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EVALUATION OF AL–F–COMPLEX CONCENTRATIONS IN ALUMINIUM SALT SOLUTIONS

Siegfried Klinger and Volker Reinsch

Forschungsinstitut für Aufbereitung der Akademie der Wissenschaften der DDR, DDR-9200 Freiberg, Strasse des Friedens 40 (G.D.R.)

Direct concentration determinations of different Al-F-complexes in aqueous solutions are only possible by ^{19}F-NMR analysis. Because this method is very expensive a computation algorithm was developed on the base of thermodynamic complex equilibrium equations and balance equations. The corresponding computer programme involves a special root finder to solve the developed polynomial equation.

The computation method is applicable to homogeneous solutions with three different centralions and one ligand for complex formations up to temperatures of 200°C. Absence of kinetic hindrances and equality of activities and concentrations are assumed.

If the total concentrations of centralions and ligand as well as the brutto stability constants of the complex equilibria are known concentrations and portions of the different complex species, free central ions and the free ligand can be computed.

This computation method was applicated to aqueous solutions of aluminium chloride and aluminium nitrate containing 0.3 - 4.4 mol/l Al and 0.2 - 4.4 mol/l F. If it is possible to determine the peak areas of the NMR spectrograms with sufficient accuracy the results are good agreement with data obtained experimentally by ^{19}F-NMR analysis.