.ins file (shelx input)

User input

WEB: International tables for crystallography

User input

SMX defaults

```
* TITL 514_RTJ_I_113_1 in P222 #16
* REM  reset to P222 #16
* CELL 0.72932 9.889 10.073 51.938 90 90 90
ZERR 4 0.00198 0.00201 0.01039 0 0 0
* LATT -1
SYMM -X,-Y,+Z
SYMM +X,-Y,-Z
SYMM -X,+Y,-Z
SFAC C N Sm
UNIT 288 48 8
TREF

HKLF 4
END
```

* Found in XSCALE.HKL

CELL	wavelength, UC
ZERR	Z (*estimated* # formula units per cell), estimated error in UC dimensions – might be able to just use all zeros here – SHELXL refinement updates this anyway
LATT	lattice type - negative if the structure is non-centrosymmetric
SYMM	symmetry operator: X, Y, Z is assumed and thus omitted.
SFAC	atom names in order of scattering factors to be employed by program
UNIT	# of each type of atom in UC in SFAC order
TREF	tells SHELX I want to use direct methods
HKLF	”n” reflection file reading instructions n = 4 is general purpose for SMX n = 3 for MX IR or anomalous

http://www.chem.gla.ac.uk/~louis/software/wingx/hlp/ch_12.htm