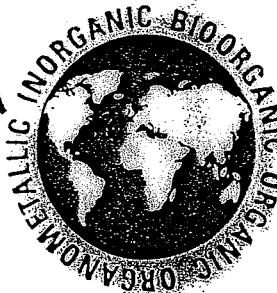


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BOOK OF ABSTRACTS

Comparative Study of Global Path-Following Methods

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Global path-following algorithms¹⁻⁴ based on the strategy of the Elber-Karplus method⁵, especially those coupled with molecular mechanics, are quite popular and widely used for the calculations of potential energy surfaces of large organic- and biomolecules. Another type of this sort is the DDRP method⁶. To have a comparison about the stability, computation time, accuracy, etc. of the different methods, calculations were performed on some mathematical test-functions (e.g. the curves of Müller-Brown⁷ and Stachó-Bán^{6,8}). The results of calculations prove our preliminary expectations, i.e. the superiority of the stability of the DDRP method over other algorithms.

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