

MSG No. 43.226 $Fd'd2'$ [Type III, orthorhombic]

Table 1: Wyckoff site: **8a**, site symmetry: $\dots 2'$

No.	position	mapping
1	$[0, 0, z]$	[1,3]
2	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{4}]$	[2,4]
3	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[5,7]
4	$[\frac{1}{4}, \frac{3}{4}, z + \frac{3}{4}]$	[6,8]
5	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[9,11]
6	$[\frac{3}{4}, \frac{1}{4}, z + \frac{3}{4}]$	[10,12]
7	$[\frac{1}{2}, \frac{1}{2}, z]$	[13,15]
8	$[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{4}]$	[14,16]

Table 2: Wyckoff site: **16b**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{4}, \frac{1}{4} - y, z + \frac{1}{4}]$	[2]
3	$[-x, -y, z]$	[3]
4	$[\frac{1}{4} - x, y + \frac{1}{4}, z + \frac{1}{4}]$	[4]
5	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x + \frac{1}{4}, \frac{3}{4} - y, z + \frac{3}{4}]$	[6]
7	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]
8	$[\frac{1}{4} - x, y + \frac{3}{4}, z + \frac{3}{4}]$	[8]
9	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[9]
10	$[x + \frac{3}{4}, \frac{1}{4} - y, z + \frac{3}{4}]$	[10]
11	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[11]
12	$[\frac{3}{4} - x, y + \frac{1}{4}, z + \frac{3}{4}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{3}{4}, \frac{3}{4} - y, z + \frac{1}{4}]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[15]
16	$[\frac{3}{4} - x, y + \frac{3}{4}, z + \frac{1}{4}]$	[16]