

MSG No. 86.71  $P4_2'/n'$  [ Type III, tetragonal ]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $-1'$

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

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

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

Table 6: Wyckoff site:  $4f$ , site symmetry:  $2..$ 

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

Table 7: Wyckoff site:  $8g$ , site symmetry:  $1$ 

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