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Computational studies of x-ray scattering from three-dimensionally-aligned asymmetric-top molecules[1]

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— We theoretically and numerically analyze x-ray scattering from asymmetric-top molecules three-dimensionally aligned using elliptically polarized laser light. A rigid-rotor model is assumed. The principal axes of the polarizability tensor are assumed to coincide with the principal axes of the moment of inertia tensor. Several symmetries in the Hamiltonian are identified and employed to enhance the efficiency of solving the time-dependent Schrödinger equation for each rotational state initially populated in a thermal ensemble. Using a phase-retrieval algorithm, the feasibility of structure reconstruction from a quasi-adiabatically-aligned sample is illustrated for the organic molecule naphthalene. The spatial resolution achievable strongly depends on the laser parameters, the initial rotational temperature, and the x-ray pulse duration. We demonstrate that for a laser peak intensity of 5 TW/cm^2, a laser pulse duration of 100 ps, a rotational temperature of 10 mK, and an x-ray pulse duration of 1 ps, the molecular structure may be probed at a resolution of 1 Å.

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