

MSG No. 52.313  $Pn'n'a'$  [ Type III, orthorhombic ]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $2. .$

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

Table 5: Wyckoff site: 8e, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[2]

*continued ...*

Table 5

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