

Non-target analysis of Murchison soluble organic matter by high-field NMR spectroscopy and FTICR mass spectrometry

N. HERTKORN*, M. HARIR AND PH. SCHMITT-KOPLIN

Helmholtz Zentrum Muenchen, German Research Center for Environmental Health, Research Unit Analytical Biogeochemistry (BGC), Ingolstaedter Landstrasse 1, D-85764 Neuherberg, Germany

(*correspondence: hertkorn@helmholtz-muenchen.de)

High field NMR spectra of Murchison meteorite methanolic extracts revealed primarily aliphatic extraterrestrial organic matter (EOM) with near statistical branching of commonly $C_{3,5}$ units separated by heteroatoms and aromatic units. Carbon NMR spectra were dominated by methylene and methyl carbon; strong apodization revealed methin carbon of which about 20% was aromatic. Extrapolation provided 5-7% aromatic carbon present in Murchison soluble EOM.

Compositional heterogeneity in Murchison methanolic extracts was visible in NMR and FTICR mass spectra obtained from a few cubic millimeters of solid Murchison meteorite; increasing sample size enhanced uniformity of NMR spectra. Intrinsic chemical diversity and pH dependent chemical shift variance contributed to the disparity of NMR spectra. FTICR mass spectra provided distinct clustering of CHO/CHOS and CHNO/CHNOS molecular series and confirmed the prevalence of aliphatic/alicyclic (73%) over single aromatic (21%) and polyaromatic (6%) molecular compositions, suggesting extensive aliphatic substitution of aromatic units as proposed by NMR.

Murchison soluble EOM molecules feature a center with enhanced aromatic and heteroatom content which provides rather diffuse and weak NMR signatures resulting from a huge overall chemical diversity. The periphery of Murchison EOM molecules comprises flexible branched aliphatic chains and aliphatic carboxylic acids. These project on narrow ranges of chemical shift, facilitating observation in one- and two-dimensional NMR spectra. The conformational entropy provided by these flexible surface moieties facilitates the solubility of EOM.