

MSG No. 27.79 $Pcc21'$ [Type II, orthorhombic]

Table 1: Wyckoff site: **2a**, site symmetry: $\dots 21'$

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

Table 2: Wyckoff site: **2b**, site symmetry: $\dots 21'$

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

Table 3: Wyckoff site: **2c**, site symmetry: $\dots 21'$

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

Table 4: Wyckoff site: **2d**, site symmetry: $\dots 21'$

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

Table 5: Wyckoff site: **4e**, site symmetry: $11'$

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