MSG No. 117.300 $P\bar{4}b21'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4..1'

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

Table 2: Wyckoff site: 2b, site symmetry: -4..1'

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

Table 3: Wyckoff site: 2c, site symmetry: 2.221'

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

Table 4: Wyckoff site: 2d, site symmetry: 2.221'

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

Table 5: Wyckoff site: 4e, site symmetry: 2..1'

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

Table 6: Wyckoff site: `4f`, site symmetry: `2..1`'

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

Table 7: Wyckoff site: `4g`, site symmetry: `..21`'

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

Table 8: Wyckoff site: `4h`, site symmetry: `..21`'

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

Table 9: Wyckoff site: `8i`, site symmetry: `11`'

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