CONFORMERS OF L-GLUTAMIC ACID: MATRIX ISOLATION FTIR AND *AB-INITIO* STUDIES.[a]

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L-glutamic acid is most abundant free amino acid in brain and it is the major excitatory neurotransmitter of the vertebrate central nervous system and known to play an important role in neural differentiation process of a developing brain. Study of the rich conformational landscape of L-glutamic acid can serve as basis to understand interactions of this amino acid with other biomolecules and receptors present in central nervous system.[c] L-glutamic acid was trapped in an inert gas matrix by employing a heated nozzle to provide an effusive molecular beam and the various conformers of the amino acid trapped in the matrix were then characterized by FTIR spectroscopy. *Ab-initio* calculations were also performed, using MP2/6-311++G(d,p) and M06-2X/6-311++G(d,p) level of theories, to corroborate with experimental observations. A comprehensive scan of the potential energy surface was performed to arrive at the various conformers of L-glutamic acid, which were further classified based on their backbone structure. The tendency of lower energy conformers to adopt certain backbone structures has been pictorially represented using a 'conformational dartboard'. Factors such as intramolecular H-bonding, delocalized orbital interactions and entropy were found to determine conformational preferences in L-glutamic acid, which will be discussed.

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[c]Tapiero, H.; Mathe, G.; Couvreur, P.; Tew, K. D. Biomed. Pharmacother. 2002, 56, 446-457.