Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Computational studies of x-ray scattering from threedimensionally- aligned asymmetric-top molecules[1] STEFAN PABST, Argonne National Laboratory, Argonne, Illinois 60439, USA; Institut fuer Theoretische Physik, Universitaet Erlangen-Nuremberg, Germany, PHAY HO, Argonne National Laboratory, Argonne, Illinois 60439, USA, ROBIN SANTRA, Argonne National Laboratory, Argonne, Illinois 60439, USA; Department of Physics, University of Chicago, Chicago, Illinois 60637, USA — We theoretically and numerically analyze x-ray scattering from asymmetric-top molecules three-dimensionally aligned using elliptically polarized laser light. 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 exploited 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. 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.

[1]This work was supported by the Office of Basic Energy Sciences, U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

Stefan Pabst
Argonne National Laboratory, Argonne, Illinois 60439, USA; Institut fuer Theoretische Physik, Universitaet Erlangen-Nuremberg, Germany

Date submitted: 27 Jan 2010 Electronic form version 1.4