

Sulfur-assisted preservation of organic matter in sediments: Evidences from a sulfur-rich crude oil by FT-ICR MS

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There are extensive interactions between carbon cycle and sulfur cycle on Earth. One well-known example is the sulfurization of organic matter in sediments. Most previous studies were limited to the analyses of GC-amenable compounds, which occupy only a small part of sedimentary organic matter. Here, Fourier transform mass spectrometry (FT-ICR MS) coupled with electrospray (ESI) provide us a excellent chance to study the sulfurization mechanism of an immature sulfur-rich crude oil in a comprehensive way. A wider range of organic species were detected in the oil, including sulfur-containing S_x , O_xS_y , N_1S_x species and non-sulfur O_x , N_1 species. We found that the distributions of most sulfur-containing species and the corresponding non-sulfur species have similarity on the plot of relative abundance-DBE-carbon number, except that sulfur-containing species usually have higher DBE (Double bond Equivalent) values than their non-sulfur counterparts. For example, under positive-ion ESI mode, there are abundant compounds with carbon number = 40 in both N_1 and N_1S_x species though their DBEs are different in that the DBEs of N_1S_x species are usually higher than N_1 species by x . We speculate that those sulfur-containing species may share common precursors with their non-sulfur counterparts, and the different DBE values can be attributed to the existence of sulfur rings. These common precursors contain reactive functional groups such as double bonds at early diagenesis. The reactive functional groups can be stabilized through either hydrogenation or sulfurization, leading to the formations of non-sulfur compounds and organic sulfur compounds containing different number of sulfur atoms. Nevertheless, not all non-sulfur species have sulfur-containing counterparts in the oil. The precursors of these non-sulfur species lack reactive functional groups for sulfurization. Thus such precursors can only produce non-sulfur species at diagenesis.