Determining the Parameters of ESR Spectra
by Computer Analysis of the Spectrum Lineshape

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Program for determine of the complexes parameters in the aqueous solution (formation constants, hyperfine coupling (HFC) constants, g-factors, relaxation parameters) by using method of analysis of spectrum lineshape was created. The main program units are the module for calculating the molar fractions of the system components by the standard procedure for solving the set of material balance equations [1]; the module for calculating the lineshape of the ESR spectrum; and the module for optimization of the parameters by the scanning and coordinate descent methods.

The experimental ESR spectrum is usually described as a convolution of the Gaussian and Lorentz lines. The theoretical spectrum was constructed by a superposition of the Lorentz curves, and this method gave a satisfactory agreement in all the cases. The correction for non-uniform broadening of the experimental signal was made by introducing the unresolved HFS. The effect of anisotropy of the HFC of an unpaired electron with the metal nucleus on the line width was calculated by the Wilson-Kivelson equation [2].

At the next step, the obtained values were refined by processing the spectra recorded at different pH and compositions of solutions, which can contain greater number of species. This calculation procedure imposes no restrictions on the number of complexes, whose parameters can be estimated simultaneously. The minimization process was stopped when the further variation of the parameters did not decrease the SSQD function and the theoretical and experimental spectra coincided visually. The reliability of the results was provided by the great number of the experimental points and by the low value of SSQD function.

[1] Beck M., Nagypal I.: Chemistry of Complex Equilibria. Budapest: Akademiai Kiado 1989.

[2] Wilson R., Kivelson D.: J. Chem. Phys. **44**, 154 (1966)