10. SHELXWAT: Automated Water Divining

A simple program **SHELXWAT** has been added that iteratively recycles SHELXL to provide automatic water divining. This may be regarded as a cheap and inadequate imitation of ARP (V. Lamzin & K.S. Wilson, *Acta Cryst.* **D49** (1993) 129-147), but is relatively easy to use and useful if you intend to take a holiday. SHELXWAT is started by means of a command line with OPTIONAL UNIX-type switches (the filename must come last):

```
shelxwat name
```

or e.g.

```
shelxwat -n10 -s4 -u0.6 -r0.8 -m50 -f name
```

These are the default settings for the switches -n (number of overall cycles), -s (scattering factor number for oxygen), -u (starting isotropic U for new waters), -r (water rejected if U refines to greater than this value), -m (maximum number of waters to be added in one cycle) and -h (half/full occupancies) or -f (full occupancies only). All switches present must come before 'name'.

Standard SHELXL files *name.ins* and name.hkl are required; the *.ins* file should contain 'CGLS 3 -20', 'FMAP 2', 'PLAN 200 2.4' or 'PLAN 200 -2.4' (half occupancies allowed), 'CONN 0 O_501 > LAST', 'BUMP' or similar instructions (the free R test is not obligatory) and MUST include at least one water at the end of the atom list. The waters will then be assigned dynamical residue numbers starting with the residue number of this water (501 in the above example) and should all have residue class 'HOH' and atom name 'O' with one atom per residue and no PART numbers. On starting, SHELXWAT makes a backup copy (*name.bak*) of the *.ins* file, since the *.ins* file is repeatedly overwritten during the recycling. The recycling may be terminated tidily before the preset number of iterations has been performed by creating a file *name.end* in the same directory; this operates like the *name.fin* file for SHELXL, but is 'deleted' by SHELXWAT once per iteration.

SHELXWAT calls SHELXL once each cycle, then edits the resulting *.res* file to prepare the *.ins* file for the next cycle. The *R*1 (and $R1_{free}$, if present) indices are extracted from the *.lst* file and included in the *.res* files as remarks; these and other remarks (REM) provide a protocol of the refinement, and may be converted to a Postscript plot using the "P" option in SHELXPRO. Note that the SHELXPRO option "U" provides the facilities necessary to update that solvent etc. interactively, in much the same way that SHELXWAT does automatically.

By changing the PLAN instruction to (say) 'PLAN 200 1 1' and leaving out the BUMP instruction it might be possible to emulate ARP in its structure extension mode; this has yet to be tested, but might be useful for completing high resolution (better than 2Å) structures.