

Table of standard unit cells appropriate for periodic boundary conditions.

Restrictions on the unit cells lengths (a, b, c) and angles (α , β , γ) are presented along with the volumes for a variety of simulation cells.

The volume of a triclinic cell is

$$V = abc * (1 - \cos(\alpha)^2 - \cos(\beta)^2 - \cos(\gamma)^2 + 2\cos(\alpha)\cos(\beta)\cos(\gamma))^{1/2}.$$

	Restrictions on unit cell parameters	volume
cubic	a=b=c $\alpha=\beta=\gamma=90.0^\circ$	a^3
tetragonal	A=b $\alpha=\beta=\gamma=90.0^\circ$	ca^2
orthorhomic	$\alpha=\beta=\gamma=90.0^\circ$	abc
monoclinic	$\alpha=\gamma=90^\circ$	abc*sin(β)
triclinic	no restrictions	(see legend)
hexagonal	A=b $\alpha=\beta=90^\circ, \gamma=120.0^\circ$	$(3/4)^{1/2}ca^2$
rhombohedral (trigonal)	a=b=c $\alpha=\beta=\gamma < 120.0^\circ$	$a^3(1-\cos(\alpha))(1+2\cos(\alpha))^{1/2}$
octahedral (truncated octahedral)	a=b=c $\alpha=\beta=\gamma=109.47122063449$	$(4(3)^{1/2}/9)a^3$
rhombic dodecahedral	a=b=c $\alpha=\gamma=60^\circ, \beta=90.0^\circ$	$(1/2)^{1/2}a^3$