

MSG No. 2.7 $P_S\bar{1}$ [Type IV, triclinic]

Table 1: Wyckoff site: **2a**, site symmetry: -1

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

Table 2: Wyckoff site: **2b**, site symmetry: $-1'$

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

Table 3: Wyckoff site: **2c**, site symmetry: -1

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

Table 4: Wyckoff site: **2d**, site symmetry: -1

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

Table 5: Wyckoff site: **2e**, site symmetry: -1

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

Table 6: Wyckoff site: **2f**, site symmetry: $-1'$

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

Table 7: Wyckoff site: $2g$, site symmetry: $-1'$

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

Table 8: Wyckoff site: $2h$, site symmetry: $-1'$

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

Table 9: Wyckoff site: $4i$, site symmetry: 1

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