

MSG No. 81.34 $P\bar{4}1'$ [Type II, tetragonal]

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

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8]

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

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

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

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

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

No.	position	mapping
1	[\mathbf{\frac{1}{2}}, \mathbf{\frac{1}{2}}, \mathbf{\frac{1}{2}}]	[1,2,3,4,5,6,7,8]

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

No.	position	mapping
1	[0, 0, z]	[1,2,5,6]
2	[0, 0, $-z$]	[3,4,7,8]

Table 6: Wyckoff site: **2f**, site symmetry: $2..1'$

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

Table 7: Wyckoff site: 2g, site symmetry: 2..1'

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

Table 8: Wyckoff site: 4h, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,5]
2	$[-x, -y, z]$	[2,6]
3	$[y, -x, -z]$	[3,7]
4	$[-y, x, -z]$	[4,8]