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 arhombohedral 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].

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- [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