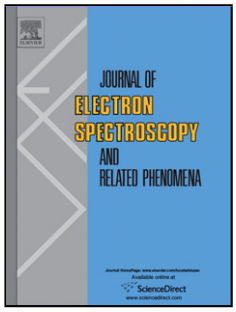


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# Rotational excitation of tetrahedral molecules by positron impact in the Born approximation

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**Abstract**

Rotational cross sections of tetrahedral molecules for low energy positron impact is the theme of this work. The scattering model is based in the Born approximation combined to multipole formulation for the scattering potential. We choose the $CH_4$ and $CF_4$ molecules as model systems to illustrate the theory. We obtain analytical expressions for octupole and hexadecapole transitions in relative momentum and partial waves formulations. The dependence of the cross sections on the molecular multipole moments, as well as the incident particle energy is directly identified. Comparison to the *ab initio* results found in literature exhibit good agreement for positron-$CH_4$ rotational cross sections.

*Keywords:* positron scattering, Born approximation, rotational excitation

## 1. Introduction

Collisions of positrons with atoms and molecules are central to the understanding of several phenomena in many branches of physics and chemistry. For example, positrons are used as a tool to identify the presence of vacancies in crystalline arrays [1]. In the same fashion, the energy loss rate of positrons in condensed matter is a theme of research [2, 3, 4, 5]. In the study of astronomical environments, positrons have remarkable role in solar flares [6, 7], supernovae [8, 9] and many other scenarios [10].

Among several collisional channels, the rotational excitation process have special role in the study of thermalization [11, 12] of positrons in gases [13, 14]. In particular, the study of rotational transitions in tetrahedral molecules induced by positron impact is of interest for plasma physics [15] and the possible development of positron traps [16].

The first model to compute rotational excitation cross sections of diatomic molecules, originally formulated for electron impact, was developed by Gerjouy and Stein [17]. After, Dalgarno and Moffett [18] improved it including polarization effects. Soon afterwards, Takayanagi and Inokuti investigated the differences [19] in the rotational excitation of nitrogen and hydrogen molecules by positrons. All these pioneering investigations were based in the Born approximation combined with some model for projectile-target interaction.

About what concerns the specific problem of rotational excitation of tetrahedral by positron impact, we were only able to find the work of Jain and Thompson on positron-$CH_4$ [20], who considered a scattering potential constructed from the superposition of the static plus an *ab initio* nonparametric polarization potential. Among molecules with this geometry, $CF_4$ is a molecular system that has attracted considerable attention of the positron-community in the last years [15]. It comes from the fact that all buffer-gas positron traps in use today rely on $N_2$ as the primary trapping gas. Recently, Marjanovic *et al* [16] suggested the use of $CF_4$ as the primary trapping gas, exploiting vibrational excitation as the main inelastic capture process. Bankovic *et al* [21] investigated the transport of positrons in $CF_4$ gas. In this specific article, they completely neglected the rotational collision channels, in the same way it is usually done in analyses for electron swarms in gaseous $CF_4$. In spite of that, they called attention to the results reported by Varella *et al* [22] for the rotational excitation of $CF_4$ by electron impact: these authors obtained relatively high cross sections ($\sim 10^{-16}$ cm$^2$ ) for rotational excitations at high energies, such that, Bankovic *et al* [21] explicitly state that "the role of rotational excitation in highly symmetric molecules is still an open issue" .

Inspired by the assertion of Bankovic *et al* [21], we decided to investigate the rotational cross sections for positron-$CH_4$ and positron-$CF_4$. In an ideal scenario, these cross sections would be computed using a methodology that simultaneously incorporate the rotational dynamics and would also take into account the correlation-polarization effects present in the low energy regime in a satisfactory way. Unfortunately, such methodology is still not available for systems with this geometry. In the absence of experimental data and of other theoretical results to compare with, it sounds reasonable to attack the problem within a simple scattering model.

We assume that the rotational cross sections can be calculated through a perturbative approach (Born approximation) since the rotational transitions are relatively weak, when compared to other stronger channels, as the elastic and vibrational ones.

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