Poster Presentation

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Structure and stability of solid oligoglycines

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Although peptides have been extensively studied within many disciplines, their solid state chemistry is not sufficiently explored. Crystalline peptide materials could present new opportunities in solid state organic synthesis as well as pharmaceutical, cosmetic and food industries. In order to facilitate these future applications, a better understanding of the relationship between the solid state structure and chemical reactivity in peptide crystals is required. In this work, a series of linear glycine oligomers was studied to see how their crystal structure and thermal reactivity changes with the chains growth. Single crystals of tetra- and pentaglycines were grown from aqueous solutions and investigated with XRD analysis (see Figure for pentaglycine). The newly collected data together with those reported previously reveal general trends likely present throughout all glycine oligomers. An antiparallel, hydrogen bound, β-sheet-like structure exists throughout the whole series and is the most stable polymorphic form in higher oligomers. Further, the thermal reactivity of this series was studied using gas chromatography – mass spectrometry (GC-MS), thermal gravimetric analysis (TGA) coupled with IR spectroscopy, differential scanning calorimetry (DSC) and bulk oven heating regimes. Finally 1H and 13C NMR and XRD analysis were used to identify key components of the thermal decomposition pathways as well as new products discovered during the thermal treatment. The results from all these studies suggest that the thermal stability of the oligomers increases with the chain length, but the decomposition pathways for the series are similar. In all cases, 2,5-diketopiperazine was formed through either condensation reactions (glycine and diglycine[1]) or depolymerisation of the peptide chain[2] in parallel with competing decomposition mechanisms. 2,5-Diketopiperazine and its derivatives are important biologically active molecules, and if this trend holds for other peptide oligomers, this solid state reaction could form a new, widely applicable synthetic method.

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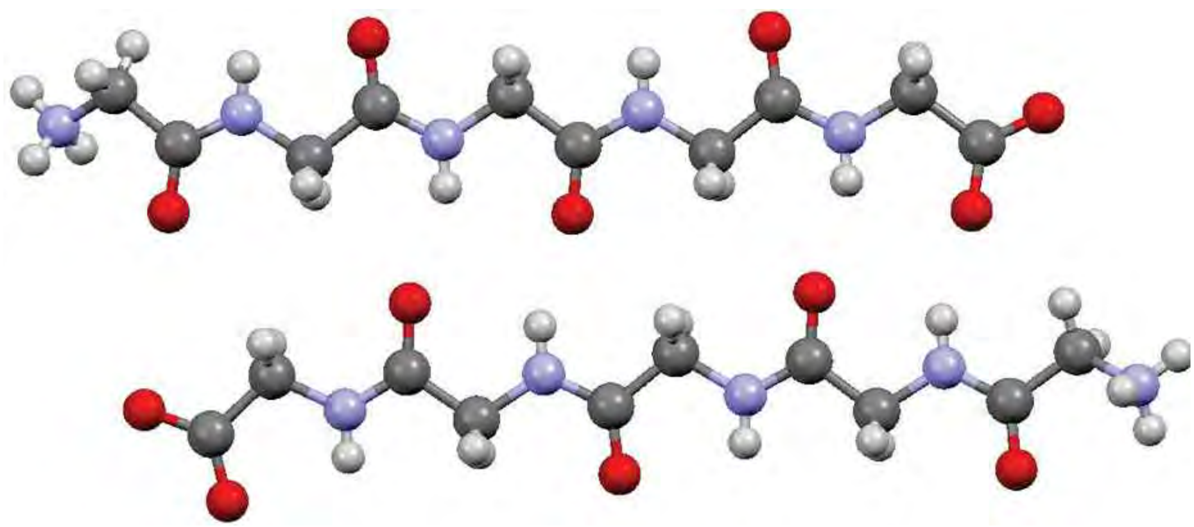

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