

MSG No. 90.96 $P4_2121'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 2..221'

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

Table 2: Wyckoff site: 2b, site symmetry: 2..221'

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

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

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: . . 21'

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

Table 7: Wyckoff site: 8g, site symmetry: 11'

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