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ESTAC- A NOVEL TOOL FOR DETERMINATION OF BINDING CONSTANTS

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For modern supramolecular chemists, the accurate evaluation of stability constants of host-guest complexes became a necessity. Among UV, potentiometry and calorimetry measurements, ¹H NMR represents a useful method of obtaining data for estimation of complexation constants. On the base of concentration of the added guest, the chemical shift of signals of the host is dependent on the equilibria between arising complex and the free molecule. Apart from the correct measurements of experimental data, the right interpretation of the results is of great importance.

A novel program ESTAC, written in FORTRAN language, represents an effective tool for processing the measured data containing uncertainty in both independent and dependent variables. The use of orthogonal distance regression package ODRPACK improves the estimation of complexation constant from experimental results. The program also offers a statistical analysis of estimated parameters with the possibility of elimination of those outlying points of the dependency, which significantly enlarge the error of calculation.

The possibilities and usefulness of this program will be discussed and the results obtained for different calixarene derivatives will be compared with the data gained using some other methods of computation.

References

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