

MSG No. 84.52  $P4_2/m1'$  [ Type II, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $2/m..1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 5, 8, 9, 12, 13, 16]$
2	$[0, 0, \frac{1}{2}]$	$[2, 3, 6, 7, 10, 11, 14, 15]$

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 4, 5, 8, 9, 12, 13, 16]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 6, 7, 10, 11, 14, 15]$

Table 3: Wyckoff site: 2c, site symmetry:  $2/m..1'$

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 4, 5, 8, 9, 12, 13, 16]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 3, 6, 7, 10, 11, 14, 15]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 4, 5, 8, 9, 12, 13, 16]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 3, 6, 7, 10, 11, 14, 15]$

Table 5: Wyckoff site: 2e, site symmetry:  $-4..1'$

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[0, 0, \frac{3}{4}]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 6: Wyckoff site: 2f, site symmetry:  $-4..1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 7: Wyckoff site: **4g**, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 9, 12]$
2	$[0, 0, z + \frac{1}{2}]$	$[2, 3, 10, 11]$
3	$[0, 0, -z]$	$[5, 8, 13, 16]$
4	$[0, 0, \frac{1}{2} - z]$	$[6, 7, 14, 15]$

Table 8: Wyckoff site: **4h**, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 4, 9, 12]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[2, 3, 10, 11]$
3	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[5, 8, 13, 16]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[6, 7, 14, 15]$

Table 9: Wyckoff site: **4i**, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4, 9, 12]$
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[2, 3, 10, 11]$
3	$[0, \frac{1}{2}, -z]$	$[5, 8, 13, 16]$
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[6, 7, 14, 15]$

Table 10: Wyckoff site: **4j**, site symmetry:  $m..1'$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 8, 9, 16]$
2	$[-y, x, \frac{1}{2}]$	$[2, 7, 10, 15]$
3	$[y, -x, \frac{1}{2}]$	$[3, 6, 11, 14]$
4	$[-x, -y, 0]$	$[4, 5, 12, 13]$

Table 11: Wyckoff site: **8k**, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[-y, x, z + \frac{1}{2}]$	$[2, 10]$
3	$[y, -x, z + \frac{1}{2}]$	$[3, 11]$
4	$[-x, -y, z]$	$[4, 12]$

*continued ...*

Table 11

No.	position	mapping
5	$[-x, -y, -z]$	$[5, 13]$
6	$[y, -x, \frac{1}{2} - z]$	$[6, 14]$
7	$[-y, x, \frac{1}{2} - z]$	$[7, 15]$
8	$[x, y, -z]$	$[8, 16]$