

Heat Capacity, Thermal Expansion Coefficient, and Grüneisen Parameter of CH₄, CO₂, and C₂H₆ Hydrates and Ice I_h via Density Functional Theory and Phonon Calculations

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Calculated Quantities

Table 1. Definitions and symbols for calculated quantities			
Symbol	Name	Equation	Definition
C_V	Constant volume heat capacity	$T \left(\frac{\partial S}{\partial T} \right)_V$ $\left(\frac{\partial U}{\partial T} \right)_V$	The amount of heat to be supplied to a material to produce a unit change in the temperature of the material undergoing an isochoric process.
C_P	Constant pressure heat capacity	$T \left(\frac{\partial S}{\partial T} \right)_P$ $\left(\frac{\partial H}{\partial T} \right)_P$	The amount of heat to be supplied to a material to produce a unit change in the temperature of the material undergoing an isobaric process.
β	Isobaric volumetric thermal	$\frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P$	A measure of the change in volume of the material per unit temperature change at constant pressure.

	expansion coefficient		
γ	Grüneisen parameter	$V \left(\frac{\partial P}{\partial E} \right)_V$ $\frac{\beta K_T}{C_V \rho}$ $\frac{\beta K_S}{C_P \rho}$ $\frac{\beta v_s^2}{C_P}$ $- \left(\frac{\partial \ln T}{\partial \ln V} \right)_S$	A measure of the effect of a volume change on vibrational properties, and therefore of the effect of temperature on vibrational properties. Using the quasi-harmonic approximation for atomic vibrations, it is a measure of the temperature effects on dynamic properties of the lattice.

V_s is the speed of sound in the particular medium, K_T is the isothermal bulk modulus, K_S is the isentropic bulk modulus.

Calculation Processes and Parameters

- The values in parentheses in each bubble represent values used for this work.
- This process is repeated at each volume above and below the ground state volume for the QHA related properties.

