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Processing of the results of quantum chemical calculations using P-Analysis Program

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Abstract

The paper describes a new computer program P-Analysis, designed to process the results of quantum chemical calculations performed using Priroda program. The program analyzes the output files of calculations and depending on the mode selected by the user creates a table containing information about the themselves calculations and corresponding thermodynamic parameters. There are two modes of operation: a separate connection and elementary act. In the first case will be presented at the output the main thermodynamic parameters of the compounds under consideration. The main value of this mode is the ability to get information directly to a large number of output files of calculations. The second mode facilitates investigation of chemical reactions. As initial information for the program, the user specifies the location of the output files of the transition state, products and reagents. The program will analyze them and provide for each of these three structures information on thermodynamic parameters and produce the calculation of the activation parameters of the researched reaction, in particular, the activation energy, activation enthalpy, Gibbs energy of activation (these characteristics will be calculated for both the forward and reverse reaction). The results of processing, depending on the user's choice can be automatically tabulated in CSV format, or MS Word. The application is a window, but it is possible to work from the command line, which allows batch processing of output files to a large number of reactions studied. For these purposes it is necessary to form a text file that contains information necessary for processing. Step of results processing can be integrated in the iterative process the PES automatic survey using program Priroda and shell P-AutoExtremum. When the transition state calculation, descents along the reaction coordinate for products and reagents, as well search of the exact lows, which correspond to them, will be ended P-AutoExtremum automatically generates a text file with processing parameters and initiates the launch of P-Analysis.