

MSG No. 77.16 P_42 [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $4'..$

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

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

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

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

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

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

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