

MSG No. 16.2  $P2221'$  [ Type II, orthorhombic ]

Table 1: Wyckoff site: 1a, site symmetry:  $2221'$

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

Table 2: Wyckoff site: 1b, site symmetry:  $2221'$

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

Table 3: Wyckoff site: 1c, site symmetry:  $2221'$

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

Table 4: Wyckoff site: 1d, site symmetry:  $2221'$

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

Table 5: Wyckoff site: 1e, site symmetry:  $2221'$

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

Table 6: Wyckoff site: 1f, site symmetry:  $2221'$

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

Table 7: Wyckoff site: 1g, site symmetry: 2221'

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

Table 8: Wyckoff site: 1h, site symmetry: 2221'

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

Table 9: Wyckoff site: 2i, site symmetry: 2..1'

No.	position	mapping
1	$[x, 0, 0]$	[1,2,5,6]
2	$[-x, 0, 0]$	[3,4,7,8]

Table 10: Wyckoff site: 2j, site symmetry: 2..1'

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

Table 11: Wyckoff site: 2k, site symmetry: 2..1'

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

Table 12: Wyckoff site: 2l, site symmetry: 2..1'

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

Table 13: Wyckoff site:  $2m$ , site symmetry:  $.2.1'$ 

No.	position	mapping
1	$[0, y, 0]$	$[1, 3, 5, 7]$
2	$[0, -y, 0]$	$[2, 4, 6, 8]$

Table 14: Wyckoff site:  $2n$ , site symmetry:  $.2.1'$ 

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

Table 15: Wyckoff site:  $2o$ , site symmetry:  $.2.1'$ 

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

Table 16: Wyckoff site:  $2p$ , site symmetry:  $.2.1'$ 

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

Table 17: Wyckoff site:  $2q$ , site symmetry:  $..21'$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 5, 8]$
2	$[0, 0, -z]$	$[2, 3, 6, 7]$

Table 18: Wyckoff site:  $2r$ , site symmetry:  $..21'$ 

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

Table 19: Wyckoff site: 2s, site symmetry:  $\dots 21'$ 

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

Table 20: Wyckoff site: 2t, site symmetry:  $\dots 21'$ 

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

Table 21: Wyckoff site: 4u, site symmetry:  $11'$ 

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