Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electronic Structure Mediated Vibrational Coherence in Methyl Acetophenone Isomers ARKAPRABHA KONAR, YINAN SHU, BENJAMIN LEVINE, VADIM LOZOVOY, MARCOS DANTUS, Michigan State University — The role of ground and excited state electronic structures in influencing the vibrational coherences in gas phase polyatomic molecules has been a hot topic for quite some time. Here we explore the time resolved dynamics of acetophenone and its methyl substituted isomer when excited by intense 800nm femtosecond pump and probe pulses. The parent ion yield show 500 fs modulations that die down within 3ps. Similar modulations having the same timescales in the parent ion yield are also observed for the p-methyl isomer. The o-methyl isomer however shows longer 1ps modulations. Interestingly enough no oscillations are observed for the meta isomer. Quantum chemical calculations at the CASSCF/6-311G level of theory predicts that upon excitation the neutral ground state is planar and the energy spacing between the levels is very small. Preliminary calculations also predict torsional motion coupled to electronic modulations on the D_0 state and further calculations are being performed to ascertain the involvement of the D_1 and D_2 states. This could help us better understand the electronic effect of substitution on a benzene ring.

Arkaprabha Konar
Michigan State University

Date submitted: 11 Nov 2013 Electronic form version 1.4