

QUANTUM-CHEMICAL SIMULATION
OF THE CLUSTER STRUCTURE
OF LIQUID *N*-HEPTANOL

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S u m m a r y

Different molecular aggregations formed in liquid heptanol due to the hydrogen bonding are investigated. Using the methods of quantum-chemical simulation, the preference of the aggregations involving more than 5 molecules is shown. The correctness of the conclusions is established by the comparison of the obtained results with experimental data.