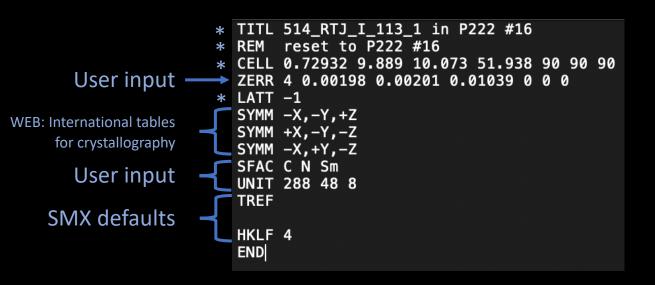
.ins file (shelx input)



* Found in XSCALE.HKL

wavelength, UC **CELL** 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 tells SHELX I want to use direct methods TREF 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