Journal of Physics: Conference Series 2012 vol.394 N1

New program for computation of the thermodynamic, spectral, and NMR relaxation parameters of coordination compounds in complex systems

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Abstract

A new approach providing a direct calculations of equilibrium constants, parameters of the chemical exchange reactions, and spectral characteristics of complexes on the basis of data of several methods including pH-potentiometry, multi-wavelength electronic spectroscopy, and NMR relaxation within a single computer program was proposed and realized in the program STALABS. Application of the STALABS program has been demonstrated on the example of investigation of the complex nickel(II) - L-histidine system by joint usage of the above three methods.

http://dx.doi.org/10.1088/1742-6596/394/1/012031