

MSG No. 94.130  $P4_22'_12'$  [ Type III, tetragonal ]

Table 1: Wyckoff site: **2a**, site symmetry:  $2.2'2'$

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

Table 2: Wyckoff site: **2b**, site symmetry:  $2.2'2'$

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

Table 3: Wyckoff site: **4c**, site symmetry:  $2..$

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

Table 4: Wyckoff site: **4d**, site symmetry:  $2..$

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

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

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

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

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

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

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