

MSG No. 77.14 $P4_21'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $2..1'$

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $2..1'$

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

Table 4: Wyckoff site: 4d, site symmetry: $11'$

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