

MSG No. 14.81  $P_b2_1/c$  [ Type IV, monoclinic ]

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

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

Table 2: Wyckoff site: **4b**, site symmetry:  $-1$

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

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

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

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

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

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

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

*continued ...*

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: 2<sup>2</sup>

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

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

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