

# Study of thermodynamic properties of Sodium carbonate, Na<sub>2</sub>CO<sub>3</sub>

Mala N. Rao<sup>1,\*</sup> and S.L. Chaplot<sup>1,†</sup>

<sup>1</sup>*Solid State Physics Division, BARC, Mumbai-400085*

Sodium carbonate (Na<sub>2</sub>CO<sub>3</sub>) has a couple of unique structural phase transitions with temperature. At high temperatures (T<sub>i</sub>760 K), the a phase is hexagonal with space group P63/mmc. With decrease in temperature, at T=760 K, through a process of lattice melting [1-4] Na<sub>2</sub>CO<sub>3</sub> transforms to the b-phase, which is monoclinic (space group C2/m). Lattice melting is a phenomenon where long-range order is reestablished on cooling below the transition temperature, by a process of continuous recrystallization. Currently, Na<sub>2</sub>CO<sub>3</sub> is the only known example in nature, in which this phenomenon occurs. We have studied the lattice dynamical and thermodynamic properties of sodium carbonate through a combination of inelastic neutron scattering experiments and potential model calculations. We carried out inelastic neutron scattering studies at Dhruva reactor, Trombay, to determine the phonon density of states of the external modes of polycrystalline sodium carbonate Na<sub>2</sub>CO<sub>3</sub> at room temperature and pressure. The experimental results have been analyzed on the basis of a lattice dynamics computation employing a rigid molecular ion model [5]. The parameters were optimized to the available experimental phonon dispersion curves of calcite and then transferred to sodium carbonate. The computed values of lattice parameters and the computed phonon density of states are in fairly good agreement with experimental data. Also, the calculated diffuse scattering corresponding to the soft mode in the high temperature a phase is consistent with published experimental observations that suggest lattice melting at the a-b phase transition. [1] M.J. Harris et al., Phys. Rev. Lett. 71 (1993) 2939; *ibid.* 79 (1997) 4846. [2] M.J. Harris et al., Phys. Rev. B51 (1995) 6758. [3] I.P. Swainson et al., J. Phys. Condens. Matter 7 (1995) 4395. [4] M.J. Harris et al., J. Phys. Condens. Matter 8 (1996) 7073. [5] K.R. Rao et al., Phys. Chem. Miner. 16 (1988) 83.

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\*Electronic address: mala@apsara.barc.ernet.in

†Electronic address: chaplot@magnum.barc.ernet.in