

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]