

عنوان مقاله:

Degradation Pathway of Volatile Organic Compounds of Bitumen in the Presence of Sulfur-Doped Phenol-Rich Bio-oils

محل انتشار:

هفتمین کنفرانس ملی شیمی و توسعه فناوری نانو (سال: 1402)

تعداد صفحات اصل مقاله: 18

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خلاصه مقاله:

We have developed an efficacious methodology for degradation of volatile organic compounds (VOCs) from the matrix of bitumen under visible-light conditions which time dependent density functional theory (TD-DFT) analysis supports the degradation of VOCs by sulfur-doped phenol-rich bio-oil ($S_{4^{\wedge}0}-WPn$ ($n = 1-3$)) prepared by C-S coupling reaction. This method involves two sequential reactions where the degradation of the VOCs is followed by sulfur-doped phenol-rich bio-oil ($S_{4^{\wedge}0}-WPn$ ($n = 1-3$)) with C-S coupling reaction. This study examines how sulfur-doped phenol-rich bio-oil ($S_{4^{\wedge}0}-WPn$ ($n = 1-3$)) reduces the emission of the VOCs from the bitumen matrix. To do so, we have evaluated the degradation pathway of two bitumen VOCs (Benzoic acid and Benzofuran) by $S_{4^{\wedge}0}-WPn$. TD-DFT results indicate that the $S_{4^{\wedge}0}-WPn$ have the potential to retain these VOCs in the bitumen matrix. Our calculations also predict that the reaction of tetrameric radical sulfur ($S_{4^{\wedge}0}$) with bio-oil (WPn) and subsequent VOCs could accelerate the degradation of VOCs while diminishing bitumen aging. To gain insight into the C-S cross-coupling mechanism, we have performed UV-Vis spectroscopic measurements for VOCs and VOCs- $S_{4^{\wedge}0}-WPn$ compounds. TD-DFT calculations also predicted a significant red shift in UV-Vis spectroscopic absorption spectrum at 400 nm albeit with a weaker absorption when $S_{4^{\wedge}0}-WPn$ and VOCs reacted and these peaks resulted from the degradation of VOCs. The study outcomes show the efficacy of sulfur-doped phenol-rich bio-oils in the degradation of selected VOCs. An interesting phenomenon was found that UV-Vis spectroscopic absorption red shift (~200 nm) occurs after the C-S coupling reaction between $S_{4^{\wedge}0}-WPn$ and VOCs. The absorption spectral of (VOCs- $S_{4^{\wedge}0}-WPn$) has been red-shifted to nearly 400 nm. The red shift enhanced the ability of these VOCs compounds to absorb light at a wavelength higher than 400 nm, thereby favoring the direct photodegradation of VOCs compounds.

کلمات کلیدی:

Volatile Organic Compounds, Bitumen, Degradation, Phenol, Sulfur, Ultraviolet Aging

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