

MSG No. 183.187 $P6'm'm$ [Type III, hexagonal]

Table 1: Wyckoff site: $1a$, site symmetry: $6'm'm$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

Table 2: Wyckoff site: $2b$, site symmetry: $3m'$.

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 10, 11, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, z]$	$[4, 5, 6, 7, 8, 9]$

Table 3: Wyckoff site: $3c$, site symmetry: $2'm'm$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	$[1, 5, 8, 10]$
2	$[0, \frac{1}{2}, z]$	$[2, 6, 9, 11]$
3	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, 4, 7, 12]$

Table 4: Wyckoff site: $6d$, site symmetry: $.m$

No.	position	mapping
1	$[x, 0, z]$	$[1, 5]$
2	$[0, x, z]$	$[2, 6]$
3	$[-x, -x, z]$	$[3, 4]$
4	$[x, x, z]$	$[7, 12]$
5	$[-x, 0, z]$	$[8, 10]$
6	$[0, -x, z]$	$[9, 11]$

Table 5: Wyckoff site: $6e$, site symmetry: $.m'$.

No.	position	mapping
1	$[x, -x, z]$	$[1, 11]$
2	$[x, 2x, z]$	$[2, 12]$
3	$[-2x, -x, z]$	$[3, 10]$
4	$[-x, -2x, z]$	$[4, 9]$
5	$[2x, x, z]$	$[5, 7]$
6	$[-x, x, z]$	$[6, 8]$

Table 6: Wyckoff site: 12f, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[-x, -x + y, z]$	[4]
5	$[x - y, -y, z]$	[5]
6	$[y, x, z]$	[6]
7	$[x - y, x, z]$	[7]
8	$[-x, -y, z]$	[8]
9	$[y, -x + y, z]$	[9]
10	$[-x + y, y, z]$	[10]
11	$[-y, -x, z]$	[11]
12	$[x, x - y, z]$	[12]