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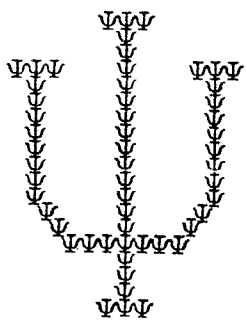

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QCMP149. **DDRP-1: Program for Determining Dynamically Defined Reaction Path (DDRP) in 3-Atom Collinear Collision**

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This program is a realization of a global path following procedure [1-5]. DDRP-1 requires the positions of atoms in internal coordinates and can be used for describing chemical reactions of collinear 3-atom systems. For treating the most general case of reacting systems using Cartesian coordinates, a modified program (DDRP-2) will follow soon. The DDRP procedure can be coupled with a conventional or quantum chemical (semiempirical or *ab initio*) method suitable for calculating the total energy of the system. In the present version, the total energy is calculated by a truncated MNDO program: QCPE 353 has been modified in order to have a simpler input and reduce computational time, and the configurational interaction has been omitted. The DDRP programs approximate the reaction path in an iterative way. A perfectly reliable choice for the first approximation of the reaction path is a closed polygon containing the probable location of the saddle point in its interior. Regarding the high stability of the method, this choice is safe but not necessary. The approximate polygons computed in consecutive steps show the rapid convergence of the procedure: the polygons will quickly turn to a line, thus giving the shape of the final reaction path. The program in its present form is to illustrate the theory laid down in the references cited and is suitable for computing systems which are composed of atoms with atomic numbers not greater than 17 and starting from polygons with a maximum of 200 vertices. This latter number is limited by the size of the RAM of PCs.

References:

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[3] L. L. Stachó and M. I. Bán, *Theor. Chim. Acta*, **84**, 535 (1993).

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[5] Gy. Dömötör. M. I. Bán and L. L. Stachó, *J. Comp. Chem.*, **14**, 1491 (1993).

Lines of Code: 3200

Microsoft FORTRAN (version 4.0 or later)