

Supplemental material for:
 Canonical magnetic insulators with isotropic
 magnetoelectric coupling

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Canonical structure: **1.** out of **30**

Space group $P2_13 \ T^4$ (#198)
 Centering primitive cubic
 Wyckoff orbit 4a
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1

Canonical structure: **2.** out of **30**

Space group $I2_13 \ T^5$ (#199)
 Centering body-centered cubic
 Wyckoff orbit 12b
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	.	1/4	1	.	.
2	-u+1/2	.	3/4	-1	.	.
3	1/4	u	.	.	1	.
4	3/4	-u+1/2	.	.	-1	.
5	.	1/4	u	.	.	1
6	.	3/4	-u+1/2	.	.	-1

Canonical structure: **3.** out of **30**

Space group $I2_13 T^5$ (#199)
 Centering body-centered cubic
 Wyckoff orbit $8a$
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	u	u	1	1	1
2	$-u+1/2$	$-u$	$u+1/2$	-1	-1	1
3	$-u$	$u+1/2$	$-u+1/2$	-1	1	-1
4	$u+1/2$	$-u+1/2$	$-u$	1	-1	-1

Canonical structure: **4.** out of **30**

Space group $Pm3 T_h^1$ (#200)
 Centering primitive cubic
 Wyckoff orbit $6f$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	$.$	$1/2$	1	$.$	$.$
2	$-u$	$.$	$1/2$	-1	$.$	$.$
3	$1/2$	u	$.$	$.$	1	$.$
4	$1/2$	$-u$	$.$	$.$	-1	$.$
5	$.$	$1/2$	u	$.$	$.$	1
6	$.$	$1/2$	$-u$	$.$	$.$	-1

Canonical structure: **5.** out of **30**

Space group $Im\bar{3} T_h^5$ (#204)
 Centering body-centered cubic
 Wyckoff orbit $12e$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	1/2	1	.	.
2	-u	.	1/2	-1	.	.
3	1/2	u	.	.	1	.
4	1/2	-u	.	.	-1	.
5	.	1/2	u	.	.	1
6	.	1/2	-u	.	.	-1

Canonical structure: **6.** out of **30**

Space group $Pa\bar{3} T_h^6$ (#205)
 Centering primitive cubic
 Wyckoff orbit $8c$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1
5	-u	-u	-u	-1	-1	-1
6	u+1/2	u	-u+1/2	1	1	-1
7	u	-u+1/2	u+1/2	1	-1	1
8	-u+1/2	u+1/2	u	-1	1	1

Canonical structure: 7. out of 30

Space group $Ia3 \bar{T}_h^7$ (#206)
 Centering body-centered cubic
 Wyckoff orbit 24d
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	1/4	1	.	.
2	-u+1/2	.	3/4	-1	.	.
3	1/4	u	.	.	1	.
4	3/4	-u+1/2	.	.	-1	.
5	.	1/4	u	.	.	1
6	.	3/4	-u+1/2	.	.	-1
7	-u	.	3/4	-1	.	.
8	u+1/2	.	1/4	1	.	.
9	3/4	-u	.	.	-1	.
10	1/4	u+1/2	.	.	1	.
11	.	3/4	-u	.	.	-1
12	.	1/4	u+1/2	.	.	1

Canonical structure: 8. out of 30

Space group $Ia3 \bar{T}_h^7$ (#206)
 Centering body-centered cubic
 Wyckoff orbit 16c
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1
5	-u	-u	-u	-1	-1	-1
6	u+1/2	u	-u+1/2	1	1	-1
7	u	-u+1/2	u+1/2	1	-1	1
8	-u+1/2	u+1/2	u	-1	1	1

Canonical structure: **9.** out of **30**

Space group $P4_332 O^6$ (#212)
 Centering primitive cubic
 Wyckoff orbit 8c
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1
5	u+1/4	u+3/4	-u+3/4	1	1	-1
6	-u+1/4	-u+1/4	-u+1/4	-1	-1	-1
7	u+3/4	-u+3/4	u+1/4	1	-1	1
8	-u+3/4	u+1/4	u+3/4	-1	1	1

Canonical structure: **10.** out of **30**

Space group $I4_132 O^8$ (#214)
 Centering body-centered cubic
 Wyckoff orbit 24f
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	.	1/4	1	.	.
2	-u+1/2	.	3/4	-1	.	.
3	1/4	u	.	.	1	.
4	3/4	-u+1/2	.	.	-1	.
5	.	1/4	u	.	.	1
6	.	3/4	-u+1/2	.	.	-1
7	3/4	u+1/4	.	.	1	.
8	3/4	-u+3/4	1/2	.	-1	.
9	u+3/4	1/2	1/4	1	.	.
10	-u+1/4	.	1/4	-1	.	.
11	.	1/4	-u+1/4	.	.	-1
12	1/2	1/4	u+3/4	.	.	1

Canonical structure: **11.** out of **30**

Space group $I4_132 \ O^8$ (#214)
 Centering body-centered cubic
 Wyckoff orbit 16e
 Magnetic moment irrep Γ^1

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1
5	u+3/4	u+1/4	-u+1/4	1	1	-1
6	-u+3/4	-u+3/4	-u+3/4	-1	-1	-1
7	u+1/4	-u+1/4	u+3/4	1	-1	1
8	-u+1/4	u+3/4	u+1/4	-1	1	1

Canonical structure: **12.** out of **30**

Space group $P\bar{4}3m \ T_d^1$ (#215)
 Centering primitive cubic
 Wyckoff orbit 4e
 Magnetic moment irrep Γ^2

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1

Canonical structure: **13.** out of **30**

Space group $F\bar{4}3m T_d^2$ (#216)
 Centering face-centered cubic
 Wyckoff orbit 16e
 Magnetic moment irrep Γ^2

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1

Canonical structure: **14.** out of **30**

Space group $I\bar{4}3m T_d^3$ (#217)
 Centering body-centered cubic
 Wyckoff orbit 8c
 Magnetic moment irrep Γ^2

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1

Canonical structure: **15.** out of **30**

Space group $\bar{1}43d$ T_d^6 (#220)
 Centering body-centered cubic
 Wyckoff orbit 24d
 Magnetic moment irrep Γ^2

	Positions			Moments		
1	u	.	1/4	1	.	.
2	-u+1/2	.	3/4	-1	.	.
3	1/4	u	.	.	1	.
4	3/4	-u+1/2	.	.	-1	.
5	.	1/4	u	.	.	1
6	.	3/4	-u+1/2	.	.	-1
7	1/4	u+1/4	1/2	.	1	.
8	1/4	-u+3/4	.	.	-1	.
9	u+1/4	1/2	1/4	1	.	.
10	-u+3/4	.	1/4	-1	.	.
11	1/2	1/4	u+1/4	.	.	1
12	.	1/4	-u+3/4	.	.	-1

Canonical structure: **16.** out of **30**

Space group $\bar{1}43d$ T_d^6 (#220)
 Centering body-centered cubic
 Wyckoff orbit 16c
 Magnetic moment irrep Γ^2

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u	u+1/2	-1	-1	1
3	-u	u+1/2	-u+1/2	-1	1	-1
4	u+1/2	-u+1/2	-u	1	-1	-1
5	u+1/4	u+1/4	u+1/4	1	1	1
6	-u+1/4	-u+3/4	u+3/4	-1	-1	1
7	u+3/4	-u+1/4	-u+3/4	1	-1	-1
8	-u+3/4	u+3/4	-u+1/4	-1	1	-1

Canonical structure: **17.** out of **30**

Space group $Pm\bar{3}m$ O_h^1 (#221)
 Centering primitive cubic
 Wyckoff orbit 12h
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	1/2	.	1	.	.
2	-u	1/2	.	-1	.	.
3	.	u	1/2	.	1	.
4	.	-u	1/2	.	-1	.
5	1/2	.	u	.	.	1
6	1/2	.	-u	.	.	-1
7	1/2	u	.	.	1	.
8	1/2	-u	.	.	-1	.
9	u	.	1/2	1	.	.
10	-u	.	1/2	-1	.	.
11	.	1/2	-u	.	.	-1
12	.	1/2	u	.	.	1

Canonical structure: **18.** out of **30**

Space group $Pm\bar{3}m$ O_h^1 (#221)
 Centering primitive cubic
 Wyckoff orbit 8g
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1
5	u	u	-u	1	1	-1
6	-u	-u	-u	-1	-1	-1
7	u	-u	u	1	-1	1
8	-u	u	u	-1	1	1

Canonical structure: **19.** out of **30**

Space group $Pm\bar{3}m$ O_h^1 (#221)
 Centering primitive cubic
 Wyckoff orbit $6e$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	.	1	.	.
2	-u	.	.	-1	.	.
3	.	u	.	.	1	.
4	.	-u	.	.	-1	.
5	.	.	u	.	.	1
6	.	.	-u	.	.	-1

Canonical structure: **20.** out of **30**

Space group $Pm\bar{3}n$ O_h^3 (#223)
 Centering primitive cubic
 Wyckoff orbit $12g$
 Magnetic moment irrep Γ^{1-}

	Positions				Moments		
1	u	.	.	1/2	1	.	.
2	-u	.	.	1/2	-1	.	.
3	1/2	u	.	.	.	1	.
4	1/2	-u	.	.	.	-1	.
5	.	1/2	u	.	.	.	1
6	.	1/2	-u	.	.	.	-1
7	1/2	u+1/2	.	.	.	1	.
8	1/2	-u+1/2	.	.	.	-1	.
9	u+1/2	.	.	1/2	1	.	.
10	-u+1/2	.	.	1/2	-1	.	.
11	.	1/2	-u+1/2	.	.	.	-1
12	.	1/2	u+1/2	.	.	.	1

Canonical structure: **21.** out of **30**

Space group $Pn\bar{3}m O_h^4$ (#224)
 Centering primitive cubic
 Wyckoff orbit $8e$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+1/2	-u+1/2	u	-1	-1	1
3	-u+1/2	u	-u+1/2	-1	1	-1
4	u	-u+1/2	-u+1/2	1	-1	-1
5	u+1/2	u+1/2	-u	1	1	-1
6	-u	-u	-u	-1	-1	-1
7	u+1/2	-u	u+1/2	1	-1	1
8	-u	u+1/2	u+1/2	-1	1	1

Canonical structure: **22.** out of **30**

Space group $Fm\bar{3}m O_h^5$ (#225)
 Centering face-centered cubic
 Wyckoff orbit $32f$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1
5	u	u	-u	1	1	-1
6	-u	-u	-u	-1	-1	-1
7	u	-u	u	1	-1	1
8	-u	u	u	-1	1	1

Canonical structure: **23.** out of **30**

Space group $Fm\bar{3}m O_h^5$ (#225)
 Centering face-centered cubic
 Wyckoff orbit 24e
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	.	1	.	.
2	-u	.	.	-1	.	.
3	.	u	.	.	1	.
4	.	-u	.	.	-1	.
5	.	.	u	.	.	1
6	.	.	-u	.	.	-1

Canonical structure: **24.** out of **30**

Space group $Fd\bar{3}m O_h^7$ (#227)
 Centering face-centered cubic
 Wyckoff orbit 48f
 Magnetic moment irrep Γ^{1-}

	Positions				Moments		
1	u	1/8	1/8	1/8	1	.	.
2	-u+3/4	1/8	5/8	5/8	-1	.	.
3	1/8	u	1/8	1/8	.	1	.
4	5/8	-u+3/4	1/8	1/8	.	-1	.
5	1/8	1/8	u	u	.	.	1
6	1/8	5/8	-u+3/4	-u+3/4	.	.	-1
7	7/8	u+1/4	3/8	3/8	.	1	.
8	7/8	-u	7/8	7/8	.	-1	.
9	u+3/4	3/8	3/8	3/8	1	.	.
10	-u+1/2	7/8	3/8	3/8	-1	.	.
11	7/8	3/8	-u+1/2	-u+1/2	.	.	-1
12	3/8	3/8	u+3/4	u+3/4	.	.	1

Canonical structure: **25.** out of **30**

Space group $Fd\bar{3}m O_h^7$ (#227)
 Centering face-centered cubic
 Wyckoff orbit 32e
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u+3/4	-u+1/4	u+1/2	-1	-1	1
3	-u+1/4	u+1/2	-u+3/4	-1	1	-1
4	u+1/2	-u+3/4	-u+1/4	1	-1	-1
5	u+3/4	u+1/4	-u+1/2	1	1	-1
6	-u	-u	-u	-1	-1	-1
7	u+1/4	-u+1/2	u+3/4	1	-1	1
8	-u+1/2	u+3/4	u+1/4	-1	1	1

Canonical structure: **26.** out of **30**

Space group $Im\bar{3}m O_h^9$ (#229)
 Centering body-centered cubic
 Wyckoff orbit 24g
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	1/2	1	.	.
2	-u	.	1/2	-1	.	.
3	1/2	u	.	.	1	.
4	1/2	-u	.	.	-1	.
5	.	1/2	u	.	.	1
6	.	1/2	-u	.	.	-1
7	.	u	1/2	.	1	.
8	.	-u	1/2	.	-1	.
9	u	1/2	.	1	.	.
10	-u	1/2	.	-1	.	.
11	1/2	.	-u	.	.	-1
12	1/2	.	u	.	.	1

Canonical structure: **27.** out of **30**

Space group $Im\bar{3}m O_h^9$ (#229)
 Centering body-centered cubic
 Wyckoff orbit 16f
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	u	u	1	1	1
2	-u	-u	u	-1	-1	1
3	-u	u	-u	-1	1	-1
4	u	-u	-u	1	-1	-1
5	u	u	-u	1	1	-1
6	-u	-u	-u	-1	-1	-1
7	u	-u	u	1	-1	1
8	-u	u	u	-1	1	1

Canonical structure: **28.** out of **30**

Space group $Im\bar{3}m O_h^9$ (#229)
 Centering body-centered cubic
 Wyckoff orbit 12e
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
1	u	.	.	1	.	.
2	-u	.	.	-1	.	.
3	.	u	.	.	1	.
4	.	-u	.	.	-1	.
5	.	.	u	.	.	1
6	.	.	-u	.	.	-1

Canonical structure: **29.** out of **30**

Space group $Ia\bar{3}d \ O_h^{10} \ (\#230)$
 Centering body-centered cubic
 Wyckoff orbit 48f
 Magnetic moment irrep Γ^{1-}

	Positions				Moments		
1	u	.	1/4	1	.	.	
2	-u+1/2	.	3/4	-1	.	.	
3	1/4	u	.	.	1	.	
4	3/4	-u+1/2	.	.	-1	.	
5	.	1/4	u	.	.	1	
6	.	3/4	-u+1/2	.	.	-1	
7	3/4	u+1/4	.	.	1	.	
8	3/4	-u+3/4	1/2	.	-1	.	
9	u+3/4	1/2	1/4	1	.	.	
10	-u+1/4	.	1/4	-1	.	.	
11	.	1/4	-u+1/4	.	.	-1	
12	1/2	1/4	u+3/4	.	.	1	
13	-u	.	3/4	-1	.	.	
14	u+1/2	.	1/4	1	.	.	
15	3/4	-u	.	.	-1	.	
16	1/4	u+1/2	.	.	1	.	
17	.	3/4	-u	.	.	-1	
18	.	1/4	u+1/2	.	.	1	
19	1/4	-u+3/4	.	.	-1	.	
20	1/4	u+1/4	1/2	.	1	.	
21	-u+1/4	1/2	3/4	-1	.	.	
22	u+3/4	.	3/4	1	.	.	
23	.	3/4	u+3/4	.	.	1	
24	1/2	3/4	-u+1/4	.	.	-1	

Canonical structure: **30.** out of **30**

Space group $Ia\bar{3}d \ O_h^{10} \ (\#230)$
 Centering body-centered cubic
 Wyckoff orbit $32e$
 Magnetic moment irrep Γ^{1-}

	Positions			Moments		
	<u>u</u>	<u>u</u>	<u>u</u>	<u>1</u>	<u>1</u>	<u>1</u>
1	<u>u</u>	<u>u</u>	<u>u</u>	<u>1</u>	<u>1</u>	<u>1</u>
2	$-u+1/2$	$-u$	$u+1/2$	-1	-1	1
3	$-u$	$u+1/2$	$-u+1/2$	-1	1	-1
4	$u+1/2$	$-u+1/2$	$-u$	1	-1	-1
5	$u+3/4$	$u+1/4$	$-u+1/4$	1	1	-1
6	$-u+3/4$	$-u+3/4$	$-u+3/4$	-1	-1	-1
7	$u+1/4$	$-u+1/4$	$u+3/4$	1	-1	1
8	$-u+1/4$	$u+3/4$	$u+1/4$	-1	1	1
9	$-u$	$-u$	$-u$	-1	-1	-1
10	$u+1/2$	<u>u</u>	$-u+1/2$	<u>1</u>	<u>1</u>	-1
11	<u>u</u>	$-u+1/2$	$u+1/2$	<u>1</u>	-1	<u>1</u>
12	$-u+1/2$	$u+1/2$	<u>u</u>	-1	<u>1</u>	<u>1</u>
13	$-u+1/4$	$-u+3/4$	$u+3/4$	-1	-1	<u>1</u>
14	$u+1/4$	$u+1/4$	$u+1/4$	<u>1</u>	<u>1</u>	<u>1</u>
15	$-u+3/4$	$u+3/4$	$-u+1/4$	-1	<u>1</u>	-1
16	$u+3/4$	$-u+1/4$	$-u+3/4$	<u>1</u>	-1	-1