

SG No. 42  $C_{2v}^{18}$   $Fmm2$  [ orthorhombic ]

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

\* Wyckoff site: **4a**, site symmetry: **mm2**

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

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

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

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

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

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

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

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: **8e@4a**

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: **8f@4a**

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: **16g@4a**

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: **8b**, site symmetry:  $\bar{4}2$

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

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

Table 9: Wyckoff bond: **8b@8b**

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

Table 10: Wyckoff bond: **16c@8b**

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

\* Wyckoff site: **8c**, site symmetry:  $m\bar{2}$

Table 11: Wyckoff bond: **8a@8c**

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

Table 12: Wyckoff bond: **8b@8c**

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

Table 13: Wyckoff bond: **16c@8c**

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: **8d**, site symmetry:  $\bar{4}2m$ .

Table 14: Wyckoff bond: **8a@8d**

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

Table 15: Wyckoff bond: **8b@8d**

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

Table 16: Wyckoff bond: **16c@8d**

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: **16e**, site symmetry:  $\bar{4}2m$ .

Table 17: Wyckoff bond: 16a@16e

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]