

MSG No. 116.292  $P\bar{4}c21'$  [ Type II, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $2.221'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $2.221'$

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

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

No.	position	mapping
1	[0, 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 4: Wyckoff site: 2d, site symmetry:  $-4..1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	[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:  $..21'$

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

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $..21'$ 

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $2..1'$ 

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $2..1'$ 

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $2..1'$ 

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

Table 10: Wyckoff site:  $8\mathbf{j}$ , site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	[1,9]
2	$[-x, -y, z]$	[2,10]
3	$[y, x, \frac{1}{2} - z]$	[3,11]
4	$[-y, -x, \frac{1}{2} - z]$	[4,12]

*continued ...*

Table 10

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