Title:	Do amino acids prefer only certain backbone structures? Steering through the conformational maze of l-threonine using matrix isolation infrared spectroscopy and ab initio studies
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Abstract:	The conformations of l-threonine have been studied using matrix isolation infrared spectroscopy and ab initio computations. Computations at the M06-2X/6–311++G(d,p) and MP2/6–311++G(d,p) levels of theory, yielded 38 conformers of l-threonine. Single point energies were also computed at the MP2/CBS and CCSD(T)/6–311++G(d,p) level. All the conformers were classified into eight groups, depending on its backbone structure. Four conformers, whose populations were computed to be in excess of ~10% or greater, were observed in our matrix isolation experiments. We further analysed the factors influencing the conformational preferences in l-threonine and it was found, through our AIM and NBO studies, that the conformational stability resulted from an interplay of intramolecular hydrogen bonding and orbital delocalisation interactions, particularly the vicinal interactions. Earlier work had alluded to a bifurcated Nsingle bondH···Odouble bondC type hydrogen bonding interactions as being important in stabilizing certain conformations. However, we do not find evidence for such interactions and it appears that those structures are stabilized more by vicinal delocalisation interactions. We have also demonstrated that a pattern seems to exist in the backbone structures adopted by the amino acids, which is displayed through a “conformational dartboard”. We have shown that the low energy conformers of l-threonine adopted only certain backbone structures out of the possible eight. Our preliminary computations seems to show that the same backbone structures are probably adopted by a number of other amino acids, pointing to a general pattern adopted by amino acids; an aspect that may have important consequences in rationalizing protein structures.
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