REVISED EQUATION OF STATE OF NACL

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Recently in the paper [1] a critical analysis of equations of state of NaCl from references Birch [1] and Decker [2] data has been made and conclusion has been drawn regarding incorrectness of the Decker [3] equation of state on isotherm 1073 K. This conclusion has been made from Figure 9 in [1], where the Decker [1] isotherm 1073 K had been wrongly shifted from its right position, which approximately fits the Birch [2] isotherm 1100 K.

Slightly before Brown [4] had published the equation of state of NaCl, which pretends to be the pressure standard after the Birch [2] and Decker [3] equations. This equation optimizes *PVT* data of Boehler and Kennedy [5], shock-wave data of Fritz et al [6] and volume at zero pressure. Spline-functions for smoothing of *PVT* relations have been used in it, therefore the behavior of the Grüneisen parameter vs. volume under expansion is inconsistent with the theory (Fig. 1 in Brown [4]).

These comments are eliminated in a new equation of state for NaCl, with accounts the input data listed in [1], shock-wave data from Shock Wave Database [7] and formalism [1]. Moreover, it should be noted that *PV* measurements under quasi-hydrostatic conditions are almost absent (see overviews in [2] and [4]), that is why we added two isotherms (298 and 1100 K) obtained from Fei [8] data using equation of state for MgO [9]. The Holzapfel [10] equation in the APL form is used instead of a third order Birch-Murnaghan equation.

$$P(V) = 3K_0 \cdot X^{-5}(1-X) \cdot \exp[c_0(1-X)] \cdot [1 + c_2 \cdot X(1-X)],$$

where $X=(V/V_0)^{1/3}$, $c_0= -\ln(3K_0/P_{FG0})$, $P_{FG0} = a_{FG}(Z/V_0)^{5/3}$, $a_{FG} = -0.02337$ GPa nm^5, $K'=3+2(c_0+c_2)/3$. For NaCl Z=28, then P_{FG0} =1074.5 GPa.

The equation of state for NaCl fits the experimental measurements in the temperature range of 10-1073 GPa and pressures up to 25GPa within the error comparable with direct measurements. The fitting parameters are given in Table 1.

Table 1. Parameters of equation of state of NaCl.

Parameters	NaCl
V_0, cm^3	27.015
K_0, GPa	23.84
K'	4.89
Θ_{B1o}, K	138.75
d_1	3.994
m_{B1}	0.569
Θ_{B2o}, K	143.49
d_2	34.280
m_{B2}	1.747
Θ_{E1o}, K	235.32
m_{E1}	3.684
γ_0	1.658
γ_∞	1.340
β	7.033
a_0, K^{-1}	–10.26E–6
g	8.653

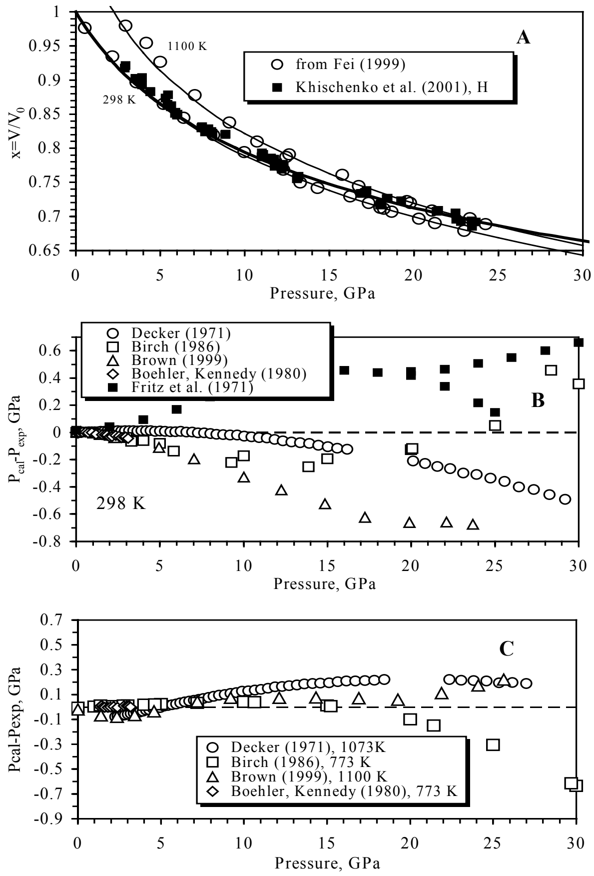

Fig.1. Comparison of the calculated isotherms and the Hugoniot adiabat with experiment (A) and deviation of calculated pressure from experiments on different isotherms (B, C).

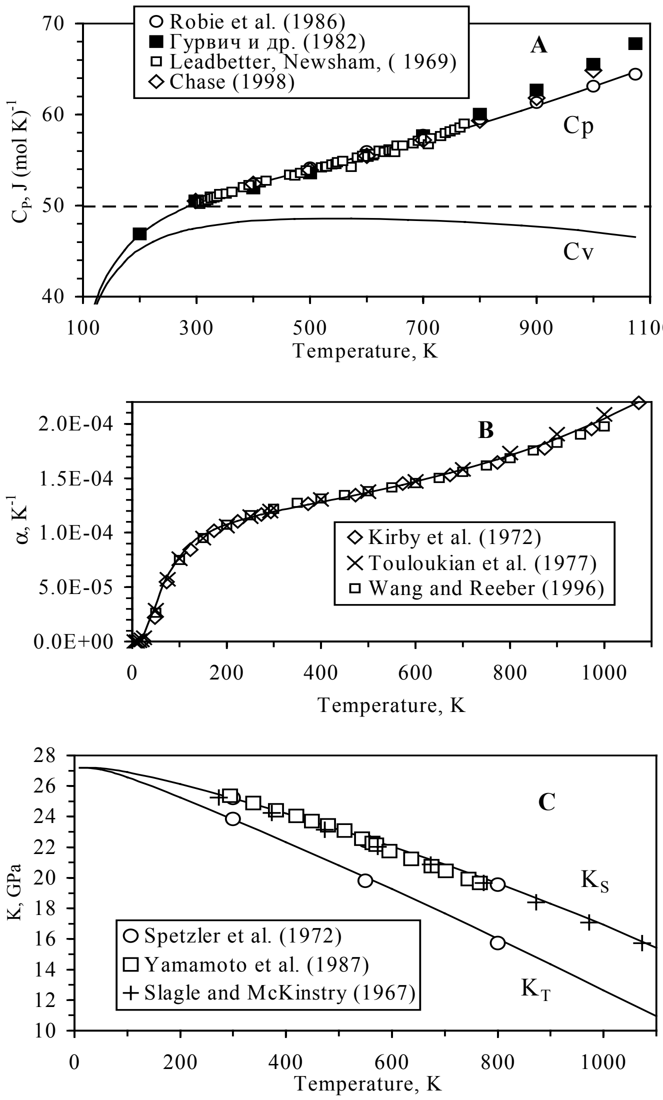

Fig. 2. Comparison of calculated heat capacity (A), thermal expansion coefficient (B) and bulk moduli (C) with experiment.

Now deviations of our calculation from theoretical one of Decker [3] are almost linear (see Fig. 1) that suggests the correctness of using the Holzapfel equation. Deviation of the Birch [2] equation of state have a non-linear character, which resulted from using a fourth order Birch-Murnaghan equation and an attempt to fit the Boehler and Kennedy [5] data with rooom-temperature isotherm from Fritz et al. [6]. Non-linear deviations of the Brown [4] equation of state are linked, on the one hand, with the use of spline-function, and on the other hand, probably as well as Birch [2] does with an attempt to fit the data of Boehler and Kennedy [5] with shock-wave data of Fritz et al. [6]. From our equation it follows that room isotherm of Decker [3] overestimates the pressure by up to 1.5% and the isotherm 1073 K, on the contrary, slightly under-estimates the pressure.

The proposed thermal equation of state for NaCl also approximates very well temperature dependence of heat capacity, thermal expansion coefficient and bulk moduli at zero pressure (Fig. 2).

Hence, the proposed equation of state for NaCl confirms as a whole the Decker [3] equation of state contrary to the statement in [1].

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