Elastic scattering of low-energy electrons by CH$_3$CN and CN$_3$NC Isomers

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INTRODUCTION

Molecules containing cyanide and isocyanide groups have many different applications in chemical industries. The CH$_3$CN (acetonitrile) molecule was detected in the interstellar clouds and can be considered an building block for amino acids. The isomers CH$_3$CN and CH$_3$NC (isoacetonitrile) have large permanent dipole moments (> 3 Debye), can form "dipole-bound" molecular anions. Theoretical and experimental studies have shown the existence of "dipole-bonded" anion for CH$_3$CN. There are also studies of dissociative electron attachment (DEA) for both CH$_3$CN and CH$_3$NC in the gas phase. The resonance features are important to understand the DEA mechanism of explain, such as, appearance energies of ions and even fragmentation patterns leading different anions. In this work we report elastic integral cross sections for low-energy (below 10 eV) electron collisions with CH$_3$CN and CH$_3$NC.

METHODS

The R-matrix theory[1] is used to describe electron scattering by molecules and the UK polyatomic Rmatrix (UKRMol) codes were employed to calculated the cross sections and quantities of interest in the nuclei-fixed frame. In this method the space is split into an inner and an outer region. The inner region is defined as the space inside of a sphere of radius r=a in which the center-of-mass of the molecule defines the origin of the coordinates. The radius a is chosen in order to have all electronic density of the target molecule inside the sphere. In the inner region, the interactions between the scattering electron and all electrons of the molecule is strong is the inner region, it is important to consider exchange, polarization and correlation effects. The cross sections were calculated in static-exchange (SE) and static-exchange-polarization (SEP) level. Due to the large permanent dipole moment for both isomers, and in order to take into account the long-range interaction, a Born closure procedure[2] was employed.

RESULTS AND DISCUSSION

First, we performed a systematic study of the convergence of eigenphase sums and in SE level, we observed sharp resonance feature near 5.0 eV and 5.5 eV for CH$_3$CN and CH$_3$NC, then in SEP level the resonance moves to 2.4 and 2.8 eV respectively. Both molecules present another broad resonance at higher energy near 6 eV.

The differential cross sections (DCS) for both molecules are very similar between them. As there is no experimental data available in the literature, we have compared our results with available results for HCN. The magnitude order of DCS are in good agreement.

The integral cross section (ICS)-SEP results have shown that the resonance converges to 2.4 and 2.8 eV and the long-range interactions are dominant effects comparing with polarization. The ICS experimental results for HCN are around 4 times smaller comparing with both isomers, and it could be partially explained by experimental extrapolation method.

CONCLUSIONS

This study presents the first study of elastic cross sections for CH$_3$CN and CH$_3$NC. The lower energy resonance (2.4 and 2.8eV) are in reasonably agreement with experimental results. The long-range interactions are dominant comparing with polarization effects.

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