Compositional Space Boundaries for Organic Compounds

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Results and Discussion

An upper elemental compositional boundary for fossil hydrocarbons has previously been established as double bond equivalents (i.e., DBE = rings plus double bonds) not exceeding 90% of the number of carbons number. For heteroatom-containing fossil compounds, the 90% rule still applies if each nitrogen atom is counted as a carbon atom. The 90% rule eliminates more than 10% of the possible elemental compositions at a given mass for fossil database molecules. However, some synthetic compounds can fall outside the upper boundary defined for naturally occurring compounds. Their inclusion defines an "absolute" upper boundary as DBE (rings plus double bonds to carbon) equal to carbon number plus one, and applies to all organic compounds including fullerenes and other molecules containing no hydrogen (see **Figure 1**). Finally, the DBE definition can fail for molecules with particular atomic valences. We therefore also present a generalized DBE definition that includes atomic valence to enable calculation of the correct total number of rings, double bonds and triple bonds for heteroatom-containing compounds.[1]

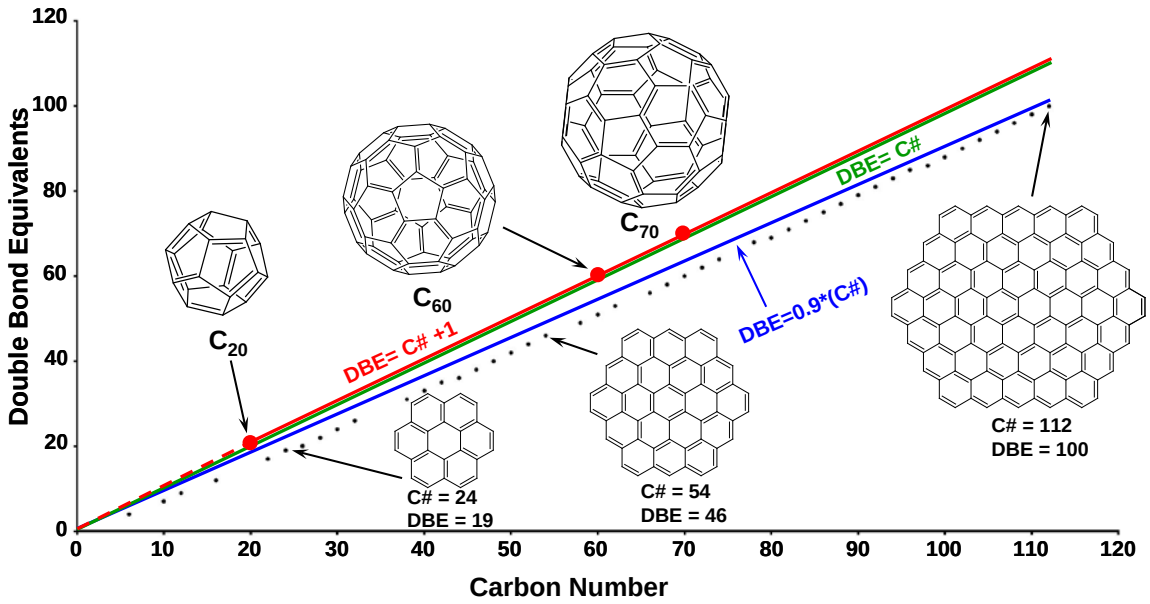

Figure 1. DBE versus carbon number plot for hydrocarbons, C_cH_h. The blue line (DBE = 0.9*C#) defines the upper compositional boundary for fossil hydrocarbons. The green line (DBE = C#) applies to all hydrocarbons (including synthetic polyynes), and the red line (DBE = C#+1) represents the absolute upper limit for organic compounds that lack H and N atoms.

Acknowledgements

Work supported by NSF Division of Materials Research (DMR-0654118) and the State of Florida. We thank Ms. Ekaterina V. Maksimova from the Department of Earth, Ocean and Atmospheric Sciences (Florida State University) for preparation of Figures 5-7 and Dr. Janne Janis (University of Eastern Finland) for providing the asphaltene sample.

References

[1] Lobodin, V. V., *et al.*, Anal. Chem. **84**, 3410-3416 (2012).