Using the transferability to predict the infrared intensities of dipeptides, from a test set of amino acids.

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Abstract

The infrared intensities of 10 essential L-amino acids were calculated through B3LYP/6-311+G(d,p) and glycylglycine, The intensities of the main characteristic absorption bands are rather transferable, capable of making predictions on dipeptides.

Introduction

For some time our research group has been working on improving and developing new applications for Quantum in Theory Atoms in Molecules (QTAIM) electronic parameters, especially for the interpretation of charge transfer and polarization effects. The objective of this work, with is in its very early stage, is to use our new developed dynamic atomic contributions (DAC) to test the transferability of infrared intensities o amino acids, and to predict the intensities of glycylglycine.

Results and Discussion

One of the new features of our work, presented for the first time in this abstract, is the use of a new, and completely updated software's. The geometric optimizations of the amino acids were performed with GAUSSIAN 09, as the vibration analysis. In both cases DFT was used, as B3LYP/6-311+G(d,p) level was chosen.

The amino acids chosen were: L-alanine, L-asparagine, L-Cysteine, L-phenylalanine, L- Aspartic acid, L-methionine, L-serine, L-glycine, L-tyrosine and L-histidine. The dipeptide that had its infrared intensities predicted was glycylglycine. Table 1 contains the average of the frequencies and intensities of these ten amino acids for their most prominent vibration groups.

Table 1. Average of the vibrational intensities and frequencies for the ten amino acids calculates through the B3LYP/6-311+G(d,p) level

Vibration	Frequencies	Intensities
O-H str	3768,5±28	71,27±8,5
NH_2 str A	3596,7±14	14,39±6,5
NH_2 str S	3511,4±10	5,34±2,7
C=O str	1810,1±6	330,68±19,7
NH_2 bend	1653,2±17	61,46±31,6

One can see from Table 1 that the frequencies of the characteristic vibrations are much more transferable than the respective intensities as the standard deviations are about 1% of the frequency average.

On analyzing the intensities becomes clear that, even though all intensities are somewhat transferable, some of the absorption bands are much more transferable than others. The most transferable absorption band is the C=O stretch, as the standard deviation is just under 10% of the average intensity. Unpublished results of our group can explain that observation with the fact that in many carbonyls the C=O stretch can be reproduced solely by the electronic alterations on the carbon and oxygen atoms.

The comparison between the transferred averages and the calculated intensities for glycylglycine is presented in Figure 1

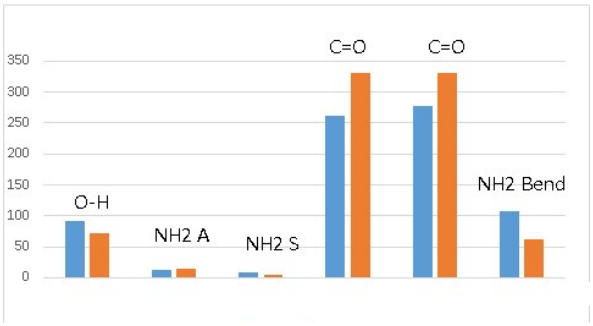

Figure 1. Comparison between the predicted values for the intensities of glycylglycine and the predicted ones from the amino acids

Conclusions

From Table 1 and Figure 1 becomes clear that the intensities of amino acids do not vary substantially among the test set, and that they are capable of making reliable predictions or a peptide.

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