#F Crystals.dat

#UT Crystals: atoms coordinates in unit cell. Cell's dimensions

#UIDL xfh

#UD

#UD The crystal structures are arranged using as a scan

#UD identifier (#S) the atomic number of the heavier atom

#UD present in the crystal. Several crystal are possible with

#UD the same scan id, but they do not conflict.

#UD

#UD The following keyword contain other information:

#UD #UCOMMENT comment

#UD #UCELL a b c alpha beta gamma

#UD The unit cell dimensions (A and deg) (\*MANDATORY, IT MUST EXIST\*)

#UD #UTEMP temperature in Kelvin at which UCELL is given

#UD #UREF reference

#UD #USYSTEM : 7 crystal system, i.e., triclinic monoclinic orthorhombic

#UD tetragonal rhombohedral(trigonal)

#UD hexagonal cubic

#UD #ULATTICE the lattice centering:

#UD P: Primitive centering: lattice points on the cell corners only

#UD I: Body centered: one additional lattice point at the center of the cell

#UD F: Face centered: one additional lattice point at center of each

#UD of the faces of the cell

#UD A,B,C Centered on a single face (A, B or C centering): one

#UD additional lattice point at the center of one of the

#UD cell faces.

#UD The 14 Bravais lattices are, then:

#UD 1 triclinic (P)

#UD 2 monoclinic (P,C)

#UD 3 orthorhombic (P,C,I,F)

#UD 2 tetragonal (P,I)

#UD 1 rhombohedral (P)

#UD 1 hexagonal (P)

#UD 3 cubic (P,I,F)

#UD

#UD #USTRUCTURE Model for structure (e.g., diamond, fcc)

#UD

#UD Data columns:

#UD 4 or 5:

#UD AtomicNumber Fraction X Y Z Biso

#UD The Biso one is optional

#UD

#UD

#UD

#S 41 LiNbO3

#UCELL 5.148 5.148 13.863 90.0000 90.0000 120.0000

#USYSTEM Trigonal

#ULATTICE R

#UREF R.S. Weis and T.K. Gaylord, Appl. Phys. 191-203 (1985)

#UCOMMENT LiNbO3 Ref:R.S. Weis and T.K. Gaylord, Appl. Phys. 191-203 (1985)

#UCOMMENT (coordinates calculated by Olivier Mathon (mathon@esrf.fr)

#N 5

#L AtomicNumber Fraction X Y Z

3 1.0 0 0 0.2829

3 1.0 0.3333 0.6667 0.9496

3 1.0 0.6667 0.3333 0.6162

3 1.0 0 0 0.7829

3 1.0 0.3333 0.6667 0.4496

3 1.0 0.6667 0.3333 0.1162

41 1.0 0 0 0

41 1.0 0.3333 0.6667 0.6667

41 1.0 0.6667 0.3333 0.3333

41 1.0 0 0 0.5

41 1.0 0.3333 0.6667 0.1667

41 1.0 0.6667 0.3333 0.8333

8 1.0 0.0492 0.3446 0.0647

8 1.0 0.3825 0.0113 0.7314

8 1.0 0.7159 0.6779 0.3980

8 1.0 0.6554 0.7046 0.0647

8 1.0 0.9887 0.3713 0.7314

8 1.0 0.3221 0.0379 0.3980

8 1.0 0.2954 0.9508 0.0647

8 1.0 0.6287 0.6175 0.7314

8 1.0 0.9621 0.2841 0.3980

8 1.0 0.6554 0.9508 0.5647

8 1.0 0.9887 0.6175 0.2314

8 1.0 0.3221 0.2841 0.8980

8 1.0 0.0492 0.7046 0.5647

8 1.0 0.3825 0.3713 0.2314

8 1.0 0.7159 0.0379 0.8980

8 1.0 0.2954 0.3446 0.5647

8 1.0 0.6287 0.0113 0.2314

8 1.0 0.9621 0.6779 0.8980