An object-oriented approach to the calculation of the inverse kinetic energy matrix.

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Streszczenie

A novel approach to the calculation of the elements of the kinetic energy matrix is presented. In the proposed method the matrix elements are calculated directly in the internal coordinate space, without determination of the intermediate matrix, using the analytical expressions given by Decius. The C++ program exploits a new method for the representation the geometry and constitution of chemical structures, which enables both molecular topology manipulation and geometry calculation. Starting with the set of internal coordinates, all possible types of the matrix elements are found for the molecule in an automatic search and subsequently evaluated. The method is exemplified by calculation on the water and cyclopentanone molecules.

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