

MSG No. 91.105 $P4'_122'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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