CHARACTERISTICS OF NO COMPOUNDS IN SOURCE ROCKS FROM TWO DIFFERENT DEPOSITIONAL ENVIRONMENTS IDENTIFIED BY ESI FT-ICR MS

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Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) has been widely used in recent years in investigating NSO compounds in various oils (Ji et al., 2018). However, the composition and relative distributions of heteroatomic compounds in potential source rocks has seldom been reported (Wan et al., 2017), and the geochemical significance of the compounds in crude oils and related source rocks is still not sufficiently clear. The intention of this study is to investigate and compare NO compounds in shale extracts from the Dalong Formation in the Sichuan Basin and the Lucaogou Formation in the Junggar Basin in China, using negative ion electrospray ionization (ESI) coupled with FT-ICR-MS. These compounds were formed in marine and lacustrine sedimentary facies, respectively.

Marine shales sampled from the Dalong Formation in the Sichuan Basin are characterized by relatively high total organic carbon (TOC =10.60%), II1 kerogen type and relatively low maturity (Ro = 0.74%). In comparison, lacustrine shales from the Dalong Formation in the southern part of the Junggar Basin also feature relatively high TOC values (7.82%) and low thermal maturity (Ro = 0.78%) while presenting a better kerogen type (Type I). Both of these types can be classified as good source rocks with excellent petroleum potential. Marine source rocks from the Dalong Formation have relatively low abundances of gammacerane and C28 steranes, a low pristine/phytane ratio (0.89), and no (or trace) amounts of β-carotane. Lucaogou source rocks have almost inverse features, suggesting a different depositional environment for their source rocks.

Detection by negative ESI FT-ICR MS, shows that marine shales of the Dalong Formation contain abundant NO compounds - including N1, N1O1, N1O2, N1O3, N1O4, N1O1S1, O1, O2, and O3. The O2 class species predominates, with a lower content of O3 and N1 species relative to that of the O2 species, and the lowest content of N1O4 and N1O1S1 species. Compared with those of the Dalong Formation, lacustrine shales from the Lucaogou Formation possess a greater variety of NO compounds, such as N1O4, N1O1S1 and O3, in addition to N1, N1O1, N1O2, N1O3, O1, and O2 species. The latter is dominated by the N1 class species with O1 species having almost the lowest abundance. The shales also feature a lower abundance of N1O1 relative to O2.

It is suggested, based on previous research (Ji et al., 2018), that shales from the Dalong Formation are composed mostly of carboxylic acids (O2 compounds), particularly fatty acids. Shales from the Lucaogou Formation are composed mostly of pyrrolic compounds (Figure 1), especially carbazole (N1 compounds). Shales in the Lucaogou Formation have probably been biodegraded slightly, according to the TIC fingerprint and the ratio of Pr/nC17 and Ph/nC18 (<1), which is much lower than that of the Dalong shales (2.10~2.72 and 2.13~2.41, respectively). Biodegradation is suggested to have had a significant controlling influence on the composition and distribution of NO compounds, especially oxygen compounds (Wan et al., 2017), which might be responsible for the relatively high abundance of naphthenic acids in Lucaogou shales compared with Dalong shales (Figure 1).
The sedimentary environment of the Dalong Formation is a kind of platform facies, with silicon and phosphorus normally developed. The main source material may be benthic-macroalgae, nematothallus, and acritarchs, which contain less protein. The Lucaogou Formation was deposited under deep to semi-deep lacustrine reduction facies, with relatively high salinity in the water. The source material may feature relatively lower content of hydrobionts and phytoplankton and a relatively high abundance of protein. This might provide an explanation for the evidently higher abundance of N1 class species detected in the Dalong Formation than that found in the Lucaogou Formation (Figure 1).

Figure 1 Plots of DBE versus carbon number of the different species for the two source rocks analysed identified by negative ESI FT-ICR MS

ESI FT-ICR MS technology worked well for the characterization of N and O compounds in marine and lacustrine source rocks in this study. The marine environment is characterized by greater quantities of oxygenated compounds, while the lacustrine environment exhibits more nitrogenous compounds. The results show that ESI FT-ICR MS, operated in negative mode, is helpful for evaluating paleoenvironment, organic source input and secondary alteration of source rocks, and would prove useful in oil-oil and oil-source rocks correlation as well as in distinguishing and assessing secondary alteration.

Acknowledgements
This study was funded by the Natural Science Funding Council of China (Grant Nos. #41673055 and #41473047).

References