Advances in molecular geochemical characterisation of NSO compounds: Insights from a natural maturity series of crude oils

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Recent innovations in analytical class-type separation procedures and advances in high resolution characterization techniques now allow the nitrogen-, sulfur- and oxygen-containg (NSO), or so-called "polar" organic compounds, ubiqutious in petroleum fluids and source-rocks to be investigated in detail. Industrial interest in these hetero-functionalized compounds covers many subject areas and challenges, spanning exploration, field-development and production issues. Their importance lies in their structural diversity, which is the basis for significant variability in their physicochemical properties, giving rise to different behaviors during important physical and chemical processes.

In this study, we examined a well constrained suite of related crude oils derived from a common marine carbonate source and spanning a range of maturities (0.6 – 1.2% vitrinite reflectance equivalent, (%R_e)), for molecular compositional changes in NSO compounds with increasing thermal maturity. Comprehensive separation of the crude oils into discrete compound classes based on functionality, was achieved using both ion exchange and normal phase chromatography, generating fractions of saturated hydrocarbons, aromatic hydrocarbons, basic compounds, naphthenic acids, and other oxygen-containing species, carbazoles, sulphones and thiophenes from small samples of crude oil (0.25g). Total recoveries from the separation of the suite of oils were excellent (96-99.6%). Isolation of these discrete fractions allowed subsequent analysis by comprehensive two-dimensional gas-chromatography mass-spectrometry (GC×GC/MS) and/or liquid-chromatography high-resolution accurate-mass mass spectrometry methods (LC-HRAM-MS). We observe that significant distributional and compositional changes in individual NSO compound classes can be monitored at the molecular level. These changes and trends can be correlated against existing bulk property and conventional biomarker maturity parameters obtained for the same samples. The approach has the potential to be applied to numerous geochemical challenges.

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