Computational methods in coordination chemistry

syllabus

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pH-metry:
calibration methods / ionic strength / pH or E / mixed solvents
Simple acid-base titrations and evalutions of them by excel.
Speciation diagram by excel.
Limit in concentrations and then error / pH-regions and the error / ligands with lots of pKa-s (n>10 / 20).
Speciation in systems with three components (excel).
Estimation of stability constants, relations with the pH-range
Speciation curve calculation with special programs (sed / psequad) the component matrix and its transformations. Predominance curves and others.
Evaluation of real pH-metric measurements, types of errors.
Minor component problems. Practicing how to make models,
Spectroscopies:
EPR / NMR (UV-VIS / CD)
Matrix rank analysis
Fitting of EPR and NMR spectra (excel)
The 2D-EPR program
PSEQUAD / HYPERQUAD and the spectroscopies.
Evaluation of low range measurements. Estimation of the error of the fitted parameters. Perturbation and robustness. Outliers.
DFT calculations (report from student(s))
X-ray measurements fitting (report from student(s))
The Mercury program.