

MSG No. 85.60 $P4/n1'$ [Type II, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $-11'$

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

Table 5: Wyckoff site: 4e, site symmetry: $-11'$

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

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

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

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

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