

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

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

Table 1: Wyckoff site: **4a**, site symmetry:  $\dots 2$

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:  $\dots 2$

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