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Comparative studies of dissociative electron attachment to CH_2Cl_2 and CF_2Cl_2 molecules SHAVKAT MAMATKULOV, University of Nebraska-Lincoln, Uzbekistan Academy of Sciences, ILYA FABRIKANT, University of Nebraska-Lincoln — Experimental studies[1] of dissociative electron attachment to dichloroalkanes and chlorofluoromethanes have established a universal relation between the peak value of the cross section and the vertical attachment energy. The CH_2Cl_2 is the only compound that is substantially removed from the trend observed for all other compounds: its peak cross section is more than one order of magnitude lower than that predicted by the universal curve. In an attempt to understand this difference we calculated energies of the LUMO states for CH_2Cl_2 and CF_2Cl_2 anions as functions of the C-Cl distance and performed dissociative electron attachment calculations using one effective reaction coordinate corresponding to the C-Cl stretch. For the potential energy curve calculations we employed MP2 theory with 6-31+G(d) and 6-311++G(3df,3pd) basis sets. The calculations show that the ionic curve for CH_2Cl_2 is much less repulsive and crosses the neutral curve at substantially larger internuclear separation than for CF_2Cl_2. This explains qualitatively and semiquantitatively the much lower dissociative attachment cross section for CH_2Cl_2. This work was supported by the US National Science Foundation. and by a Fullbright fellowship.

[1]K. Aflatooni and P. D. Burrow, Int. J. Mass Spectrom. **205**, 149 (2001).

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