

SG No. 45 C_{2v}^{21} $Iba2$ [orthorhombic]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

Table 1: Wyckoff site: 4a, site symmetry: ...2

No.	position	mapping
1	$[0, 0, z]$	[1,2]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[3,4]

Table 2: Wyckoff site: 4b, site symmetry: ...2

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1,2]
2	$[\frac{1}{2}, 0, z]$	[3,4]

Table 3: Wyckoff site: 8c, site symmetry: 1

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