

Table 1: Wyckoff site: 1o, site symmetry:  $m\bar{3}1'$ 

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]

 Table 2: Wyckoff site: 6a, site symmetry:  $2mm$ .

No.	position	mapping
1	[ $x$ , 0, 0]	[1, 2, 15, 16, 25, 26, 39, 40]
2	[ $-x$ , 0, 0]	[3, 4, 13, 14, 27, 28, 37, 38]
3	[0, $x$ , 0]	[9, 11, 22, 24, 33, 35, 46, 48]
4	[0, $-x$ , 0]	[10, 12, 21, 23, 34, 36, 45, 47]
5	[0, 0, $x$ ]	[5, 8, 18, 19, 29, 32, 42, 43]
6	[0, 0, $-x$ ]	[6, 7, 17, 20, 30, 31, 41, 44]

 Table 3: Wyckoff site: 8b, site symmetry:  $\bar{3}$ .

No.	position	mapping
1	[ $x$ , $x$ , $x$ ]	[1, 5, 9, 25, 29, 33]
2	[ $-x$ , $-x$ , $x$ ]	[4, 8, 12, 28, 32, 36]
3	[ $-x$ , $x$ , $-x$ ]	[3, 7, 11, 27, 31, 35]
4	[ $x$ , $-x$ , $-x$ ]	[2, 6, 10, 26, 30, 34]
5	[ $-x$ , $-x$ , $-x$ ]	[13, 17, 21, 37, 41, 45]
6	[ $x$ , $x$ , $-x$ ]	[16, 20, 24, 40, 44, 48]
7	[ $x$ , $-x$ , $x$ ]	[15, 19, 23, 39, 43, 47]
8	[ $-x$ , $x$ , $x$ ]	[14, 18, 22, 38, 42, 46]

 Table 4: Wyckoff site: 12c, site symmetry:  $m\bar{3}$ .

No.	position	mapping
1	[0, $y$ , $z$ ]	[1, 14, 25, 38]
2	[0, $-y$ , $z$ ]	[4, 15, 28, 39]
3	[0, $y$ , $-z$ ]	[3, 16, 27, 40]
4	[0, $-y$ , $-z$ ]	[2, 13, 26, 37]
5	[ $z$ , 0, $y$ ]	[9, 23, 33, 47]
6	[ $z$ , 0, $-y$ ]	[10, 24, 34, 48]
7	[ $-z$ , 0, $y$ ]	[12, 22, 36, 46]
8	[ $-z$ , 0, $-y$ ]	[11, 21, 35, 45]
9	[ $y$ , $z$ , 0]	[5, 20, 29, 44]

*continued ...*

Table 4

No.	position	mapping
10	$[-y, z, 0]$	$[7, 18, 31, 42]$
11	$[y, -z, 0]$	$[6, 19, 30, 43]$
12	$[-y, -z, 0]$	$[8, 17, 32, 41]$

Table 5: Wyckoff site: 24d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1, 25]$
2	$[-x, -y, z]$	$[4, 28]$
3	$[-x, y, -z]$	$[3, 27]$
4	$[x, -y, -z]$	$[2, 26]$
5	$[z, x, y]$	$[9, 33]$
6	$[z, -x, -y]$	$[10, 34]$
7	$[-z, -x, y]$	$[12, 36]$
8	$[-z, x, -y]$	$[11, 35]$
9	$[y, z, x]$	$[5, 29]$
10	$[-y, z, -x]$	$[7, 31]$
11	$[y, -z, -x]$	$[6, 30]$
12	$[-y, -z, x]$	$[8, 32]$
13	$[-x, -y, -z]$	$[13, 37]$
14	$[x, y, -z]$	$[16, 40]$
15	$[x, -y, z]$	$[15, 39]$
16	$[-x, y, z]$	$[14, 38]$
17	$[-z, -x, -y]$	$[21, 45]$
18	$[-z, x, y]$	$[22, 46]$
19	$[z, x, -y]$	$[24, 48]$
20	$[z, -x, y]$	$[23, 47]$
21	$[-y, -z, -x]$	$[17, 41]$
22	$[y, -z, x]$	$[19, 43]$
23	$[-y, z, x]$	$[18, 42]$
24	$[y, z, -x]$	$[20, 44]$