NAME

quatfit – superimpose atoms of two molecules given in XYZ format

SYNOPSIS

quatfit [**-r** *ref-mol*] [**-f** *fit-mol*] [**-p** *pairs*] [**-o** *fit-out*] [**-s** *statfile*]

DESCRIPTION

Program **quatfit** superimposes specified atoms of two molecules so they are as close as possible (in a least squares sense). The orientation of the reference molecule is kept fixed, while the fitted molecule is rotated and translated as a rigid body to fulfill the fit. As the first step, the reference and fitted molecule are translated, so their geometric centers are located at the origin of the coordinate system. Then the rotation matrix is found by the quaternion method and the fitted molecule is rotated. Then both molecules are translated to the original center of the reference molecule. If normal modes are present, they are also rotated. The pairs of atoms to be fitted may have assigned weights (the weights represent the onverse of the atom pair distance, a larger weight will force a thighter fit for the pair). The XYZ format used in the Xmol program (Xmol is a product of Research Equipment Inc. and Minnesota Supercomputer Center, Inc., and is available via anonymous ftp at ftp.msc.edu in /pub/xmol) was chosen to represent input files for the reference and fitted molecules. The format is:

line 1: **number of atoms**
line 2: **descriptive title**
line 3, etc.: **Atomic-Symbol X Y Z** [**Charge**] [**Mode-X Mode-Y Mode-Z**]

If **Charge** is present, it is in 5th column. If normal modes are present, they occupy last 3 columns. The file specifying atom pairs starts with a line containing the number of fitted pairs; the next lines have the format:

ref-atom fit-atom weight

where **ref-atom** is the atom number in the reference molecule, **fit-atom** is the corresponding atom in the fitted molecule, and **weight** represents the tightness of the fit for this pair. Coordinates of the superimposed fitted molecule (and normal modes, if present) are stored in the *fit-out* file and information about the goodness of fit is stored in the *statfile* which lists distances between fitted atom pairs, the RMS, and dot product of normal modes from the reference and the fitted molecule. When any of the I/O options is omitted, the corresponding file is read from(sent to) standard input(standard output). The order of files in the standard input stream is *ref-mol*, *fit-mol*, *pairs*. The order of files in the standard output is *fit-out, statfile*.

OPTIONS

-r *ref-mol*
The *ref-mol* is a file name of XYZ file for reference molecule. If this option is absent, the information is taken from standard input.

-f *fit-mol*
The *fit-mol* is an XYZ file with fitted molecule, i.e., the molecule which will be translated and rotated. If this option is missing, the information is taken from the standard input.

-p *pairs* The *pairs* is the file with atom pairs and their weights. It starts with the number of fitted pairs as a top line and is followed by 3 columns: 1st column is a list of reference molecule atoms, 2nd is a list of fitted molecule atoms, and 3rd column represents weights. If **-p** *none* is specified, the weights are not read in but they are all set to 1.0, and fitted atom pairs are set to consecutive natural numbers, i.e., 1 — 1, 2 — 2, 3 — 3 ..., up to the number of atoms in the smaller molecule. You might want to use **-p** *none* option if you compare geometry of the same molecule calculated by different methods, provided that atom numbering is the same.

-o *fit-out*
This option specifies the output file for the transformed fitted molecule. If absent, the file is sent to standard output.

-s *statfile*
The file name for fit statistics. If this option is absent, this information is sent to standard output.

EXAMPLE

cat rm.xyz fm.xyz | quatfit -o fmmod.xyz -p none > stat.txt
is equivalent to
quatfit -r rm.xyz -f fm.xyz -p none -o fmmod.xyz -s stat.txt
i.e., the reference molecule (kept fixed) file is rm.xyz, the fitted molecule file is fm.xyz, file for translated and rotated coordinates of fitted molecule is fmmod.xyz, and stat.txt contains the information about goodness of the fit. Atom pairs to be fitted and their weights are assigned automatically by the program in this example. If the weights were given explicitly, the command could look like:
cat rm.xyz fm.xyz pairs.tab | quatfit -o fmmod.xyz > stat.txt
which is equivalent to:
quatfit -r rm.xyz -f fm.xyz -p pairs.tab -o fmmod.xyz -s stat.txt
where pairs.tab is the file with fitted pairs and weights.

DIAGNOSTICS

Most error messages are self-explanatory.

BUGS

Report bugs to the authors.

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