

MSG No. 103.195 $P4cc$ [Type I, tetragonal]

Table 1: Wyckoff site: **2a**, site symmetry: 4..

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

Table 2: Wyckoff site: **2b**, site symmetry: 4..

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

Table 3: Wyckoff site: **4c**, site symmetry: 2..

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

Table 4: Wyckoff site: **8d**, site symmetry: 1

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