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README for fit_dihedral_parameters_paper.plx

Author: Chad Hopkins
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Implementation of pseudo-code in Appendix of:
Hopkins, C. and Roitberg, A. "Fitting of dihedral terms in classical force fields as an
analytic linear least squares problem"

Usage:
fit_dihedral_parameters_paper.plx DATA_FILE TYPES_FILE d phase nmax [INI_FILE]

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INPUT:

-DATA_FILE
File that encodes the arrays qme, mme, ang (in degrees), and optionally w.
Column format, where each row represents one data point.
For row i (see paper for array specifications):
        Columns 1 to d  = ang[1:d][i]
        Column d+1      = mme[i]
        Column d+2      = qme[i]
        Column d+3      = w[i]          (Optional)
If Column d+3 is not present for row i, data point i is given weight w[i] = 1.

-TYPES_FILE
File that encodes the array type.
Each row represents a unique dihedral type.
        Row i           = array type[i]

-d
Same as d in paper: Integer. Number of dihedral angles being fit in the molecule.

-phase
Same as phase in paper: Flag (specified here as "0" (off) or "1" (on)). Specifies
whether the phase constants are varied (on) or
held fixed at 0 or pi (off).

-nmax
Same as nmax in paper: Integer. Maximum multiplicity being fit.

-INI_FILE (Optional)
File that encodes the array ini (phase constants in degrees).
        Row i           = ini[1:2][i]
If the second column is left blank, a harmonic restraint of 0 (free fit) is assumed for
that term
Only the harmonic restraints read on the dihedral force constant rows (first half) are
used for restraint of linearized parameters
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!                                       IMPORTANT
NOTE                                                                  !
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! There is a numerical issue when restraining the force constant to be 0 for a dihedral
using the harmonic          !
! restraint in the LLS scheme.  If you restrain a force constant to 0, THE
CORRESPONDING PHASE CONSTANT WILL NOT BE !
! RESTRAINED, and the force constant restraint tends to act unpredictably. The best way
to keep the force           !
! constant close to 0 is to give a small (non-zero) initial value, and set the force
constant very high. In         !
! conclusion, YOU SHOULD NOT SET THE INITIAL FORCE CONSTANT TO EXACTLY ZERO IF YOU ARE
PUTTING A HARMONIC RESTRAINT !
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IT.
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OUTPUT:

-fit.out
File that encodes the array a (phase constants in degrees).
        Row i           = a[i]
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