

MSG No. 90.96 $P42_121'$ [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: $4\mathbf{f}$, 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: $8\mathbf{g}$, 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]