

P-V-T Equation of state of a- and b-rhombohedral boron

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In our paper [1], we propose *P-V-T* equations of state (EoS) for a-rhombohedral boron (a-B12) and b-rhombohedral boron (b-B106) up to 100 GPa for the temperature ranges of 298-1280 K and 300-2500 K, respectively, based on the EoS obtained from the Anderson-Grüneisen model. To determine the *P-V-T* parameters, experimental and calculated data taken from the literature were used. The derived EoS for a-B12 and b-B106 are consistent with the data obtained using density functional theory molecular dynamics calculations in Ref. [2] with an accuracy of more than 98

The derived *P-V-T* EoS allow one to analytically determine the values of molar volume and density in the range of 0-100 GPa, which are necessary for thermodynamic calculations of reactions occurring under HPHT conditions, such as synthesis of diamonds at high pressure (7 GPa) and temperature (1500 oC) from C-O-H fluids without metal catalysts [3].

The work was supported by Ioffe Institute, FFUG-2024-0019.

- [1] Ruchkin I A and Shakhov F M 2024 *SSRN* **1**
<https://ssrn.com/abstract=5041946>
- [2] Zhang S, Whitley H D and Ogitsu T 2020 *Solid State Sci.* **108**(111260) 106376
- [3] Shakhov F M, Ruchkin I A, Prilezhaev K S and Oshima R 2024 *Diamond Relat. Mater.* **147**(111260) <https://doi.org/10.1016/j.diamond.2024.111260>