

MSG No. 53.322  $Pmna1'$  [ Type II, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $2/m..1'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $2/m..1'$

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

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

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

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

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 2, 5, 6, 9, 10, 13, 14]$
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:  $2..1'$

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

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $2..1'$ 

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $.2.1'$ 

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $m..1'$ 

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

Table 9: Wyckoff site:  $8\mathbf{i}$ , site symmetry:  $11'$ 

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