

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: . . 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 . . 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 . . 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 . . 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: 11'

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]