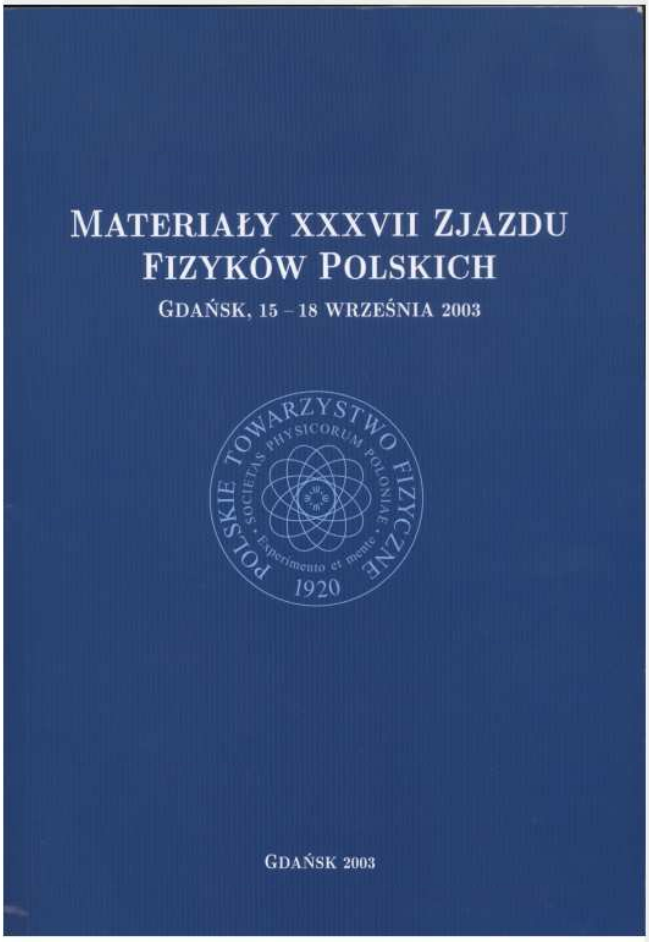

Stability of water clusters: group theory view

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A new study of the problem of stability of the water clusters is presented. We use the group theoretical method. Dependence of stability from symmetry and type of structure is discussed.

Numerous configurations of neutral and protonated clusters with n up to 8 have been calculated by Hartree-Fock *ab-initio* method with 6-311G** and 6-31G** molecular-basis sets. Theoretical dissociation energies diminish from about 24kcal/mol for protonated clusters containing $n = 3H_2O$ molecules down to about 5–6kcal/mol for $n = 7$ and then rises again.

Group theory allows dividing obtained structures into several (approximate) symmetry classes. The water clusters of higher symmetry and ice-liked structure are more stable than other. Reduction of the symmetry group of the bigger clusters to the symmetry group of the smaller clusters results on the possibility of the paths of dissociation of the water clusters.