A Deconvolution Model to Approach the Functional Interpretation of ^{13}C-NMR spectra of Charcoals.

M. Melguizo[1], M. D. López[1], O. del Pico[2]

[1]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071-Jaén, Spain.
[2]Servicios Técnicos de Investigación, Universidad de Jaén, 23071-Jaén, Spain.

Charcoals are carbonaceous materials of high degree of aromaticity. Their ^{13}C-NMR spectra suffers from low sensitivity, and a lack of resolution arising, at least in a great part, from the extremely high anisotropy caused by the graphite content of these materials, that increases with the final temperature at which they are subjected.[1] Although the CP-MAS technique has been used to obtain ^{13}C spectra of coals, the direct polarization (DP) MAS has proven to produce more reliable quantitative information for charcoals, as well as for other highly graphitized carbons of low hydrogen content.[2] But even under the best acquisition conditions, the spectra of charcoals largely consists of a main broad peak at around 120 ppm (attributable to aromatic carbons) having a width-at-half-high (WHH) of several tens of ppm, accompanied by some other small broad peaks, some of which overlap with the referred main band.

Due to such notable lack of resolution, the structural interpretation of ^{13}C- NMR spectra of charcoals and other carbonaceous materials has been approached through deconvolution models that decompose the original broad signal into resonance peaks assignable to chemical functions commonly found in carbons.[3,4] However no general agreement exists about the set of peaks that better fit the measured curves and its correlation with chemical groups present in the analysed material. Then, based on previous models and on detailed analysis of chemical shift of polycyclic aromatic hydrocarbons[5, 6] a new deconvolution model is proposed whose consistency and usefulness for the analysis of chemical functionality in charcoals is discussed.

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