FTIR quantification of the functional C groups in coals and extraterrestrial kerogens: a calibration procedure

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Introduction: Kerogens and coals are complex polyaromatic carbonaceous solids that formed in Earth sediments from the thermal maturation and preservation of living organisms [1]. Kerogen-like polyaromatic materials are also present in primitive meteorites, presumably formed in the proto-solar disk through thermal and/or radiolytic reactions and were further processed in their parent bodies [2]. Though decades of analytical investigations, the composition and chemical structure of those materials remain not fully elucidated. FTIR (Fourier-Transform Infrared Spectroscopy) has been proved to be a powerful technique for characterizing coals, peats, terrestrial and meteoritic kerogens [2]–[4]. However, the quantification of functional C groups by calculating of the integrated cross-section of each functional C groups is hampered by the lack of precise knowledge of their integrated cross-sections.

Our present work aims to investigate the infrared spectra using the different standards as known polymers [5] and synthetic polyaromatic materials (e.g. tholin), produced by thermal degradations of a ^{13}C-substituted precursor. It was synthesized in a cold plasma reactor (PAMPRE, Latmos, Guyancourt) from a $^{13}CH_4$: ^{13}CO = 7: 3 gas mixture with 90% of Ar [6]. Characterization of known molecular polymer and the carbonized tholin were performed and Nuclear Magnetic Resonance (NMR) measurements were then run, providing estimates of the integrated cross-sections ratio of the aromatic, C=C, C=O and CH_x groups. The carbonization process can increase the polyaromatic character in the tholin composition toward a structure similar to that observed in these terrestrial and extraterrestrial materials.

We will present the whole calibration procedure and applications to the quantification of the above-mentioned functional groups for coal and meteoritic kerogen samples. A series of coals with different vitrinite reflectances and some FTIR data of IOM samples from chondrites will be re-calculated to compare with the previous data to see the contribution of the relative abundance of carbon atoms regrading to the C=C, C=O, CH_3, CH_2 and aromatic groups.

References:

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