

MSG No. 50.279 *Pb'an* [ Type III, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $22'2'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $22'2'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $22'2'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $22'2'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $-1'$

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

Table 6: Wyckoff site: **4f**, site symmetry:  $-1'$ 

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

Table 7: Wyckoff site: **4g**, site symmetry:  $2..$ 

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

Table 8: Wyckoff site: **4h**, site symmetry:  $2..$ 

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

Table 9: Wyckoff site: **4i**, site symmetry:  $.2'$ 

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

Table 10: Wyckoff site: **4j**, site symmetry:  $.2'$ 

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

Table 11: Wyckoff site:  $4\mathbf{k}$ , site symmetry:  $\bar{3}2'$ 

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

Table 12: Wyckoff site:  $4\mathbf{l}$ , site symmetry:  $\bar{3}2'$ 

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

Table 13: Wyckoff site:  $8\mathbf{m}$ , site symmetry:  $1$ 

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