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Shell P-AutoExtremum(G) for automation of iterative algorithm for PES research with program Gaussian

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Abstract

In the study of the mechanisms of chemical reactions, the most laborious calculations are connected with the study of the potential energy surface (PES), in particular, with the construction of reaction paths (RP) from the found transition states (TS) to the reactants and reaction products. The authors of this work suggested using several programs in the research process of reactions mechanisms in order to take advantage of each of them. A P-AutoExtremum shell program was created for the Priroda program, which automates the process of investigating an elementary chemical reaction event, including searching for a PS, building an OL from a PS to reagents and products, and optimizing the geometry of the latter. For the Priroda program a P-AutoExtremum shell program was created, which automates the process of investigating an elementary chemical reaction stage, including searching for a TS, building an RP from a TS to reagents and products, and optimizing the geometry of the latter. The final step in calculating the elementary stage of a chemical reaction is to compile a report using the P-Analysis program. The next step in investigating the reaction mechanism is to calculate the elementary act by a more accurate density functional method using Gaussian 09W (G09W). Unfortunately, at this stage there were technical problems associated with looping in calculating the reaction paths and optimizing the geometry of the reagents and reaction products. In part, they were overcome by applying the LQA option for the IRC keyword when *ω*B97X when ωB97XD method with calculating the RP and replacing the calculating the PES. To reduce the computer time and increase the reliability of calculations when searching for extremes on the PES, the authors created the P-AutoExtremum (G) shell program. It runs a series of G09W program runs with CalcFC and MaxCycle=N options, in which N is specified by the control shell according to a user-defined rule. The geometry of the molecule at the origin is specified by the user, and is taken from the calculation that was completed earlier. If the specified number of geometry optimization iterations in G09W is exceeded, the shell computes the new value of N and calls G09W again. The process stops when the extremum is localized to the PES with the specified accuracy, or when the maximum number of calls G09W specified in the shell is exceeded. The experience of using the described shell to search for extrema in poorly convergent problems of aquathermolysis of sulfur-containing compounds has shown its effectiveness: the algorithm used successfully works, and the number of analytical calculations of the matrix of second derivatives decreases by a factor of 5-10 when the localization of extremum.

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