ABSORPTION INTENSITIES OF THE MULTIPOLE-INDUCED ZERO-PHONON TRANSITIONS IN SOLID HD, HT AND DT

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Solid hydrogen as the archetypical molecular quantum crystal, seems to provide endless opportunities and challenges to experimentalists and theorists alike. The absorption process in solid hydrogens (H_2, D_2, HD, etc.) results primarily from induced dipole moments, although the small non-adiabatic allowed dipole contributes to the R-branch transitions for heteronuclear isotopomers. General and special expressions for the integrated absorption coefficients of all types of zero-phonon single and double transitions in solid H_2 have been derived earlier by different groups[a]. These expressions would also be valid for D_2 and T_2 but the definition of ortho- and para-modifications with respect to J (rotational quantum number) will be different. For heteronuclear molecules, the ortho-para distinction does not exist and all the molecules in solid HD, HT and DT are normally in the J=0 state, thus simplifying the infrared spectra and theoretical analysis. However, extra complications arise due to the non-coincidence of the geometric charge center with the center of mass of the molecule. Further, since these molecules are not perfectly centrosymmetric, odd ΔJ transitions are also allowed in addition to even ΔJ transitions, which alone are possible in homonuclear counterparts like H_2. Although theoretical expressions for the intensities of certain transitions in HD have been derived by Poll and co-workers[b], so far no attempt is made to give general expressions valid for all transitions of similar types. Currently, we are attempting to derive closed-form expressions for the absorption intensities of single and double transitions in solid HD, HT and DT. The details will be discussed in the present paper.

[a] A. P. Mishra and T. K. Balasubramanian *Phys. Rev.* **B59** (6002), 1999 and references therein.
[b] J. D. Poll, M. Attia and R. H. Tipping *Phys. Rev.* **B39** (11378), 1989 and references therein.