

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: $2\mathbf{g}$, 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: $4\mathbf{h}$, site symmetry: 1

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