

Flowchart

- 1) Obtain crystallographic primitive cell (Table 3), “reduced” cell for triclinic, Sec.4.2.4.
- 2) Derive “extended Bravais” symbol: Bravais symbol (check space group number range) + “type” (depends on either space group range or axial ratio) + inversion (Y or N, check space group number range!)
- 3) Force inversion in extended Bravais symbol if time-reversal symmetry is enforced.
- 4) Look up relevant table of definition of labels, coordinates, band path (Table 69-92, kpx, kpy, kpz); don’t forget to include “inverted wedge” if there is no inversion! Except for triclinic: One band path per one extended Bravais symbol. Two extended Bravais symbols for one table only if the type specifies whether then extra path is included or not. Triclinic: determine acute or obtuse by looking at a reciprocal interaxial angle, and use labels, coordinates, and band path in the relevant table.
- 5) Optional: give kpoint coordinates along the band path along with identifiers for labelled points. My preference for kpoint intervals is $0.025/2\pi$ ($2\pi/\text{angstrom}$), but it depends on how much resources you can afford.

Extended Bravais definition

Extended Bravais symbol: Bravais lattice + type (1-3) + inversion (Y/N)

Bravais lattice, type, definition

cP1: #195-206 (extra path)

cP2: #207-230 (no extra path)

cF1: #195-206 (extra path)

cF2: #207-230 (no extra path)

cI1

tP1

tI1:c<a

tI2:c>a

oP1

oF1: $a^2 > b^2 + c^2$

oF2: $c^2 > a^2 + b^2$
 oF3: a^2, b^2, c^2 edges of triangle
 oI1: c largest
 oI2: a largest
 oI3: b largest
 oC1: $a < b$
 oC2: $a > b$
 oA1: $b < c$
 oA2: $b > c$
 hP1: #143-149, 151, 153, 157, 159-163 (extra path)
 hP2: Other (no extra path)
 hR1: $\sqrt{3}a < \sqrt{2}c$
 hR2: $\sqrt{3}a > \sqrt{2}c$
 mP1
 mC1: $b < \sin(\beta)$
 mC2: $b > \sin(\beta)$ BZ 12-face
 mC3: $b > \sin(\beta)$ BZ 14-face
 aP1

Example of an extended Bravais symbol is oP1Y or mP1N.