

MSG No. 16.3 $P2'2'2$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 1c, site symmetry: $2'2'2$

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

Table 4: Wyckoff site: 1d, site symmetry: $2'2'2$

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

Table 5: Wyckoff site: 1e, site symmetry: $2'2'2$

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

Table 6: Wyckoff site: 1f, site symmetry: $2'2'2$

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

Table 7: Wyckoff site: $1g$, site symmetry: $2'2'2$

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

Table 8: Wyckoff site: $1h$, site symmetry: $2'2'2$

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	$[x, 0, 0]$	$[1, 3]$
2	$[-x, 0, 0]$	$[2, 4]$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 20: Wyckoff site: $2t$, site symmetry: $\dots 2$

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

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]