

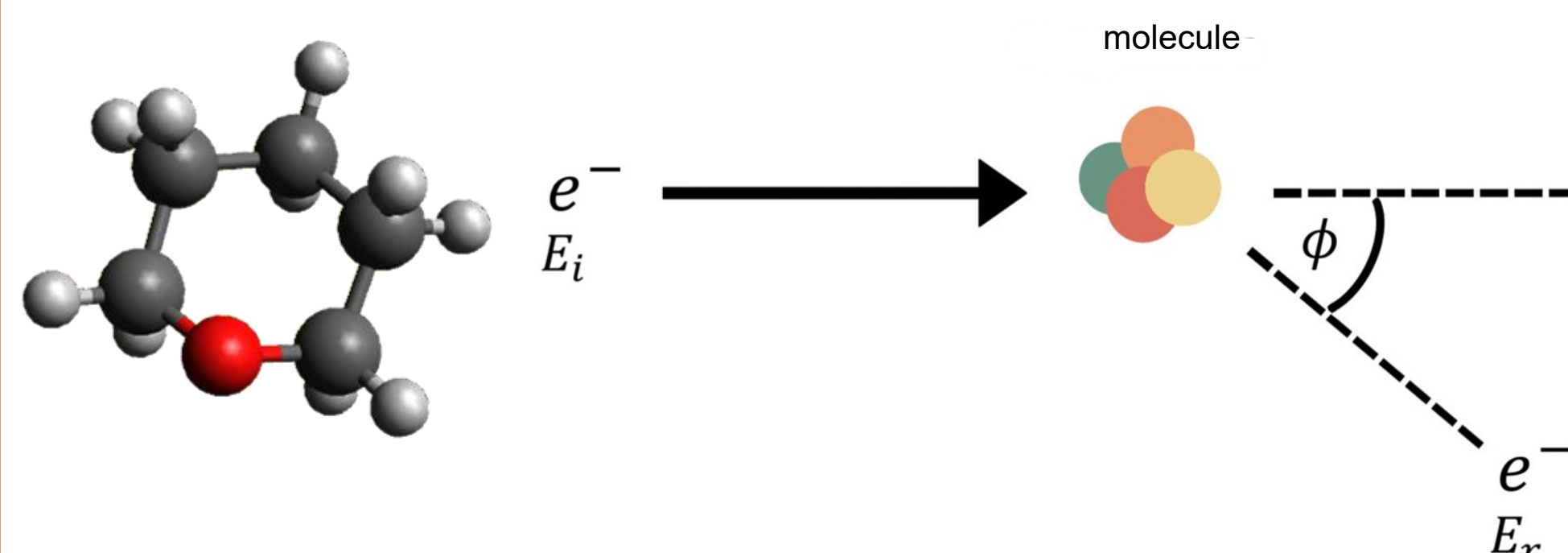
Exploring the Excited States of Tetrahydropyran using Electron Energy Loss Spectroscopy

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INTRODUCTION

Heterocyclic molecules play a crucial role in modern science due to their unique structural characteristics, which have inspired a wide range of research. Among these, a particularly intriguing group is the pyranoses – compounds containing rings composed of carbon and oxygen atoms. Their composition makes them especially relevant in the context of combustion science, where the presence of oxygenated structures is of notable interest. One representative member of this family is tetrahydropyran (THP, $C_5H_{10}O$), a six-membered saturated ring consisting solely of single bonds [1]. THP is non-carcinogenic, biodegradable, and does not form peroxides, making it a promising alternative to many traditionally used, hazardous chemicals. Furthermore, THP plays a vital role in nature, as it forms the structural backbone of several biologically significant molecules, such as glucose and ribose [2]. In recent years, scientific interest in the sustainable production of THP has grown considerably. It can be synthesized from lignocellulosic biomass, positioning it as an environmentally friendly alternative to conventional, less sustainable compounds [3]. Notably, THP has been identified as a potential next-generation biofuel – a development that could not only reduce reliance on fossil fuels but also help mitigate issues such as deforestation. As its production utilizes biomass, often considered a waste product, THP represents a sustainable solution with significant implications for the transportation sector [4]. Beyond its potential as a fuel, THP may also contribute to addressing the global plastic pollution crisis. It has been shown to act as a solvent for certain plastic materials. Thanks to its low toxicity and biodegradability, THP could replace traditional, more harmful solvents in industrial and environmental applications [3]. This fascinating molecule also finds extensive application in medicine, as it constitutes one of the most commonly utilized ring structures in pharmaceuticals [5].



Electron Energy Loss Spectroscopy focuses on the investigation of phenomena occurring during the electron scattering with molecules. This technique provides crucial information about the energies of excited states of the studied species, thereby offering insights into their electronic structure. A schematic representation of the experimental idea is shown in the figure below. An electron beam with an initial energy E_i is directed at a target molecule, and the scattered electrons are detected at an angle ϕ with a final energy E_r . Depending on the energy difference, calculated using the relation $\Delta E = E_i - E_r$, the collisions can be classified as either elastic, when $\Delta E = 0$, or inelastic, when $\Delta E > 0$. This value corresponds to the energy lost by the electron, which is simultaneously absorbed by the molecule. This energy is equal to the excitation energy of the species that are studied. One of the significant advantages of this type of measurement is its ability to probe optically forbidden states, such as triplet states. This is possible because the interaction mechanisms in electron scattering differ fundamentally from those involved in photon absorption. [6]

SUMMARY AND OUTLOOK

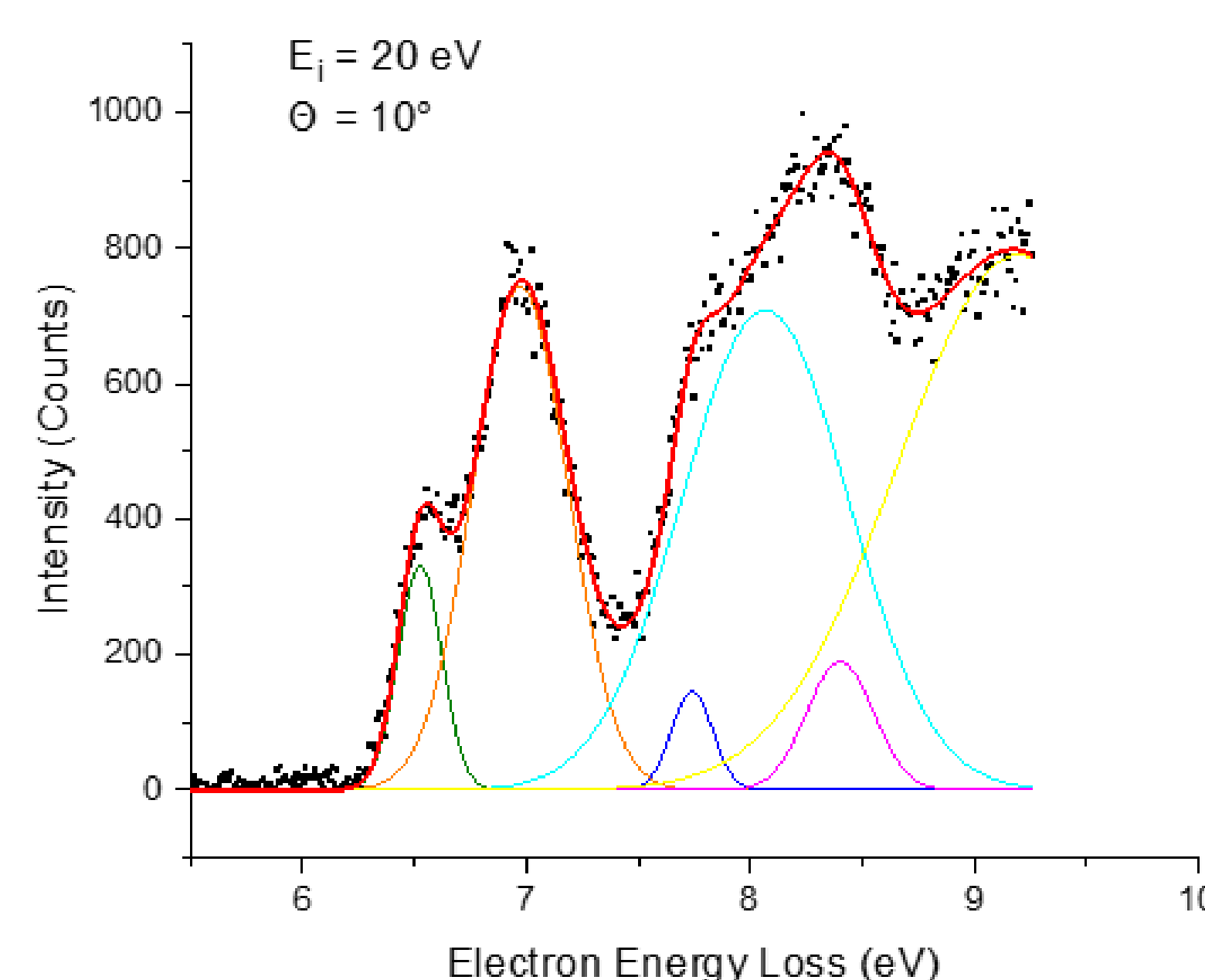
This work explores how electrons interact with tetrahydropyran (THP) molecules, using electron energy loss spectroscopy. By tuning the electron beam energy and scattering angle, it was possible to observe both singlet and triplet excited states, depending on the conditions. The energies of excited states in tetrahydropyran were determined. Future studies could expand on these findings by investigating related molecules and environmental effects to better understand the excited-state behavior of heterocyclic compounds.

REFERENCES

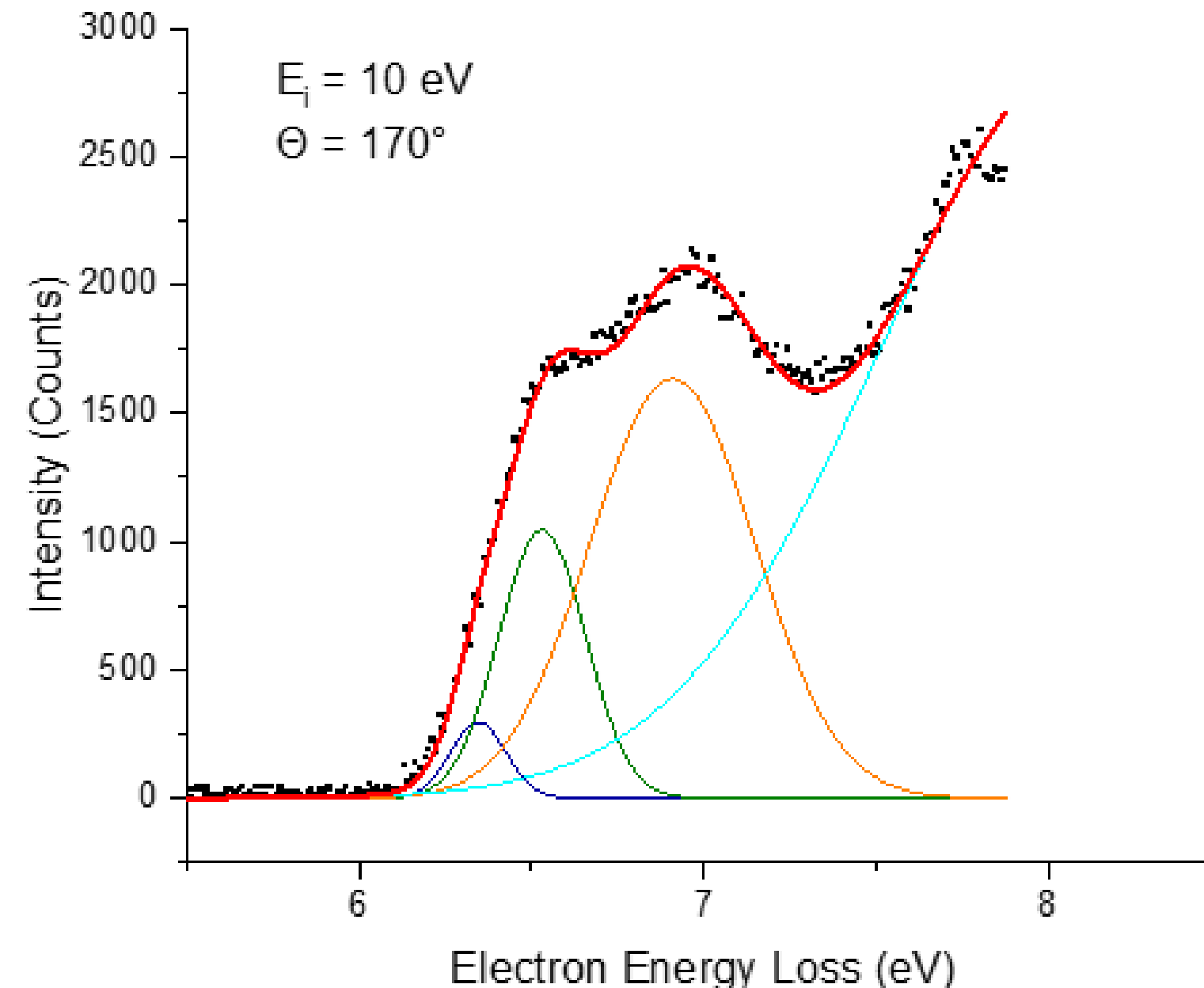
- [1] Avogadro: an open-source molecular builder and visualization tool. Version 1.2. <http://avogadro.cc/>
- [2] Gruet, S. et al. *Physical Chemistry Chemical Physics* 2019, 21 (6), 3016.
- [3] Dastidar, R. G et al. *Green Chemistry* 2022, 24 (23), 9101.
- [4] Labbe, N. J. et al. *Proceedings of the Combustion Institute* 2012, 34 (1), 259.

- [5] Shearer, J. *Journal of Medicinal Chemistry* 2022, 65, 13, 8699–8712
- [6] Linert, I.; Zubek, M. *Journal of Electron Spectroscopy and Related Phenomena* 2019, 233, 69.
- [7] <https://electronoptics.com/>
- [8] M. Wojdyr, *J. Appl. Cryst.* 2010, 43, 1126–1128

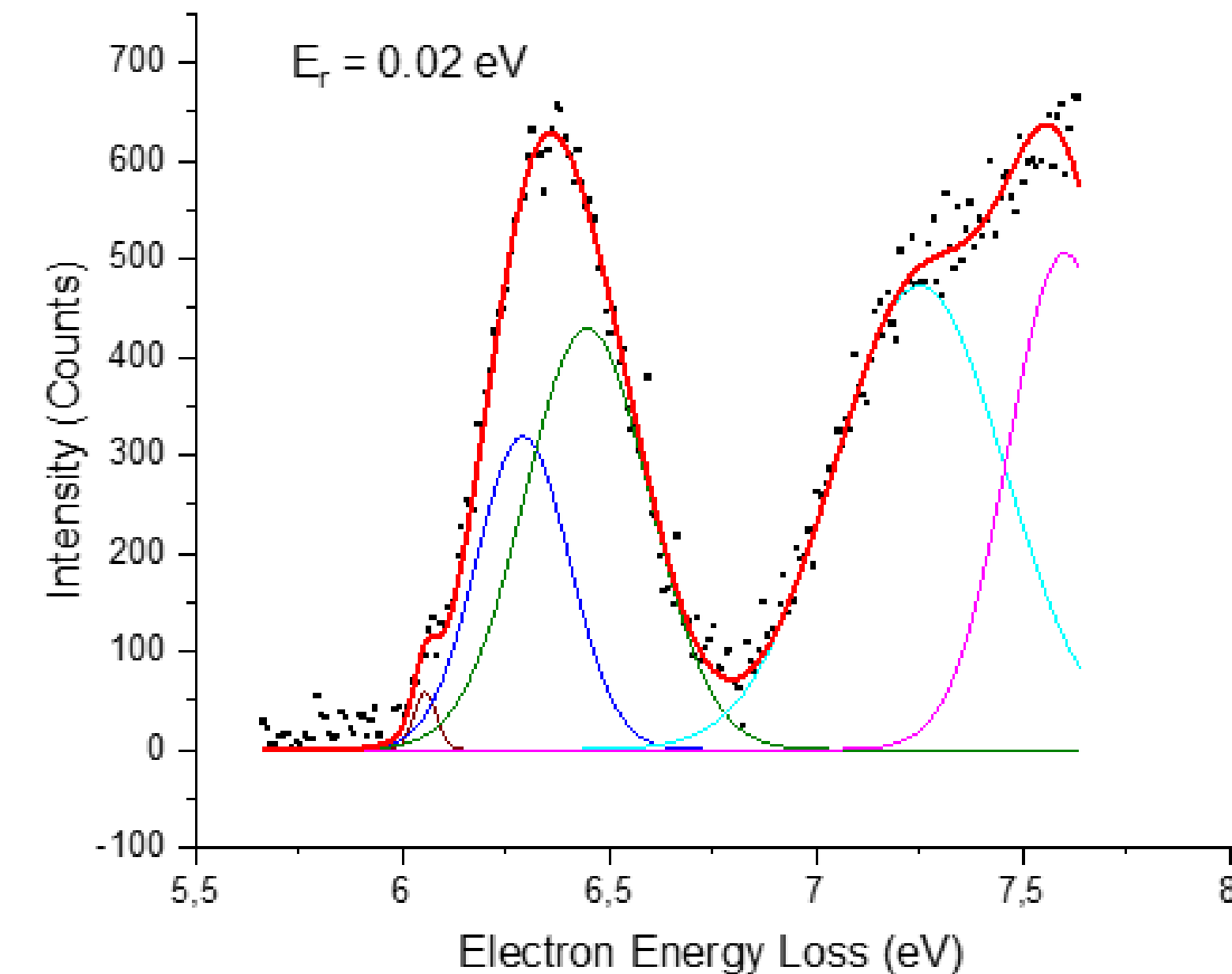
RESULTS



a) The spectrum shown in the first figure was recorded in constant primary energy mode. The incident energy was high but the scattering angle was small. Such experimental parameters promote the excitation of singlet states, which are exclusively observed in this case.



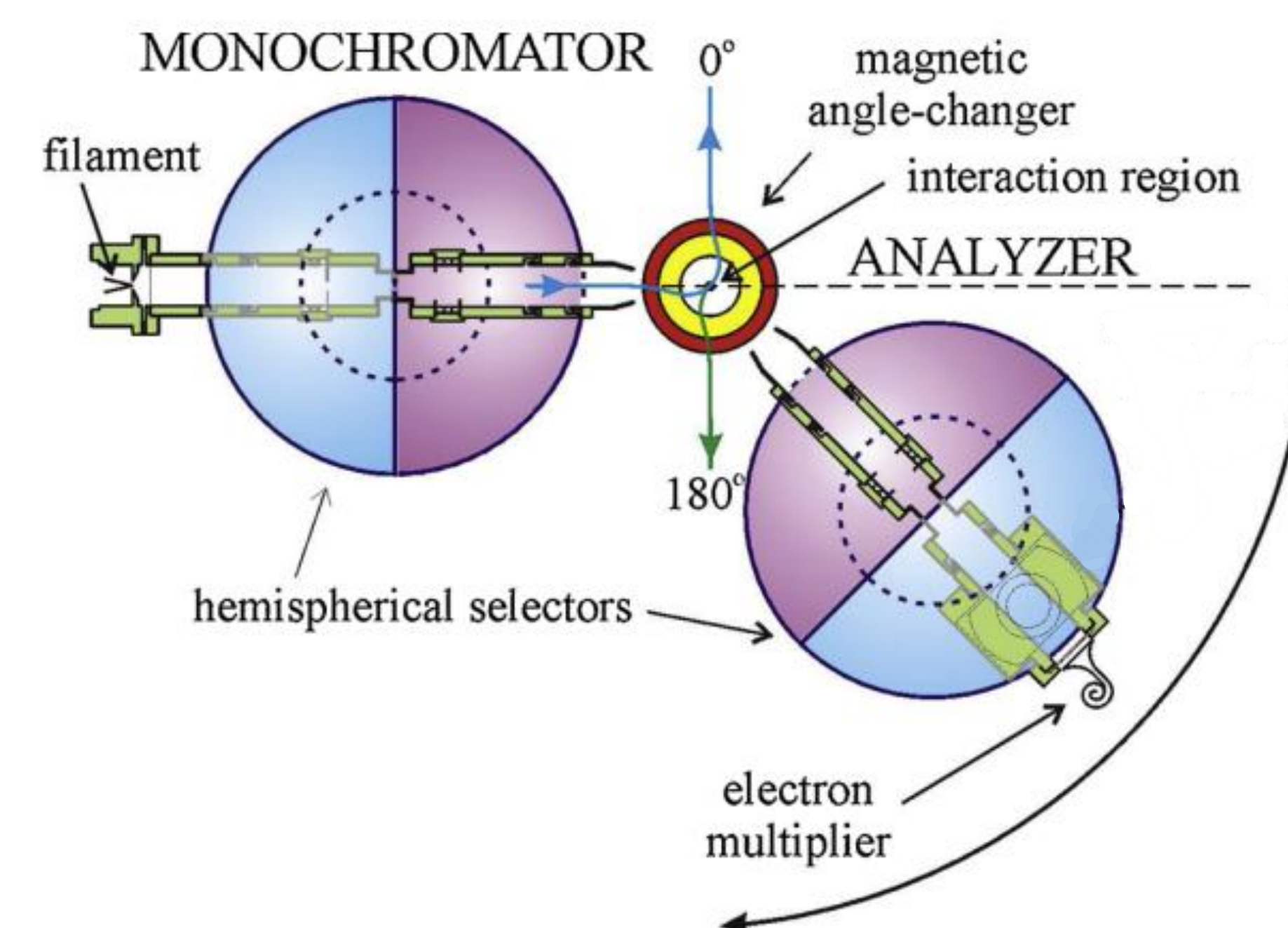
b) To enable the observation of triplet states, the experimental conditions were adjusted. In the spectrum presented in this figure, the primary energy was reduced and the scattering angle increased. Although singlet states are still present, the lowest-energy visible excitation corresponds to a triplet state.



c) Triplet states appeared more prominently in the threshold mode, where the residual energy was kept constant. In this mode, the entire energy of the incident electron is transferred to the molecule. Notably, the orange-colored triplet state observed previously is no longer present in the spectrum.

EXPERIMENTAL METHODS

Schematic diagram of experimental apparatus



The electron energy loss spectra of tetrahydropyran were measured using an electron spectrometer at the Laboratory of Complex Systems Spectroscopy, Gdańsk University of Technology. The spectrometer comprises three main sections: a monochromator, a scattering center, and an analyzer. The monochromator includes key components such as an electron gun, electrostatic lenses, and hemispherical energy selectors. Its primary function is to generate and select electrons based on their energy. The experimental setup features a magnetic angle changer, located in the scattering center. A capillary, positioned perpendicular to the electron beam, is used to produce the target gas beam. The electron analyzer can rotate around the axis of the gas beam in the range of 0° to 90° . Moreover, with the aid of the magnetic angle changer, this range can be extended up to 180° [6]. The trajectory of the electron beam was simulated using CPO program [7]. For threshold measurements, an electrostatic field technique was employed, utilizing an extracting electrode. The spectra were recorded in two modes: (a) at constant initial energy (E_i), and (b,c) at constant residual energy (E_r). Spectral fitting was performed using the Fityk software [8].

RESULTS

A list of experimentally determined excitation energies for tetrahydropyran, including both singlet and triplet states derived from fits to observed spectra measured under various experimental conditions.

State Type	Triplet	Triplet	Singlet	Singlet
Vertical Excitation Energy [eV]	6.08 ± 0.05	6.37 ± 0.07	6.55 ± 0.02	7.01 ± 0.05
FWHM of the peak	0.15 ± 0.06	0.26 ± 0.04	0.32 ± 0.08	0.60 ± 0.08

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