عنوان مقاله:

Computational study on energetics and structure of coronene as one of ingredients of the petroleum-refining process

محل انتشار:

چهارمین همایش بین المللی نفت،گاز و پتروشیمی (سال: 1396)

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خلاصه مقاله:

Quantum chemistry methods were used to study energy data and geometry of coronene. Also, curved coronenes was considered to examine role of structure on molecular properties of polycyclic aromatic hydrocarbons (PAHs). Indeed, aromaticity at 1 Å above and 1 Å below of central rings of coronene and curved coronenes was calculated using nucleus independent chemical shift (NICS) criterion. Moreover, binary complexes which are formed from interactions of coronene with curved coronenes (or interactions of curved coronenes with each other) were considered to determine in what ways change of structure influences on π-π stacking interactions. Results indicate that curvature of coronene leads to structural changes and influences on binding energy values of the complexes.

کلمات کلیدی:

coronene, PAHs, π-π stacking, aromaticity, NICS