

SG No. 44  $C_{2v}^{20}$   $Imm2$  [ orthorhombic ]

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

\* Wyckoff site: **2a**, site symmetry: **mm2**

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2, 3, 4]$

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

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, z]$	$[1, -2, -3, 4]$

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

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, z]$	$[1, -2, 3, -4]$

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

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	$[1, -2]$
2	$[X, -Y, 0]$	$[0, 0, z]$	$[3, -4]$

Table 5: Wyckoff bond: **4e@2a**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, z]$	$[1, 3]$
2	$[-X, 0, Z]$	$[0, 0, z]$	$[2, 4]$

Table 6: Wyckoff bond: **4f@2a**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, z]$	$[1, 4]$
2	$[0, -Y, Z]$	$[0, 0, z]$	$[2, 3]$

Table 7: Wyckoff bond: **8g@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, z]$	$[2]$
3	$[X, -Y, Z]$	$[0, 0, z]$	$[3]$
4	$[-X, Y, Z]$	$[0, 0, z]$	$[4]$

\* Wyckoff site: **2b**, site symmetry: **mm2**

Table 8: Wyckoff bond: **2a@2b**

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

Table 9: Wyckoff bond: **2b@2b**

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

Table 10: Wyckoff bond: **2c@2b**

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

Table 11: Wyckoff bond: **4d@2b**

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

Table 12: Wyckoff bond: **4e@2b**

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

Table 13: Wyckoff bond: **4f@2b**

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

Table 14: Wyckoff bond: **8g@2b**

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

\* Wyckoff site: **4c**, site symmetry:  $\bar{4}2m$ .

Table 15: Wyckoff bond: **4a@4c**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	$[1, 3]$
2	$[-X, 0, Z]$	$[-x, 0, z]$	$[2, 4]$

Table 16: Wyckoff bond: **4b@4c**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, z]$	$[1, -3]$
2	$[0, -Y, 0]$	$[-x, 0, z]$	$[2, -4]$

Table 17: Wyckoff bond: **8c@4c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, z]$	$[2]$
3	$[X, -Y, Z]$	$[x, 0, z]$	$[3]$
4	$[-X, Y, Z]$	$[-x, 0, z]$	$[4]$

\* Wyckoff site: **4d**, site symmetry:  $m\bar{3}m$ .

Table 18: Wyckoff bond: **4a@4d**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, z]$	$[1, 4]$
2	$[0, -Y, Z]$	$[0, -y, z]$	$[2, 3]$

Table 19: Wyckoff bond: **4b@4d**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	$[1, -4]$
2	$[-X, 0, 0]$	$[0, -y, z]$	$[2, -3]$

Table 20: Wyckoff bond: **8c@4d**

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

\* Wyckoff site: **8e**, site symmetry: 1

Table 21: Wyckoff bond: **8a@8e**

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