Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Radiative electron attachment to molecules of astrophysical interest. Benchmark study of CN^-.[1] VIATCHESLAV KOKOOULINE, Dep. of Physics, University of Central Florida, NICOLAS DOUGUET, Dep. of Chemical Engineering and Materials Science, Univ. of California at Davis, OLIVIER DULIEU, MAURICE RAOULT, Laboratoire Aime Cotton, Universite Paris XI, ANN E. OREL, Dep. of Chemical Engineering and Materials Science, Univ. of California at Davis — We develop a first-principles approach to study the process of radiative electron attachment (REA) to linear molecules of astrophysical interest $Mol + e^- \rightarrow Mol^- + \hbar\omega$. ($Mol^- = C_nH^-$, C_nN^-). The approach is based on accurate ab initio calculations of electronic bound and continuum states of the negative ion. The electronic continuum states are obtained with the complex-Kohn variational method. A preliminary calculation for the formation of the simplest observed ion, CN^-, by REA gave a low rate coefficient. We will present also a preliminary result for the C_4H^- formation by REA. For this molecule, the REA rate coefficient is expected to be somewhat larger due to the Renner-Teller non-adiabatic coupling that should enhance electron capture. The goal of this study is to answer the question if negative molecular ions C_nH^- and C_nN^- recently observed in the interstellar space could indeed be formed by REA as previously suggested.

[1]This work is supported by the DOE Office of Basic Energy Science and the National Science Foundation, Grant No's PHY-08-55092 and PHY-08-55622.

Viatcheslav Kokoouline
Dep. of Physics, University of Central Florida

Date submitted: 27 Jan 2012 Electronic form version 1.4