

MSG No. 31.133 P_Cmn2_1 [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: **8b**, site symmetry: **1**

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