

PG No. 27 D_{6h} $6/mmm$ [hexagonal]

Table 1: Wyckoff site: **1o**, site symmetry: **6/mmm**

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]

Table 2: Wyckoff site: **2a**, site symmetry: **6mm**

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 4, 5, 6, 19, 20, 21, 22, 23, 24]
2	[0, 0, $-z$]	[7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]

Table 3: Wyckoff site: **6b**, site symmetry: **m2m**

No.	position	mapping
1	[x , 0, 0]	[1, 8, 16, 23]
2	[0, x , 0]	[2, 7, 17, 22]
3	[$-x$, $-x$, 0]	[3, 9, 18, 24]
4	[$-x$, 0, 0]	[4, 11, 13, 20]
5	[0, $-x$, 0]	[5, 10, 14, 19]
6	[x , x , 0]	[6, 12, 15, 21]

Table 4: Wyckoff site: **6c**, site symmetry: **mm2**

No.	position	mapping
1	[x , $2x$, 0]	[1, 11, 16, 20]
2	[$-2x$, $-x$, 0]	[2, 10, 17, 19]
3	[x , $-x$, 0]	[3, 12, 18, 21]
4	[$-x$, $-2x$, 0]	[4, 8, 13, 23]
5	[$2x$, x , 0]	[5, 7, 14, 22]
6	[$-x$, x , 0]	[6, 9, 15, 24]

Table 5: Wyckoff site: **12d**, site symmetry: **. . m**

No.	position	mapping
1	[x , 0, z]	[1, 23]
2	[0, x , z]	[2, 22]
3	[$-x$, $-x$, z]	[3, 24]

continued ...

Table 5

No.	position	mapping
4	$[-x, 0, z]$	$[4, 20]$
5	$[0, -x, z]$	$[5, 19]$
6	$[x, x, z]$	$[6, 21]$
7	$[0, x, -z]$	$[7, 17]$
8	$[x, 0, -z]$	$[8, 16]$
9	$[-x, -x, -z]$	$[9, 18]$
10	$[0, -x, -z]$	$[10, 14]$
11	$[-x, 0, -z]$	$[11, 13]$
12	$[x, x, -z]$	$[12, 15]$

Table 6: Wyckoff site: $12\mathbf{e}$, site symmetry: $\bar{6}m$.

No.	position	mapping
1	$[x, 2x, z]$	$[1, 20]$
2	$[-2x, -x, z]$	$[2, 19]$
3	$[x, -x, z]$	$[3, 21]$
4	$[-x, -2x, z]$	$[4, 23]$
5	$[2x, x, z]$	$[5, 22]$
6	$[-x, x, z]$	$[6, 24]$
7	$[2x, x, -z]$	$[7, 14]$
8	$[-x, -2x, -z]$	$[8, 13]$
9	$[-x, x, -z]$	$[9, 15]$
10	$[-2x, -x, -z]$	$[10, 17]$
11	$[x, 2x, -z]$	$[11, 16]$
12	$[x, -x, -z]$	$[12, 18]$

Table 7: Wyckoff site: $12\mathbf{f}$, site symmetry: $m\bar{3}m$.

No.	position	mapping
1	$[x, y, 0]$	$[1, 16]$
2	$[-y, x - y, 0]$	$[2, 17]$
3	$[-x + y, -x, 0]$	$[3, 18]$
4	$[-x, -y, 0]$	$[4, 13]$
5	$[y, -x + y, 0]$	$[5, 14]$
6	$[x - y, x, 0]$	$[6, 15]$
7	$[y, x, 0]$	$[7, 22]$
8	$[x - y, -y, 0]$	$[8, 23]$
9	$[-x, -x + y, 0]$	$[9, 24]$
10	$[-y, -x, 0]$	$[10, 19]$
11	$[-x + y, y, 0]$	$[11, 20]$
12	$[x, x - y, 0]$	$[12, 21]$

Table 8: Wyckoff site: $24g$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[y, -x + y, z]$	[5]
6	$[x - y, x, z]$	[6]
7	$[y, x, -z]$	[7]
8	$[x - y, -y, -z]$	[8]
9	$[-x, -x + y, -z]$	[9]
10	$[-y, -x, -z]$	[10]
11	$[-x + y, y, -z]$	[11]
12	$[x, x - y, -z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[y, -x + y, -z]$	[14]
15	$[x - y, x, -z]$	[15]
16	$[x, y, -z]$	[16]
17	$[-y, x - y, -z]$	[17]
18	$[-x + y, -x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[-x + y, y, z]$	[20]
21	$[x, x - y, z]$	[21]
22	$[y, x, z]$	[22]
23	$[x - y, -y, z]$	[23]
24	$[-x, -x + y, z]$	[24]