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Comments about the CIF file format

The International Union of Crystallography (`http://www.iucr.org/resources/cif`) has defined the CIF "Crystallographic Information Framework" in order to facilitate data exchange. Many results are available in the open database `http://www.crystallography.net/new.html` as well as from supplementary materials in some journal articles. You can also create a CIF file from information you have. The following example shows a minimal number of key words and data that can produce a CIF file readable by the program *mercury*:

```
# s1-Li2PO2N structure Calculated
# Calculated using PWscf
data_s1Li2PO2N
_chemical_formula_iupac  'Li2 P O2 N'
_chemical_formula_sum  'Li2 N O2 P'
_space_group_IT_number  57
_symmetry_cell_setting  orthorhombic
_symmetry_space_group_name_H-M  'P b c m'
_cell_angle_alpha 90.0
_cell_angle_beta  90.0
_cell_angle_gamma  90.0
_cell_length_a  5.35
_cell_length_b  4.68
_cell_length_c  9.16
_cell_formula_units_Z  4
#Fractional coordinates
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
 Li  0.167   -0.454    -0.408
 P   0.341    0.456     0.250
 O   0.184   -0.039    -0.386
 N  -0.387   -0.388     0.250
```