

MSG No. 42.219 *Fmm2* [Type I, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: **mm2**

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 4]
2	[0, $\frac{1}{2}$, $z + \frac{1}{2}$]	[5, 6, 7, 8]
3	[$\frac{1}{2}$, 0, $z + \frac{1}{2}$]	[9, 10, 11, 12]
4	[$\frac{1}{2}$, $\frac{1}{2}$, z]	[13, 14, 15, 16]

Table 2: Wyckoff site: **8b**, site symmetry: **..2**

No.	position	mapping
1	[$\frac{1}{4}$, $\frac{1}{4}$, z]	[1, 14]
2	[$\frac{3}{4}$, $\frac{3}{4}$, z]	[2, 13]
3	[$\frac{3}{4}$, $\frac{1}{4}$, z]	[3, 16]
4	[$\frac{1}{4}$, $\frac{3}{4}$, z]	[4, 15]
5	[$\frac{1}{4}$, $\frac{3}{4}$, $z + \frac{1}{2}$]	[5, 10]
6	[$\frac{3}{4}$, $\frac{1}{4}$, $z + \frac{1}{2}$]	[6, 9]
7	[$\frac{3}{4}$, $\frac{3}{4}$, $z + \frac{1}{2}$]	[7, 12]
8	[$\frac{1}{4}$, $\frac{1}{4}$, $z + \frac{1}{2}$]	[8, 11]

Table 3: Wyckoff site: **8c**, site symmetry: **m..**

No.	position	mapping
1	[0, y, z]	[1, 3]
2	[0, -y, z]	[2, 4]
3	[0, $y + \frac{1}{2}$, $z + \frac{1}{2}$]	[5, 7]
4	[0, $\frac{1}{2} - y$, $z + \frac{1}{2}$]	[6, 8]
5	[$\frac{1}{2}$, y, $z + \frac{1}{2}$]	[9, 11]
6	[$\frac{1}{2}$, -y, $z + \frac{1}{2}$]	[10, 12]
7	[$\frac{1}{2}$, $y + \frac{1}{2}$, z]	[13, 15]
8	[$\frac{1}{2}$, $\frac{1}{2} - y$, z]	[14, 16]

Table 4: Wyckoff site: **8d**, site symmetry: **.m.**

No.	position	mapping
1	[x, 0, z]	[1, 4]
2	[-x, 0, z]	[2, 3]
3	[x, $\frac{1}{2}$, $z + \frac{1}{2}$]	[5, 8]
4	[-x, $\frac{1}{2}$, $z + \frac{1}{2}$]	[6, 7]
5	[$x + \frac{1}{2}$, 0, $z + \frac{1}{2}$]	[9, 12]

continued ...

Table 4

No.	position	mapping
6	$[\frac{1}{2} - x, 0, z + \frac{1}{2}]$	[10,11]
7	$[x + \frac{1}{2}, \frac{1}{2}, z]$	[13,16]
8	$[\frac{1}{2} - x, \frac{1}{2}, z]$	[14,15]

Table 5: Wyckoff site: 16e, 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]
5	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]
9	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[11]
12	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[16]