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Elastic low-energy electron collisions with methylamine

Kedong Wang*, and Ju Meng

College of Physics and Electronical Engineering, Henan Normal University, Xinxiang 453007, People's Republic of China

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Abstract. We present *ab initio* scattering calculations results of low-energy electron collision with methylamine using *R*-matrix approach within the static-exchange (SE) and static-exchange-polarization (SEP) approximations. The elastic integral, momentum transfer and differential cross sections are reported. The calculated elastic integral cross sections are in agreement with the available experimental and theoretical data. A σ^* shape resonances of ^{2}A' symmetry located at 8.9 eV are detected within SEP model. For this dipole molecule Born-closure procedure was used to account for the higher partial waves ($l > 4$) to obtain the convergence of the cross section.

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Key words: electron collision, elastic cross section, momentum transfer cross section, differential cross section.

1 Introduction

Studies of low-energy electron collisions with molecules are motivated by their importance in the understanding of radiation damage [1], in the investigating physic-chemistry of interstellar and plasma-based processing. Methylamine, like ammonia, is a molecule of fundamental interest in photochemistry. It is a low-energy source of the fluorescent NH_2 and NH radical species. It has been included in models of the atmospheres of Uranus and Saturn [2-3] and detected in that of Halley's comet [4].

A variety of experimental studies on electron collisions with methylamine are available with some theoretical work. In early experiments, Schmieder and Elektrochem [5] investigated total electron cross section of methylamine. Subsequently, Szmytkowski and Krzysztofowicz [6] measured total cross sections for methylamine in a linear electron-transmission experiment for impact energies from nearly 1 eV up to 250 eV. Samardzic

*Corresponding author. *Email address:* wangkd@htu.cn (K. D. Wang)

et al. [7] measured the complete valence shell electron separation energy spectra and momentum distributions for methylamine by high-resolution electron momentum spectroscopy at a total energy of 1500 eV. Recently, Silva *et al.* [8] investigated low-energy electrons and positrons scattering by methylamine using the Schwinger multichannel (SMC) method. They presented integral (ICS), momentum transfer (MTCS) and differential cross sections for positrons and electrons collision with methylamine. And they found a σ^* shape resonance at around 9.0 eV.

In the present paper we report *R*-matrix calculations of elastic collision with methylamine. We present both differential and integral cross sections at energies ranging from 0.01 to 20 eV. The electron scattering calculations are performed at static exchange (SE), static-exchange-polarization (SEP) using UK molecular *R*-matrix code [9-10]. This method has been proven to be a reliable method to study electron scattering in the low energy region [11-14]. During the course of electron-molecule scattering, the formed shape resonances which can cause enhancements in the cross sections are explored. The differential cross sections are calculated using the code POLYDCS [15].

2 Method

2.1 Theory

The UK molecular *R*-matrix method has been described carefully elsewhere [11], thus here we just present some relevant details of the calculations. This method is a variational technique that relies on the partitioning of configuration space into an inner and an outer part. The boundary is a sphere whose center is located at the center of mass of the molecule. The radii is chosen so that the molecular electron cloud is fully contained within the sphere. In the inner region, exchange and electron-electron correlations are considerable. As a result, the collision problem within a finite volume can be treated as a molecular bound state problem, by constructing and diagonalizing a Hamiltonian matrix. To meet the boundary conditions, the Bloch operator is added to the diagonalized inner region Hamiltonian. In the outer region, exchange and electron-electron correlations are not important and are negligible, and one need only account for the long-range multi-polar interactions between the scattering electrons and the target. Hence the problem can be reduced to solving a set coupled second order equations, which is in practice done by propagating the *R*-matrix and matching to the asymptotic expansion of the solution to obtain the scattering observables.

In inner region, the wave function of the scattering system is written using the configuration interaction (CI) expression

$$\psi_k^{N+1} = A\sum_{ij} a_{ijk}\phi_i^N(x_1,\cdots,x_N)u_{ij}(x_{N+1}) + \sum_i b_{ik}\chi_i^{N+1}(x_1,\cdots,x_{N+1}) \quad (1)$$

where A is an antisymmetrization operator, x_N is the spatial and spin coordinate of the Nth electron, ϕ_i^N represents the ith state of the N-electron target, μ_{ij} is a continuum-