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THEORETICAL DEVELOPMENT OF NEW METHODOLOGIES FOR ILLICT DRUG ANALYSIS

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Ion mobility is a technique for the separation and structural analysis of molecules, in which a buffer gas is used to determine the flight time of a specific substance in a dedicated equipment. Coupling ion mobility with computational chemistry, precise structural information can be achieved. For this, ruge calculations of the collision cross-section (CCS) must be performed, being calculated with the trajectory method (TM). The interpretation of results, is still an arduous task, depending on the development of specific methodologies.

The objective of this work is to obtain CCS information for illicit drugs, contributing to the development of more effective analytical methods for the detection and quantification of these substances, as well as, provide accurate data for toxicological tests and other scientific applications.

For this purpose, relevant molecules were selected, then prepared and optimized using the Density Functional Theory (DFT), M06-2X. Single-point calculations, at the MP2 high-level, were performed to obtain atomic charges. The CCS calculations were performed using the HPCCS[2] software, allowing a direct comparison with the experimental data available in the literature. The results are presented in Figure 1.

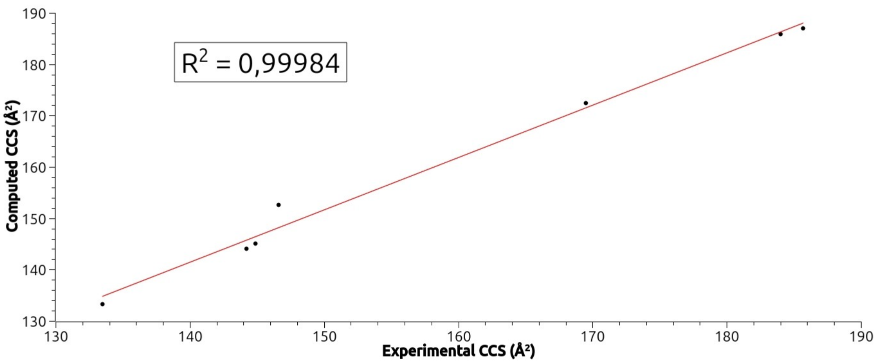

Figure 1: Experimental versus theoretical CCS data, in Å².

This analysis revealed a high correlation between theoretical and experimental values, average deviation 1.2%, validating the accuracy of the applied methodology . The database is being expanded, other molecules can be analyzed and detected from ionic mobility experiments.

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