Theoretical study of the gas-phase decomposition of neutral ?-amino acid ethyl esters. Part 1 - The elimination of N,N-dimethylglycine ethyl ester and ethyl 1-piperidineacetate

Quijano, Jairo

Notario, Rafael

Chamorro, Eduardo

León, Luis A.

Sánchez, Claudia

Alarcón, Gustavo

Quijano, J. Camilo

Chuchani, Gabriel

Theoretical studies of the thermolysis of two ?-amino acid ethyl esters in the gas phase were carried out using ab initio theoretical methods, at the HF/6-31G(d) and the MP2/6-311 + G(2d,p)//MP2/6-31G(d) levels of theory. The reactions studied have two steps: the first one corresponds to the formation of ethylene and a neutral amino acid intermediate via a six-membered cyclic transition state, and the second is the rapid decarboxylation of this intermediate via a five-membered cyclic transition state. The progress of the first step of the reactions was followed by means of the Wiberg bond indices. The results indicate that the transition states have an intermediate character between reactants and products, and the calculated synchronicities show that the reactions are concerted and slightly asynchronous. The bond-breaking processes are more advanced than the bond-forming processes, indicating a bond deficiency in the transition states. The kinetic parameters calculated for both reactio