

# MSG No. 16.1 $P\bar{2}2\bar{2}$ [ Type I, orthorhombic ]

Table 1: Wyckoff site: **1a**, site symmetry: 222

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4]

Table 2: Wyckoff site: **1b**, site symmetry: 222

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

Table 3: Wyckoff site: **1c**, site symmetry: 222

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

Table 4: Wyckoff site: **1d**, site symmetry: 222

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

Table 5: Wyckoff site: **1e**, site symmetry: 222

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

Table 6: Wyckoff site: **1f**, site symmetry: 222

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

Table 7: Wyckoff site: 1g, site symmetry: 222

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

Table 8: Wyckoff site: 1h, site symmetry: 222

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

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

No.	position	mapping
1	$[x, 0, 0]$	[1,2]
2	$[-x, 0, 0]$	[3,4]

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

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

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

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

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

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

Table 13: Wyckoff site:  $2\bar{m}$ , site symmetry:  $.2.$ 

No.	position	mapping
1	$[0, y, 0]$	$[1,3]$
2	$[0, -y, 0]$	$[2,4]$

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

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

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

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

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

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

Table 17: Wyckoff site:  $2q$ , site symmetry:  $\dots 2$ 

No.	position	mapping
1	$[0, 0, z]$	$[1,4]$
2	$[0, 0, -z]$	$[2,3]$

Table 18: Wyckoff site:  $2r$ , site symmetry:  $\dots 2$ 

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

Table 19: Wyckoff site: 2s, site symmetry: . . 2

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

Table 20: Wyckoff site: 2t, site symmetry: . . 2

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

Table 21: Wyckoff site: 4u, site symmetry: 1

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