

MSG No. 113.268  $P\bar{4}2_1m1'$  [ Type II, tetragonal ]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 2..mm1'

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: ..m1'

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

Table 6: Wyckoff site: 8f, site symmetry: 11'

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