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Supporting information for article:

Group theoretical analysis of structural instability, vacancy ordering and magnetic transitions in the system troilite (FeS) – pyrrhotite (Fe_{1-x}S)

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Supplementary Material

S1. Tables in full

S1.1. 4C

S1.1.1. 4C $U_1(1/2,0,1/4)$

Table S1 Order parameter components and unit cell configurations for subgroups of $P6_3/mmc$ which can arise from phase transitions in which irrep $U_1(1/2,0,1/4)$ is the active representation. SGN = space group number.

SGN	Space Group	OPD Name	OPD Vector	Basis Vectors	Origin
12	$C2/m$	P1	(a,0,0,0,0,0)	(2,1,-4),(0,1,0),(2,1,0)	(0,0,0)
44	$Imm2$	P2	(a,-0.414a,0,0,0,0)	(0,0,4),(0,1,0),(-2,-1,0)	(-7/8,1/16,-7/4)
12	$C2/m$	P3	(a,0,a,0,0,0)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
15	$C2/c$	P4	(a,0,0,a,0,0)	(2,-2,0),(2,2,0),(-1,1,2)	(0,1/2,0)
42	$Fmm2$	P5	(a,-0.414a,a,-0.414a,0,0)	(0,0,4),(2,2,0),(-2,2,0)	(-1/8,1/8,1/4)
43	$Fdd2$	P6	(a,-0.414a,0.414a,a,0,0)	(0,0,4),(2,2,0),(-2,2,0)	(-7/8,7/8,7/4)
164	$P\bar{3}m1$	P7	(a,0,a,0,a,0)	(2,0,0),(0,2,0),(0,0,4)	(0,0,0)
187	$P\bar{6}m2$	P8	(a,-0.414a,a,-0.414a,a,-0.414a)	(0,-2,0),(2,2,0),(0,0,4)	(0,0,1/4)
8	Cm	C1	(a,b,0,0,0,0)	(2,1,-4),(0,1,0),(2,1,0)	(0,0,0)
5	$C2$	C2	(a,b,a,-b,0,0)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
5	$C2$	C3	(a,b,0.707a,0.707b,-0.707a,0.707b,0,0)	(2,2,0),(-2,2,0),(1,1,2)	(1/8,15/8,1/4)
2	$P\bar{1}$	C4	(a,0,b,0,0,0)	(1,1,2),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	C5	(a,0,0,b,0,0)	(1,1,2),(0,2,0),(-2,0,0)	(0,1/2,0)
8	Cm	C6	(a,-0.414a,b,-0.414b,0,0)	(-2,-2,0),(0,0,4),(-2,0,0)	(-1/8,-1/8,1/4)

9	<i>Cc</i>	C7	(a,-0.414a,b,2.414b,0,0)	(-2,-2,0),(0,0,4),(-2,0,0)	(-5/8,-5/8,5/4)
8	<i>Cm</i>	C8	(a,b,a,b,0,0)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
9	<i>Cc</i>	C9	(a,b,b,-a,0,0)	(2,-2,0),(2,2,0),(-1,1,2)	(3/2,0,0)
156	<i>P3m1</i>	C10	(a,b,a,b,a,b)	(2,0,0),(0,2,0),(0,0,4)	(0,0,0)
12	<i>C2/m</i>	C11	(a,0,b,0,a,0)	(-2,-4,0),(2,0,0),(0,0,4)	(0,0,0)
12	<i>C2/m</i>	C12	(0,a,b,0,0,-a)	(-2,-4,0),(2,0,0),(0,0,4)	(1/2,0,0)
38	<i>Amm2</i>	C13	(a,-0.414a,b,-0.414b,b,- 0.414b)	(0,0,4),(0,2,0),(-4,-2,0)	(0,0,1/4)
39	<i>Abm2</i>	C14	(a,-0.414a,b,2.414b,- b,2.414b)	(0,0,4),(0,2,0),(-4,-2,0)	(0,0,1/4)
5	<i>C2</i>	S1	(a,b,c,0,a,-b)	(-2,-4,0),(2,0,0),(0,0,4)	(0,0,0)
5	<i>C2</i>	S2	(a,- 0.414a,b,c,0.707b0.707c,- 0.707b0.707c)	(0,-2,0),(4,2,0),(0,0,4)	(0,0,1/4)
2	$P\bar{1}$	S3	(a,0,b,0,c,0)	(0,0,4),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	S4	(a,0,0,b,0,c)	(0,0,4),(0,2,0),(-2,0,0)	(0,1/2,0)
6	<i>Pm</i>	S5	(a,-0.414a,b,- 0.414b,c,-0.414c)	(-2,0,0),(0,0,4),(0,2,0)	(0,0,1/4)
7	<i>Pc</i>	S6	(a,- 0.414a,b,2.414b,c,2.414c)	(-2,0,0),(0,0,4),(0,2,0)	(0,0,1/4)
1	<i>P1</i>	4D1	(a,b,c,d,0,0)	(1,1,2),(0,2,0),(-2,0,0)	(0,0,0)
8	<i>Cm</i>	4D2	(a,b,c,d,a,b)	(-2,-4,0),(2,0,0),(0,0,4)	(0,0,0)
1	<i>P1</i>	6D1	(a,b,c,d,e,f)	(0,0,4),(0,2,0),(-2,0,0)	(0,0,0)

S1.1.2. 4C $m\Gamma_4^+$ with U_1

Table S2 Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/4)$, with respect to the parent space group $P6_3/mmc$. SGN.M = magnetic space group number.

SGN.M	Space Group	OPD Name		Basis Vectors	Origin
		$U_1(1/2,0,1/4)$	OPD Vector $U_1(1/2,0,1/4), m\Gamma_4^+$		
12.62	$C2'/m'$	P1(1)P1(1)	(a,0,0,0,0,0),(b)	(2,1,- 4),(0,1,0),(2,1,0)	(0,0,0)

44.232	$Im'm'2$	P2(1)P1(1)	(a,-0.414a,0,0,0,0),(b)	(0,0,4),(0,1,0),(-2,-1,0)	(-7/8,1/16,-7/4)
12.62	$C2'/m'$	P3(1)P1(1)	(a,0,a,0,0,0),(b)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
15.89	$C2'/c'$	P4(1)P1(1)	(a,0,0,a,0,0),(b)	(2,-2,0),(2,2,0),(-1,1,2)	(0,1/2,0)
42.222	$Fm'm'2$	P5(1)P1(1)	(a,-0.414a,a,-0.414a,0,0),(b)	(0,0,4),(2,2,0),(-2,2,0)	(-1/8,1/8,1/4)
43.227	$Fd'd'2$	P6(1)P1(1)	(a,-0.414a,0.414a,a,0,0),(b)	(0,0,4),(2,2,0),(-2,2,0)	(-7/8,7/8,7/4)
164.89	$P\bar{3}m'1$	P7(1)P1(1)	(a,0,a,0,a,0),(b)	(0,-2,0),(2,2,0),(0,0,4)	(0,0,0)
187.211	$P\bar{6}m'2$	P8(1)P1(1)	(a,-0.414a,a,-0.414a,a,-0.414a),(b)	(2,2,0),(-2,0,0),(0,0,4)	(0,0,1/4)
8.34	Cm'	C1(1)P1(1)	(a,b,0,0,0,0),(c)	(2,1,-4),(0,1,0),(2,1,0)	(0,0,0)
5.15	$C2'$	C2(1)P1(1)	(a,b,a,-b,0,0),(c)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
5.13	$C2$	C3(1)P1(1)	(a,b,0.707a-0.707b,-0.707a-0.707b,0,0),(c)	(2,2,0),(-2,2,0),(1,1,2)	(1/8,15/8,1/4)
2.4	$P\bar{1}$	C4(1)P1(1)	(a,0,b,0,0,0),(c)	(1,1,2),(0,2,0),(-2,0,0)	(0,0,0)
2.4	$P\bar{1}$	C5(1)P1(1)	(a,0,0,b,0,0),(c)	(1,1,2),(0,2,0),(-2,0,0)	(0,1/2,0)
8.34	Cm'	C6(1)P1(1)	(a,-0.414a,b,-0.414b,0,0),(c)	(-2,-2,0),(0,0,4),(-2,0,0)	(-1/8,-1/8,1/4)
9.39	Cc'	C7(1)P1(1)	(a,-0.414a,b,2.414b,0,0),(c)	(-2,-2,0),(0,0,4),(-2,0,0)	(-5/8,-5/8,5/4)
8.34	Cm'	C8(1)P1(1)	(a,b,a,b,0,0),(c)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
9.39	Cc'	C9(1)P1(1)	(a,b,b,-a,0,0),(c)	(2,-2,0),(2,2,0),(-1,1,2)	(3/2,0,0)
156.51	$P3m'1$	C10(1)P1(1)	(a,b,a,b,a,b),(c)	(0,-2,0),(2,2,0),(0,0,4)	(0,0,0)

12.62	$C2'/m'$	C11(1)P1(1)	(a,0,b,0,a,0),(c)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
12.62	$C2'/m'$	C12(1)P1(1)	(0,a,b,0,0,-a),(c)	(-2,- 4,0),(2,0,0),(0,0,4)	(1/2,0,0)
38.191	$Am'm'2$	C13(1)P1(1)	(a,-0.414a,b,-0.414b,b,- 0.414b),(c)	(0,0,4),(0,2,0),(-4,- 2,0)	(0,0,1/4)
39.199	$Ab'm'2$	C14(1)P1(1)	(a,-0.414a,b,2.414b,-b,- 2.414b),(c)	(0,0,4),(0,2,0),(-4,- 2,0)	(0,0,1/4)
5.15	$C2'$	S1(1)P1(1)	(a,b,c,0,a,-b),(d)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
5.13	$C2$	S2(1)P1(1)	(a,-0.414a,b,c,0.707b- 0.707c,-0.707b-0.707c),(d)	(0,- 2,0),(4,2,0),(0,0,4)	(0,0,1/4)
2.4	$P\bar{1}$	S3(1)P1(1)	(a,0,b,0,c,0),(d)	(0,0,4),(0,2,0),(- 2,0,0)	(0,0,0)
2.4	$P\bar{1}$	S4(1)P1(1)	(a,0,0,b,0,c),(d)	(0,0,4),(0,2,0),(- 2,0,0)	(0,1/2,0)
6.2	Pm'	S5(1)P1(1)	(a,-0.414a,b,-0.414b,c,- 0.414c),(d)	(- 2,0,0),(0,0,4),(0,2, 0)	(0,0,1/4)
7.26	Pc'	S6(1)P1(1)	(a,- 0.414a,b,2.414b,c,2.414c),(d)	(- 2,0,0),(0,0,4),(0,2, 0)	(0,0,1/4)
1.1	$P1$	4D1(1)P1(1)	(a,b,c,d,0,0),(e)	(1,1,2),(0,2,0),(- 2,0,0)	(0,0,0)
8.34	Cm'	4D2(1)P1(1)	(a,b,c,d,a,b),(e)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
1.1	$P1$	6D1(1)P1(1)	(a,b,c,d,e,f),(g)	(0,0,4),(0,2,0),(- 2,0,0)	(0,0,0)

S1.1.3. 4C $m\Gamma_5^+$ and U_1

Table S3 Magnetic subgroups arising from coupling of irreps $m\Gamma_5^+$ and $U_1(1/2,0,1/4)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space Group	OPD Name	OPD Vector	Basis Vectors	Origin
		$U_1(1/2,0,1/4)$	$m\Gamma_5^+$	$U_1(1/2,0,1/4)$	$m\Gamma_5^+$

12.58	<i>C2/m</i>	P1(1)P1(1)	(a,0,0,0,0),(b,-1.732b)	(2,1,-4),(0,1,0),(2,1,0)	(0,0,0)
44.229	<i>Imm2</i>	P2(1)P1(1)	(a,-0.414a,0,0,0),(b,-1.732b)	(0,1,0),(0,0,4),(2,1,0)	(0,0,1/4)
12.58	<i>C2/m</i>	P3(1)P1(3)	(a,0,a,0,0),(b,1.732b)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
15.85	<i>C2/c</i>	P4(1)P1(3)	(a,0,0,a,0),(b,1.732b)	(2,-2,0),(2,2,0),(-1,1,2)	(0,1/2,0)
42.219	<i>Fmm2</i>	P5(1)P1(3)	(a,-0.414a,a,-0.414a,0,0),(b,1.732b)	(2,2,0),(0,0,4),(2,-2,0)	(1/8,-1/8,1/4)
43.224	<i>Fdd2</i>	P6(1)P1(3)	(a,-0.414a,0.414a,a,0,0),(b,1.732b)	(2,2,0),(0,0,4),(2,-2,0)	(11/8,-3/8,3/4)
8.32	<i>Cm</i>	C1(1)P1(1)	(a,b,0,0,0),(c,-1.732c)	(2,1,-4),(0,1,0),(2,1,0)	(0,0,0)
5.13	<i>C2</i>	C2(1)P1(3)	(a,b,a,-b,0,0),(c,1.732c)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
5.13	<i>C2</i>	C3(1)P1(3)	(a,b,0.707a-0.707b,-0.707a-0.707b,0,0),(c,1.732c)	(2,2,0),(-2,2,0),(1,1,2)	(1/8,15/8,1/4)
8.32	<i>Cm</i>	C8(1)P1(3)	(a,b,a,b,0,0),(c,1.732c)	(2,-2,0),(2,2,0),(-1,1,2)	(0,0,0)
9.37	<i>Cc</i>	C9(1)P1(3)	(a,b,b,-a,0,0),(c,1.732c)	(2,-2,0),(2,2,0),(-1,1,2)	(3/2,0,0)
12.58	<i>C2/m</i>	C11(1)P1(2)	(a,0,b,0,a,0),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,4)	(0,0,0)
12.58	<i>C2/m</i>	C12(1)P1(2)	(0,a,b,0,0,-a),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,4)	(1/2,0,0)
38.187	<i>Amm2</i>	C13(1)P1(1)	(a,-0.414a,b,-0.414b,b,-0.414b),(c,-1.732c)	(0,0,4),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.195	<i>Abm2</i>	C14(1)P1(1)	(a,-0.414a,b,2.414b,-b,-2.414b),(c,-1.732c)	(0,0,4),(0,2,0),(-4,-2,0)	(0,0,1/4)
5.13	<i>C2</i>	S1(1)P1(2)	(a,b,c,0,a,-b),(-2d,0)	(-2,-4,0),(2,0,0),(0,0,4)	(0,0,0)
5.13	<i>C2</i>	S2(1)P1(1)	(a,-0.414a,b,c,0.707b-0.707c,-0.707b-0.707c),(d,-1.732d)	(0,-2,0),(4,2,0),(0,0,4)	(0,0,1/4)

8.32	<i>Cm</i>	4D2(1)P1(2)	(a,b,c,d,a,b),(-2e,0)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
12.62	<i>C2'/m'</i>	P1(1)P2(1)	(a,0,0,0,0,0),(b,0.577b)	(2,1,- 4),(0,1,0),(2,1,0)	(0,0,0)
44.231	<i>Im'm2'</i>	P2(1)P2(1)	(a,-0.414a,0,0,0,0),(b,0.577b)	(0,1,0),(0,0,4),(2,1,0)	(0,0,1/4)
12.62	<i>C2'/m'</i>	P3(1)P2(3)	(a,0,a,0,0,0),(-b,0.577b)	(2,-2,0),(2,2,0),(- 1,1,2)	(0,0,0)
15.89	<i>C2'/c'</i>	P4(1)P2(3)	(a,0,0,a,0,0),(-b,0.577b)	(2,-2,0),(2,2,0),(- 1,1,2)	(0,1/2,0)
42.221	<i>Fm'm2'</i>	P5(1)P2(3)	(a,-0.414a,a,-0.414a,0,0),(- b,0.577b)	(2,2,0),(0,0,4),(2,- 2,0)	(1/8,-1/8,1/4)
43.226	<i>Fd'd2'</i>	P6(1)P2(3)	(a,-0.414a,0.414a,a,0,0),(- b,0.577b)	(2,2,0),(0,0,4),(2,- 2,0)	(11/8,- 3/8,3/4)
8.34	<i>Cm'</i>	C1(1)P2(1)	(a,b,0,0,0,0),(c,0.577c)	(2,1,- 4),(0,1,0),(2,1,0)	(0,0,0)
5.15	<i>C2'</i>	C2(1)P2(3)	(a,b,a,-b,0,0),(-c,0.577c)	(2,-2,0),(2,2,0),(- 1,1,2)	(0,0,0)
5.15	<i>C2'</i>	C3(1)P2(3)	(a,b,0.707a-0.707b,-0.707a- 0.707b,0,0),(-c,0.577c)	(2,2,0),(- 2,2,0),(1,1,2)	(1/8,15/8,1/4)
8.34	<i>Cm'</i>	C8(1)P2(3)	(a,b,a,b,0,0),(-c,0.577c)	(2,-2,0),(2,2,0),(- 1,1,2)	(0,0,0)
9.39	<i>Cc'</i>	C9(1)P2(3)	(a,b,b,-a,0,0),(-c,0.577c)	(2,-2,0),(2,2,0),(- 1,1,2)	(3/2,0,0)
12.62	<i>C2'/m'</i>	C11(1)P2(2)	(a,0,b,0,a,0),(0,-1.155c)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
12.62	<i>C2'/m'</i>	C12(1)P2(2)	(0,a,b,0,0,-a),(0,-1.155c)	(-2,- 4,0),(2,0,0),(0,0,4)	(1/2,0,0)
38.19	<i>Amm'2'</i>	C13(1)P2(1)	(a,-0.414a,b,-0.414b,b,- 0.414b),(c,0.577c)	(0,0,4),(0,2,0),(-4,- 2,0)	(0,0,1/4)
39.198	<i>Abm'2'</i>	C14(1)P2(1)	(a,-0.414a,b,2.414b,-b,- 2.414b),(c,0.577c)	(0,0,4),(0,2,0),(-4,- 2,0)	(0,0,1/4)
5.15	<i>C2'</i>	S1(1)P2(2)	(a,b,c,0,a,-b),(0,-1.155d)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)

5.15	$C2'$	S2(1)P2(1)	(a,-0.414a,b,c,0.707b-0.707c,- 0.707b-0.707c),(d,0.577d)	(0,- 2,0),(4,2,0),(0,0,4)	(0,0,1/4)
8.34	Cm'	4D2(1)P2(2)	(a,b,c,d,a,b),(0,-1.155e)	(-2,- 4,0),(2,0,0),(0,0,4)	(0,0,0)
2.4	$P\bar{1}$	P1(1)C1(1)	(a,0,0,0,0),(b,c)	(1,0,2),(0,1,0),(- 2,0,0)	(0,0,0)
8.32	Cm	P2(1)C1(1)	(a,-0.414a,0,0,0),(b,c)	(- 2,0,0),(0,0,4),(0,1,0)	(-1/8,0,1/4)
1.1	$P1$	C1(1)C1(1)	(a,b,0,0,0),(c,d)	(1,0,2),(0,1,0),(- 2,0,0)	(0,0,0)
2.4	$P\bar{1}$	C4(1)C1(1)	(a,0,b,0,0),(c,d)	(1,1,2),(0,2,0),(- 2,0,0)	(0,0,0)
2.4	$P\bar{1}$	C5(1)C1(1)	(a,0,0,b,0,0),(c,d)	(1,1,2),(0,2,0),(- 2,0,0)	(0,1/2,0)
8.32	Cm	C6(1)C1(1)	(a,-0.414a,b,-0.414b,0,0),(c,d)	(-2,-2,0),(0,0,4),(- 2,0,0)	(-1/8,- 1/8,1/4)
9.37	Cc	C7(1)C1(1)	(a,-0.414a,b,2.414b,0,0),(c,d)	(-2,-2,0),(0,0,4),(- 2,0,0)	(-5/8,- 5/8,5/4)
2.4	$P\bar{1}$	S3(1)C1(1)	(a,0,b,0,c,0),(d,e)	(0,0,4),(0,2,0),(- 2,0,0)	(0,0,0)
2.4	$P\bar{1}$	S4(1)C1(1)	(a,0,0,b,0,c),(d,e)	(0,0,4),(0,2,0),(- 2,0,0)	(0,1/2,0)
6.18	Pm	S5(1)C1(1)	(a,-0.414a,b,-0.414b,c,- 0.414c),(d,e)	(- 2,0,0),(0,0,4),(0,2,0)	(0,0,1/4)
7.24	Pc	S6(1)C1(1)	(a,- 0.414a,b,2.414b,c,2.414c),(d,e)	(- 2,0,0),(0,0,4),(0,2,0)	(0,0,1/4)
1.1	$P1$	4D1(1)C1(1)	(a,b,c,d,0,0),(e,f)	(1,1,2),(0,2,0),(- 2,0,0)	(0,0,0)
1.1	$P1$	6D1(1)C1(1)	(a,b,c,d,e,f),(g,h)	(0,0,4),(0,2,0),(- 2,0,0)	(0,0,0)

S2. 5C**S2.1. U_1**

Table S4 Order parameter components and unit cell configurations for subgroups of $P6_3/mmc$ which can arise from phase transitions in which irrep $U_1(1/2,0,1/5)$ is the active representation.

SGN	Space Group	OPD Name	OPD Vector	Basis Vectors	Origin
58	$Pnmm$	P1	(a,0,0,0,0)	(0,0,5),(2,1,0),(0,1,0)	(0,0,0)
59	$Pmnn$	P2	(0,a,0,0,0)	(0,0,5),(0,-1,0),(2,1,0)	(1/2,1/2,0)
164	$P\bar{3}m1$	P3	(a,0,a,0,a)	(2,0,0),(0,2,0),(0,0,5)	(0,0,0)
187	$P\bar{6}m2$	P4	(a,-0.325a,a,-0.325a,a,-0.325a)	(0,-2,0),(2,2,0),(0,0,5)	(0,0,1/4)
64	$Cmca$	P5	(a,0,0,0,a)	(2,0,0),(2,4,0),(0,0,5)	(0,0,0)
63	$Cmcm$	P6	(0,a,0,0,-a)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
31	$Pmn2_1$	C1	(a,b,0,0,0)	(0,-1,0),(2,1,0),(0,0,5)	(1/2,1/4,0)
156	$P3m1$	C2	(a,b,a,b,a,b)	(2,0,0),(0,2,0),(0,0,5)	(0,0,0)
20	$C222_1$	C3	(a,b,0,0,a,-b)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
14	$P2_1/c$	C4	(0,0,a,0,b,0)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,0)
11	$P2_1/m$	C5	(0,0,0,a,0,b)	(-2,0,0),(0,0,5),(0,2,0)	(0,1/2,0)
14	$P2_1/c$	C6	(a,0,0,0,0,b)	(-2,0,0),(0,0,5),(2,2,0)	(0,1/2,0)
12	$C2/m$	C7	(a,0,b,0,a,0)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
12	$C2/m$	C8	(0,a,b,0,0,-a)	(-2,-4,0),(2,0,0),(0,0,5)	(1/2,0,0)
38	$Amm2$	C9	(a,-0.325a,b,-0.325b,b,-0.325b)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
39	$Abm2$	C10	(a,-0.325a,b,3.078b,-b,-3.078b)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
36	$Cmc2_1$	C11	(a,b,0,0,a,b)	(2,0,0),(2,4,0),(0,0,5)	(1/2,-1,0)
5	$C2$	S1	(a,b,c,0,a,-b)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
5	$C2$	S2	(a,-0.325a,b,c,0.809b-0.588c,-0.588b-0.809c)	(0,-2,0),(4,2,0),(0,0,5)	(0,0,1/4)
2	$P\bar{1}$	S3	(a,0,b,0,c,0)	(0,0,5),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	S4	(a,0,0,b,0,c)	(0,0,5),(0,2,0),(-2,0,0)	(0,1/2,0)
6	Pm	S5	(a,-0.325a,b,-0.325b,c,-0.325c)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,1/4)

7	Pc	S6	(a,- 0.325a,b,3.078b,c,3.078c)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,1/4)
4	$P2_1$	4D1	(0,0,a,b,c,d)	(-2,0,0),(0,0,5),(0,2,0)	(0,1/2,0)
8	Cm	4D2	(a,b,c,d,a,b)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
1	$P1$	6D1	(a,b,c,d,e,f)	(0,0,5),(0,2,0),(-2,0,0)	(0,0,0)
58	$Pnmm$	P1	(a,0,0,0,0,0)	(0,0,5),(2,1,0),(0,1,0)	(0,0,0)
59	$Pmmn$	P2	(0,a,0,0,0,0)	(0,0,5),(0,-1,0),(2,1,0)	(1/2,1/2,0)
164	$P\bar{3}m1$	P3	(a,0,a,0,a,0)	(2,0,0),(0,2,0),(0,0,5)	(0,0,0)

S2.2. U_1 and $m\Gamma_4^+$

Table S5 Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/5)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space Group	OPD Name $U_1(1/2,0,1/5)$ $m\Gamma_4^+$	OPD Vector $U_1(1/2,0,1/5)$, $m\Gamma_4^+$	Basis Vectors	Origin
58.398	$Pnn'm'$	P1(1)P1(1)	(a,0,0,0,0,0),(b)	(-2,-1,0),(0,0,5),(0,1,0)	(0,0,0)
59.409	$Pm'm'n$	P2(1)P1(1)	(0,a,0,0,0,0),(b)	(0,0,5),(0,-1,0),(2,1,0)	(1/2,1/2,0)
164.89	$P\bar{3}m'1$	P3(1)P1(1)	(a,0,a,0,a,0),(b)	(0,-2,0),(2,2,0),(0,0,5)	(0,0,0)
187.211	$P\bar{6}'m'2$	P4(1)P1(1)	(a,-0.325a,a,- 0.325a,a,- 0.325a),(b)	(2,2,0),(-2,0,0),(0,0,5)	(0,0,1/4)
64.476	$Cm'ca'$	P5(1)P1(1)	(a,0,0,0,a,0),(b)	(2,0,0),(2,4,0),(0,0,5)	(0,0,0)
63.464	$Cm'cm'$	P6(1)P1(1)	(0,a,0,0,0,-a),(b)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
31.125	$Pm'n2_1'$	C1(1)P1(1)	(a,b,0,0,0,0),(c)	(0,-1,0),(2,1,0),(0,0,5)	(1/2,1/4,0)
156.51	$P3m'1$	C2(1)P1(1)	(a,b,a,b,a,b),(c)	(0,-2,0),(2,2,0),(0,0,5)	(0,0,0)
20.34	$C22'2_1'$	C3(1)P1(1)	(a,b,0,0,a,-b),(c)	(2,4,0),(-2,0,0),(0,0,5)	(3/2,2,5/4)
14.79	$P2_1'/c'$	C4(1)P1(1)	(0,0,a,0,b,0),(c)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,0)
11.54	$P2_1'/m'$	C5(1)P1(1)	(0,0,0,a,0,b),(c)	(-2,0,0),(0,0,5),(0,2,0)	(0,1/2,0)
14.79	$P2_1'/c'$	C6(1)P1(1)	(a,0,0,0,0,b),(c)	(-2,0,0),(0,0,5),(2,2,0)	(0,1/2,0)

12.62	$C2'/m'$	C7(1)P1(1)	(a,0,b,0,a,0),(c)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
12.62	$C2'/m'$	C8(1)P1(1)	(0,a,b,0,0,-a),(c)	(-2,-4,0),(2,0,0),(0,0,5)	(1/2,0,0)
38.191	$Am'm'2$	C9(1)P1(1)	(a,-0.325a,b,- 0.325b,b,- 0.325b),(c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.199	$Ab'm'2$	C10(1)P1(1)	(a,- 0.325a,b,3.078b,- b,-3.078b),(c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
36.174	$Cm'c2_1'$	C11(1)P1(1)	(a,b,0,0,a,b),(c)	(2,0,0),(2,4,0),(0,0,5)	(1/2,-1,0)
5.15	$C2'$	S1(1)P1(1)	(a,b,c,0,a,-b),(d)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
5.13	$C2$	S2(1)P1(1)	(a,- 0.325a,b,c,0.809b -0.588c,-0.588b- 0.809c),(d)	(0,-2,0),(4,2,0),(0,0,5)	(0,0,1/4)
2.4	$P\bar{1}$	S3(1)P1(1)	(a,0,b,0,c,0),(d)	(0,0,5),(0,2,0),(-2,0,0)	(0,0,0)
2.4	$P\bar{1}$	S4(1)P1(1)	(a,0,0,b,0,c),(d)	(0,0,5),(0,2,0),(-2,0,0)	(0,1/2,0)
6.2	Pm'	S5(1)P1(1)	(a,-0.325a,b,- 0.325b,c,- 0.325c),(d)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,1/4)
7.26	Pc'	S6(1)P1(1)	(a,- 0.325a,b,3.078b,c, 3.078c),(d)	(-2,0,0),(0,0,5),(0,2,0)	(0,0,1/4)
4.9	$P2_1'$	4D1(1)P1(1)	(0,0,a,b,c,d),(e)	(-2,0,0),(0,0,5),(0,2,0)	(0,1/2,0)
8.34	Cm'	4D2(1)P1(1)	(a,b,c,d,a,b),(e)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
1.1	$P1$	6D1(1)P1(1)	(a,b,c,d,e,f),(g)	(0,0,5),(0,2,0),(-2,0,0)	(0,0,0)

S2.3. U_1 and $m\Gamma_5^+$

Table S6 Magnetic subgroups arising from coupling of irreps $m\Gamma_5^+$ and $U_1(1/2,0,1/5)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space Group	OPD Name $U_1(1/2,0,1/5)$ $m\Gamma_5^+$	OPD Vector $U_1(1/2,0,1/5)$, $m\Gamma_5^+$	Basis Vectors	Origin
58.393	$Pnmm$	P1(1)P1(1)	(a,0,0,0,0,0),(b,-1.732b)	(-2,-1,0),(0,0,5),(0,1,0)	(0,0,0)
59.405	$Pmmm$	P2(1)P1(1)	(0,a,0,0,0,0),(b,-1.732b)	(0,1,0),(0,0,5),(2,1,0)	(1/2,0,0)

64.469	<i>Cmca</i>	P5(1)P1(2)	(a,0,0,0,a,0),(-2b,0)	(2,0,0),(2,4,0),(0,0,5)	(0,0,0)
63.457	<i>Cmcm</i>	P6(1)P1(2)	(0,a,0,0,0,-a),(-2b,0)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
31.123	<i>Pmn</i> ₂ ₁	C1(1)P1(1)	(a,b,0,0,0,0),(c,-1.732c)	(0,-1,0),(2,1,0),(0,0,5)	(1/2,1/4,0)
20.31	<i>C222</i> ₁	C3(1)P1(2)	(a,b,0,0,a,-b),(-2c,0)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
12.58	<i>C2/m</i>	C7(1)P1(2)	(a,0,b,0,a,0),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
12.58	<i>C2/m</i>	C8(1)P1(2)	(0,a,b,0,0,-a),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,5)	(1/2,0,0)
38.187	<i>Amm</i> ₂	C9(1)P1(1)	(a,-0.325a,b,-0.325b,b,-0.325b),(c,-1.732c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.195	<i>Abm</i> ₂	C10(1)P1(1)	(a,-0.325a,b,3.078b,-b,-3.078b),(c,-1.732c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
36.172	<i>Cmc</i> ₂ ₁	C11(1)P1(2)	(a,b,0,0,a,b),(-2c,0)	(2,0,0),(2,4,0),(0,0,5)	(1/2,-1,0)
5.13	<i>C2</i>	S1(1)P1(2)	(a,b,c,0,a,-b),(-2d,0)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
5.13	<i>C2</i>	S2(1)P1(1)	(a,-0.325a,b,c,0.809b-0.588c,-0.588b-0.809c),(d,-1.732d)	(0,-2,0),(4,2,0),(0,0,5)	(0,0,1/4)
8.32	<i>Cm</i>	4D2(1)P1(2)	(a,b,c,d,a,b),(-2e,0)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
58.398	<i>Pnn'm'</i>	P1(1)P2(1)	(a,0,0,0,0,0),(b,0.577b)	(0,0,5),(2,1,0),(0,1,0)	(0,0,0)
59.41	<i>Pmm'n'</i>	P2(1)P2(1)	(0,a,0,0,0,0),(b,0.577b)	(0,0,5),(0,-1,0),(2,1,0)	(1/2,1/2,0)
64.474	<i>Cm'c'a</i>	P5(1)P2(2)	(a,0,0,0,a,0),(0,-1.155b)	(2,0,0),(2,4,0),(0,0,5)	(0,0,0)
63.462	<i>Cm'c'm</i>	P6(1)P2(2)	(0,a,0,0,0,-a),(0,-1.155b)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
31.127	<i>Pm'n'</i> ₂ ₁	C1(1)P2(1)	(a,b,0,0,0,0),(c,0.577c)	(0,-1,0),(2,1,0),(0,0,5)	(1/2,1/4,0)
20.33	<i>C2'2'</i> ₂ ₁	C3(1)P2(2)	(a,b,0,0,a,-b),(0,-1.155c)	(2,0,0),(2,4,0),(0,0,5)	(1/2,0,0)
12.62	<i>C2'/m'</i>	C7(1)P2(2)	(a,0,b,0,a,0,0),(-1.155c)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
12.62	<i>C2'/m'</i>	C8(1)P2(2)	(0,a,b,0,0,-a),(0,-1.155c)	(-2,-4,0),(2,0,0),(0,0,5)	(1/2,0,0)
38.19	<i>Amm'2'</i>	C9(1)P2(1)	(a,-0.325a,b,-0.325b,b,-0.325b),(c,0.577c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.198	<i>Abm'2'</i>	C10(1)P2(1)	(a,-0.325a,b,3.078b,-b,-3.078b),(c,0.577c)	(0,0,5),(0,2,0),(-4,-2,0)	(0,0,1/4)
36.176	<i>Cm'c'2'</i> ₁	C11(1)P2(2)	(a,b,0,0,a,b),(0,-1.155c)	(2,0,0),(2,4,0),(0,0,5)	(1/2,-1,0)
5.15	<i>C2'</i>	S1(1)P2(2)	(a,b,c,0,a,-b),(0,-1.155d)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)

5.15	$C2'$	S2(1)P2(1)	(a,-0.325a,b,c,0.809b- 0.588c,-0.588b- 0.809c),(d,0.577d)	(0,-2,0),(4,2,0),(0,0,5)	(0,0,1/4)
8.34	Cm'	4D2(1)P2(2)	(a,b,c,d,a,b),(0,-1.155e)	(-2,-4,0),(2,0,0),(0,0,5)	(0,0,0)
14.75	$P2_1/c$	P1(1)C1(1)	(a,0,0,0,0),(b,c)	(0,1,0),(0,0,5),(2,0,0)	(0,0,0)
11.50	$P2_1/m$	P2(1)C1(1)	(0,a,0,0,0),(b,c)	(0,-1,0),(0,0,5),(-2,-1,0)	(-1/2,0,0)
4.7	$P2_1$	C1(1)C1(1)	(a,b,0,0,0),(c,d)	(0,-1,0),(0,0,5),(-2,-1,0)	(-1/2,0,0)
14.75	$P2_1/c$	C4(1)C1(1)	(0,0,a,0,b),(c,d)	(-2,0,0),(0,0,-5),(0,-2,0)	(0,0,0)
11.50	$P2_1/m$	C5(1)C1(1)	(0,0,0,a,0,b),(c,d)	(-2,0,0),(0,0,-5),(0,-2,0)	(0,1/2,0)
14.75	$P2_1/c$	C6(1)C1(1)	(a,0,0,0,b),(c,d)	(-2,0,0),(0,0,5),(2,2,0)	(0,1/2,0)
2.4	$P\bar{1}$	S3(1)C1(1)	(a,0,b,0,c),(d,e)	(0,2,0),(-2,0,0),(0,0,5)	(0,0,0)
2.4	$P\bar{1}$	S4(1)C1(1)	(a,0,0,b,0,c),(d,e)	(0,2,0),(-2,0,0),(0,0,5)	(0,1/2,0)
6.18	Pm	S5(1)C1(1)	(a,-0.325a,b,0.325b,c,- 0.325c),(d,e)	(-2,0,0),(0,0,-5),(0,-2,0)	(0,0,1/4)
7.24	Pc	S6(1)C1(1)	(a,- 0.325a,b,3.078b,c,3.078c),(d ,e)	(-2,0,0),(0,0,-5),(0,-2,0)	(0,0,1/4)
4.7	$P2_1$	4D1(1)C1(1)	(0,0,a,b,c,d),(e,f)	(-2,0,0),(0,0,-5),(0,-2,0)	(0,1/2,0)
1.1	$P1$	6D1(1)C1(1)	(a,b,c,d,e,f),(g,h)	(0,2,0),(-2,0,0),(0,0,5)	(0,0,0)

S3. 6C

S3.1. U_1

Table S7 Order parameter components and unit cell configurations for subgroups of $P6_3/mmc$ which can arise from phase transitions in which irrep $U_1(1/2,0,1/6)$ is the active representation.

SGN	Space Group	OPD Name	OPD Vector	Basis Vectors	Origin
12	$C2/m$	P1	(a,0,0,0,0)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)
44	$Imm2$	P2	(a,-0.268a,0,0,0)	(0,0,6),(0,1,0),(-2,-1,0)	(-11/12,1/24,- 11/4)
12	$C2/m$	P3	(a,0,a,0,0)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
15	$C2/c$	P4	(a,0,0,a,0)	(2,2,0),(-2,2,0),(1,1,3)	(0,1/2,0)
43	$Fdd2$	P5	(a,-0.268a,0.268a,a,0)	(0,0,6),(-2,2,0),(-2,-2,0)	(-4/3,-1/3,1)
42	$Fmm2$	P6	(a,-0.268a,a,-0.268a,0)	(0,0,6),(2,2,0),(-2,2,0)	(-1/12,1/12,1/4)

164	$P\bar{3}m1$	P7	(a,0,a,0,a,0)	(2,0,0),(0,2,0),(0,0,6)	(0,0,0)
187	$P\bar{6}m2$	P8	(a,-0.268a,a,-0.268a,a,- 0.268a)	(0,-2,0),(2,2,0),(0,0,6)	(0,0,1/4)
152	$P3_121$	P9	(a,1.732a,-2a,0,a,-1.732a)	(2,0,0),(0,2,0),(0,0,6)	(0,0,1)
151	$P3_112$	P10	(a,a,- 1.366a,0.366a,0.366a,1.366a)	(0,-2,0),(2,2,0),(0,0,6)	(0,0,5/4)
8	Cm	C1	(a,b,0,0,0,0)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)
5	$C2$	C2	(a,b,a,-b,0,0)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
5	$C2$	C3	(a,b,0.866a,0.500b,- 0.500a,0.866b,0,0)	(2,2,0),(-2,2,0),(1,1,3)	(1/12,23/12,1/4)
2	$P\bar{1}$	C4	(a,0,b,0,0,0)	(1,1,3),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	C5	(a,0,0,b,0,0)	(1,1,3),(0,2,0),(-2,0,0)	(0,1/2,0)
8	Cm	C6	(a,-0.268a,b,-0.268b,0,0)	(-2,-2,0),(0,0,6),(-2,0,0)	(-1/12,-1/12,1/4)
9	Cc	C7	(a,-0.268a,b,3.732b,0,0)	(-2,-2,0),(0,0,6),(-2,0,0)	(-7/12,-7/12,7/4)
8	Cm	C8	(a,b,a,b,0,0)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
9	Cc	C9	(a,b,b,-a,0,0)	(2,2,0),(-2,2,0),(1,1,3)	(0,3/2,0)
156	$P3m1$	C10	(a,b,a,b,a,b)	(2,0,0),(0,2,0),(0,0,6)	(0,0,0)
12	$C2/m$	C11	(a,0,b,0,a,0)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
12	$C2/m$	C12	(0,a,b,0,0,-a)	(-2,-4,0),(2,0,0),(0,0,6)	(1/2,0,0)
38	$Amm2$	C13	(a,-0.268a,b,-0.268b,b,- 0.268b)	(0,0,6),(0,2,0),(-4,-2,0)	(0,0,1/4)
39	$Abm2$	C14	(a,-0.268a,b,3.732b,- b,3.732b)	(0,0,6),(0,2,0),(-4,-2,0)	(0,0,1/4)
144	$P3_1$	C15	(a,b,-0.500a,0.866b,0.866a- 0.500b,-0.500a+0.866b,- 0.866a-0.500b)	(2,2,0),(-2,0,0),(0,0,6)	(0,0,0)
5	$C2$	S1	(a,b,c,0,a,-b)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
5	$C2$	S2	(a,-0.268a,b,c,0.866b,0.500c,- 0.500b,0.866c)	(0,-2,0),(4,2,0),(0,0,6)	(0,0,1/4)
2	$P\bar{1}$	S3	(a,0,b,0,c,0)	(0,0,6),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	S4	(a,0,0,b,0,c)	(0,0,6),(0,2,0),(-2,0,0)	(0,1/2,0)
6	Pm	S5	(a,-0.268a,b,-0.268b,c,- 0.268c)	(-2,0,0),(0,0,6),(0,2,0)	(0,0,1/4)
7	Pc	S6	(a,-0.268a,b,3.732b,c,3.732c)	(-2,0,0),(0,0,6),(0,2,0)	(0,0,1/4)
1	$P1$	4D1	(a,b,c,d,0,0)	(1,1,3),(0,2,0),(-2,0,0)	(0,0,0)

8	<i>Cm</i>	4D2	(a,b,c,d,a,b)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
1	<i>P1</i>	6D1	(a,b,c,d,e,f)	(0,0,6),(0,2,0),(-2,0,0)	(0,0,0)

S3.1.1. U_1 and $m\Gamma_4^+$

Table S8 Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/6)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space group	OPD Name $U_1(1/2,0,1/6)$	OPD Vector $m\Gamma_4^+$ $U_1(1/2,0,1/6)$	Basis Vectors $m\Gamma_4^+$	Origin
12.62	$C2'/m'$	P1(1)P1(1)	(a,0,0,0,0,0),(b)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)
44.232	$Im'm'2$	P2(1)P1(1)	(a,-0.268a,0,0,0,0),(b)	(0,0,6),(0,1,0),(-2,-1,0)	(-11/12,1/24,-11/4)
12.62	$C2'/m'$	P3(1)P1(1)	(a,0,a,0,0,0),(b)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
15.85	$C2/c$	P4(1)P1(1)	(a,0,0,a,0,0),(b)	(2,2,0),(-2,2,0),(1,1,3)	(0,1/2,0)
43.226	$Fd'd2'$	P5(1)P1(1)	(a,-0.268a,0.268a,a,0,0),(b)	(0,0,6),(-2,2,0),(-2,2,0)	(-4/3,-1/3,1)
42.222	$Fm'm'2$	P6(1)P1(1)	(a,-0.268a,a,-0.268a,0,0),(b)	(0,0,6),(2,2,0),(-2,2,0)	(-1/12,1/12,1/4)
164.89	$P\bar{3}m'1$	P7(1)P1(1)	(a,0,a,0,a,0),(b)	(0,-2,0),(2,2,0),(0,0,6)	(0,0,0)
187.211	$P\bar{6}'m'2$	P8(1)P1(1)	(a,-0.268a,a,-0.268a,a,-0.268a),(b)	(2,2,0),(-2,0,0),(0,0,6)	(0,0,1/4)
152.35	$P3_12'1$	P9(1)P1(1)	(a,1.732a,-2a,0,a,-1.732a),(b)	(0,-2,0),(2,2,0),(0,0,6)	(0,0,0)
151.29	$P3_112$	P10(1)P1(1)	(a,a,-1.366a,0.366a,0.366a,-1.366a),(b)	(2,2,0),(-2,0,0),(0,0,6)	(0,0,1/4)
8.34	Cm'	C1(1)P1(1)	(a,b,0,0,0,0),(c)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)
5.15	$C2'$	C2(1)P1(1)	(a,b,a,-b,0,0),(c)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
5.13	$C2$	C3(1)P1(1)	(a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(c)	(2,2,0),(-2,2,0),(1,1,3)	(1/12,23/12,1/4)

2.4	<i>P</i>	C4(1)P1(1)	(a,0,b,0,0,0),(c)	(1,1,3),(0,2,0),(-2,0,0)	(0,0,0)
2.4	<i>P</i>	C5(1)P1(1)	(a,0,0,b,0,0),(c)	(1,1,3),(0,2,0),(-2,0,0)	(0,1/2,0)
8.34	<i>Cm'</i>	C6(1)P1(1)	(a,-0.268a,b,-0.268b,0,0),(c)	(-2,-2,0),(0,0,6),(-2,0,0)	(-1/12,-1/12,1/4)
9.39	<i>Cc'</i>	C7(1)P1(1)	(a,-0.268a,b,3.732b,0,0),(c)	(-2,-2,0),(0,0,6),(-2,0,0)	(-7/12,-7/12,7/4)
8.34	<i>Cm'</i>	C8(1)P1(1)	(a,b,a,b,0,0),(c)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
9.37	<i>Cc</i>	C9(1)P1(1)	(a,b,b,-a,0,0),(c)	(2,2,0),(-2,2,0),(1,1,3)	(0,3/2,0)
156.51	<i>P3m'1</i>	C10(1)P1(1)	(a,b,a,b,a,b),(c)	(0,-2,0),(2,2,0),(0,0,6)	(0,0,0)
12.62	<i>C2'/m'</i>	C11(1)P1(1)	(a,0,b,0,a,0),(c)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
12.62	<i>C2'/m'</i>	C12(1)P1(1)	(0,a,b,0,0,-a),(c)	(-2,-4,0),(2,0,0),(0,0,6) (0,0,6),(0,2,0),(-4,-2,0)	(1/2,0,0)
38.191	<i>Am'm'2</i>	C13(1)P1(1)	(a,-0.268a,b,-0.268b,b,-0.268b),(c)	2,0)	(0,0,1/4)
39.199	<i>Ab'm'2</i>	C14(1)P1(1)	(a,-0.268a,b,3.732b,-b,-3.732b),(c)	(0,0,6),(0,2,0),(-4,-2,0) (2,2,0),(-	(0,0,1/4)
144.4	<i>P3₁</i>	C15(1)P1(1)	(a,b,-0.500a-0.866b,0.866a-0.500b,-0.500a+0.866b,-0.866a-0.500b),(c)	2,0,0),(0,0,6)	(0,0,0)
5.15	<i>C2'</i>	S1(1)P1(1)	(a,b,c,0,a,-b),(d)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
5.13	<i>C2</i>	S2(1)P1(1)	(a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866c),(d)	(0,-2,0),(4,2,0),(0,0,6)	(0,0,1/4)
2.4	<i>P</i>	S3(1)P1(1)	(a,0,b,0,c,0),(d)	(0,0,6),(0,2,0),(-2,0,0)	(0,0,0)

2.4	<i>P</i>	S4(1)P1(1)	(a,0,0,b,0,c),(d)	(0,0,6),(0,2,0),(- 2,0,0)	(0,1/2,0)
6.2	<i>Pm'</i>	S5(1)P1(1)	(a,-0.268a,b,-0.268b,c,- 0.268c),(d)	(- 2,0,0),(0,0,6),(0,2,0)	(0,0,1/4)
7.26	<i>Pc'</i>	S6(1)P1(1)	(a,- 0.268a,b,3.732b,c,3.732c),(d)	(- 2,0,0),(0,0,6),(0,2,0)	(0,0,1/4)
1.1	<i>P1</i>	4D1(1)P1(1)	(a,b,c,d,0,0),(e)	(1,1,3),(0,2,0),(- 2,0,0)	(0,0,0)
8.34	<i>Cm'</i>	4D2(1)P1(1)	(a,b,c,d,a,b),(e)	(-2,- 4,0),(2,0,0),(0,0,6)	(0,0,0)
1.1	<i>P1</i>	6D1(1)P1(1)	(a,b,c,d,e,f),(g)	(0,0,6),(0,2,0),(- 2,0,0)	(0,0,0)

S3.2. U_1 and $m\Gamma_5^+$

Table S9 Magnetic subgroups arising from coupling of irreps $m\Gamma_5^+$ and $U_1(1/2,0,1/6)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space Group	OPD Name $U_1(1/2,0,1/6)$	OPD Vector $m\Gamma_5^+$ $U_1(1/2,0,1/6)$	Basis Vectors	Origin
12.58	<i>C2/m</i>	P1(1)P1(1)	(a,0,0,0,0,0),(b,-1.732b)	(2,1,- 6),(0,1,0),(2,1,0)	(0,0,0)
44.229	<i>Imm2</i>	P2(1)P1(1)	(a,-0.268a,0,0,0,0),(b,-1.732b)	(0,1,0),(0,0,6),(2,1,0)	(0,0,1/4)
12.58	<i>C2/m</i>	P3(1)P1(3)	(a,0,a,0,0,0),(b,1.732b)	(2,-2,0),(2,2,0),(- 1,1,3)	(0,0,0)
15.85	<i>C2/c</i>	P4(1)P1(3)	(a,0,0,a,0,0),(b,1.732b)	(2,2,0),(- 2,2,0),(1,1,3)	(0,1/2,0)
43.224	<i>Fdd2</i>	P5(1)P1(3)	(a,- 0.268a,0.268a,a,0,0),(b,1.732b)	(- 2,2,0),(0,0,6),(2,2,0)	(5/6,5/6,5/2)
42.219	<i>Fmm2</i>	P6(1)P1(3)	(a,-0.268a,a,- 0.268a,0,0),(b,1.732b)	(2,2,0),(0,0,6),(2,- 2,0)	(1/12,-1/12,1/4)
8.32	<i>Cm</i>	C1(1)P1(1)	(a,b,0,0,0,0),(c,-1.732c)	(2,1,- 6),(0,1,0),(2,1,0)	(0,0,0)
5.13	<i>C2</i>	C2(1)P1(3)	(a,b,a,-b,0,0),(c,1.732c)	(2,-2,0),(2,2,0),(- 1,1,3)	(0,0,0)

5.13	<i>C2</i>	C3(1)P1(3)	(a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(c,1.732c)	(2,2,0),(-2,2,0),(1,1,3)	(1/12,23/12,1/4)
8.32	<i>Cm</i>	C8(1)P1(3)	(a,b,a,b,0,0),(c,1.732c)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
9.37	<i>Cc</i>	C9(1)P1(3)	(a,b,b,-a,0,0),(c,1.732c)	(2,2,0),(-2,2,0),(1,1,3)	(0,3/2,0)
12.58	<i>C2/m</i>	C11(1)P1(2)	(a,0,b,0,a,0),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
12.58	<i>C2/m</i>	C12(1)P1(2)	(0,a,b,0,0,-a),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,6)	(1/2,0,0)
38.187	<i>Amm2</i>	C13(1)P1(1)	(a,-0.268a,b,-0.268b,b,-0.268b),(c,-1.732c)	(0,0,6),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.195	<i>Abm2</i>	C14(1)P1(1)	(a,-0.268a,b,3.732b,-b,-3.732b),(c,-1.732c)	(0,0,6),(0,2,0),(-4,-2,0)	(0,0,1/4)
5.13	<i>C2</i>	S1(1)P1(2)	(a,b,c,0,a,-b),(-2d,0)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
5.13	<i>C2</i>	S2(1)P1(1)	(a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866c),(d,-1.732d)	(0,-2,0),(4,2,0),(0,0,6)	(0,0,1/4)
8.32	<i>Cm</i>	4D2(1)P1(2)	(a,b,c,d,a,b),(-2e,0)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
12.62	<i>C2'/m'</i>	P1(1)P2(1)	(a,0,0,0,0,0),(b,0.577b)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)
44.231	<i>Im'm2'</i>	P2(1)P2(1)	(a,-0.268a,0,0,0,0),(b,0.577b)	(0,1,0),(0,0,6),(2,1,0)	(0,0,1/4)
12.62	<i>C2'/m'</i>	P3(1)P2(3)	(a,0,a,0,0,0),(-b,0.577b)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
15.89	<i>C2'/c'</i>	P4(1)P2(3)	(a,0,0,a,0,0),(-b,0.577b)	(2,2,0),(-2,2,0),(1,1,3)	(0,1/2,0)
43.226	<i>Fd'd2'</i>	P5(1)P2(3)	(a,-0.268a,0.268a,a,0,0),(-b,0.577b)	(-2,2,0),(0,0,6),(2,2,0)	(5/6,5/6,5/2)
42.221	<i>Fm'm2'</i>	P6(1)P2(3)	(a,-0.268a,a,-0.268a,0,0),(-b,0.577b)	(2,2,0),(0,0,6),(2,-2,0)	(1/12,-1/12,1/4)
8.34	<i>Cm'</i>	C1(1)P2(1)	(a,b,0,0,0,0),(c,0.577c)	(2,1,-6),(0,1,0),(2,1,0)	(0,0,0)

5.15	$C2'$	C2(1)P2(3)	(a,b,a,-b,0,0),(-c,0.577c)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
5.15	$C2'$	C3(1)P2(3)	(a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(-c,0.577c)	(2,2,0),(-2,2,0),(1,1,3)	(1/12,23/12,1/4)
8.34	Cm'	C8(1)P2(3)	(a,b,a,b,0,0),(-c,0.577c)	(2,-2,0),(2,2,0),(-1,1,3)	(0,0,0)
9.39	Cc'	C9(1)P2(3)	(a,b,b,-a,0,0),(-c,0.577c)	(2,2,0),(-2,2,0),(1,1,3)	(0,3/2,0)
12.62	$C2'/m'$	C11(1)P2(2)	(a,0,b,0,a,0),(0,-1.155c)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
12.62	$C2'/m'$	C12(1)P2(2)	(0,a,b,0,0,-a),(0,-1.155c)	(-2,-4,0),(2,0,0),(0,0,6)	(1/2,0,0)
38.19	$Amm'2'$	C13(1)P2(1)	(a,-0.268a,b,-0.268b,b,-0.268b),(c,0.577c)	(0,0,6),(0,2,0),(-4,2,0)	(0,0,1/4)
39.198	$Abm'2'$	C14(1)P2(1)	(a,-0.268a,b,3.732b,-b,-3.732b),(c,0.577c)	(0,0,6),(0,2,0),(-4,2,0)	(0,0,1/4)
5.15	$C2'$	S1(1)P2(2)	(a,b,c,0,a,-b),(0,-1.155d)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
5.15	$C2'$	S2(1)P2(1)	(a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866c),(d,0.577d)	(0,-2,0),(4,2,0),(0,0,6)	(0,0,1/4)
8.34	Cm'	4D2(1)P2(2)	(a,b,c,d,a,b),(0,-1.155e)	(-2,-4,0),(2,0,0),(0,0,6)	(0,0,0)
2.4	$P\bar{1}$	P1(1)C1(1)	(a,0,0,0,0,0),(b,c)	(1,0,3),(0,1,0),(-2,0,0)	(0,0,0)
8.32	Cm	P2(1)C1(1)	(a,-0.268a,0,0,0,0),(b,c)	(-2,0,0),(0,0,6),(0,1,0)	(-1/12,0,1/4)
1.1	$P1$	C1(1)C1(1)	(a,b,0,0,0,0),(c,d)	(1,0,3),(0,1,0),(-2,0,0)	(0,0,0)
2.4	$P\bar{1}$	C4(1)C1(1)	(a,0,b,0,0,0),(c,d)	(1,1,3),(0,2,0),(-2,0,0)	(0,0,0)
2.4	$P\bar{1}$	C5(1)C1(1)	(a,0,0,b,0,0),(c,d)	(1,1,3),(0,2,0),(-2,0,0)	(0,1/2,0)
8.32	Cm	C6(1)C1(1)	(a,-0.268a,b,-0.268b,0,0),(c,d)	(-2,-2,0),(0,0,6),(-2,0,0)	(-1/12,-1/12,1/4)

9.37	Cc	$C7(1)C1(1)$	$(a,-0.268a,b,3.732b,0,0),(c,d)$	$(-2,-2,0),(0,0,6),(-2,0,0)$	$(-7/12,-7/12,7/4)$
				$(0,0,6),(0,2,0),(-2,0,0)$	$(0,0,0)$
2.4	$P\bar{1}$	$S3(1)C1(1)$	$(a,0,b,0,c,0),(d,e)$	$(0,0,6),(0,2,0),(-2,0,0)$	$(0,1/2,0)$
2.4	$P\bar{1}$	$S4(1)C1(1)$	$(a,0,0,b,0,c),(d,e)$	$(0,0,6),(0,2,0),(-2,0,0)$	$(0,0,0)$
6.18	Pm	$S5(1)C1(1)$	$(a,-0.268a,b,-0.268b,c,-0.268c),(d,e)$	$(-2,0,0),(0,0,6),(0,2,0)$	$(0,0,1/4)$
7.24	Pc	$S6(1)C1(1)$	$(a,-0.268a,b,3.732b,c,3.732c),(d,e)$	$(-2,0,0),(0,0,6),(0,2,0)$	$(0,0,1/4)$
1.1	$P1$	$4D1(1)C1(1)$	$(a,b,c,d,0,0),(e,f)$	$(1,1,3),(0,2,0),(-2,0,0)$	$(0,0,0)$
1.1	$P1$	$6D1(1)C1(1)$	$(a,b,c,d,e,f),(g,h)$	$(0,0,6),(0,2,0),(-2,0,0)$	$(0,0,0)$

S3.3. 3C

S3.3.1. U_1

Table S10 Order parameter components and unit cell configurations for subgroups of $P6_3/mmc$ which can arise from phase transitions in which irrep $U_1(1/2,0,1/3)$ is the active representation.

SGN	Space Group	OPD Name	OPD Vector	Basis Vectors	Origin
58	$Pnmm$	P1	$(a,0,0,0,0,0)$	$(0,0,3),(2,1,0),(0,1,0)$	$(0,0,0)$
59	$Pmnn$	P2	$(0,a,0,0,0,0)$	$(0,0,3),(0,-1,0),(2,1,0)$	$(1/2,1/2,0)$
164	$P\bar{3}m1$	P3	$(a,0,a,0,a,0)$	$(2,0,0),(0,2,0),(0,0,3)$	$(0,0,0)$
187	$P\bar{6}m2$	P4	$(a,-0.577a,a,-0.577a,a,-0.577a)$	$(0,-2,0),(2,2,0),(0,0,3)$	$(0,0,1/4)$
64	$Cmca$	P5	$(a,0,0,0,a,0)$	$(2,0,0),(2,4,0),(0,0,3)$	$(0,0,0)$
63	$Cmcm$	P6	$(0,a,0,0,0,-a)$	$(2,0,0),(2,4,0),(0,0,3)$	$(1/2,0,0)$
152	$P3_121$	P7	$(a,1.732a,-2a,0,a,-1.732a)$	$(2,0,0),(0,2,0),(0,0,3)$	$(0,0,1/2)$
151	$P3_112$	P8	$(a,0.577a,-a,0.577a,0,-1.155a)$	$(0,-2,0),(2,2,0),(0,0,3)$	$(0,0,3/4)$
31	$Pmn2_1$	C1	$(a,b,0,0,0,0)$	$(0,-1,0),(2,1,0),(0,0,3)$	$(1/2,1/4,0)$
156	$P3m1$	C2	(a,b,a,b,a,b)	$(2,0,0),(0,2,0),(0,0,3)$	$(0,0,0)$
20	$C222_1$	C3	$(a,b,0,0,a,-b)$	$(2,0,0),(2,4,0),(0,0,3)$	$(1/2,0,0)$

14	$P2_1/c$	C4	(0,0,a,0,b,0)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,0)
11	$P2_1/m$	C5	(0,0,0,a,0,b)	(-2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
14	$P2_1/c$	C6	(a,0,0,0,0,b)	(-2,0,0),(0,0,3),(2,2,0)	(0,1/2,0)
12	$C2/m$	C7	(a,0,b,0,a,0)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
12	$C2/m$	C8	(0,a,b,0,0,-a)	(-2,-4,0),(2,0,0),(0,0,3)	(1/2,0,0)
38	$Amm2$	C9	(a,-0.577a,b,- 0.577b,b,-0.577b)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)
39	$Abm2$	C10	(a,-0.577a,b,1.732b,-b,1.732b)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)
36	$Cmc2_1$	C11	(a,b,0,0,a,b)	(2,0,0),(2,4,0),(0,0,3)	(1/2,-1,0)
144	$P3_1$	C12	(a,b,-0.500a0.866b,0.866a- 0.500b,-0.500a+0.866b,- 0.866a-0.500b)	(2,2,0),(-2,0,0),(0,0,3)	(0,0,0)
5	$C2$	S1	(a,b,c,0,a,-b)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
5	$C2$	S2	(a,-0.577a,b,c,0.500b0.866c,- 0.866b0.500c)	(0,-2,0),(4,2,0),(0,0,3)	(0,0,1/4)
2	$P\bar{1}$	S3	(a,0,b,0,c,0)	(0,0,3),(0,2,0),(-2,0,0)	(0,0,0)
2	$P\bar{1}$	S4	(a,0,0,b,0,c)	(0,0,3),(0,2,0),(-2,0,0)	(0,1/2,0)
6	Pm	S5	(a,-0.577a,b,- 0.577b,c,-0.577c)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
7	Pc	S6	(a,-0.577a,b,1.732b,c,1.732c)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
4	$P2_1$	4D1	(0,0,a,b,c,d)	(-2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
8	Cm	4D2	(a,b,c,d,a,b)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
1	$P1$	6D1	(a,b,c,d,e,f)	(0,0,3),(0,2,0),(-2,0,0)	(0,0,0)

S3.3.2. U_1 and $m\Gamma_4^+$

Table S11 Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/3)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space group	OPD Name $U_1(1/2,0,1/3)$	OPD Vector $m\Gamma_4^+$	Basis Vectors $U_1(1/2,0,1/3)$	Origin $m\Gamma_4^+$
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58.398	$Pnn'm'$	P1(1)P1(1)	(a,0,0,0,0),(b)	(-2,- 1,0),(0,0,3),(0,1,0)	(0,0,0)
59.409	$Pm'm'n$	P2(1)P1(1)	(0,a,0,0,0),(b)	(0,0,3),(0,-1,0),(2,1,0)	(1/2,1/2,0)
164.89	$P\bar{3}m'1$	P3(1)P1(1)	(a,0,a,0,a),(b)	(0,-2,0),(2,2,0),(0,0,3)	(0,0,0)
187.211	$P'm'2$	P4(1)P1(1)	(a,-0.577a,a,-0.577a,a,- 0.577a),(b)	(2,2,0),(-2,0,0),(0,0,3)	(0,0,1/4)
64.476	$Cm'ca'$	P5(1)P1(1)	(a,0,0,0,a),(b)	(2,0,0),(2,4,0),(0,0,3)	(0,0,0)
63.464	$Cm'cm'$	P6(1)P1(1)	(0,a,0,0,0,-a),(b)	(2,0,0),(2,4,0),(0,0,3)	(1/2,0,0)
152.35	$P312'1$	P7(1)P1(1)	(a,1.732a,-2a,0,a,-1.732a),(b)	(0,-2,0),(2,2,0),(0,0,3)	(0,0,0)
151.29	$P3112$	P8(1)P1(1)	(a,0.577a,-a,0.577a,0,- 1.155a),(b)	(2,2,0),(-2,0,0),(0,0,3)	(0,0,1/4)
31.125	$Pm'n2_1'$	C1(1)P1(1)	(a,b,0,0,0),(c)	(0,-1,0),(2,1,0),(0,0,3)	(1/2,1/4,0)
156.51	$P3m'1$	C2(1)P1(1)	(a,b,a,b,a,b),(c)	(0,-2,0),(2,2,0),(0,0,3)	(0,0,0)
20.34	$C22'2_1'$	C3(1)P1(1)	(a,b,0,0,a,-b),(c)	(2,4,0),(-2,0,0),(0,0,3)	(3/2,2,3/4)
14.79	$P2_1'/c'$	C4(1)P1(1)	(0,0,a,0,b,0),(c)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,0)
11.54	$P2_1'/m'$	C5(1)P1(1)	(0,0,0,a,0,b),(c)	(-2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
14.79	$P2_1'/c'$	C6(1)P1(1)	(a,0,0,0,0,b),(c)	(-2,0,0),(0,0,3),(2,2,0)	(0,1/2,0)
12.62	$C2'/m'$	C7(1)P1(1)	(a,0,b,0,a,0),(c)	(-2,- 4,0),(2,0,0),(0,0,3)	(0,0,0)
12.62	$C2'/m'$	C8(1)P1(1)	(0,a,b,0,0,-a),(c)	(-2,- 4,0),(2,0,0),(0,0,3)	(1/2,0,0)
38.191	$Am'm'2$	C9(1)P1(1)	(a,-0.577a,b,-0.577b,b,- 0.577b),(c)	(0,0,3),(0,2,0),(-4,- 2,0)	(0,0,1/4)
39.199	$Ab'm'2$	C10(1)P1(1)	(a,-0.577a,b,1.732b,-b,- 1.732b),(c)	(0,0,3),(0,2,0),(-4,- 2,0)	(0,0,1/4)
36.174	$Cm'c2_1'$	C11(1)P1(1)	(a,b,0,0,a,b),(c)	(2,0,0),(2,4,0),(0,0,3)	(1/2,-1,0)
144.4	$P3_1$	C12(1)P1(1)	(a,b,-0.500a-0.866b,0.866a- 0.500b,-0.500a+0.866b,- 0.866a-0.500b),(c)	(2,2,0),(-2,0,0),(0,0,3)	(0,0,0)
5.15	$C2'$	S1(1)P1(1)	(a,b,c,0,a,-b),(d)	(-2,- 4,0),(2,0,0),(0,0,3)	(0,0,0)

5.13	$C2$	S2(1)P1(1)	(a,-0.577a,b,c,0.500b-0.866c,-0.866b-0.500c),(d)	(0,-2,0),(4,2,0),(0,0,3)	(0,0,1/4)
2.4	$P\bar{1}$	S3(1)P1(1)	(a,0,b,0,c,0),(d)	(0,0,3),(0,2,0),(-2,0,0)	(0,0,0)
2.4	$P\bar{1}$	S4(1)P1(1)	(a,0,0,b,0,c),(d)	(0,0,3),(0,2,0),(-2,0,0)	(0,1/2,0)
6.2	Pm'	S5(1)P1(1)	(a,-0.577a,b,-0.577b,c,-0.577c),(d)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
7.26	Pc'	S6(1)P1(1)	(a,-0.577a,b,1.732b,c,1.732c),(d)	(-2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
4.9	$P2_1'$	4D1(1)P1(1)	(0,0,a,b,c,d),(e)	(-2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
8.34	Cm'	4D2(1)P1(1)	(a,b,c,d,a,b),(e)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
1.1	$P1$	6D1(1)P1(1)	(a,b,c,d,e,f),(g)	(0,0,3),(0,2,0),(-2,0,0)	(0,0,0)

S3.3.3. U_1 and $m\Gamma_5^+$ **Table S12** Magnetic subgroups arising from coupling of irreps $m\Gamma_5^+$ and $U_1(1/2,0,1/3)$, with respect to the parent space group $P6_3/mmc$.

SGN.M	Space Group	OPD Name $U_1(1/2,0,1/3)$	OPD Vector $m\Gamma_5^+$ $U_1(1/2,0,1/3)$	Basis Vectors	Origin
58.393	$Pnmm$	P1(1)P1(1)	(a,0,0,0,0),(b,-1.732b)	(-2,-1,0),(0,0,3),(0,1,0)	(0,0,0)
59.405	$Pmmm$	P2(1)P1(1)	(0,a,0,0,0),(b,-1.732b)	(0,1,0),(0,0,3),(2,1,0)	(1/2,0,0)
64.469	$Cmca$	P5(1)P1(2)	(a,0,0,0,a,0),(-2b,0)	(2,0,0),(2,4,0),(0,0,3)	(0,0,0)
63.457	$Cmcm$	P6(1)P1(2)	(0,a,0,0,0,-a),(-2b,0)	(2,0,0),(2,4,0),(0,0,3)	(1/2,0,0)
31.123	$Pmn2_1$	C1(1)P1(1)	(a,b,0,0,0),(c,-1.732c)	(0,-1,0),(2,1,0),(0,0,3)	(1/2,1/4,0)
20.31	$C222_1$	C3(1)P1(2)	(a,b,0,0,a,-b),(-2c,0)	(2,0,0),(2,4,0),(0,0,3)	(1/2,0,0)
12.58	$C2/m$	C7(1)P1(2)	(a,0,b,0,a,0),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
12.58	$C2/m$	C8(1)P1(2)	(0,a,b,0,0,-a),(-2c,0)	(-2,-4,0),(2,0,0),(0,0,3)	(1/2,0,0)
38.187	$Amm2$	C9(1)P1(1)	(a,-0.577a,b,-0.577b,b,-0.577b),(c,-1.732c)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)

39.195	<i>Abm2</i>	C10(1)P1(1)	(a,-0.577a,b,1.732b,-b,-1.732b),(c,-1.732c)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)
36.172	<i>Cmc2₁</i>	C11(1)P1(2)	(a,b,0,0,a,b),(-2c,0)	(2,0,0),(2,4,0),(0,0,3)	(1/2,-1,0)
5.13	<i>C2</i>	S1(1)P1(2)	(a,b,c,0,a,-b),(-2d,0)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
5.13	<i>C2</i>	S2(1)P1(1)	(a,-0.577a,b,c,0.500b-0.866c,-0.866b-0.500c),(d,-1.732d)	(0,-2,0),(4,2,0),(0,0,3)	(0,0,1/4)
8.32	<i>Cm</i>	4D2(1)P1(2)	(a,b,c,d,a,b),(-2e,0)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
58.398	<i>Pnn'm'</i>	P1(1)P2(1)	(a,0,0,0,0,0),(b,0.577b)	(0,0,3),(2,1,0),(0,1,0)	(0,0,0)
59.41	<i>Pmm'n'</i>	P2(1)P2(1)	(0,a,0,0,0,0),(b,0.577b)	(0,0,3),(0,-1,0),(2,1,0)	(1/2,1/2,0)
64.474	<i>Cm'c'a</i>	P5(1)P2(2)	(a,0,0,0,a,0),(0,-1.155b)	(2,0,0),(2,4,0),(0,0,3)	(0,0,0)
63.462	<i>Cm'c'm</i>	P6(1)P2(2)	(0,a,0,0,0,-a),(0,-1.155b)	(2,0,0),(2,4,0),(0,0,3)	(1/2,0,0)
31.127	<i>Pm'n'2₁</i>	C1(1)P2(1)	(a,b,0,0,0,0),(c,0.577c)	(0,-1,0),(2,1,0),(0,0,3)	(1/2,1/4,0)
20.33	<i>C2'2'2₁</i>	C3(1)P2(2)	(a,b,0,0,a,-b),(0,-1.155c)	(2,0,0),(2,4,0),(0,0,3)	(1/2,0,0)
12.62	<i>C2'/m'</i>	C7(1)P2(2)	(a,0,b,0,a,0),(0,-1.155c)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
12.62	<i>C2'/m'</i>	C8(1)P2(2)	(0,a,b,0,0,-a),(0,-1.155c)	(-2,-4,0),(2,0,0),(0,0,3)	(1/2,0,0)
38.19	<i>Amm'2'</i>	C9(1)P2(1)	(a,-0.577a,b,-0.577b,b,-0.577b),(c,0.577c)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)
39.198	<i>Abm'2'</i>	C10(1)P2(1)	(a,-0.577a,b,1.732b,-b,-1.732b),(c,0.577c)	(0,0,3),(0,2,0),(-4,-2,0)	(0,0,1/4)
36.176	<i>Cm'c'2₁</i>	C11(1)P2(2)	(a,b,0,0,a,b),(0,-1.155c)	(2,0,0),(2,4,0),(0,0,3)	(1/2,-1,0)
5.15	<i>C2'</i>	S1(1)P2(2)	(a,b,c,0,a,-b),(0,-1.155d)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
5.15	<i>C2'</i>	S2(1)P2(1)	(a,-0.577a,b,c,0.500b-0.866c,-0.866b-0.500c),(d,0.577d)	(0,-2,0),(4,2,0),(0,0,3)	(0,0,1/4)
8.34	<i>Cm'</i>	4D2(1)P2(2)	(a,b,c,d,a,b),(0,-1.155e)	(-2,-4,0),(2,0,0),(0,0,3)	(0,0,0)
14.75	<i>P2₁/c</i>	P1(1)C1(1)	(a,0,0,0,0,0),(b,c)	(0,1,0),(0,0,3),(2,0,0)	(0,0,0)

11.5	<i>P21/m</i>	P2(1)C1(1)	(0,a,0,0,0),(b,c)	(- 2,0,0),(0,0,3),(0,1,0)	(-1/2,0,0)
4.7	<i>P21</i>	C1(1)C1(1)	(a,b,0,0,0),(c,d)	(- 2,0,0),(0,0,3),(0,1,0)	(-1/2,0,0)
14.75	<i>P21/c</i>	C4(1)C1(1)	(0,0,a,0,b,0),(c,d)	(- 2,0,0),(0,0,3),(0,2,0)	(0,0,0)
11.5	<i>P21/m</i>	C5(1)C1(1)	(0,0,0,a,0,b),(c,d)	(- 2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
14.75	<i>P21/c</i>	C6(1)C1(1)	(a,0,0,0,b),(c,d)	(- 2,0,0),(0,0,3),(2,2,0)	(0,1/2,0)
2.4	<i>P$\bar{1}$</i>	S3(1)C1(1)	(a,0,b,0,c,0),(d,e)	(0,0,3),(0,2,0),(- 2,0,0)	(0,0,0)
2.4	<i>P$\bar{1}$</i>	S4(1)C1(1)	(a,0,0,b,0,c),(d,e)	(0,0,3),(0,2,0),(- 2,0,0)	(0,1/2,0)
6.18	<i>Pm</i>	S5(1)C1(1)	(a,-0.577a,b,-0.577b,c,- 0.577c),(d,e)	(- 2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
7.24	<i>Pc</i>	S6(1)C1(1)	(a,- 0.577a,b,1.732b,c,1.732c),(d,e)	(- 2,0,0),(0,0,3),(0,2,0)	(0,0,1/4)
4.7	<i>P2₁</i>	4D1(1)C1(1)	(0,0,a,b,c,d),(e,f)	(- 2,0,0),(0,0,3),(0,2,0)	(0,1/2,0)
1.1	<i>P1</i>	6D1(1)C1(1)	(a,b,c,d,e,f),(g,h)	(0,0,3),(0,2,0),(- 2,0,0)	(0,0,0)
