

MSG No. 149.21  $P312$  [ Type I, trigonal ]

Table 1: Wyckoff site: 1a, site symmetry:  $3.2$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6]$

Table 2: Wyckoff site: 1b, site symmetry:  $3.2$

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

Table 3: Wyckoff site: 1c, site symmetry:  $3.2$

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

Table 4: Wyckoff site: 1d, site symmetry:  $3.2$

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

Table 5: Wyckoff site: 1e, site symmetry:  $3.2$

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

Table 6: Wyckoff site: 1f, site symmetry:  $3.2$

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

Table 7: Wyckoff site:  $2\mathbf{g}$ , site symmetry:  $3..$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3]$
2	$[0, 0, -z]$	$[4, 5, 6]$

Table 8: Wyckoff site:  $2\mathbf{h}$ , site symmetry:  $3..$ 

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

Table 9: Wyckoff site:  $2\mathbf{i}$ , site symmetry:  $3..$ 

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

Table 10: Wyckoff site:  $3\mathbf{j}$ , site symmetry:  $..2$ 

No.	position	mapping
1	$[x, -x, 0]$	$[1, 6]$
2	$[x, 2x, 0]$	$[2, 4]$
3	$[-2x, -x, 0]$	$[3, 5]$

Table 11: Wyckoff site:  $3\mathbf{k}$ , site symmetry:  $..2$ 

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

Table 12: Wyckoff site:  $6\mathbf{l}$ , site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$

*continued ...*

Table 12

No.	position	mapping
3	$[-x + y, -x, z]$	[3]
4	$[x, x - y, -z]$	[4]
5	$[-x + y, y, -z]$	[5]
6	$[-y, -x, -z]$	[6]