Calculation of trans-hydrogen-bond ^{13}C-^{15}N three-bond and other scalar *J*-couplings in cooperative peptide models. A density functional theory study.

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We report B3LYP DFT calculations on peptide models that consider the effects of cooperative interactions with proximate H-bonds and local geometry at the H-bonding site upon trans-H-bond $^{13}C–^{15}N$ three-bond scalar *J*-couplings. The calculations predict that cooperative interactions with other H-bonds within a H-bonding chain can significantly increase the magnitude of these couplings. Such increases are due to a combination of the presence of the neighboring H-bonds and the slight increase in CO distances expected for peptide H-bonds near the centers of H-bonding chains. The energies of H-bonds inferred from H-bonding distances, alone, could be significantly in error if the effects of neighboring H-bonds are ignored.

Słowa kluczowe

Chemical calculations, Coupling reactions, Mathematical methods, Oligomers

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