

MSG No. 122.334  $I\bar{4}2d1'$  [ Type II, tetragonal ]

Table 1: Wyckoff site: 4a, site symmetry: -4..1'

No.	position	mapping
1	[0, 0, 0]	[1,4,5,6,17,20,21,22]
2	[0, $\frac{1}{2}$ , $\frac{1}{4}$ ]	[2,3,7,8,18,19,23,24]
3	[ $\frac{1}{2}$ , $\frac{1}{2}$ , $\frac{1}{2}$ ]	[9,12,13,14,25,28,29,30]
4	[ $\frac{1}{2}$ , 0, $\frac{3}{4}$ ]	[10,11,15,16,26,27,31,32]

Table 2: Wyckoff site: 4b, site symmetry: -4..1'

No.	position	mapping
1	[0, 0, $\frac{1}{2}$ ]	[1,4,5,6,17,20,21,22]
2	[0, $\frac{1}{2}$ , $\frac{3}{4}$ ]	[2,3,7,8,18,19,23,24]
3	[ $\frac{1}{2}$ , $\frac{1}{2}$ , 0]	[9,12,13,14,25,28,29,30]
4	[ $\frac{1}{2}$ , 0, $\frac{1}{4}$ ]	[10,11,15,16,26,27,31,32]

Table 3: Wyckoff site: 8c, site symmetry: 2..1'

No.	position	mapping
1	[0, 0, $z$ ]	[1,4,17,20]
2	[0, $\frac{1}{2}$ , $\frac{1}{4} - z$ ]	[2,3,18,19]
3	[0, 0, $-z$ ]	[5,6,21,22]
4	[0, $\frac{1}{2}$ , $z + \frac{1}{4}$ ]	[7,8,23,24]
5	[ $\frac{1}{2}$ , $\frac{1}{2}$ , $z + \frac{1}{2}$ ]	[9,12,25,28]
6	[ $\frac{1}{2}$ , 0, $\frac{3}{4} - z$ ]	[10,11,26,27]
7	[ $\frac{1}{2}$ , $\frac{1}{2}$ , $\frac{1}{2} - z$ ]	[13,14,29,30]
8	[ $\frac{1}{2}$ , 0, $z + \frac{3}{4}$ ]	[15,16,31,32]

Table 4: Wyckoff site: 8d, site symmetry: .2.1'

No.	position	mapping
1	[ $x$ , $\frac{1}{4}$ , $\frac{1}{8}$ ]	[1,2,17,18]
2	[ $-x$ , $\frac{3}{4}$ , $\frac{1}{8}$ ]	[3,4,19,20]
3	[ $\frac{1}{4}$ , $-x$ , $\frac{7}{8}$ ]	[5,15,21,31]
4	[ $\frac{3}{4}$ , $x$ , $\frac{7}{8}$ ]	[6,16,22,32]
5	[ $\frac{3}{4}$ , $\frac{1}{2} - x$ , $\frac{3}{8}$ ]	[7,13,23,29]
6	[ $\frac{1}{4}$ , $x + \frac{1}{2}$ , $\frac{3}{8}$ ]	[8,14,24,30]
7	[ $x + \frac{1}{2}$ , $\frac{3}{4}$ , $\frac{5}{8}$ ]	[9,10,25,26]
8	[ $\frac{1}{2} - x$ , $\frac{1}{4}$ , $\frac{5}{8}$ ]	[11,12,27,28]

Table 5: Wyckoff site: 16e, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[x, \frac{1}{2} - y, \frac{1}{4} - z]$	[2,18]
3	$[-x, y + \frac{1}{2}, \frac{1}{4} - z]$	[3,19]
4	$[-x, -y, z]$	[4,20]
5	$[y, -x, -z]$	[5,21]
6	$[-y, x, -z]$	[6,22]
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	[7,23]
8	$[y, x + \frac{1}{2}, z + \frac{1}{4}]$	[8,24]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9,25]
10	$[x + \frac{1}{2}, -y, \frac{3}{4} - z]$	[10,26]
11	$[\frac{1}{2} - x, y, \frac{3}{4} - z]$	[11,27]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,28]
13	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[13,29]
14	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[14,30]
15	$[\frac{1}{2} - y, -x, z + \frac{3}{4}]$	[15,31]
16	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	[16,32]