Association of diphenylguanidine molecules and quntum-chemical calculations of the structure of its cyclic dimers.

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The frequencies and intensities of the two tautomeric structures of the N,\(N'\)-diphenylguanidine monomer and its hydrogen-bonded cyclic dimers were calculated for structure elucidation of the monomer and dimer forms of this compound and identification of the stretching vibration band νNH of this molecule in solution. *Ab initio* HF/3-21G and B3LYP/6-31G(d,p) calculations of DPG monomers and cyclic associates suggest that the asymmetric tautomer is dominant, proving that the dimer structures with two C=(Ph)N...H–NPh hydrogen bonds prevail in solution. An assignment of IR absorption frequencies of DPG in solution is suggested.

Adres publiczny

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