UNCERTAINTY, PRECISION AND ROUNDING IN THE PRESENTATION OF FITTED (DIATOMIC SPECTRA) PARAMETERS

ROBERT J. LE ROY, *Guelph-Waterloo Centre for Graduate Work in Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

In multiparameter fits of models to experimental data sets, the spectroscopic literature has seen very inconsistent treatments of the rounding of fitted parameters. In attempting to minimize the clutter of unnecessary digits to be reported, the simplest approach is to round off all parameters at the first or second digit of their uncertainty; however, experience shows that predictions generated from the resulting constants may disagree with the input data by *orders of magnitude* more than the experimental uncertainties. The alternate approach of blindly reporting all constants to maximum computer precision removes this difficulty, but requires tediously large numbers of digits to be listed, making such results inconvenient to use and prone to transcription error by users. A strategy for optimal rounding of all the parameters determined in a fit is presented, and is illustrated by applications to band data for the A-X system of I_2 and to infrared and microwave data for HF. This automatic sequential rounding procedure is incorporated in a general program for performing simultaneous single- or combined-isotope fits to all possible types of diatomic molecule data involving one or more singlet electronic states.