OPTIMIZATION MONITORING OF MOLECULAR CLUSTERS MATHEMATICAL MODELING

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In the study of molecular clusters, the simultaneous completion of processing of computational tasks is required, which is dictated by the need to compare the thermochemical properties of isomers. Systematization of data on the costs of computational time makes it possible to increase the effectiveness of research. In this paper, a tool is developed for statistical analysis of the time characteristics of computational experiments conducted using quantum chemical methods [1].

An embedded computing environment module [2] has been developed that allows to obtain interval estimates of the processing time of computational tasks on the basis of which the parameters of automatic means for generating the initial geometries of the studied structures can be selected.

The module is a universal means of postmonitoring large-scale computational experiments, using both different problem-oriented software and heterogeneous computer complexes. The development is used in the Laboratory of Molecular Modeling of Nanostructured Systems of MGTU "STANKIN" for balancing the computational load. The work was supported by the Ministry of Education and Science of the Russian Federation, project No. 1.7706.2017 / BC, and RFBR, grant No. 15-08-4969a.

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