Thermodynamic database for the computer modeling of cosmochemistry and comparative planetology tasks: heat capacity of minerals

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For a description of the thermodynamic behavior of crystalline materials is necessary to have the equations of the temperature dependence of heat capacity over a wide range of temperatures. The choice of form of these equations, it is advisable to conduct such a way as to meet the maximum limits are theoretical relations and the number of empirical coefficients would be minimal. In this case, these equations can be used not only to interpolate the results of experimental measurements and reasonable extrapolations to the unexplored range of temperatures (usually higher).

The progress in the high-precision measurements of Cp of solids in the wide temperature range allow to propose a simple semi-empirical equation for the lattice heat capacity (Khodakovsky, 2012):

$$C_p = R\mathrm{n}[k\mathrm{L_D} + (3-k)\mathrm{L_E})] + \alpha_T^2 V_T K_T T \quad (1),$$

where is $\mathrm{L_D} = [1 - 1/(1 + b\mathrm{T}^3)]$, $\mathrm{L_E} = [1 - 1/(1 + c\mathrm{T}^2)]$, R − the gas constant, n − number of atoms in the molecule, α_T – thermal expansion coeffcient, V_T – the molar volume, K_T – the bulk modulus, k, b, c − empirical coefficients.

The empirical parameter k varies from 3 to 0. For $k = 3$ and $T \rightarrow 0$ the first term in square brackets of equation (1) gives the Debye equation ($C_V = AT^3$). At $T > 10 – 40$ K, becomes a significant contribution to the heat capacity is described by Einstein's theory.

Semi-empirical equation (1) with reasonable accuracy have reproduced the corresponding experimental points with the smallest number of coefficients and fitting parameters.