Construction of Energetic Complexes Based on LLM-105 and Transition Metal Cations (Ni, Co, Mn, and Cu)

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Supporting Information

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S1: Bond lengths between non-hydrogen atoms

Table S1 Bond lengths between non-hydrogen atoms in compound **1**.

Type	*d* / Å	Type	*d* / Å	Type	*d* / Å
Ni1—N9	1.841(2)	C4—N2	1.388(3)	C7—N12	1.445(4)
Ni1—O1	1.843(2)	N2—O1	1.347(2)	C8—N10	1.324(4)
Ni1—N3	1.848(2)	N5—O3	1.234(3)	C8—N7	1.351(3)
Ni1—O6	1.8625(19)	N5—O2	1.229(3)	N7—O6	1.360(3)
C1—N1	1.325(3)	N6—O5	1.215(3)	N11—O7	1.215(4)
C1—N5	1.423(3)	N6—O4	1.223(3)	N11—O8	1.221(3)
C1—C2	1.427(3)	C5—N8	1.302(4)	N12—O10	1.218(3)
C2—N4	1.310(3)	C5—C6	1.437(4)	N12—O9	1.227(4)
C2—N2	1.348(3)	C5—N11	1.447(4)	O11—C9	1.231(4)
C3—N1	1.292(3)	C6—N9	1.289(3)	N13—C9	1.306(4)
C3—C4	1.443(3)	C6—N7	1.387(3)	N13—C11	1.438(6)
C3—N6	1.463(3)	C7—N8	1.306(4)	N13—C10	1.456(5)
C4—N3	1.289(3)	C7—C8	1.427(4)		

Table S2 Bond lengths between non-hydrogen atoms in compound **2**.

Type	*d* / Å	Type	*d* / Å	Type	*d* / Å
Co1—O1	2.0413(12)	C2—N5	1.442(2)	N6—O5	1.215(2)
Co1—N4	2.0968(18)	C3—N4	1.287(2)	N6—O4	1.222(2)
Co1—O6	2.2084(14)	C3—N1	1.406(2)	O6—C5	1.240(2)
O1—N1	1.3474(18)	C3—C4	1.449(2)	C5—N7	1.318(2)
C1—N3	1.317(2)	C4—N2	1.303(2)	N7—C6	1.451(3)
C1—N1	1.352(2)	C4—N6	1.456(2)	N7—C7	1.453(3)
C1—C2	1.427(2)	N5—O3	1.211(2)		
C2—N2	1.309(2)	N5—O2	1.226(2)		

Table S3 Bond lengths between non-hydrogen atoms in compound **3**.

Type	*d* / Å	Type	*d* / Å	Type	*d* / Å
Mn1—N4	1.893(3)	C3—N3	1.323(5)	N5—O3	1.232(5)
Mn1—O1	1.906(2)	C3—N1	1.352(4)	N6—O4	1.217(6)
C1—N4	1.292(4)	C3—C4	1.414(6)	N6—O5	1.223(6)
C1—N1	1.383(4)	C4—N2	1.308(5)	O6—C5	1.1993(10)
C1—C2	1.426(5)	C4—N6	1.452(5)	N7—C5	1.4489(10)

C2—N2	1.302(4)	N1—O1	1.350(4)	N7—C6'	1.4996(10)
C2—N5	1.440(5)	N5—O2	1.221(5)	N7—C6	1.4999(10)

Table S4 Bond lengths between non-hydrogen atoms in compound **4**.

Type	*d* / Å	Type	*d* / Å	Type	*d* / Å
Cu1—N3	1.920(3)	N4—O3	1.212(5)	N9—O5	1.230(5)
Cu1—N7	1.924(3)	N4—O2	1.213(5)	N9—O6	1.234(5)
Cu1—O1	1.9960(12)	C3—N7	1.287(5)	N10—O7	1.215(5)
Cu1—O4	2.016(3)	C3—N5	1.390(5)	N10—O8	1.237(6)
Cu1—O9	2.353(3)	C3—C4	1.436(5)	O9—C7	1.247(5)
Cu2—N8	1.907(4)	C4—N6	1.292(5)	C7—N11	1.297(6)
Cu2—O4	1.984(2)	C4—N9	1.438(5)	N11—C9	1.429(7)
C1—N2	1.303(4)	C5—N6	1.296(6)	N11—C8	1.445(6)
C1—N4	1.447(5)	C5—N10	1.436(6)	N12—C10	1.310(11)
C1—C2	1.447(5)	C5—C6	1.450(5)	N12—C11	1.325(16)
C2—N3	1.283(5)	C6—N8	1.274(5)	O10—C10	1.218(14)
C2—N1	1.385(4)	C6—N5	1.365(5)		
N1—O1	1.362(5)	N5—O4	1.389(4)		

S2: Geometric parameters of hydrogen bond interactions.

Table S5 Geometric parameters of hydrogen bond interactions in compound **1**.

Type	*d* (D-H) / Å	*d* (D···A) / Å	*d* (H···A) / Å	Angle (D—H···A) / º
N10—H10A···O3	0.86	3.118	2.374	145.00
N4—H4A···O2	0.86	2.944	2.086	176.09
N4—H4B···O4	0.86	2.983	2.196	152.11
N9—H9···O11	0.86	2.967	2.197	148.95
N3—H3···O11	0.86	2.886	2.099	151.89
C9—H91···O9	0.93	3.260	2.674	121.73
C11—H11A···O8	0.96	3.305	2.711	120.64

Table S6 Geometric parameters of hydrogen bond interactions in compound **2**.

Type	*d* (D-H) / Å	*d* (D···A) / Å	*d* (H···A) / Å	Angle (D—H···A) / º

C6−H6A···O2	0.96	3.239	2.540	129.79
N3−H3B···O6	0.86	2.877	2.235	131.42
N3−H3A···O1	0.86	2.836	2.261	124.30
C7−H7C···O3	0.96	3.309	2.544	136.68
C7−H7A···O3	0.96	3.328	2.577	135.28

Table S7 Geometric parameters of hydrogen bond interactions in compound **3**.

Type	*d* (D-H) / Å	*d* (D···A) / Å	*d* (H···A) / Å	Angle (D—H···A) / º
N3−H3B···O2	0.86	3.253	2.477	150.42
N3−H3B···O3	0.86	3.137	2.630	118.85
N3−H3A···O6	0.86	2.860	2.035	160.69

Table S8 Geometric parameters of hydrogen bond interactions in compound **4**.

Type	*d* (D-H) / Å	*d* (D···A) / Å	*d* (H···A) / Å	Angle (D—H···A) / º
C8−H8C···O3	0.96	3.103	2.600	112.91
C9−H9A···O7	0.96	3.166	2.650	114.10
N8−H8···O10	0.86	3.044	2.265	150.68

S3: Geometric parameters of π–stacking interactions.

Table S9. Geometric parameters of π–stacking interactions in compounds **1** and **4**.

1	**O5···Center**
Distance / Å	3.315 Å
4	**C3···Center**
Distance / Å	3.276

S4: Figures of the π–stacking and electrostatic interactions in compound 4.

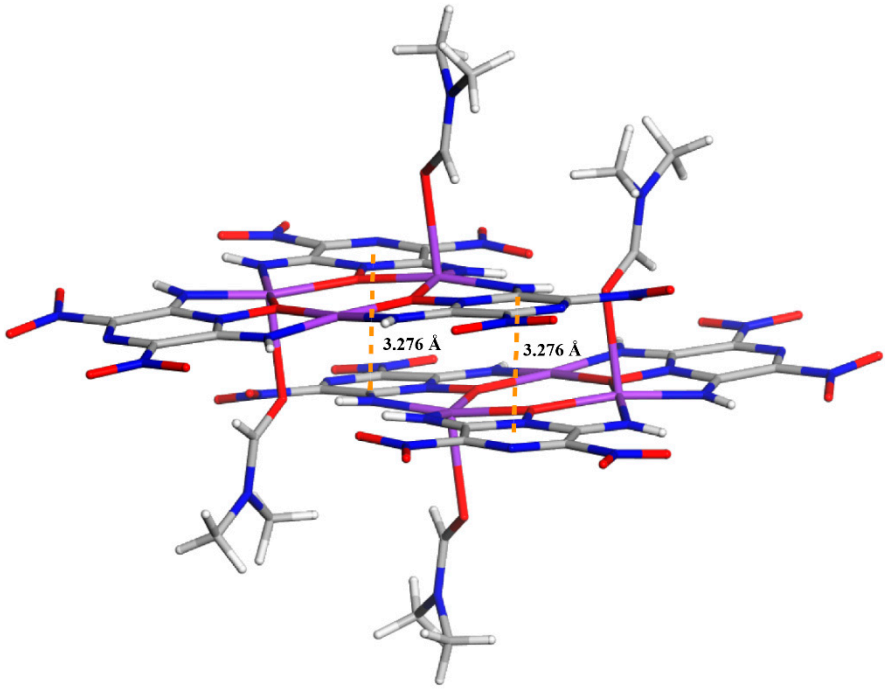

Figure S1. The π–stacking interactions between C3 atoms and pyrazine rings.

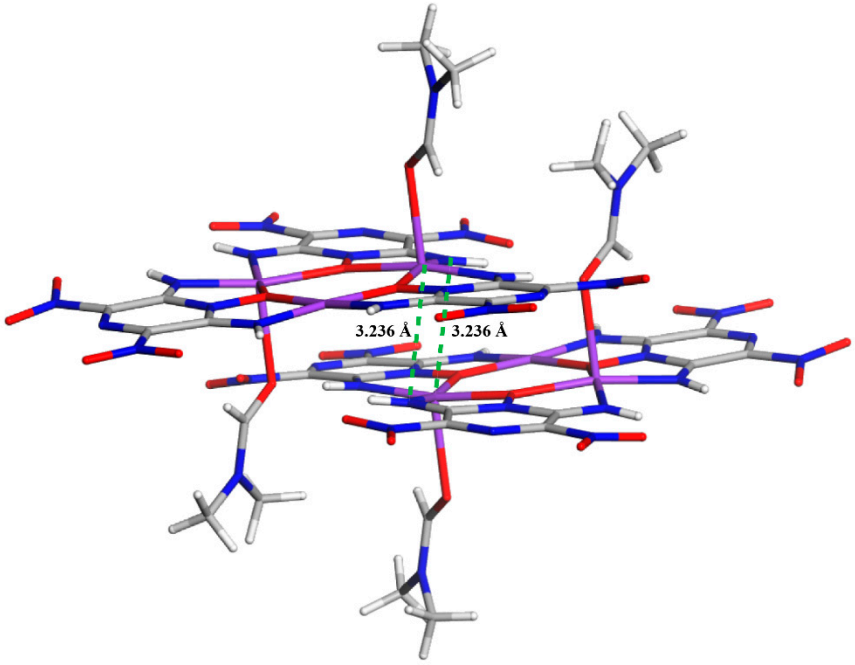

Figure S2. The electrostatic interactions between Cu1 atoms and N3 atoms.

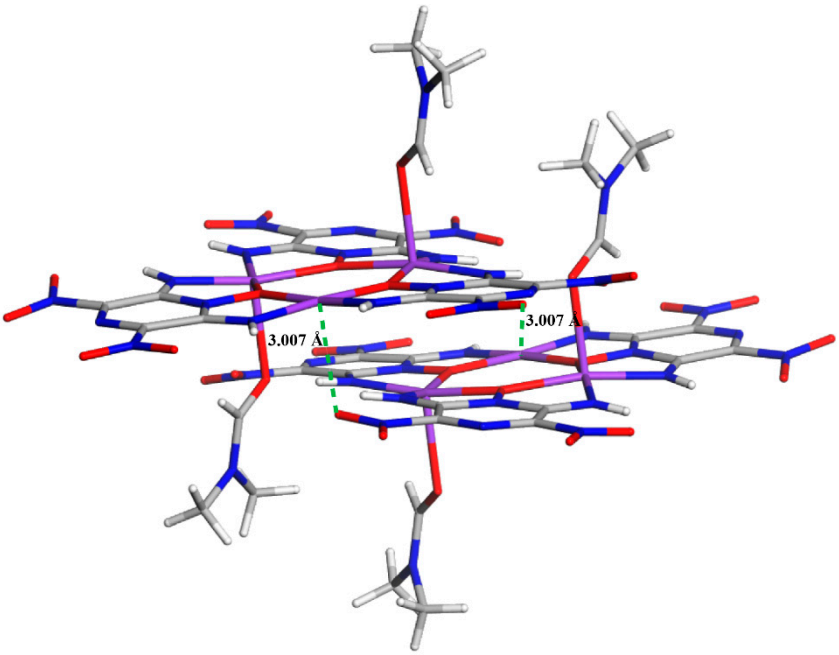

Figure S3. The electrostatic interactions between Cu2 atoms and O2 atoms.