Compositional Analysis of Oil Residues by Ultrahigh Resolution Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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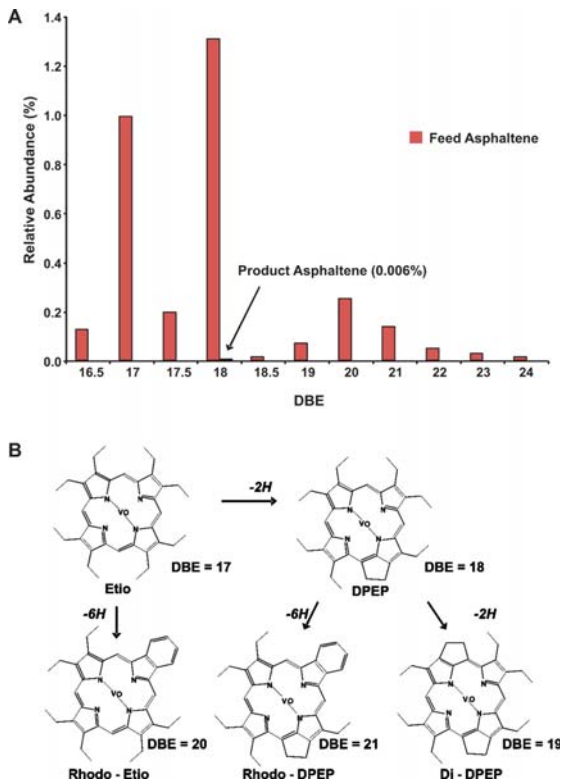
Results and Discussion

Ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry was used for compositional analysis of polar and asphaltene fractions of complex oil residues. The samples were collected before and after the processing of oil in a residue hydrocracking unit, in which the feed oil was the vacuum distillation residue of the crude oil, and the product sample was the residue collected after the processing. From the asphaltene fraction, as many as ~26 000 peaks were detected by atmospheric pressure photoionization and more than ~33 000 peaks by positive-ion electrospray ionization (ESI), with up to 18 distinct heteroatom classes identified. Negative-ion ESI provided complementary information through selective ionization of acidic compounds. The detected species were sorted based on heteroatom class, carbon number, and aromaticity (double bond equivalents, i.e., number of rings + double bonds to carbon). The N_1 class compounds were predominant in both fractions of the feed and product oils. The sulfur-containing compounds were mainly degraded or removed during the processing as expected. Vanadyl porphyrins (heteroatom class $N_4O_1V_1$), detected in the asphaltene fraction of the feed oil, were not observed in the product oil fractions, consistent with their efficient removal **(Figure 1)**. Increase in the aromaticity for the most heteroatom classes was generally noted in both polar and asphaltene fractions.



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References

[1] Kekäläinen, T., *et al*., Energy & Fuels., **27**, 2002-2009 (2013)