

Exploration of the (ethanol)₄-water heteropentamers potential energy surface by simulated annealing and Ab initio molecular dynamics

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A DFT electronic structure study of the (ethanol)₄-water heteropentamers at the B3LYP/6-31+G(d) model chemistry was carried out. To get determine possible configurations, the potential energy surface (PES) was explored with two methods: simulated annealing and ab initio molecular dynamics. The results suggest that the PES is very flat. A total of 81 stable structures were determined. These structures were classified into 16 different geometric patterns according to geometric criteria like the number of hydrogen bonds and their spatial arrangement: cyclic, bicyclic, or lineal patterns. Thermodynamic stability was used for defining the order of such classification. Hydrogen bonds are mutually disturbed due to the existence of cooperative effects. Cooperativity affects the nature of the hydrogen bonds and the overall stability of the ethanol-water system given that the strongest interactions are markedly covalent and the most stable geometric pattern corresponds to the pentagonal arrangement