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Experimental Evidence for Stable Ethane Dication in the Gas Phase*

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Abstract

The first experimental proof of the existence of stable ethane dication is reported. This $C_2H_6^{2+}$ species was generated by charge-stripping reaction in a mass spectrometer.

Ab initio calculations on $C_2H_6^{2+}$ have been reported recently [1, 2]. The authors pointed out that there was no experimental evidence so far for this species, but concluded that this ion might be observable under appropriate experimental conditions. Charge-stripping mass spectrometry [3] is a powerful technique for observing doubly charged ions and for measuring the energy needed to remove one electron from a singly charged ion (denoted as $Q_{min} = IE(m^+) - IE(m)$).

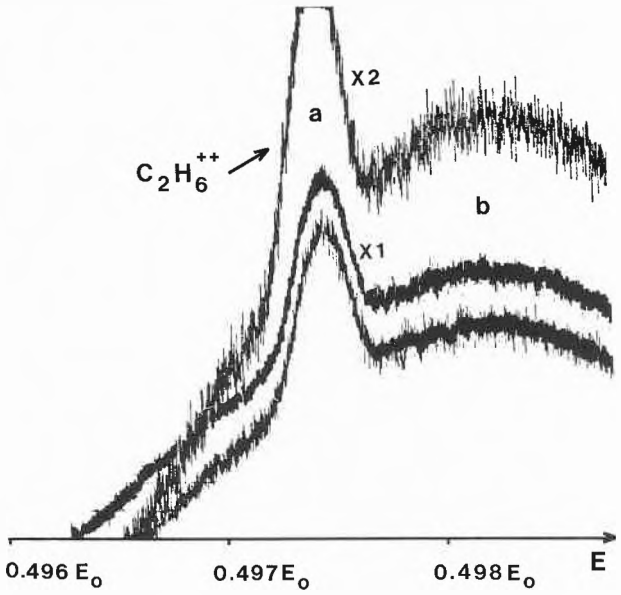

Fig. 1: Mass analyzed ion kinetic energy spectrum (MIKES) in the $E_0/2$ region.

A beam of $C_2H_6^+$ ions formed by electron impact of ethane in the ion source of a double focusing mass spectrometer of reverse geometry [4] was allowed to collide

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section of interest of the mass analyzed ion kinetic energy spectrum (MIKES) in the $E_0/2$ region [6]. The charge-stripping peak appears as a small bump (a) on the top of a large peak (b) corresponding to the collisional induced fragmentation of $C_2H_6^+$ into $CH_3^+ + CH_3^\cdot$. In spite of the composite nature of this signal it is possible to estimate quite accurately the minimum energy required for the process $C_2H_6^+ \rightarrow C_2H_6^{2+} + e^-$. Taking $Q_{min} = 15.7$ eV for the toluene molecule as a reference value for the calibration of the energy scale, the difference between single and double ionisation energies is found to be 18.4 ± 0.2 eV for the ethane molecule. In a forth-coming paper this experimental value will be compared with results of theoretical calculations and the properties of this doubly charged ion will be discussed [7].

Acknowledgement

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5 The experiments have been carried out on a VG-Analytical ZAB-2F mass spectrometer. $C_2H_6^+$ ions are produced by 70 eV electrons. They are accelerated by a potential of 8 kV and selected by the magnetic sector before colliding with O_2 at a pressure of about 10^{-4} T. Products of collisional induced reactions are studied by scanning the electrostatic analyzer.

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