ELUCIDATING THE EFFECTS OF AMIDE SIDE CHAIN INTERACTIONS IN FLEXIBLE BIOMOLECULES

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Preliminary investigations of *O*-(acetamidoethyl)-*N*-acetyltyramine (OANAT), a *para*-substituted benzene with two flexible side chains, allowed the assignment of the six resolved conformations seen in the jet-cooled electronic spectrum into two classes, interacting and non-interacting chains. In the conformations with interacting chains, the amide groups in each of the chains are hydrogen-bonded to one another. In order to gain more insight into the potential energy surface and attempt to make more detailed structural assignments, molecules similar to OANAT have been studied. These include the single chain molecules 2-phenoxyethylacetamide (POEA), *p*-methoxyphenethylacetamide (MPEA), and *N*-methyl-benzenepropanamide (NMBPA). The two alkyl chains from MPEA and NMBPA can be combined to form three different *para* substituted double chain molecules, *N*,*N*′-(1,4-phenylenedi-2,1-ethanediyl)bis acetamide (NPEBA), 3,3′-(1,4-phenylenedi)bis-(*N*-methylpropanamide) (PBNMP), and 1,4-(*N*-methylpropanamide-*N*′-ethylacetamide)benzene (NMPNEA). Experimental results of several of these molecules are compared with *ab initio* calculations of the entire set in order to elucidate the possibilities of interchain interactions and the effect on the observed spectra.