New aspects of weak C-Hp bonds: intermolecular interactions between alicyclic and aromatic rings in crystals of small compounds, peptides and proteins.

Autorzy

Zbigniew Ciunik

Sławomir Berski

Zdzisław Latajka

Jerzy Leszczyński

Rok wydania

1998

Czasopismo

Journal of Molecular Structure

Numer woluminu

442

Strony

125-134

DOI

10.1016/S0022-2860(97)00288-3

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The geometry of intermolecular contacts between alicyclic and aromatic rings in a number of crystal structures suggests an attractive interaction between the rings. An analysis of molecular packing of 444 different crystal structures collected in the Cambridge Structural Database shows that phenyl… cyclohexanonyl, cyclohexyl, and/or cyclopentyl ring interactions occur in 59-82% of studied crystals. Similar interactions are observed between aromatic rings and heterocyclic pyrrolidine rings of proline in peptides and proteins. An analysis of data collected in the Brookhaven Protein Data Bank reveals that interactions between proline C□H groups and aromatic rings of phenylalanine, tyrosine, and tryptophan as acceptors are frequently observed in proteins. Based on these results, several geometric models of these interactions are proposed. Two of these models are fully optimized using quantum chemical calculations at the density functional theory level. Calculated energies suggest that the most important interaction between the cyclohexanone and benzene rings is described by the face-to-face model, in which three axial hydrogen atoms are directed toward the aromatic partner.

Adres publiczny

http://dx.doi.org/10.1016/S0022-2860(97)00288-3

Strona internetowa wydawcy

http://www.elsevier.com