Mathematics 11: Band Structures

We look at a few three-dimensional geometries, analysing the bandstructures generic to them. We place the atoms in the correct places in space, but we do not use the correct atomic states for the electron. Each atom is permitted a single s-electron which hops to only the closest neighbours, so-called *tight-binding theory.*

Bloch's theorem ensures that the electronic states only pick up a phase of $e^{i\mathbf{k}.\mathbf{R}}$ in translating from any cell to another cell at a position lattice vector $\mathbf{R}$ away. The permissable eigenstates are then controlled by the matrix:

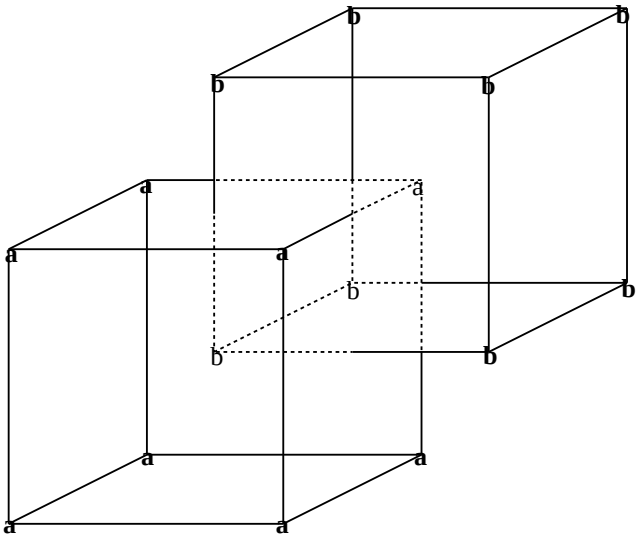
$$\gamma_{\mathbf{k}\alpha\alpha'} = -\frac{1}{N}\sum_{ij} t_{ij}^{\alpha\alpha'} e^{i\mathbf{k}.(\mathbf{R}_i+\mathbf{c}_\alpha-\mathbf{R}_j-\mathbf{c}_{\alpha'})}$$

where α, α' are labels denoting the particular atom in the cell, $\mathbf{R}_i + \mathbf{c}_\alpha$ is the position of the α'th atom, $\mathbf{c}_\alpha$, in the i'th cell, $\mathbf{R}_i$, and the $t_{ij}^{\alpha\alpha'}$ are the hopping strengths. It is not crucial to understand the details, only the basic idea.

(i) *Simple Cubic*
(i.1) One atom per unit cell:

$$\gamma_{\mathbf{k}} = \frac{1}{3}\left[\cos k_1 + \cos k_2 + \cos k_3\right]$$

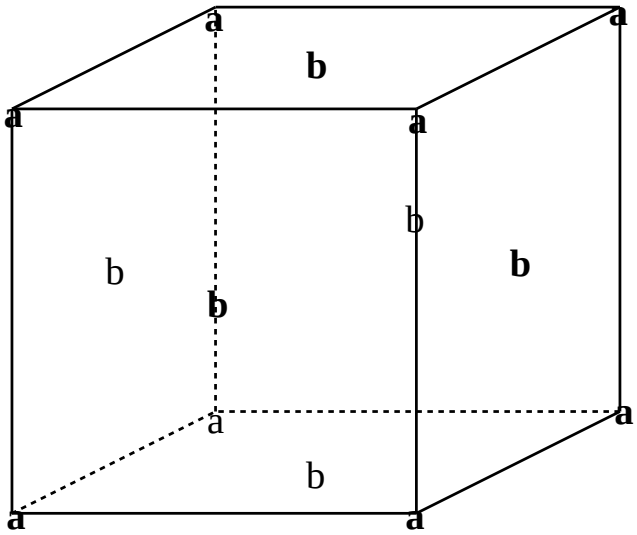
(i.2) Cesium-Chloride Structure: CsCl



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -8t\cos\frac{k_1}{2}\cos\frac{k_2}{2}\cos\frac{k_3}{2} \\ -8t\cos\frac{k_1}{2}\cos\frac{k_2}{2}\cos\frac{k_3}{2} & e \end{bmatrix}$$

with the special case that:
$e = 0 \mapsto$ Body-centre cubic.

(i.3) Copper-Gold Structure: Cu_3Au



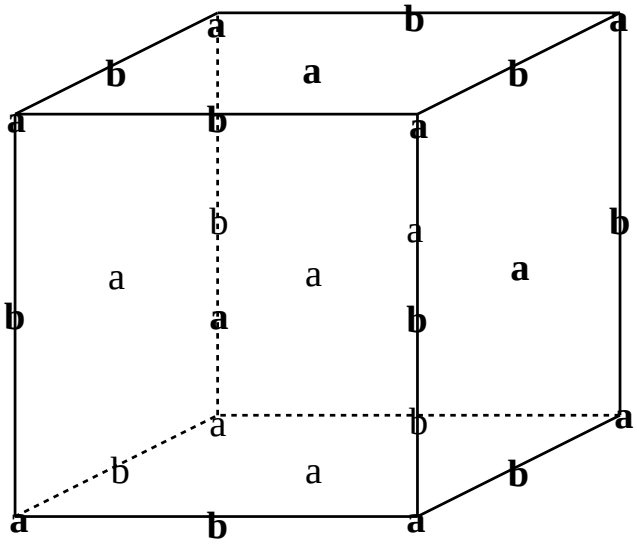
$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -4t\cos\frac{k_2}{2}\cos\frac{k_3}{2} & -4t\cos\frac{k_3}{2}\cos\frac{k_1}{2} & -4t\cos\frac{k_1}{2}\cos\frac{k_2}{2} \\ -4t\cos\frac{k_2}{2}\cos\frac{k_3}{2} & e & -4s\cos\frac{k_1}{2}\cos\frac{k_2}{2} & -4s\cos\frac{k_3}{2}\cos\frac{k_1}{2} \\ -4t\cos\frac{k_3}{2}\cos\frac{k_1}{2} & -4s\cos\frac{k_1}{2}\cos\frac{k_2}{2} & e & -4s\cos\frac{k_2}{2}\cos\frac{k_3}{2} \\ -4t\cos\frac{k_1}{2}\cos\frac{k_2}{2} & -4s\cos\frac{k_3}{2}\cos\frac{k_1}{2} & -4s\cos\frac{k_2}{2}\cos\frac{k_3}{2} & e \end{bmatrix}$$

with the special case that:
$e = 0$ and $t = s \mapsto$ Face-centre cubic.

(ii) *Face-centre cubic:*
(ii.1) One atom per unit cell

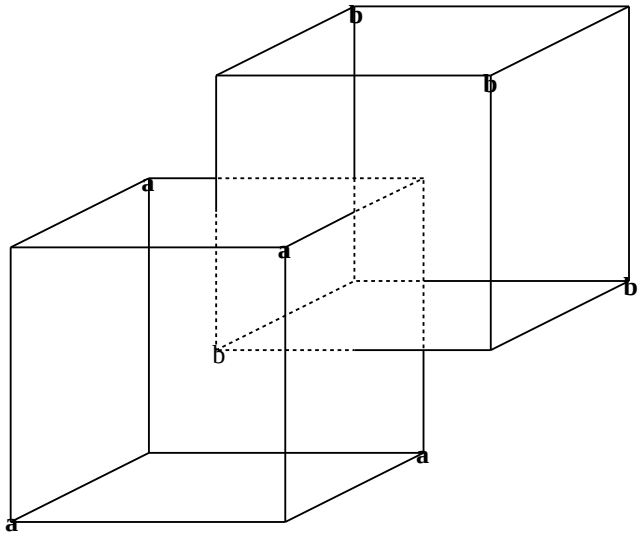
$$\gamma_{\mathbf{k}} = \frac{1}{3}\left[\cos k_2 \cos k_3 + \cos k_3 \cos k_1 + \cos k_1 \cos k_2\right]$$

(ii.2) Sodium-Chloride: NaCl



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -2t\left[\cos\frac{k_1}{2} + \cos\frac{k_2}{2} + \cos\frac{k_3}{2}\right] \\ -2t\left[\cos\frac{k_1}{2} + \cos\frac{k_2}{2} + \cos\frac{k_3}{2}\right] & e \end{bmatrix}$$

with the special case that:
$e = 0 \mapsto$ Simple cubic.
(ii.3) Zincblende: Diamond

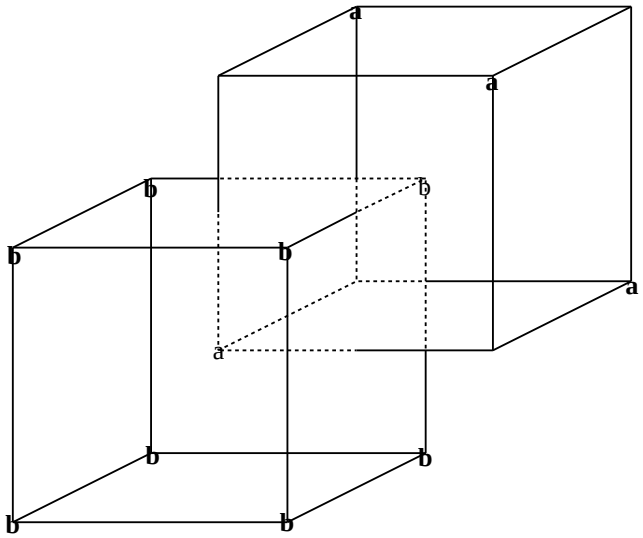


$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -t\gamma_{\mathbf{k}}^{D} \\ -t\gamma_{\mathbf{k}}^{D*} & e \end{bmatrix}$$

in terms of:

$$\gamma_{\mathbf{k}}^{D} = \left[e^{i(k_1+k_2+k_3)/2} + e^{i(k_1-k_2-k_3)/2} + e^{i(-k_1+k_2-k_3)/2} + e^{i(-k_1-k_2+k_3)/2}\right]$$

with no special case.
(ii.4) Uranium-dioxide structure: UO_2

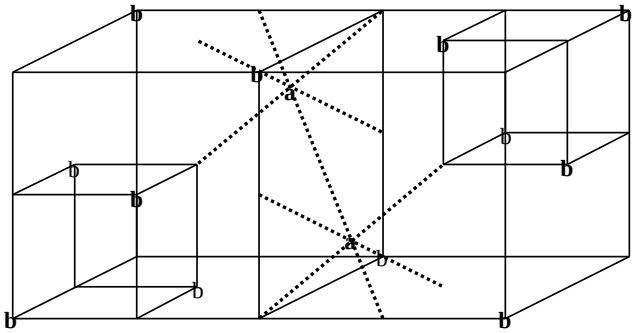


$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -t\gamma_{\mathbf{k}}^{D} & -t\gamma_{\mathbf{k}}^{D*} \\ -t\gamma_{\mathbf{k}}^{D*} & e & -2s\left[\cos\frac{k_1}{2}+\cos\frac{k_2}{2}+\cos\frac{k_3}{2}\right] \\ -t\gamma_{\mathbf{k}}^{D} & -2s\left[\cos\frac{k_1}{2}+\cos\frac{k_2}{2}+\cos\frac{k_3}{2}\right] & e \end{bmatrix}$$

in terms of:

$$\gamma_{\mathbf{k}}^{D} = \left[e^{i(k_1+k_2+k_3)/2} + e^{i(k_1-k_2-k_3)/2} + e^{i(-k_1+k_2-k_3)/2} + e^{i(-k_1-k_2+k_3)/2}\right]$$

with the special case that:
$e = 0 = t \mapsto$ Simple cubic.
(ii.5) Pyrochlore lattice: YMn_2



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & 0 & -t\gamma_0 & -t\gamma_1 & -t\gamma_2 & -t\gamma_3 \\ 0 & 0 & -t\gamma_0^* & -t\gamma_1^* & -t\gamma_2^* & -t\gamma_3^* \\ -t\gamma_0^* & -t\gamma_0 & e & -2sc_1 & -2sc_2 & -2sc_3 \\ -t\gamma_1^* & -t\gamma_1 & -2sc_1 & e & -2s\bar{c}_3 & -2s\bar{c}_2 \\ -t\gamma_2^* & -t\gamma_2 & -2sc_2 & -2s\bar{c}_3 & e & -2s\bar{c}_1 \\ -t\gamma_3^* & -t\gamma_3 & -2sc_3 & -2s\bar{c}_2 & -2s\bar{c}_1 & e \end{bmatrix}$$

where:

$$\begin{aligned} \gamma_0 &= e^{i[x+y+z]}\left[e^{-4ix} + e^{-4iy} + e^{-4iz}\right] \\ \gamma_1 &= e^{i[x-y-z]}\left[e^{-4ix} + e^{4iy} + e^{4iz}\right] \\ \gamma_2 &= e^{i[-x+y-z]}\left[e^{4ix} + e^{-4iy} + e^{4iz}\right] \\ \gamma_3 &= e^{i[-x-y+z]}\left[e^{4ix} + e^{4iy} + e^{-4iz}\right] \end{aligned}$$

and:

$$c_1 = \cos(2y+2z) \qquad c_2 = \cos(2z+2x) \qquad c_3 = \cos(2x+2y)$$

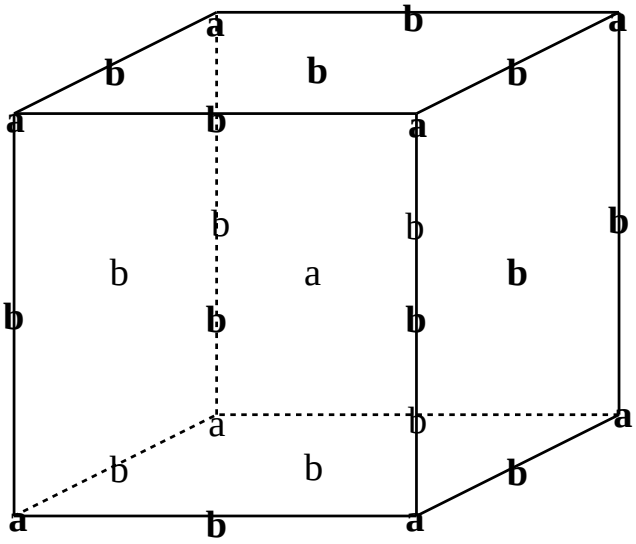
$$\bar{c}_1 = \cos(2y-2z) \qquad \bar{c}_2 = \cos(2z-2x) \qquad \bar{c}_3 = \cos(2x-2y)$$

interms of $k_1 = 4x$, $k_2 = 4y$ and $k_3 = 4z$, and with no special case.

(iii) *Body-centre cubic*
(iii.1) One atom per unit cell

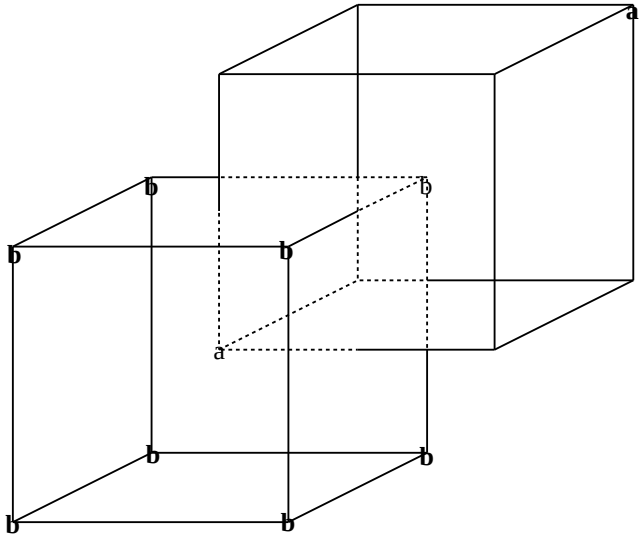
$$\gamma_{\mathbf{k}} = \cos k_1 \cos k_2 \cos k_3$$

(iii.2)



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -2t\cos k_1 & -2t\cos k_2 & -2t\cos k_3 \\ -2t\cos k_1 & e & -2s\cos k_3 & -2s\cos k_2 \\ -2t\cos k_2 & -2s\cos k_3 & e & -2s\cos k_1 \\ -2t\cos k_3 & -2s\cos k_2 & -2s\cos k_1 & e \end{bmatrix}$$

with the special case that:
$e = 0$ and $s = t \mapsto$ Simple cubic.
(iii.3)

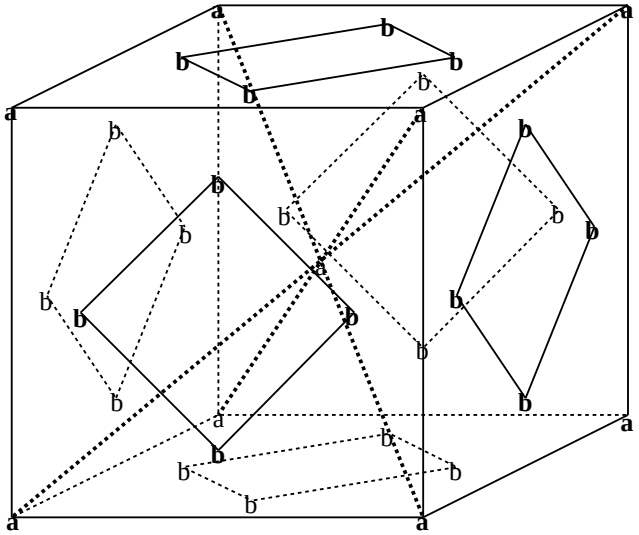


$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -2tc_0 & -2tc_1 & -2tc_2 & -2tc_3 \\ -2tc_0 & e & -2s\cos k_1 & -2s\cos k_2 & -2s\cos k_3 \\ -2tc_1 & -2s\cos k_1 & e & -2s\cos k_3 & -2s\cos k_2 \\ -2tc_2 & -2s\cos k_2 & -2s\cos k_3 & e & -2s\cos k_1 \\ -2tc_3 & -2s\cos k_3 & -2s\cos k_2 & -2s\cos k_1 & e \end{bmatrix}$$

where:

$$c_0 = \cos\frac{k_1 + k_2 + k_3}{2}$$
$$c_1 = \cos\frac{k_1 - k_2 - k_3}{2}$$
$$c_2 = \cos\frac{-k_1 + k_2 - k_3}{2}$$
$$c_3 = \cos\frac{-k_1 - k_2 + k_3}{2}$$

with the special case that:
$e = 0 = t \mapsto$ Simple cubic.
(iii.4) UBe_{12} 'U'



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -2t\gamma_1 & -2t\gamma_2 & -2t\gamma_3 & -2t\gamma_1^* & -2t\gamma_2^* & -2t\gamma_3^* \\ -2t\gamma_1^* & e & -sxy & -sz^{-1}x^{-1} & 0 & -sxy^{-1} & -szx^{-1} \\ -2t\gamma_2^* & -sx^{-1}y^{-1} & e & -syz & -sxy^{-1} & 0 & -syz^{-1} \\ -2t\gamma_3^* & -szx & -sy^{-1}z^{-1} & e & -szx^{-1} & -syz^{-1} & 0 \\ -2t\gamma_1 & 0 & -sx^{-1}y & -sz^{-1}x & e & -sx^{-1}y^{-1} & -szx \\ -2t\gamma_2 & -sx^{-1}y & 0 & -sy^{-1}z & -sxy & e & -sy^{-1}z^{-1} \\ -2t\gamma_3 & -sz^{-1}x & -sy^{-1}z & 0 & -sz^{-1}x^{-1} & -syz & e \end{bmatrix}$$

in terms of:

$$\gamma_1 = xc_2 + x^{-1}c_3$$
$$\gamma_2 = yc_3 + y^{-1}c_1$$
$$\gamma_3 = zc_1 + z^{-1}c_2$$

where:

$$c_1 = \frac{1}{2}\left[x^2 + x^{-2}\right] \qquad c_2 = \frac{1}{2}\left[y^2 + y^{-2}\right] \qquad c_3 = \frac{1}{2}\left[z^2 + z^{-2}\right]$$

and:

$$x = e^{ik_1/2} \qquad y = e^{ik_2/2} \qquad z = e^{ik_3/2}$$

(iv) *Simple Hexagonal*
(iv.1) Hexagonal close-packing:

$$\gamma_{\mathbf{k}\pm} = \frac{\gamma^T_{\mathbf{k}\parallel}}{2} \pm \frac{\cos\frac{k_3}{2}}{6}\sqrt{[3 + 6\gamma^T_{\mathbf{k}\parallel}]}$$

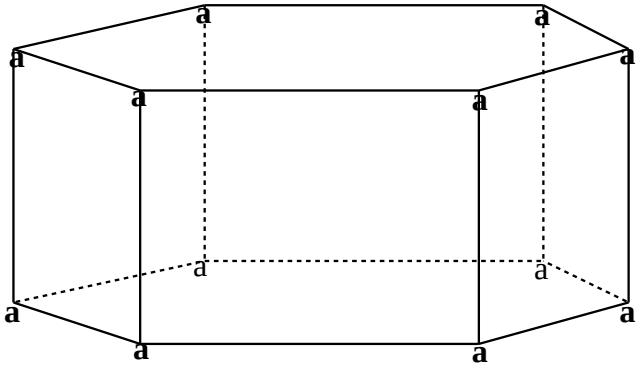
in terms of the triangular lattice structure factor:

$$\gamma^T_{\mathbf{k}\parallel} = \frac{1}{3}\left[2\cos\frac{k_1}{2}\left(\cos\frac{k_1}{2} + \cos\frac{\sqrt{3}k_2}{2}\right) - 1\right]$$

(iv.2) Simple Hexagonal:

$$\gamma_{\mathbf{k}} = -6t\gamma^T_{\mathbf{k}\parallel} - 2s\cos\frac{k_3}{2}$$

(iv.3) Graphite:

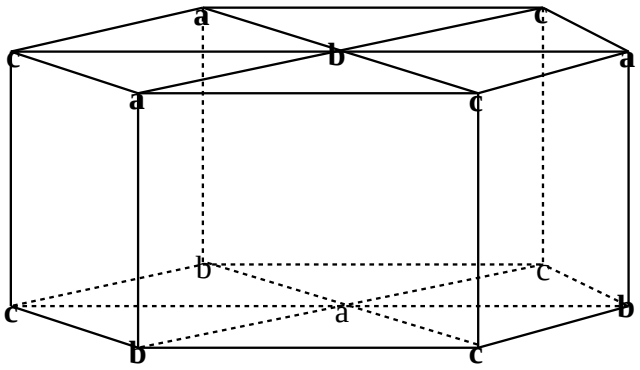


$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -t\gamma^t_{\mathbf{k}\parallel} - 2s\cos k_3 \\ -t\gamma^{t*}_{\mathbf{k}\parallel} - 2s\cos k_3 & e \end{bmatrix}$$

in terms of:

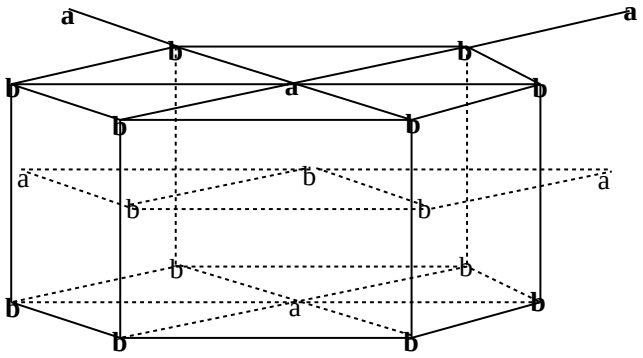
$$\gamma^t_{\mathbf{k}\parallel} = e^{ik_1} + e^{-i(k_1+\sqrt{3}k_2)/2} + e^{-i(k_1-\sqrt{3}k_2)/2}$$

with no special case.
(iv.4)



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & -t\gamma^{t}_{\mathbf{k}\|} & -t\gamma^{t*}_{\mathbf{k}\|} & 0 & -2t\cos\frac{k_3}{2} & 0 \\ -t\gamma^{t*}_{\mathbf{k}\|} & e & -s\gamma^{t}_{\mathbf{k}\|} & -2t\cos\frac{k_3}{2} & 0 & 0 \\ -t\gamma^{t}_{\mathbf{k}\|} & -s\gamma^{t*}_{\mathbf{k}\|} & e & 0 & 0 & -2t\cos\frac{k_3}{2} \\ 0 & -2t\cos\frac{k_3}{2} & 0 & 0 & -t\gamma^{t*}_{\mathbf{k}\|} & -t\gamma^{t}_{\mathbf{k}\|} \\ -2t\cos\frac{k_3}{2} & 0 & 0 & -t\gamma^{t}_{\mathbf{k}\|} & e & -s\gamma^{t*}_{\mathbf{k}\|} \\ 0 & 0 & -2t\cos\frac{k_3}{2} & -t\gamma^{t*}_{\mathbf{k}\|} & -s\gamma^{t}_{\mathbf{k}\|} & e \end{bmatrix}$$

with the special case that:
$e = 0$ and $s = t \mapsto$ Simple Hexagonal.
(iv.5) Uranium Platinide: UPt_3



$$\gamma_{\mathbf{k}\alpha\alpha'} = \begin{bmatrix} 0 & 0 & -2tc_1 & -2tc_2 & -2tc_3 & -2txc_0 & -2tyc_0 & -2tzc_0 \\ 0 & 0 & -2tx^{-1}c_0 & -2ty^{-1}c_0 & -2tz^{-1}c_0 & -2tc_1 & -2tc_2 & -2tc_3 \\ -2tc_1 & -2txc_0 & e & -2sc_3 & -2sc_2 & 0 & -2szc_0 & -2syc_0 \\ -2tc_2 & -2tyc_0 & -2sc_3 & e & -2sc_1 & -2szc_0 & 0 & -2sxc_0 \\ -2tc_3 & -2tzc_0 & -2sc_2 & -2sc_1 & e & -2syc_0 & -2sxc_0 & 0 \\ -2tx^{-1}c_0 & -2tc_1 & 0 & -2sz^{-1}c_0 & -2sy^{-1}c_0 & e & -2sc_3 & -2sc_2 \\ -2ty^{-1}c_0 & -2tc_2 & -2sz^{-1}c_0 & 0 & -2sx^{-1}c_0 & -2sc_3 & e & -2sc_1 \\ -2tz^{-1}c_0 & -2tc_3 & -2sy^{-1}c_0 & -2sx^{-1}c_0 & 0 & -2sc_2 & -2sc_1 & e \end{bmatrix}$$

in terms of:

$$2c_1 = \frac{y}{z} + \frac{z}{y} \qquad 2c_2 = \frac{z}{x} + \frac{x}{z} \qquad 2c_3 = \frac{x}{y} + \frac{y}{x}$$

where:

$$x = \exp\left[\frac{i}{3}\left(\frac{-k_1 + \sqrt{3}k_2}{2} - \frac{-k_1 - \sqrt{3}k_2}{2}\right)\right]$$
$$y = \exp\left[\frac{i}{3}\left(k_1 - \frac{-k_1 - \sqrt{3}k_2}{2}\right)\right]$$
$$z = \exp\left[\frac{i}{3}\left(\frac{-k_1 - \sqrt{3}k_2}{2} - k_1\right)\right]$$

and:

$$c_0 = \cos\frac{k_3}{2}$$