AN INVESTIGATION OF THE STRUCTURE AND GAS PHASE ION CHEMISTRY OF THE HERBICIDE CHLORSULFURON BY HIGH FIELD FOURIER TRANSFORM ICR MASS SPECTROMETRY

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The environmental protection agencies of many countries now require full and detailed analysis of pesticides that occur in ground water and soil samples. Further, such agencies also now require that, throughout the development of new pesticides, the manufacturers of such compounds identify and quantify the active ingredient and its metabolites in various matrices. It is expected then that mass spectrometry will play an ever increasing role in active compound and impurity analysis in this industry.

In this paper we report on a high field (7 Tesla) Fourier transform ICR mass spectrometry study of the common herbicide, 2-Chloro-N-[[4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl] benzenesulfonamide commonly known as - *Chlorsulfuron.* As a sulfonamide, chlorsulfuron is widely used as a herbicide to control broad leaf weeds that can plague cereal crops. This herbicide acts by inhibiting certain enzymatic transformations in the weed after which it is hydrolyzed to a soluble chlorosulfonic acid, urea (a fertilizer) and a cyanuric acid derivative which is a fungicide.

The chemical structure of chlorsulfuron is shown in Fig. 1. This compound has previously been studied extensively by GC and LC chromatography[1] and also by mass spectrometry.[2] In this paper we report the electrospray ionization, laser desorption ionization and matrix assisted laser desorption ionisation FT/ICR mass spectrometry of this material. We will also present results from high resolution and tandem mass spectrometry studies on this compound.

FT/ICR mass spectrometry affords the opportunity to examine the gas phase ion-chemistry of such pesticides with various solvents thereby providing fundamental reactivity data devoid of external forces such as solvation and acidity.

A positive-ion ESI-FT/ICR mass spectrum of chlorsulfuron is shown in Figure 2. In this experiment a solution of chlorsulfuron in a (10:1) methanol:dimethylformamide mixture was used.

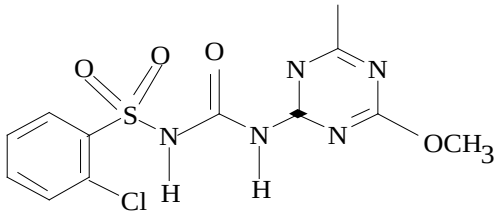

Figure 1. *The chemical structure of chlorsulfuron.*

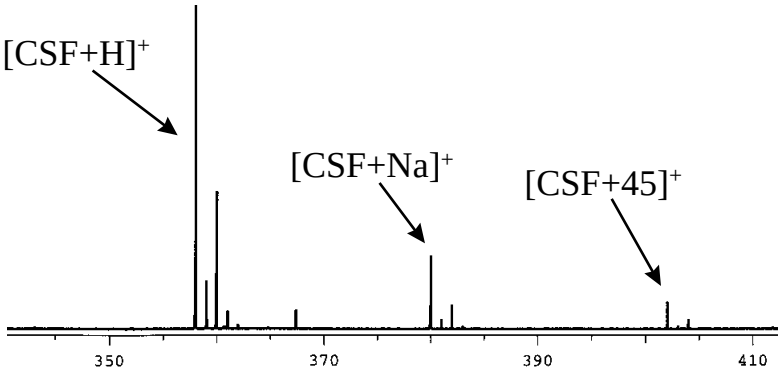

Figure 2. *Positive-ion electrospray ionisation FT/ICR mass spectrum of chlorsulfuron.*

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