Abstract Submitted
for the DAMOP13 Meeting of
The American Physical Society

Formation of negative ions in the interstellar medium by dissociative electron attachment to the H_2CN molecule[1] VIATCHESLAV KOKOOULINE, Dept. of Physics, U Central Florida, SAMANTHA FONSECA DOS SANTOS, NICOLAS DOUGUET, ANN E. OREL, Dept. of Chem. Eng and Mat. Sci., UCDavis — The methylene amidogen radical (H_2CN) was first discovered, in 1962 by Cochran *et al.* [1], and since then it has received considerable attention from both experimentalists and theoreticians. It is considered an important intermediate in the combustion of nitramine propellants and proposed to play a role in extraterrestrial atmospheres. It was detected in interstellar clouds in 1994 [2], and its dissociative electron attachment (DEA) process may be responsible for the formation of the CN^- and the H^- negative ions: e^-+$H_2CN \rightarrow CN^- + H_2$; e^-+$H_2CN \rightarrow H^- + HCN$. We report here the results of our ab initio quantum chemical studies of the geometrical and electronic structure of the methylene amidogen and and its negative ion H_2CN^- in the theoretical of DEA in H_2CN. The scattering calculations are carried out using the complex Kohn variational method. The nuclear dynamics, including dissociation, will later be treated using the MCTDH code [3] with a three-dimensional potential energy surface, in which the distance of CN is kept frozen. [1] E. L. Cochran *et al.* J. Chem. Phys., 1962, 36, 1938. [2] M. Ohishi *et al.*, Astrophys. J., 1994, 427, L51. [3] G. A. Worth *et al.*, MCTDH package, Version 8.4

[1]This work is supported by the DOE Office of Basic Energy Science and the National Science Foundation, Grant No's PHY-11-60611 and PHY-10-68785

Viatcheslav Kokoouline
Department of Physics, University of Central Florida

Date submitted: 25 Jan 2013 Electronic form version 1.4