

SG No. 31 C_{2v}^7 $Pmn2_1$ [orthorhombic]

* plus set: $+ [0, 0, 0]$

* Wyckoff site: **2a**, site symmetry: **m** . .

Table 1: Wyckoff bond: **2a@2a**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, z]$	$[1, 4]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	$[2, 3]$

Table 2: Wyckoff bond: **2b@2a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	$[1, -4]$
2	$[-X, 0, 0]$	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	$[2, -3]$

Table 3: Wyckoff bond: **4c@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	$[2]$
3	$[X, -Y, Z]$	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	$[3]$
4	$[-X, Y, Z]$	$[0, y, z]$	$[4]$

* Wyckoff site: **4b**, site symmetry: **1**

Table 4: Wyckoff bond: **4a@4b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	$[2]$
3	$[X, -Y, Z]$	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	$[3]$
4	$[-X, Y, Z]$	$[-x, y, z]$	$[4]$