Isomerization and dissociation of CHNS : quantum mechanical study.

Autorzy

Maria Wierzejewska

Jerzy Moc

Rok wydania

2003

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

107

Strony

11209-11216

DOI

10.1021/jp030971b

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

An extensive quantum mechanical study of the potential energy surface for the isomerization and dissociation reactions of CHNS is reported. The calculations were performed using density functional theory and correlated ab initio methods and employing large aug-cc-pVTZ basis set. Nine CHNS isomers and eleven transition states linking them have been found on the singlet PES. Dissociation energies of the singlet most stable open chain CHNS isomers have been evaluated. On the triplet PES, eight mostly highly energetic CHNS isomers and five transition states for their interconversion and dissociation have been also found. Several available routes for isomerization and dissociation have been identified. A prediction has been made for the possible mechanism explaining the formation of the singlet HSCN and HSNC during UV photolysis of HNCS/Ar and HNCS/N_2 low-temperature matrixes observed recently by one of us.

Słowa kluczowe

Molecular structure, Isomerization, Potential energy, Dissociation, Transition states

Adres publiczny

https://doi.org/10.1021/jp030971b

Strona internetowa wydawcy

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