Basis vectors for Tb1 sites ATOM 1: (.05, .25, .65), ATOM 2: (.95, .75, .35), ATOM 3: (.45, .75, .15)

ATOM 4: (.55, .25, .85), 2-dimensional irrep, contained 6 times in GAMMA (12 BVs)

$\mathbf{k}_{13}$ = (½ □ 0), □=0.29

	Atom #1	Atom #2	Atom #3	Atom #4
ψ1	(1 0 0)	(1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ2	(0 1 0)	(0 -1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ3	(0 0 1)	(0 0 1) exp[iπ□]	(0 0 0)	(0 0 0)
ψ4	(0 0 0)	(0 0 0)	(1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ5	(0 0 0)	(0 0 0)	(0 -1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ6	(0 0 0)	(0 0 0)	(0 0 -1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ7	(0 0 0)	(0 0 0)	(-1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ8	(0 0 0)	(0 0 0)	(0 1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ9	(0 0 0)	(0 0 0)	(0 0 1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ10	(1 0 0)	(-1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ11	(0 1 0)	(0 1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ12	(0 0 1)	(0 0 -1) exp[iπ□]	(0 0 0)	(0 0 0)

$$Sk\ (x) = C1*\psi_1 + C4*\psi_4 + C7*\psi_7 + C10*\psi_{10}$$

$$Sk(y) = C2*\psi_2 + C5*\psi_5 + C8*\psi_8 + C11*\psi_{11}$$

$$Sk(z) = C3*\psi_3 + C6*\psi_6 + C9*\psi_9 + C12*\psi_{12}$$

Basis vectors for Tb2 sites ATOM 1: (.18, .065, .821), ATOM 2: (.82, .565, .179), ATOM 3: (.32, .565, .321), ATOM 4: (.68, .065, .679), 2-dimensional irrep, contained 6 times in GAMMA (12 BVs)

$\mathbf{k}_{13}$ = (½ □ 0), □=0.29

	Atom #1	Atom #2	Atom #3	Atom #4
ψ1	(1 0 0)	(1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ2	(0 1 0)	(0 -1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ3	(0 0 1)	(0 0 1) exp[iπ□]	(0 0 0)	(0 0 0)
ψ4	(0 0 0)	(0 0 0)	(1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ5	(0 0 0)	(0 0 0)	(0 -1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ6	(0 0 0)	(0 0 0)	(0 0 -1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ7	(0 0 0)	(0 0 0)	(-1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ8	(0 0 0)	(0 0 0)	(0 1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ9	(0 0 0)	(0 0 0)	(0 0 1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ10	(1 0 0)	(-1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ11	(0 1 0)	(0 1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ12	(0 0 1)	(0 0 -1) exp[iπ□]	(0 0 0)	(0 0 0)

$$Sk\ (x) = C1*\psi_1 + C4*\psi_4 + C7*\psi_7 + C10*\psi_{10}$$

$$Sk(y) = C2*\psi_2 + C5*\psi_5 + C8*\psi_8 + C11*\psi_{11}$$

$$Sk(z) = C3*\psi_3 + C6*\psi_6 + C9*\psi_9 + C12*\psi_{12}$$

Basis vectors for Tb2_2 sites ATOM 1: (.32, .935, .321), ATOM 2: (.68, .435, .679), ATOM 3: (.18, .435, .821)

ATOM 4: (.82, .935, .179) 2-dimensional irrep, contained 6 times in GAMMA (12 BVs)

$\mathbf{k}_{13}$ = (½ □ 0), □=0.29

	Atom #1	Atom #2	Atom #3	Atom #4
ψ1	(1 0 0)	(1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ2	(0 1 0)	(0 -1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ3	(0 0 1)	(0 0 1) exp[iπ□]	(0 0 0)	(0 0 0)
ψ4	(0 0 0)	(0 0 0)	(1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ5	(0 0 0)	(0 0 0)	(0 -1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ6	(0 0 0)	(0 0 0)	(0 0 -1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ7	(0 0 0)	(0 0 0)	(-1 0 0) exp[iπ(□–0.5)]	(-1 0 0) exp[iπ/2]
ψ8	(0 0 0)	(0 0 0)	(0 1 0) exp[iπ(□–0.5)]	(0 -1 0) exp[iπ/2]
ψ9	(0 0 0)	(0 0 0)	(0 0 1) exp[iπ(□–0.5)]	(0 0 1) exp[iπ/2)]
ψ10	(1 0 0)	(-1 0 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ11	(0 1 0)	(0 1 0) exp[iπ□]	(0 0 0)	(0 0 0)
ψ12	(0 0 1)	(0 0 -1) exp[iπ□]	(0 0 0)	(0 0 0)

$$Sk\ (x) = C1*\psi_1 + C4*\psi_4 + C7*\psi_7 + C10*\psi_{10}$$

$$Sk(y) = C2*\psi_2 + C5*\psi_5 + C8*\psi_8 + C11*\psi_{11}$$

$$Sk(z) = C3*\psi_3 + C6*\psi_6 + C9*\psi_9 + C12*\psi_{12}$$