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Characterization of Nitrogen Compounds in Vacuum Residues by Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

Keiko Miyabayashi[1)], Yasuhide Naito[1)], Kazuo Tsujimoto[1)] and Mikio Miyake[1)]

1) School of Materials Science, Japan Advanced Institute of Science and Technology

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The structural characteristics of the components of several vacuum residues from different geological sources (Taching, Sumatra light, Iranian heavy, Arabian mix, and Murban vacuum residues) were investigated by electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI FT-ICR MS) without chromatographic pre-separation. The present approach can detect basic nitrogen compounds in vacuum residues with high selectivity. The mass spectra showed differences in both average and range of molecular weights depending on the origin. Accurate masses were used to estimate molecular formulas. All observed peaks were assigned to mononitrogen-containing compounds (major components) or both mononitrogen- and monosulfur- containing compounds (minor components). Homologue analysis for all estimated molecular formulas showed the analogies and peculiarities in components of the five vacuum residues. Every observed compound was sorted by hydrogen deficiency index (Z-value: $[C_nH_{2n+Z}N_mS_s+H]^+$) and carbon number. The distribution center of the Z-values depended on the vacuum residue origin and the maximum value decreased as follows: Taching (−17) > Sumatra light (−19) > Iranian heavy (−21) ≥ Arabian mix (−21) > Murban (−25). Taching vacuum residue contained low absolute Z-values compared to the other vacuum residues from the Middle East. The results obtained by ESI FT-ICR MS were in good accordance with reported findings of highly condensed aromatic compounds in Middle East vacuum residues contains compared to Chinese vacuum residues.

Keywords: Vacuum residue, Structural characterization, Nitrogen compound, Electrospray ionization, FT-ICR, MS

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