Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Effect of the rotational motion between ionization and fragmentation for non-linear molecules in MFPAD studies JESUS LOPEZ-DOMINGUEZ, ROBERT LUCCHESE, Texas A&M University — Molecular-frame photoelectron angular distributions (MFPADs) are one of the most useful quantities to measure when probing the dynamics of dissociation in photoionization. Being able to make accurate theoretical calculations of MFPADs to accompany experimental measurements is of great importance to better understand and explain the mechanisms and phenomena underlying molecular ionization and fragmentation events. One of the key approximations in determining the MFPADs assumes that the dissociative event occurs faster than the rotational motion of the molecule i.e., the axial recoil approximation. In the present work, we derived expressions for computing the usual MFPADs but including the rotational motion by accounting for the extra angular momentum dependence in non-linear molecules. This allows for the study of the recoil frame photoelectron angular distributions (RFPAD) for molecules with dissociative states where the lifetime of metastable molecular ions is not short compared to the rotational periods of the molecule. Under this consideration the number of states that can be studied is extended and a better agreement between experiment and theory is to be expected. After presenting the formalism for non-linear molecules, we used it to study the core photoionization of CH_4, and compared the results with experimental measurements and with previous works that did not include the rotational motion in the computation of the MFPADs.

Robert Lucchese
Texas A&M Univ

Date submitted: 19 Feb 2014 Electronic form version 1.4