

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: 4f, 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: 4g, 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: 4h, 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: 8i, 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]