Abstract Submitted
for the DAMOP07 Meeting of
The American Physical Society

Resonances and threshold effects in low-energy electron collisions with methyl halides[1] ILYA FABRIKANT, GORDON GALLUP, University of Nebraska — Cross sections for elastic and inelastic electron collisions with CH_3X (X=Cl, Br, I) molecules are calculated. For the lowest partial wave the resonance R-matrix theory, and for the higher partial waves the theory of scattering by dipolar plus polarization potential, are used. It is shown that the rotationally elastic scattering amplitude for a polar molecule in the fixed-nuclei approximation is logarithmically divergent for the forward direction, and a new closure formula is derived to speed up the convergence at small angles. The dipole moment as a function of the C–X distance is modeled semiempirically. This is supplemented by *ab initio* calculations of the dipole moment function for CH_3Br using the multi-configurational valence bond method. The results for scattering cross sections show pronounced features caused by vibrational Feshbach resonances and threshold cusps. The features are most noticeable at the $v = 6$, 7, and 8 thresholds in CH_3Cl, at the $v = 3$ and 4 thresholds in CH_3Br and at the $v = 1$ threshold in CH_3I. The authors are grateful to H. Hotop for many stimulating discussions.

[1]Supported by NSF, grant No. PHY-0354688.

Ilya Fabrikant
University of Nebraska

Date submitted: 05 Feb 2007 Electronic form version 1.4