

A quantum chemical study of the 5-aminomethinimino-3-methylisoxazole-4-carboxylic acid phenylamides-A new lead structure in the immunosuppressing agents.

Autorzy

Stanisław Ryng

Michał Zimecki

Adam Fedorowicz

Aleksander Koll

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Streszczenie

Infrared spectra of HCl-doped CO solutions have been studied at $T \sim 140-90$ K. First overtone and combination bands of the $\text{OC}\cdots\text{HCl}$ complex were revealed at the lowest temperature of the liquid solution. Ab initio calculations utilizing the 6-311++G(3df,3pd) basis set with electron correlation at the n th-order Møller–Plesset (MP n , $n \leq 4$) levels of approximation predict minima for the $\text{CO}\cdots\text{HCl}$ and $\text{OC}\cdots\text{HCl}$ linear structures. Based on simplified treatment of anharmonic interactions between CO and HCl constituents, the model estimations of the dipole transition moments have been performed.

Adres publiczny

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