

MSG No. 81.35 $P\bar{4}'$ [Type III, 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	$[-y, x, -z]$	$[4]$