

Measured and Simulated Electronic Absorption and Emission Spectra of Asphaltenes

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The electronic absorption and emission spectra of petroleum asphaltenes are distinct and characteristic; indeed, asphaltene “color” is one of the canonical properties of asphaltenes. Moreover, each π -electron has a fixed oscillator strength; thus, each aromatic carbon and nitrogen is represented in the absorption spectrum. Nevertheless, these spectral origins have not previously been thoroughly explored. Most importantly, there has been significant controversy regarding the types of polycyclic aromatic hydrocarbons (PAHs) contained in asphaltenes, with grossly different PAH distributions being reported. Here, we show that the main features of the absorption and emission spectra of asphaltenes are accounted for using a distribution of 523 PAH model compounds incorporating heteroatom substitution. This distribution is discussed in terms of PAH classes. In particular, we have used a distribution with 7 fused aromatic rings as most likely along with a slow drop off for contributions from smaller and larger PAHs. In addition, a “tail” of large PAHs is assumed. Another PAH distribution consisting of very small PAHs proposed in the literature is shown to be very inconsistent with measured asphaltene spectra. In particular, small PAHs absorb strongly in the UV spectrum but not in the visible spectrum; asphaltenes show a much smaller contrast between UV and visible absorption as shown herein. That is, if the π -oscillator strength is not in the near-infrared and visible spectra, then it must be in the UV spectrum.