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

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Kerogens and coals are complex polyaromatic carbonaceous solids that formed in Earth sediments from the thermal decomposition of living organisms. 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 [1]. 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 [1]–[3]. 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. In this study, we have used standards as simple polymers and synthetic polyaromatic materials, produced by thermal degradations of a ^{13}C-substituted precursor. It was synthesized in a cold plasma reactor, named PAMPRE experiment (Latmos, Guyancourt) from a $^{13}CH_4$: ^{13}CO = 7: 3 gas mixture with 90% of Ar [4]. Nuclear Magnetic Resonance measurements were then run, providing estimates of the integrated cross-sections ratio of the aromatic, C=C, C=O and CH_x groups. We will present the whole calibration procedure and applications to the quantification of the above-mentioned functional groups for coal and meteoritic kerogen samples.

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