

Figure 1: optimized structure of the dipeptide Asn Gly.

The radical anions and cations were then considered. Figure 2 displays the result concerning the radical cation.

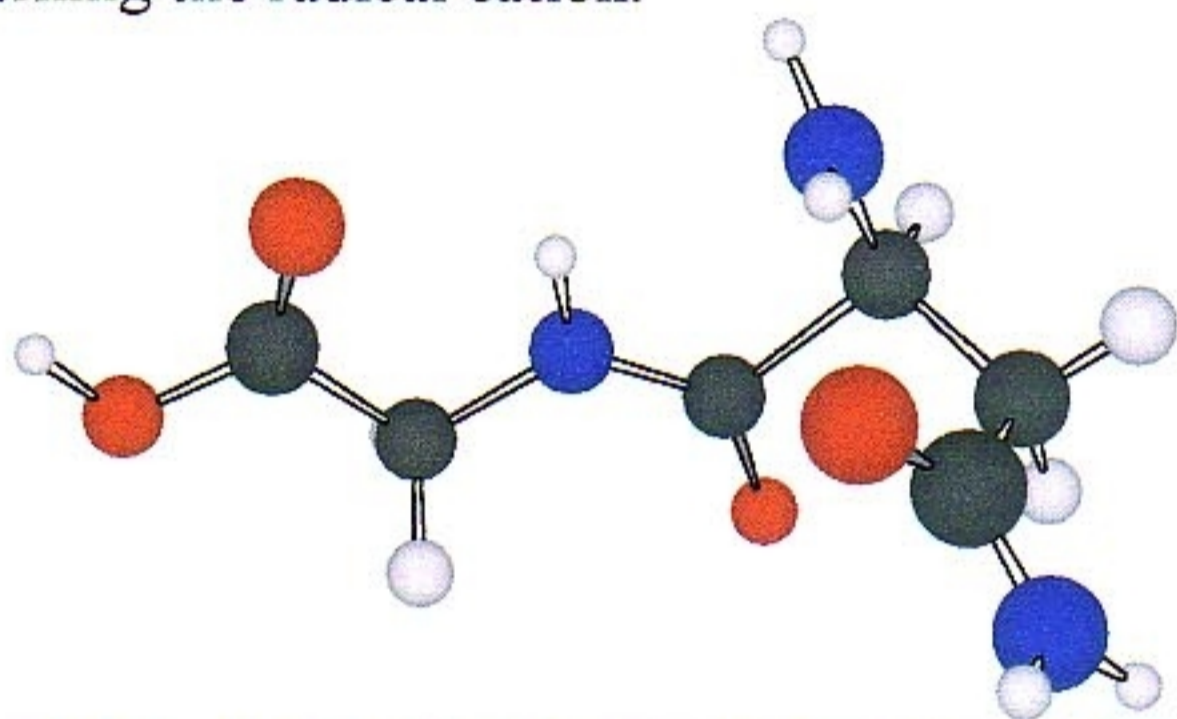


Figure 2: optimized structure of the dipeptide Asn Gly radical cation

In the radical cations from Asn Gly and Gly Asn, the spin density is mostly on the N-terminal. As for the radical anion, it is mostly on the carboxylic acid function.

We intend to continue this work by studying the following five dipeptides (Gly-Asn, Val-Asn, Met-Asn and Asn-Val and Asn-Met). These peptides were selected in order to study the influence of neighboring aminoacids and a sequence of amino acid residues on the character of radicals formed in asparagine residue. Some mechanism of formation and decay of free radicals can be deduced.

In addition, Prof. K. Bobrowski delivered a talk on Friday, May 12th. The title of his presentation was "Stabilization of sulfide radical cation: mechanisms relevant to oxidation of peptides and proteins containing Methionine". The support of the COST action was also acknowledged.