 1. Error on volume is smaller than the symbol. Bottom: Residuals in pressure to the fit of all the data (300 K and room temperature).

static experiments and the available shockwave data.[19] By assuming q is 1 and C_V is equal to the Debye limit, $3nR$, the value of γ_0 can be solved for based on the published parameters of Refs. 6 and 7 to be 1.47 and 1.78, respectively, using the relationship $\frac{\gamma}{V}=\frac{\gamma_0}{V_0}=\frac{\alpha K_T}{C_V}$. The thermal parameters in Ref. 6 were obtained from high-temperature molecular dynamics simulations, not experiments. Additionally, the data in Ref. 7 were measured only up to 8 GPa and <1000 K, and one should not expect those results to be well-extrapolated over the much wider P–T range covered here. The γ_0 value measured acoustically in Ref. 8 is closer

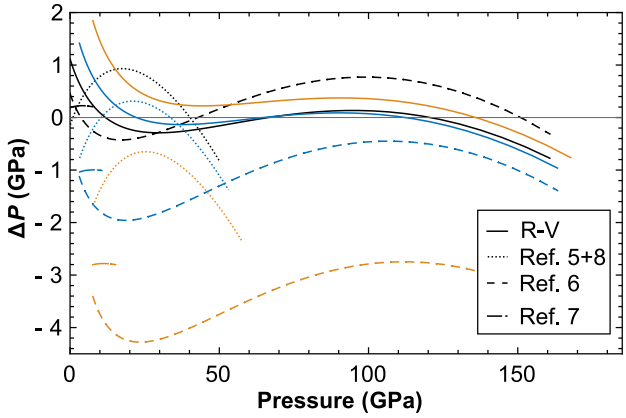

FIG. 4. Differences in calculated equations of state, $\Delta P = P - P_{Birch-Murnaghan\ (This\ study)}$, as a function of pressure. Black curves are calculated at 300 K, blue at 1000 K and gold at 2000 K. Different studies are represented by different dash formatting and are noted on the plot. Curves are plotted over the range of volume measured in each study. R-V = Rydberg-Vinet fit from this study.

to our value, at 2.3, but that study was also limited in pressure and temperature. Figure 4 shows the comparison between the thermal equations of state reported in the literature and our fit up to 170 GPa. The R-V fit from this study generally matches our B-M EOS to ± 1 GPa, but overestimates the pressure slightly at low pressures and high temperatures. All of the thermal EOSs available in the literature do a reasonable job reproducing the data at room temperature, but underestimate the pressure at high temperatures by as much as 4 GPa at 2000 K.

Figure 5 shows the 300 K isotherm resulting from this study, along with the principal isentrope and the principal shock Hugoniot calculated using our thermal equation of state and equation 5.

$$P_H = \frac{\frac{V}{\gamma}P_S + \int_{V_0}^{V} P_S dV - \Delta E_{\rm tr}}{\frac{V}{\gamma} - \frac{V_{00}-V}{2}}. \quad (5)$$

P_H is the Hugoniot pressure, P_S is the principal isentropic compression curve, $\Delta E_{\rm tr}$ is the change in energy due to the B1–B2 phase transition (31.4 J/mole)[8], and V_{00} is the ambient pressure volume of the B1 phase (37.55 cm^3/mole)[6]. The available shockwave data from Ref. 19 are also included in Fig. 5. It is clear that our predicted Hugoniot overestimates the pressure when compared with the shockwave data, corresponding to the higher Grüneisen

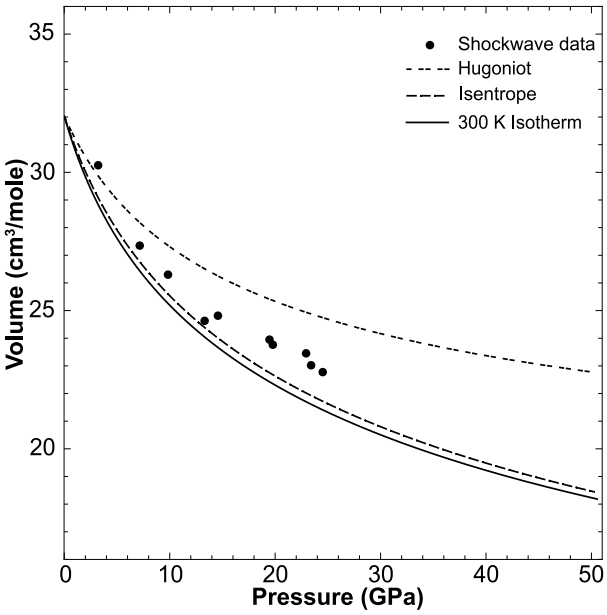

FIG. 5. The 300 K isotherm, principal isentrope and Hugoniot curves for KCl calculated from the high-temperature EOS. The measured shockwave data are shown for comparison. The B2 data end at ∼25 GPa, at which point the material melts on the Hugoniot.

parameter in our equation of state. The shock wave data are better described using a γ_0 of 1.6 to 1.7, depending on the reference equation of state used. These values are more compatible with those in Refs. 6 and 7. However, Ref. 8 reported a similar discrepancy to the one observed here between the γ_0 measured statically and the one extracted from the shockwave data. While the root cause of this discrepancy is unclear, possible causes may be differences in sample configuration or contamination of any of the samples by water.

IV. CONCLUSIONS

We have measured high P–T synchrotron X-ray diffraction on KCl in the laser-heated diamond anvil cell. These data, combined with the room temperature data from Ref. 6, were used to determine the Mie-Grüneisen-Debye equation of state for B2 KCl. The 300 K Birch-Murnaghan equation of state parameters measured here are very similar to those reported in the literature. There is a marked trade-off between the inferred V_0 term and the compressibility, which is exceptionally noticeable when comparing between Birch-Murnaghan and Rydberg-Vinet type fits. The thermal parameters, γ_0 and q, for KCl were found to be

2.9(4) and 1.0(1), respectively. This γ_0 value is higher than expected based on the calculations from Ref. 6 and the available shockwave data from Ref. 19, but is consistent with that measured acoustically by Ref. 8. The measurements here extend the available data to >100 GPa and several thousand degrees Kelvin. This greatly-expanded dataset has made a more robust high P–T equation of state possible, which will allow KCl to be used as an *in situ* pressure standard for high pressure-temperature XRD experiments in the laser-heated diamond anvil cell.

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[1] D. L. Decker, W. A. Bassett, L. Merrill, H. T. Hall, and J. D. Barnett, Journal of Physical and Chemical Reference Data **1**, 773 (1972).

[2] R. Boehler, M. Ross, and D. B. Boercker, Physical Review Letters **78**, 4589 (1997).

[3] S. N. Vaidya, G. C. Kennedy, P. Physics, and L. Angeles, Journal of Physics and Chemistry of Solids **32**, 951 (1971).

[4] T. Yagi, Solid State Communications **25**, vi (1978).

[5] A. J. Campbell and D. L. Heinz, Journal of Physics and Chemistry of Solids **52**, 495 (1991).

[6] A. Dewaele, A. B. Belonoshko, G. Garbarino, F. Occelli, P. Bouvier, M. Hanfland, and M. Mezouar, Physical Review B - Condensed Matter and Materials Physics **85**, 214105 (2012).

[7] D. Walker, L. M. D. Cranswick, P. K. Verma, S. M. Clark, and S. Buhre, American Mineralogist **87**, 805 (2002).

[8] A. J. Campbell and D. L. Heinz, Journal of Geophysical Research **99**, 11,765 (1994).

[9] A. J. Campbell, L. Danielson, K. Righter, C. T. Seagle, Y. Wang, and V. B. Prakapenka, Earth and Planetary Science Letters **286**, 556 (2009).

[10] V. B. Prakapenka, a. Kubo, a. Kuznetsov, a. Laskin, O. Shkurikhin, P. Dera, M. L. Rivers, and S. R. Sutton, High Pressure Research **28**, 225 (2008).

[11] Y. Meng, G. Shen, and H. K. Mao, Journal of physics. Condensed matter : an Institute of Physics journal **18**, S1097 (2006).

[12] A. J. Campbell, C. T. Seagle, D. L. Heinz, G. Shen, and V. B. Prakapenka, Physics of the Earth and Planetary Interiors **162**, 119 (2007).

[13] C. Prescher and V. B. Prakapenka, High Pressure Research , 1 (2015).

[14] K. Takemura and A. Dewaele, Physical Review B - Condensed Matter and Materials Physics **78**, 1 (2008).

[15] P. I. Dorogokupets and A. R. Oganov, Physical Review B - Condensed Matter and Materials Physics **75**, 1 (2007).

[16] *See Supplementary Material at ¡url¿ for the measured pressure-volume-temperature data of KCl from this study.*

[17] S. M. Arveson, B. Kiefer, J. Deng, Z. Liu, and K. K. M. Lee, Physical Review B **97**, 094103 (2018).

[18] F. Birch, J. Geophys. Res. **83**, 1257 (1978).

[19] M. van Thiel, in *Rep. UCRL - 50108* (Lawrence Livermore National Laboratory, Livermore, CA, 1977).