

ZHANG Yahe, LU Hong, REN Limin, SHI Quan, XU Chunming, and GUO Shaohui, 2015. Determination of Unknown Compound in Aromatics by FT-ICR MS with Various Ionization Techniques. *Acta Geologica Sinica* (English Edition), 89(supp.): 439.

Determination of Unknown Compound in Aromatics by FT-ICR MS with Various Ionization Techniques

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Electrospray ionization (ESI) coupled with Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is a powerful technique capable of detecting heteroatom compounds, present in trace quantities in crude oil and its products without prior sample pretreatment. It enables the assignment of a unique elemental composition to each peak in the mass spectrum of petroleum samples. Compounds can be characterized by class (number of N, O, and S heteroatoms), type [double-bond equivalent (DBE) values, i.e., rings plus double bonds], and carbon number. The compositional differences of petroleum samples obtained by ESI FT-ICR MS can be used to identify the geochemical origins of crude oils and determine the degree of thermal maturity and biodegradation.

Unknown compound in petroleum aromatics was determined by Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) coupled with electrospray ionization (ESI), direct analysis in real time (DART) ionization, and atmospheric pressure photoionization (APPI). It was deduced as tris(2,4-di-tert-butylphenyl)phosphate (TDTBPP) by the accurate mass of FT-ICR MS and collision-activated dissociation (CAD). The characteristic spectra of TDTBPP in various ionization sources were demonstrated. APPI FT-ICR MS could determine the polycyclic aromatic hydrocarbons (PAHs) with a relative higher molecular-weight which could not be determined by gas chromatography-mass

spectrometry. FT-ICR MS will play an important role in geochemistry and exploration.

Acknowledgments

This work was supported by China Postdoctoral Science Foundation funded project (No. 2015M571226).

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