Analysis of radiative emissions from collisions of O⁶⁺ with Ar, H₂O, and CH₄

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Synopsis Total capture cross sections were obtained from a quantum-mechanical analysis of slow O^{6+} -Ar, -H₂O, and -CH₄ collisions. Radiative emission spectra corresponding to single-electron capture were also obtained from this analysis. The present results are compared to previous measurements and calculations.

Interactions of highly-charged solar wind ions with comet neutrals are known to produce strong x-ray emissions through the process of chargeexchange [1]. A recent study by Machacek *et al.* [2] examined such interactions in the laboratory where they measured total cross sections from single, double, and triple-electron capture in O^{6+} collisions with neutral argon and various molecules including H₂O and CH₄. The collisions under investigation were performed at impact energies of 1.17 and 2.33 keV/amu, which corresponds to the low and high solar wind speeds. Calculations using the classical trajectory Monte Carlo (CTMC) method were also reported and compared with measurements. In addition, CTMC results of radiative spectra from singlecapture were provided.

In the present study, we examine collisions of O^{6+} with Ar, H_2O and CH_4 using a quantum mechanical analysis performed within an independent electron model. Specifically, we use the two-center basis generator method (TC-BGM) [3] to solve a set of single-particle Schrödinger equations.

The multi-center problem of the molecular collision system was addressed using a spectral representation of the molecular Hamiltonian [4]. We found that the use of a closure approximation on the molecular Hamiltonian [5] was necessary to produce reliable capture cross sections at these low impact energies. A sample set of these results for the O^{6+} -CH₄ system are shown in Table 1.

Table 1. Total capture cross sections (in 10^{-16} cm²) for O^{6+} -CH₄ at 1.17 keV/amu.

| Capture | Expt. [2] | CTMC [2] | TC-BGM |
|---------|--------------|----------|--------|
| single | 42.9 ± 2.9 | 54.2 | 52.7 |
| double | 17.8 ± 1.3 | 6.76 | 26.6 |
| triple | 2.7 ± 0.2 | 0.659 | 4.94 |

Using our calculated capture cross sections as initial conditions and radiative decay rates for the ra-

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diative cascade problem, we calculate the spectral counts resulting from single-electron capture. The spectral lines of interest for the present study correspond to energies of approximately 60 to 110 eV (or wavelengths between 10 to 20 nm). Figure 1 shows an example of the present TC-BGM emission spectra being compared with CTMC results by Machacek *et al.* [2]. Results for the other collision systems will be presented at the conference.



Figure 1. Emission spectra for O^{6+} -CH₄ collisions at 1.17 keV/amu impact energy. CTMC calculations are by Machacek *et al.* [2] (\diamond), and present TC-BGM results (\bullet).

References

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