

Chapter 2.8

CELL

Unit Cell Reduction

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The programs under this menu item are useful in checking whether the proposed unit cell is consistent with higher symmetry, or if two cells are related.

- **LEPAGE** This program carries out an analysis of metric symmetry, and can optionally search for subcells and supercells, based on the Lepage MISSYM algorithm.
- **REDUCE** This program carries out the standard Derichlet reduction of the given unit cell, and calculates all lattice vectors up to the desired limit.

A summary output is sent to the TextServer and a more extensive output is given in the listing file (*LEPAGE.LST*). Sample output

```

THE CRITICAL VALUES USED ARE:
=====
BETWEEN THE AXES  =>  1.000 DEGREE
PSEUDO/METRICAL   =>  0.100 DEGREE
=====

Cell      Latt   a       b       c       Alpha  Beta   Gamma  Vol
-----
Input     P       8.103  14.844  14.582  90.00  100.65  90.00  1723.62
Primitive P       8.103  14.844  14.582  90.00  100.65  90.00  1723.62
Reduced   P       8.103  14.582  14.844  90.00   90.00  100.65  1723.61

Transformation matrix:  input to reduced cell      Niggli matrix
=====
(A')  (-1.00 0.00 0.00) (A)                      (A.A, B.B, C.C/B.C, A.C, A.B)
(B')  ( 0.00 0.00-1.00) (B).                      65.655  212.635  220.332
(C')  ( 0.00-1.00 0.00) (C)                      0.000   0.000  -21.842

Sorted axial lengths of the reduced cell
-----
1   1  0  0   8.103   13   2  0 -1   21.976   25   1 -2  0   31.679
2   0  1  0  14.582   14   2  0  1   21.976   26   1  2 -1   32.391

```

```

3   0  0  1  14.844   15   1 -1 -1  23.287   27   1  2  1  32.391
4   1  1  0  15.317   16   1 -1  1  23.287   28   0  2 -1  32.724

```

Inter-vector angles (deg) for reduced cell

```

1  2    1  0  0    0  1  0    100.65
1  3    1  0  0    0  0  1    90.00
1  4    1  0  0    1  1  0    69.33
1  5    1  0  0    1  0 -1    61.37
1  6    1  0  0    1  0  1    61.37

```

Number of possible 2-fold axes found = 1. Max. delta = 0.000

Nr	D	N	Rows			Products			Angle between two direct axes
			Direct	Reciprocal	Dot	Delta	Angle between two direct axes		
1	14.844	0	0 0 1	0 0 1	1	0.000	0.0		

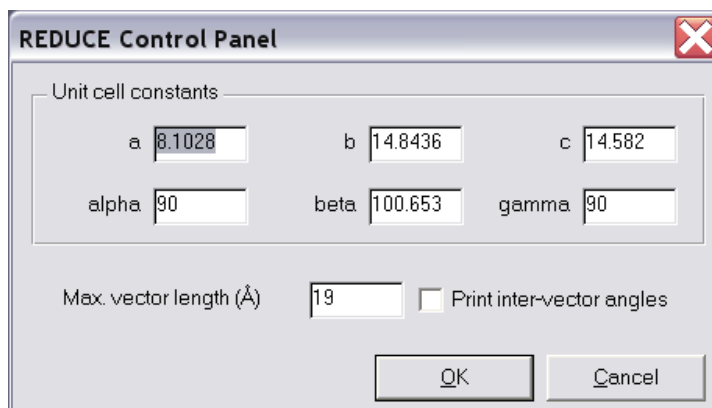
=== Transformation matrix: input (A,B,C) to conventional cell (A', B', C') ===

```

=====
(A')  (-1.00 0.00 0.00) (A)  (X')  (-1.00 0.00 0.00) (X)  metrically
(B')  ( 0.00 1.00 0.00) (B)  (Y')  ( 0.00 1.00 0.00) (Y)  monoclinic
(C')  ( 0.00 0.00-1.00) (C)  (Z')  ( 0.00 0.00-1.00) (Z)  FOM: 0.000
=====

```

Cell	Latt	a	b	c	Alpha	Beta	Gamma	Vol
Input	P	8.103	14.844	14.582	90.00	100.65	90.00	1723.62
Reduced	P	8.103	14.582	14.844	90.00	90.00	100.65	1723.61



A summary output is sent to the TextServer and a more extensive output is given in the listing file (*REDUCE.LST*). Sample output

Starting CELL *****

```

Real CELL
Edges      8.1028  14.8436  14.5820
Cosines    0.00000  -0.18486  0.00000
Angles     90.00    100.65    90.00
Volume     1723.62

Reciprocal CELL
Edges      0.1255785  0.0673691  0.0697804
Cosines    0.00000    0.18486    0.00000
Angles     90.00     79.35     90.00
Volume     0.0005802

Real and reciprocal metric tensors

   65.655   0.000  -21.842   0.015770  0.000000  0.001620
   0.000  220.332   0.000   0.000000  0.004539  0.000000
 -21.842   0.000  212.635   0.001620  0.000000  0.004869

```

```

Reduced CELL *****

Real CELL
Edges      8.1028  14.5820  14.8436
Cosines    0.00000  0.00000  -0.18486
Angles     90.00   90.00   100.65
Volume     1723.62

Reciprocal CELL
Edges      0.1255785  0.0697804  0.0673691
Cosines    0.00000  0.00000  0.18486
Angles     90.00   90.00   79.35
Volume     0.0005802

Real and reciprocal metric tensors

    65.655  -21.842   0.000   0.015770  0.001620  0.000000
   -21.842  212.635   0.000   0.001620  0.004869  0.000000
    0.000   0.000  220.332   0.000000  0.000000  0.004539

A(reduced)=J*A where J is
  1.  0.  0.
  0.  0.  1.
  0. -1.  0.

Reduced CELL is Delaunay cell

Lattice vectors
no  h  k  l      length
 1  1  0  0      8.103
 2  0  0  1     14.582
 3  0  1  0     14.844
 4  1  0  1     15.317
 5  2  0  0     16.206
 6  1 -1  0     16.911
 7  1  1  0     16.911
 8 -1  0  1     17.944

Angles between vectors
 1  2      1  0  0      0  0  1     100.65
 1  3      1  0  0      0  1  0      90.00
 1  4      1  0  0      1  0  1      69.33
 1  5      1  0  0      2  0  0       1.00
 1  6      1  0  0      1 -1  0      61.37
 1  7      1  0  0      1  1  0      61.37

```