

MSG No. 81.33 $P\bar{4}$ [Type I, tetragonal]

Table 1: Wyckoff site: **1a**, site symmetry: $-4..$

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

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

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

Table 3: Wyckoff site: **1c**, site symmetry: $-4..$

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

Table 4: Wyckoff site: **1d**, site symmetry: $-4..$

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

Table 5: Wyckoff site: **2e**, site symmetry: $2..$

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

Table 6: Wyckoff site: **2f**, site symmetry: $2..$

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

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

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

Table 8: Wyckoff site: 4h, 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]