MSG No. 81.37 $P_C\bar{4}$ [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: -4'..

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

Table 4: Wyckoff site: 2d, site symmetry: -4'..

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: 2..

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

Table 7: Wyckoff site: 4g, site symmetry: 2'..

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,6]
2	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[2,5]
3	$\left[\frac{1}{4}, \frac{1}{4}, -z\right]$	[3,8]
4	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[4,7]

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

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