

MSG No. 118.311  $P\bar{4}n'2'$  [ Type III, tetragonal ]

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[5, 6, 7, 8]$

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

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[5, 6, 7, 8]$

Table 3: Wyckoff site: 2c, site symmetry:  $2.2'2'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, 5, 6]$
2	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[3, 4, 7, 8]$

Table 4: Wyckoff site: 2d, site symmetry:  $2.2'2'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{3}{4}]$	$[1, 2, 5, 6]$
2	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[3, 4, 7, 8]$

Table 5: Wyckoff site: 4e, site symmetry:  $2..$

No.	position	mapping
1	$[0, 0, z]$	$[1, 2]$
2	$[0, 0, -z]$	$[3, 4]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[5, 6]$
4	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8]$

Table 6: Wyckoff site:  $4f$ , site symmetry:  $\dots 2'$ 

No.	position	mapping
1	$[x, \frac{1}{2} - x, \frac{1}{4}]$	[1, 6]
2	$[-x, x + \frac{1}{2}, \frac{1}{4}]$	[2, 5]
3	$[\frac{1}{2} - x, -x, \frac{3}{4}]$	[3, 7]
4	$[x + \frac{1}{2}, x, \frac{3}{4}]$	[4, 8]

Table 7: Wyckoff site:  $4g$ , site symmetry:  $\dots 2'$ 

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	[1, 5]
2	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	[2, 6]
3	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[3, 8]
4	$[\frac{1}{2} - x, x, \frac{3}{4}]$	[4, 7]

Table 8: Wyckoff site:  $4h$ , site symmetry:  $2 \dots$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1, 2]
2	$[\frac{1}{2}, 0, -z]$	[3, 4]
3	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[5, 6]
4	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[7, 8]

Table 9: Wyckoff site:  $8i$ , site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[y, -x, -z]$	[3]
4	$[-y, x, -z]$	[4]
5	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[6]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]