

ZMATH 2013b.00960

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Titration calculations with computer algebra software.

PRIMUS, Probl. Resour. Issues Math. Undergrad. Stud. 22, No. 4, 317-337 (2012).

Summary: This article examines the symbolic algebraic solution of the titration equations for a diprotic acid, as obtained using Mathematica, Maple, and Mathcad. The equilibrium and conservation equations are solved symbolically by the programs to eliminate the approximations that normally would be performed by the student. Of the three programs, Maple performs the best in terms of precision and speed. Mathcad is unable to arrive at a symbolic solution for the system of equations as posed. Mathematica can solve the algebraic problem, but requires additional programming effort to handle instabilities that arise during the calculation of numerical output.

Classification: U75 M65

Keywords: equilibrium chemistry; aqueous; titration; diprotic acid; computer algebra; nonlinear equations
doi:10.1080/10511970.2010.538135