

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	$[x, -y, z + \frac{1}{2}]$	$[4, 8]$