VIBRATIONAL RELAXATION OF THE CH STRETCH FUNDAMENTAL IN $CHBr_3$

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In continuation of our work on haloforms, we have modelled the decay of CH stretch excitation in bromoform using molecular dynamics simulations. An intermolecular force field has been obtained by fitting *ab initio* energies at select $CHBr_3$ dimer geometries to a potential function. The solvent forces on vibrational modes obtained in the simulation have been used to compute relaxation rates. The Landau-Teller approach points to a single acceptor state in the initial step of CH stretch relaxation. The timescale for this process has been calculated to be 50-90 ps, which agrees well with the experimental value of 50 ps. The reason for the selectivity of the acceptor will be elaborated. Results from a time dependent approach to the decay rates will also be discussed.