Dynamical nonplanarity of benzene. Evidences from the Car-Parrinello molecular dynamics study.

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Rok wydania

2011

Czasopismo

Journal of Physical Chemistry Letters

Numer woluminu

2

Strony

2881-2884

DOI

10.1021/jz201327t

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Car–Parrinello molecular dynamics simulation of an isolated benzene molecule unextectedly revealed very low population of a planar geometry of the ring (less than 10%) despite the ideal aromatic character of a cyclic conjugated system. Analysis of nonplanar conformations of benzene in terms of puckering parameters demonstrates that benzene in the gas phase exists mainly as a mixture of two mirror-symmetrical families of flattened boat and twist boat conformations with a total population of more than 70%. The average conformation of the ring is nonplanar with values of endocyclic torsion angles of 6.7°.

Słowa kluczowe

benzene, confomational flexibility, Car−Parrinello molecular dynamics, nonplanarity

Adres publiczny

https://doi.org/10.1021/jz201327t

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html