

MSG No. 116.292 $P\bar{4}c21'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $2.221'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2.221'$

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

Table 3: Wyckoff site: 2c, site symmetry: $-4..1'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $..21'$

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

Table 6: Wyckoff site: **4f**, site symmetry: $\bar{3}21'$

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

Table 7: Wyckoff site: **4g**, site symmetry: $2\bar{1}1'$

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

Table 8: Wyckoff site: **4h**, site symmetry: $2\bar{1}1'$

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

Table 9: Wyckoff site: **4i**, site symmetry: $2\bar{1}1'$

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

Table 10: Wyckoff site: **8j**, site symmetry: $\bar{1}1'$

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

continued ...

Table 10

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