

LATT and SYMM instructions in SHELXL input files

The “LATT” instruction specifies (1) whether a space group is centrosymmetric, or not and (2) whether there are any additional translations due to centering that need to be included in the list of symmetry-related positions.

If LATT is negative, the space group is **not** centrosymmetric and no additional symmetry related positions due to a center-of-symmetry are present. If LATT is positive, the space group **is** centrosymmetric and each of the symmetry-related positions on the SYMM instructions need to be multiplied by $-1, -1, -1$ to produce another set of positions. Thus, space group P2(1)/c (#14) would have LATT and SYMM instructions:

```
LATT 1
SYMM  -X, .50+Y, .50-Z
```

It is always understood that the identity symmetry-related position (X, Y, Z) is present, in addition to those listed on the SYMM instruction(s). Therefore, space group P2(1)/c (#14) has four symmetry operations:

```
  X, Y, Z
-X, .50+Y, .50-Z
plus two more related to these by the center of symmetry (LATT is positive):
-X, -Y, -Z
  X, -.50-Y, -.50+Z
```

Because LATT=1, there is no additional centering (the cell is said to be “Primitive”).

The possible values of LATT and their interpretations are:

<u>LATT</u>	<u>centering</u>	<u>additional translation</u>
1	Primitive (no centering)	
2	I-centered (body-centered)	+ .50, + .50, + .50
3	Rhombohedral (R)	+ .333, + .666, + .666 and + .666, + .333, + .333
4	F-centered (face centered)	+0, + .50, + .50 and + .50, +0, + .50 and + .50, + .50, +0
5	A-centered	+0, + .50, + .50
6	B-centered	+ .50, +0, + .50
7	C-centered	+ .50, + .50, +0

For example, space group C2/c (#15) would have LATT and SYMM instructions:

```
LATT 7  
SYMM -X, +Y, .50-Z
```

This would lead to eight symmetry-related positions:

```
      X, Y, Z  
-X, +Y, .50-Z      from the SYMM instruction  
plus  
-X, -Y, -Z  
X, -Y, -.50+Z     from the center-of-symmetry specified by positive LATT  
Plus  
.50+X, .50+Y, Z  
.50-X, .50+Y, .50-Z  
.50-X, .50-Y, -Z  
.50+X, .50-Y, -.50+Z     from the C-centering
```