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Structures and energetics of hydrocarbon molecules in the full hydrogen chemical potential range YONGXIN YAO, TZU-LIANG CHAN, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University — Hydrocarbons, especially polycyclic aromatic hydrocarbons (PAH), attract much interest as candidates for the unidentified infrared bands (UIRs), UV extinction curve and diffuse interstellar bands in the interstellar medium. While many experiments and quantum chemical calculations of the infrared spectra on human-selected hydrocarbons have been done, it remains an open question. A key reason may be the complicated phase space of hydrocarbons originated from the enormous bonding ability of carbon. Here we present a series of unbiased global search for hydrocarbon molecules (CnHm, 1<n<50) in the full hydrogen chemical potential range. The search is based on Genetic Algorithm (GA) combined with Brenner's hydrocarbon empirical potential and our new tight-binding potential. The structures and energies from GA are checked at both DFT and MP2 level. Such a mini database is reported, which is supposed to give more helpful information on hydrocarbon-related researches.

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