

# Model for “C2h1”

Generated on 2026-02-01 11:15:31 by MultiPie 2.0.7

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## General Condition

- Basis type: **lgs**
- SAMB selection:
  - Type: [Q, G]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
  - Spin (s): [0, 1]
- Atomic selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [ $A_g$ ,  $B_g$ ,  $A_u$ ,  $B_u$ ]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: **false**

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## Group and Unit Cell

- Group: SG No. 10  $C_{2h}^1$   $P2/m$  (b-axis setting) [ monoclinic ]
- Associated point group: PG No. 10  $C_{2h}$   $2/m$  (b-axis setting) [ monoclinic ]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.20000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ 0.00000, 1.20000, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 1.00000 ]$

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## Symmetry Operation

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{2_{010} 0\}$	3	$\{-1 0\}$	4	$\{m_{010} 0\}$		

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## Harmonics

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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$Q_0(A_g)$	$A_g$	0	$Q, T$	-	-	1
2	$G_1(A_g)$	$A_g$	1	$G, M$	-	-	$y$
3	$Q_2(A_g, 3)$	$A_g$	2	$Q, T$	3	-	$\sqrt{3}xz$
4	$G_0(A_u)$	$A_u$	0	$G, M$	-	-	1
5	$Q_1(A_u)$	$A_u$	1	$Q, T$	-	-	$y$
6	$G_2(A_u, 2)$	$A_u$	2	$G, M$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$G_1(B_g, 1)$	$B_g$	1	$G, M$	1	-	$x$
8	$G_1(B_g, 2)$	$B_g$	1	$G, M$	2	-	$z$
9	$Q_2(B_g, 1)$	$B_g$	2	$Q, T$	1	-	$\sqrt{3}yz$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
10	$\mathbb{Q}_2(B_g, 2)$	$B_g$	2	$Q, T$	2	-	$\sqrt{3}xy$
11	$\mathbb{Q}_1(B_u, 1)$	$B_u$	1	$Q, T$	1	-	$x$
12	$\mathbb{Q}_1(B_u, 2)$	$B_u$	1	$Q, T$	2	-	$z$
13	$\mathbb{G}_2(B_u, 2)$	$B_u$	2	$G, M$	2	-	$\sqrt{3}xy$

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Basis in full matrix

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Table 3: dimension = 4

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ s, \uparrow\rangle @A(1)$	1	$ s, \downarrow\rangle @A(1)$	2	$ s, \uparrow\rangle @B(1)$	3	$ s, \downarrow\rangle @B(1)$

Table 4: Atomic basis (orbital part only)

orbital	definition
$ s\rangle$	1

34 (all 34) SAMBs

• 'A' site-cluster : A

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: 1a

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(s)}(A_g)$$

• 'B' site-cluster : B

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: 1e

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(s)}(A_g)$$

• 'A'-'A' bond-cluster : A;A\_001\_1

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: 1a@1d

$$\boxed{\text{z3}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z16}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$$

• 'A'-'A' bond-cluster : A;A\_001\_2

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: 1a@1c

$$\boxed{\text{z4}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z18}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1) \mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g) \mathbb{T}_1^{(b)}(B_u, 1)$$

• 'A'-'B' bond-cluster : B;A\_001\_1

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: 4a@4o

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g) \mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_g) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1) \mathbb{M}_1^{(b)}(B_g, 1)$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_g, 3) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2) \mathbb{M}_1^{(b)}(B_g, 1)$$

$$\boxed{\text{z8}} \quad \mathbb{G}_1^{(1,-1;c)}(A_g) = \mathbb{M}_1^{(1,-1;a)}(A_g) \mathbb{T}_0^{(b)}(A_g)$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_1^{(c)}(A_u) = \mathbb{Q}_0^{(a)}(A_g) \mathbb{Q}_1^{(b)}(A_u)$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2) \mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z13}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \frac{\sqrt{2} \mathbb{M}_1^{(1,-1;a)}(A_g) \mathbb{T}_1^{(b)}(A_u)}{2} + \frac{\sqrt{2} \mathbb{M}_1^{(1,-1;a)}(B_g, 1) \mathbb{T}_1^{(b)}(B_u, 1)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{G}_2^{(1,-1;c)}(A_u, 2) = -\frac{\sqrt{2} \mathbb{M}_1^{(1,-1;a)}(A_g) \mathbb{T}_1^{(b)}(A_u)}{2} + \frac{\sqrt{2} \mathbb{M}_1^{(1,-1;a)}(B_g, 1) \mathbb{T}_1^{(b)}(B_u, 1)}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_2^{(c)}(B_g, 1) = \mathbb{Q}_0^{(a)}(A_g) \mathbb{Q}_2^{(b)}(B_g, 1)$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_g, 2) = \mathbb{M}_1^{(1,-1;a)}(A_g) \mathbb{M}_1^{(b)}(B_g, 1)$$

$$\boxed{\text{z21}} \quad \mathbb{G}_1^{(1,-1;c)}(B_g, 1) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1) \mathbb{T}_0^{(b)}(A_g)$$

$$\boxed{\text{z22}} \quad \mathbb{G}_1^{(1,-1;c)}(B_g, 2) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2) \mathbb{T}_0^{(b)}(A_g)$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_1^{(c)}(B_u, 1) = \mathbb{Q}_0^{(a)}(A_g) \mathbb{Q}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 1) = -\mathbb{M}_1^{(1,-1;a)}(B_g, 2) \mathbb{T}_1^{(b)}(A_u)$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(A_u)}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{G}_2^{(1,-1;c)}(B_u, 2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(A_u)}{2}$$

- 'B'-'B' bond-cluster : B;B\_001\_1

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **1a@1b**

$$\boxed{\text{z9}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z24}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$$

- 'B'-'B' bond-cluster : B;B\_001\_2

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **1a@1h**

$$\boxed{\text{z10}} \quad \mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 2)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z26}} \quad \mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_g, 1)\mathbb{T}_1^{(b)}(B_u, 1)$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_u, 2) = -\mathbb{M}_1^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_u, 1)$$

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## Atomic SAMB

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- bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

- ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_g) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{M}_1^{(1, -1; a)}(A_g) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{M}_1^{(1, -1; a)}(B_g, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{M}_1^{(1, -1; a)}(B_g, 2) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

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## Cluster SAMB

- Site cluster

\*\* Wyckoff: **1e**

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

\*\* Wyckoff: **1a**

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

- Bond cluster

\*\* Wyckoff: **1a@1h**

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{\text{y4}} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

\*\* Wyckoff: **1a@1d**

$$\boxed{\text{y5}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{\text{y6}} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

\*\* Wyckoff: **1a@1c**

$$\boxed{\text{y7}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{\text{y8}} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

\*\* Wyckoff: **1a@1b**

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A_g) = [1]$$

$$\boxed{\text{y10}} \quad \mathbb{T}_1^{(s)}(B_u, 1) = [i]$$

\*\* Wyckoff: **4a@4o**

$$\boxed{\text{y11}} \quad \mathbb{Q}_0^{(s)}(A_g) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{T}_0^{(s)}(A_g) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{Q}_1^{(s)}(A_u) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{T}_1^{(s)}(A_u) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{M}_1^{(s)}(B_g, 1) = \left[ \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{Q}_2^{(s)}(B_g, 1) = \left[ \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{Q}_1^{(s)}(B_u, 1) = \left[ \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{T}_1^{(s)}(B_u, 1) = \left[ \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

— Site and Bond —



Table 5: Orbital of each site

#	site	orbital
1	A	$ s, \uparrow\rangle,  s, \downarrow\rangle$
2	B	$ s, \uparrow\rangle,  s, \downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	[1]	[s]	[s]
2	A	B	[1]	[s]	[s]
3	B	B	[1]	[s]	[s]

## — Site in Unit Cell —

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: 'A' (#1) site cluster (1a), 2/m

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4]

Table 8: 'B' (#2) site cluster (1e), 2/m

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.50000, 0.50000, 0.00000]	[1,2,3,4]

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**Bond in Unit Cell**


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Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 9: 1-th 'A'-'A' [1] (#1) bond cluster (1a@1d), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[1,-2,-3,4]	(1,1)	(1,1)	[1,0,0]

Table 10: 1-th 'A'-'A' [2] (#2) bond cluster (1a@1c), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000, 0.00000,-1.00000]	[ 0.00000, 0.00000, 0.50000]	[1,-2,-3,4]	(1,1)	(1,1)	[0,0,1]

Table 11: 1-th 'A'-'B' [1] (#3) bond cluster (4a@4o), D,  $|\mathbf{v}|=0.78102$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.50000,-0.50000, 0.00000]	[ 0.25000, 0.25000, 0.00000]	[1]	(1,1)	(1,1)	[0,0,0]
2	[ 0.50000,-0.50000, 0.00000]	[ 0.75000, 0.25000, 0.00000]	[2]	(1,1)	(1,1)	[-1,0,0]
3	[ 0.50000, 0.50000, 0.00000]	[ 0.75000, 0.75000, 0.00000]	[3]	(1,1)	(1,1)	[-1,-1,0]
4	[-0.50000, 0.50000, 0.00000]	[ 0.25000, 0.75000, 0.00000]	[4]	(1,1)	(1,1)	[0,-1,0]

Table 12: 1-th 'B'-'B' [1] (#4) bond cluster (1a@1b), ND,  $|\mathbf{v}|=1.0$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[1,-2,-3,4]	(1,1)	(1,1)	[1,0,0]

Table 13: 1-th 'B'-'B' [2] (#5) bond cluster (**1a01h**), ND,  $|\boldsymbol{v}|=1.0$  (cartesian)

SL	vector ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[ 0.00000, 0.00000,-1.00000]	[ 0.50000, 0.50000, 0.50000]	[1,-2,-3,4]	(1,1)	(1,1)	[0,0,1]