



“Gheorghe Asachi” Technical University of Iasi, Romania



SYNTHON CHEMISTRY: THEORETICAL STUDY ON THE FORMATION OF PROLINE, PHENYLALANINE AND TYROSINE

**Gheorghe Surpățeanu¹, Ana-Maria Georgescu^{2*}, Ileana-Denisa Nistor²,
Neculai Catalin Lungu³**

¹Academy of Romanian Scientists (ARS), 3 Ilfov Street, District 5, Bucharest, Romania

²“Vasile Alecsandri” University of Bacău, Department of Chemical
and Food Engineering, 157 Calea Marasesti, 600115, Bacau, Romania

³A.I. Cuza University of Iasi, Faculty of Chemistry, Department of Organic Chemistry
and Biochemistry, 11 Carol I Blvd., 700506, Iasi, Romania

Abstract

According to the "synthon theory" on the formation of the first proteinogenic amino acids from three synthons: methylene, nitrene and carbon monoxide, at low temperatures, aziridinone would have formed. This, in contact with the same three synthons, forms the precursors of the 20 proteinogenic amino acids. These precursors, on contact with the components of the primary atmosphere, formed the first proteinogenic amino acids. The aim of this paper is to find the interradical reactions, which would have formed the precursors of proline, phenylalanine and tyrosine. The paper is a continuation of other studies on obtaining these amino acids in order to correlate them with their essential and non-essential character. As procedure, the quantitative results: enthalpies of formation, enthalpies of reaction, free energies, profile of reaction pathways were obtained by DFT calculations (B88-LYP).

Keywords: aziridinone, aziridinone radicals, phenylalanine, proline, tyrosine

Received: June, 2020; *Revised final:* November, 2020; *Accepted:* December, 2020

* Authors to whom all correspondence should be addressed: e-mail: ana.georgescu@ub.ro; Phone: +40740311286