

MSG No. 44.229 *Imm2* [Type I, orthorhombic]

Table 1: Wyckoff site: **2a**, site symmetry: **mm2**

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

Table 2: Wyckoff site: **2b**, site symmetry: **mm2**

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

Table 3: Wyckoff site: **4c**, site symmetry: **.m.**

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

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

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

Table 5: Wyckoff site: **8e**, 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 + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]	[5]
6	[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]	[6]

continued ...

Table 5

No.	position	mapping
7	$\left[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[7]
8	$\left[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[8]