Molecular characterization of atmospheric particulates using Fourier transform ion cyclotron resonance mass spectrometry

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A significant component of the organic matter in atmospheric particulates is composed of “humic-like substances”. Molecular level charaterization of these has been limited in the past to compounds that are either extracted by organic solvents or chemically and thermally degraded from macromolecular precursors. We have recently introduced a new approach to molecular-level studies of humic substances from soils and natural waters-use of ultrahigh-resolution mass spectrometry available only from Fourier transform ion cyclotron resonance mass spectrometers [1]. This instrumentation allows us to identify unique elemental formulas for the types of organic molecules existing in atmospheric particulates. We also can evaluate the major compound classes to which these molecules belong and essentially provide an avenue for molecular characterization that has not been possible previously.

Our studies of aerosols collected in the Eastern USA [2], diesel exhaust, and aerosols from a plume of natural vegetation fires identify molecules of clear combustion origin intermixed with compounds having a clear vegetative or soil origin. Many of these soot or black carbon-derived compounds appear to be sulfur or nitrogen-substituted. Nitric acid oxidation of diesel exhaust and atmospheric particulates tends to enhance the production of these compounds.

It is obvious that a new approach for molecular characterization of the humic-like molecules in atmospheric particulates will revolutionize our understanding of the chemistry of these substances and can lead us to better understanding of their chemistry and role in atmospheric processes.

[1] Sleighter and Hatcher (2007) *J. Mass Spectrom*, **42**, 559–574. [2] Wozniak *et al.* (2008) *Atmos. Chem. Phys* **8**, 5099-5111.

Isotopic investigation of Hamamayagı hot water spring (Samsun, Turkey)

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In this investigation Ladik (Samsun) hot water spring has been studied from the point of geology and environmental ısotopes. The study area is located around middle-north of Turkey. In the studied area, Permian to Pliocene age, sedimentary unites interbedded with volcanic rocks are crop out. $\delta\ ^{18}O$, $\delta\ ^{2}H$ and $\delta^{3}H$ isotope analyses were carried out to determine the origin of waters, recharge altitude, precipitation types, groundwater circulation. In the ^{18}O, $\delta\ ^{2}H$ diagram all of the waters in the study area situated near the Globol Meteoric Water Line (MWL) and indicate meteoric origin. According to the ^{18}O- temperature relation all water samples recharged the same elevation in the plain. Due to the snowfall on the river in the winter a variation is occurred in ^{18}O values of the river water. Low tritium and high electrical conductivity value in the Hamamayağı Thermal Spring indicate that this spring has deep circulation. High tritium and low EC values in the in the Kocapınar Spring and Hamamayağı River show that these spring waters have shallow circulation. Tritium values of the Hamamayağı Thermal Spring is near the zero indicated that this spring water has deeply circulation. In order to determinate the origin of sulpher (SO_4) and carbon in the waters, all waters were analysed for their $^{13}C_{VPDB}$ (Bee Pee Belemnite) and $^{34}S_{CDT}$ (Canyon Diablo Triolite). According to the HCO_3-^{13}C relation in the thermal spring and cold spring, while HCO_3 contend of the cold spring is reduced, $\delta^{13}C$ value is increased. This situation in the thermal spring has opposite. Carbon in the Hamamayağı Thermal Spring has come different origins that are marine carbonates and fresh water carbonates, CO_2 gas from mantle origin. Carbon in the Kocapınar Spring and Hamamayağı River has controlled by CO_2 in the soil and subsurface pores. $\delta^{34}S_{CDT}$ values show that the sulphure has come different sources in cold and hot springs. $\delta^{34}S$ isotope compositions in Hamamayağı Thermal Spring come from rocks which are reduced sulphur compounds with respect to $\delta^{34}S_{CDT}$. Source of the sulpher in Kocapınar Spring and Hamamayağı River are formed limestone and shale in the study area.

[1] Craig, H., 1961. Isotopic Variations in Meteoric Water, *Science*, **133**, 1702-1703. [2] Clark, I. ve Fritz, P., 1997. *Environmental Isotopes in Hydrogeology, Lewis publıshers*, New York. 328 p.