FIT1D

A simple code for fitting near-equilibrium potential energy curves and calculation of ro-vibrational constants of diatomic molecules

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I. Version History

First Release: March 1989 , University of Wisconsin-Madison
Language: Fortran
Compiled for: WindowsX

This is a slightly modified version of FIT1D for being compatible to "NUMEROV" code.

II. What Does FIT1D do?

FIT1D performs a least squares fit of a Taylor series in one variable and calculates vibrational second order perturbation theory spectroscopic constants. The derivative with respect to R is taken and the minimum is found by the Newton-Raphson method. ΔR is defined as $R - R_e$, where R_e (equilibrium bond length) is input as an initial guess. The data file specifies the number of terms in the expansion in an array form. Maximum size of expansion is limited to 15 terms which corresponds to a polynomial of degree 14 (see below equations). The number of points that can be fitted is set to a maximum of 200. Atomic units are used throughout.

$$E(R) = \sum_{n=0}^{norder} a_n (R - R_e)^n$$

$$a_n = \frac{1}{n!}\left(\frac{d^n E}{dR^n}\right)_{R_e}$$

III. Input file

Following is the sample of the input file for CO molecule.

```
1                       One fit to perform
CO molecule             Title
10,3,0,1                Npts, Norder, Nexpnd(0=min,1=fixed), Npert(0=yes,1=no)
2.0821                  Guess for Re or fixed expansion geometry ( in bohr)
1.970,-112.7817023      Set of Npts. - R, E, in atomic units
2.000,-112.7870190
2.030,-112.7904977
2.080,-112.7926997
2.132,-112.7909072
2.180,-112.7861712
2.200,-112.7834466
2.230,-112.7786284
2.280,-112.7688851
2.330,-112.7573427
12,16                   Mass numbers of atoms (for Npert=0)
```

Npts : number of points (pairs)
Norder: number of terms in the Taylor series
Nexpnd: whether to find minimum and re-expand or leave fixed

Npert: whether to carry out vibrational perturbation theory analysis or not

IV. Running the Program

FIT1D is executed by the following command line in the DOS shell of the Windows

FIT1D.exe <filename.inp> filename.out

V. Output files

Our code produces five different kinds of output files, each contains useful data and helps to check the correctness of the calculations.

a) filename. out

This is the main output file and contains the final results of calculations.

b) numerov. inp

This file contains the potential energy coefficients in the final Taylor series, R_e and reduced mass of the diatomic molecule. For more details please check the Numerov online manual.