Appendix

Abbreviation and symbols

$[A]$	concentration of component A
$[A]_0$	initial concentration of component A
$[B]$	concentration of component B
$[B]_0$	initial concentration of component B
$[X]$	concentration of any component
K_{11}	step-wise stability constant for a 1:1 complex
K_{21}	step-wise stability constant for a 2:1 complex
K_{12}	step-wise stability constant for a 1:2 complex
lgK	log_{10} of stability constant K
a, b	equivalent of component A or B
r_i	stoichiometric ratio
n_i	nuclearity
x	independent data, random number
y	observed signal or physical property, dependent data
θ	parameter in general
$\hat{\theta}$	estimated parameter / best-fit parameter
$[\theta_-, \theta_+]$	confidence interval, range within $\tilde{\theta}$ is expected to be
SSE	sum of squared errors
SE_y	standard error
MC	Monte Carlo simulation
BS	Bootstrapping
CV	Cross Validation
L1O	Leave-One-Out
L2O	Leave-Two-Out
LXO	Leave-X-Out
X	Number of data points to leave out during CV
RA	Reduction Analysis
S	number of MC or CV steps
S_{max}	maximal number of CV steps
N	number of data points
σ	standard deviation of normal distribution
σ_{MC}	standard deviation used to set up Monte Carlo simulations
σ_{dist}	σ of a distribution after Monte Carlo simulation or Cross Validation
$H(x)$	Shannon entropy of a distribution of random numbers (eg. after Monte Carlo simulation)
σ_{pt}	Partial standard deviation calculated from the results of a RA