

SG No. 83  $C_{4h}^1$   $P4/m$  [ tetragonal ]

\* plus set:  $+ [0, 0, 0]$

Table 1: Wyckoff site: 1a, site symmetry:  $4/m..$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 2: Wyckoff site: 1b, site symmetry:  $4/m..$

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

Table 3: Wyckoff site: 1c, site symmetry:  $4/m..$

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

Table 4: Wyckoff site: 1d, site symmetry:  $4/m..$

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

Table 5: Wyckoff site: 2e, site symmetry:  $2/m..$

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

Table 6: Wyckoff site: 2f, site symmetry:  $2/m..$

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

Table 7: Wyckoff site:  $2\mathbf{g}$ , site symmetry:  $4.$ .

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4]$
2	$[0, 0, -z]$	$[5, 6, 7, 8]$

Table 8: Wyckoff site:  $2\mathbf{h}$ , site symmetry:  $4.$ .

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $2.$ .

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

Table 10: Wyckoff site:  $4\mathbf{j}$ , site symmetry:  $\mathbf{m}.$ .

No.	position	mapping
1	$[x, y, 0]$	$[1, 6]$
2	$[-x, -y, 0]$	$[2, 5]$
3	$[-y, x, 0]$	$[3, 8]$
4	$[y, -x, 0]$	$[4, 7]$

Table 11: Wyckoff site:  $4\mathbf{k}$ , site symmetry:  $\mathbf{m}.$ .

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 6]$
2	$[-x, -y, \frac{1}{2}]$	$[2, 5]$
3	$[-y, x, \frac{1}{2}]$	$[3, 8]$
4	$[y, -x, \frac{1}{2}]$	$[4, 7]$

Table 12: Wyckoff site: **81**, site symmetry: **1**

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