Chapter 9.6

MOLFIT

Automatic Residue Fitting

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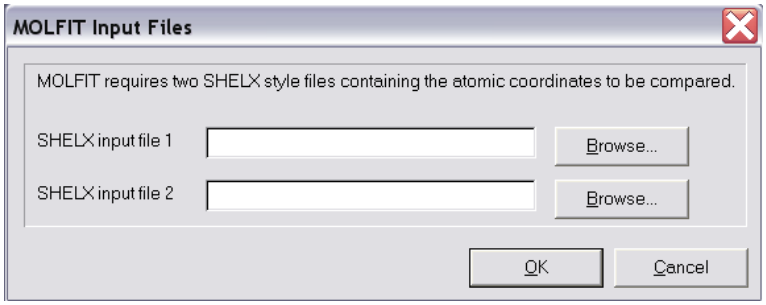
An automatic attempt is made to fit two crystallographically independent molecules (e.g. two steroid molecules) in the crystal structure on one another. Both molecules should be chemically equivalent (i.e. equal number of atoms, the correct atom type assigned, no hydrogen atoms missing). This option is implemented in the PLATON program [1]. In the WinGX environment, the two sets of coordinates should be given in two separate SHELX styles INS files, and the input files are created automatically.



The automatic fitting algorithm involves unique numbers based on the network topology assigned to all atoms in the structure. Topology numbers are listed in the connectivity table under the heading 'tnr'. Automatic fitting is attempted using the quaternion fit technique [2], on the basis of atoms with a unique and equivalent topology number for each molecule to be fitted. Atoms that are not topologically unique are not included in the fit calculation (but shown in the subsequent plot).

The published Mackay procedure fails for (close to) 180 degree fit rotations about an axis. The 180 degree situation is of course quite common in the crystallographic setting. PLATON/FIT implements a special 'work-around' for this problem. The fit is done of the first residue (or its inverted image) onto the second residue: the best fit is retained and displayed (along with the number of atoms on which the fit was done). By default (i.e. without the specification of residue numbers), residue #1 is fitted on residue #2. Other fits should be specified explicitly from the keyboard, *e.g.*

```
FIT 2 3
```

Hydrogen atoms are not included in the automatic fit, but included in the subsequent PLUTON style display. Details on the fitting results are written to the listing files. In the case that the molecules to be fitted do not have enough unique atom pairs, a fitting is then attempted assuming consistent atom numbering in both molecules. The Quaternion fit algorithm is also part of the NONSYM function. Assignment of equivalent (corresponding) atoms is done differently there. Symmetrical molecules may often be fitted automatically via that path.
A fit on an explicit subset (at least 5 pairs) of atoms can be done as well, *e.g.*

```
FIT N1 N2 O1 O5 O2 O6 O3 O7 O4 O8
```

The fitted coordinate sets are written to a file 'compound_fit.spf'.

Molecules from different origins may also be fitted by concatenation of their corresponding PDB files. In this case the number of atoms in both molecules may differ.

REFERENCES

1. Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7-13.

2. Mackay, A. L. (1984) *Acta Cryst.* **A40**, 165-166