

SG No. 80  $C_4^6$   $I4_1$  [ tetragonal ]

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

\* Wyckoff site: **4a**, site symmetry:  $2..$

Table 1: Wyckoff bond: **4a@4a**

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

Table 2: Wyckoff bond: **4b@4a**

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

Table 3: Wyckoff bond: **8c@4a**

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

\* Wyckoff site: **8b**, site symmetry:  $1$

Table 4: Wyckoff bond: **8a@8b**

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