

SG No. 101 C_{4v}^3 $P4_2cm$ [tetragonal]

* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 2a, site symmetry: 2.m̄m

No.	position	mapping
1	[0, 0, z]	[1,2,7,8]
2	[0, 0, $z + \frac{1}{2}$]	[3,4,5,6]

Table 2: Wyckoff site: 2b, site symmetry: 2.m̄m

No.	position	mapping
1	[$\frac{1}{2}$, $\frac{1}{2}$, z]	[1,2,7,8]
2	[$\frac{1}{2}$, $\frac{1}{2}$, $z + \frac{1}{2}$]	[3,4,5,6]

Table 3: Wyckoff site: 4c, site symmetry: 2..

No.	position	mapping
1	[0, $\frac{1}{2}$, z]	[1,2]
2	[$\frac{1}{2}$, 0, $z + \frac{1}{2}$]	[3,4]
3	[0, $\frac{1}{2}$, $z + \frac{1}{2}$]	[5,6]
4	[$\frac{1}{2}$, 0, z]	[7,8]

Table 4: Wyckoff site: 4d, site symmetry: ..m̄

No.	position	mapping
1	[x, x, z]	[1,8]
2	[-x, -x, z]	[2,7]
3	[-x, x, $z + \frac{1}{2}$]	[3,6]
4	[x, -x, $z + \frac{1}{2}$]	[4,5]

Table 5: Wyckoff site: 8e, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[-x, -y, z]	[2]
3	[-y, x, $z + \frac{1}{2}$]	[3]
4	[y, -x, $z + \frac{1}{2}$]	[4]
5	[x, -y, $z + \frac{1}{2}$]	[5]

continued ...

Table 5

No.	position	mapping
6	$[-x, y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]