Electronic supplementary information

A series of metal-organic frameworks based on a semi-rigid bifunctional ligand 5-((1H-1,2,4-triazol-1-yl)methoxy) isophthalic acid and flexible N-donor bridging ligands

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Table S1. Selected bond distances (Å) and angles (°) for **1**.

Co(1)-O(1W)	2.0673(15)	Co(1)-N(4)	2.0949(17)
Co(1)-O(3)$^{\#1}$	2.1308(13)	Co(1)-O(4)$^{\#2}$	2.1523(14)
Co(1)-N(3)$^{\#3}$	2.1602(17)	Co(1)-O(1)	2.1791(13)
O(1W)-Co(1)-N(4)	91.01(7)	O(1W)-Co(1)-O(3)$^{\#1}$	86.92(6)
N(4)-Co(1)-O(3)$^{\#1}$	88.26(6)	O(1W)-Co(1)-O(4)$^{\#2}$	165.53(6)
N(4)-Co(1)-O(4)$^{\#2}$	87.82(6)	O(3)$^{\#1}$-Co(1)-O(4)$^{\#2}$	107.46(5)
O(1W)-Co(1)-N(3)$^{\#3}$	100.92(7)	N(4)-Co(1)-N(3)$^{\#3}$	167.04(7)
O(3)$^{\#1}$-Co(1)-N(3)$^{\#3}$	87.37(6)	O(4)$^{\#2}$-Co(1)-N(3)$^{\#3}$	81.87(6)
O(1W)-Co(1)-O(1)	85.36(6)	N(4)-Co(1)-O(1)	100.40(6)
O(3)$^{\#1}$-Co(1)-O(1)	168.48(5)	O(4)$^{\#2}$-Co(1)-O(1)	80.67(5)
N(3)$^{\#3}$-Co(1)-O(1)	85.71(6)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x, -y+2, z-1/2; $^{\#2}$ x, -y+1, z-1/2; $^{\#3}$ -x+2, -y+1, -z+2.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Mn(1)-O(1W)	2.1693(16)	Mn(1)-O(2)	2.1783(14)
Mn(1)-O(1)$^{\#1}$	2.2041(15)	Mn(1)-N(4)	2.2119(19)
Mn(1)-O(4)$^{\#2}$	2.2357(14)	Mn(1)-N(3)$^{\#3}$	2.2902(18)
O(1W)-Mn(1)-O(2)	87.17(6)	O(1W)-Mn(1)-O(1)$^{\#1}$	165.50(6)
O(2)-Mn(1)-O(1)$^{\#1}$	107.31(5)	O(1W)-Mn(1)-N(4)	92.34(7)
O(2)-Mn(1)-N(4)	87.46(7)	O(1)$^{\#1}$-Mn(1)-N(4)	87.62(7)
O(1W)-Mn(1)-O(4)$^{\#2}$	83.96(6)	O(2)-Mn(1)-O(4)$^{\#2}$	167.24(6)
O(1)$^{\#1}$-Mn(1)-O(4)$^{\#2}$	81.87(5)	N(4)-Mn(1)-O(4)$^{\#2}$	102.02(7)
O(1W)-Mn(1)-N(3)$^{\#3}$	100.86(7)	O(2)-Mn(1)-N(3)$^{\#3}$	87.44(6)
O(1)$^{\#1}$-Mn(1)-N(3)$^{\#3}$	81.05(6)	N(4)-Mn(1)-N(3)$^{\#3}$	165.59(7)
O(4)$^{\#2}$-Mn(1)-N(3)$^{\#3}$	85.25(6)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x, y+1, z; $^{\#2}$ x, -y+2,

z-1/2; #3 -x, y+1, -z+3/2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Mn(1)-O(4)#1	2.1131(13)	Mn(1)-O(3)#2	2.1308(14)
Mn(1)-N(4)	2.2271(17)	Mn(1)-O(2)	2.2533(13)
Mn(1)-N(3)#3	2.2727(17)	Mn(1)-O(1)	2.2775(14)
O(4)#1-Mn(1)-O(3)#2	107.70(5)	O(4)#1-Mn(1)-N(4)	89.08(6)
O(3)#2-Mn(1)-N(4)	84.34(6)	O(4)#1-Mn(1)-O(2)	151.14(5)
O(3)#2-Mn(1)-O(2)	100.95(5)	N(4)-Mn(1)-O(2)	90.42(6)
O(4)#1-Mn(1)-N(3)#3	101.13(6)	O(3)#2-Mn(1)-N(3)#3	86.50(6)
N(4)-Mn(1)-N(3)#3	167.99(6)	O(2)-Mn(1)-N(3)#3	83.70(6)
O(4)#1-Mn(1)-O(1)	93.33(5)	O(3)#2-Mn(1)-O(1)	158.92(5)
N(4)-Mn(1)-O(1)	94.99(6)	O(2)-Mn(1)-O(1)	57.97(5)
N(3)#3-Mn(1)-O(1)	90.77(6)		

Symmetry transformations used to generate equivalent atoms: #1 x, y+1, z; #2 -x, -y, -z; #3 x-1, y, z.

Table S4a. Selected bond distances (Å) and angles (°) for **4**.

Ni(1)-N(7)	2.012(4)	Ni(1)-N(10)#1	2.015(4)
Ni(1)-O(1)	2.091(3)	Ni(1)-O(6)	2.125(3)
Ni(1)-O(7)	2.140(3)	Ni(1)-O(2)	2.153(3)
Ni(2)-N(3)#1	2.070(3)	Ni(2)-O(4)	2.075(3)
Ni(2)-O(1W)	2.091(3)	Ni(3)-O(9)	2.046(3)
Ni(3)-N(6)#5	2.085(3)	Ni(3)-O(2W)	2.090(3)
N(7)-Ni(1)-N(10)#1	95.61(17)	N(7)-Ni(1)-O(1)	103.04(15)
N(10)#1-Ni(1)-O(1)	98.61(15)	N(7)-Ni(1)-O(6)	99.71(15)
N(10)#1-Ni(1)-O(6)	103.84(14)	O(1)-Ni(1)-O(6)	146.10(11)
N(7)-Ni(1)-O(7)	93.05(15)	N(10)#1-Ni(1)-O(7)	164.09(15)
O(1)-Ni(1)-O(7)	92.39(12)	O(6)-Ni(1)-O(7)	61.43(11)
N(7)-Ni(1)-O(2)	164.64(15)	N(10)#1-Ni(1)-O(2)	90.27(15)
O(1)-Ni(1)-O(2)	61.96(11)	O(6)-Ni(1)-O(2)	92.61(12)
O(7)-Ni(1)-O(2)	84.77(13)	N(3)#2-Ni(2)-O(4)	88.10(12)
N(3)#1-Ni(2)-O(4)	91.90(12)	O(4)-Ni(2)-O(1W)#3	88.30(12)
N(3)#2-Ni(2)-O(1W)	92.85(13)	N(3)#1-Ni(2)-O(1W)	87.15(13)
O(4)-Ni(2)-O(1W)	91.70(12)	O(9)-Ni(3)-N(6)#5	89.53(12)
O(9)-Ni(3)-N(6)#6	90.47(12)	O(9)-Ni(3)-O(2W)#4	89.90(13)
O(9)-Ni(3)-O(2W)	90.10(13)	N(6)#5-Ni(3)-O(2W)	91.35(15)
N(6)#6-Ni(3)-O(2W)	88.65(15)		

Symmetry transformations used to generate equivalent atoms: #1 x-1, y, z; #2 -x+1, -y, -z+1; #3 -x, -y, -z+1; #4 -x+1, -y, -z+2; #5 -x, -y, -z+2; #6 x+1, y, z.

Table S4b. Hydrogen bonds for **4** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)...O(3)	0.848(10)	1.91(3)	2.676(4)	149(5)
O(3W)-H(3A)...O(1)	0.853(10)	1.96(3)	2.770(5)	157(8)
O(1W)-H(1A)...O(3W)#7	0.848(10)	1.98(2)	2.797(6)	160(5)

O(2W)-H(2A)...O(6)[#8]	0.851(10)	2.08(4)	2.835(4)	147(6)
O(2W)-H(2B)...O(8)[#4]	0.847(10)	1.90(3)	2.660(4)	148(5)
O(3W)-H(3B)...O(4W)[#6]	0.854(10)	2.07(6)	2.813(8)	146(10)

Symmetry transformations used to generate equivalent atoms: [#4] -x+1, -y, -z+2; [#6] x+1, y, z; [#7] x-1, y-1, z; [#8] -x+1, -y+1, -z+2.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Cu(1)-O(1)	1.956(3)	Cu(1)-N(7)	1.957(4)
Cu(1)-N(6)	1.976(4)	Cu(1)-O(4)[#1]	1.984(3)
Cu(2)-O(9)[#2]	1.954(3)	Cu(2)-O(6)	1.967(3)
Cu(2)-N(9)	1.989(4)	Cu(2)-N(3)[#2]	2.015(4)
Cu(2)-O(1W)	1.278(5)		
O(1)-Cu(1)-N(7)	90.14(14)	O(1)-Cu(1)-N(6)	86.76(14)
N(7)-Cu(1)-N(6)	171.62(15)	O(1)-Cu(1)-O(4)[#1]	175.83(12)
N(7)-Cu(1)-O(4)[#1]	91.56(14)	N(6)-Cu(1)-O(4)[#1]	92.06(14)
O(9)[#2]-Cu(2)-O(6)	173.52(12)	O(9)[#2]-Cu(2)-N(9)	93.32(14)
O(6)-Cu(2)-N(9)	90.26(14)	O(9)[#2]-Cu(2)-N(3)[#2]	87.15(13)
O(6)-Cu(2)-N(3)[#2]	88.15(14)	N(9)-Cu(2)-N(3)[#2]	166.99(15)
O(9)[#2]-Cu(2)-O(1W)	92.51(11)	O(6)-Cu(2)-O(1W)	92.41(11)
N(9)-Cu(2)-O(1W)	97.08(16)	N(3)[#2]-Cu(2)-O(1W)	95.89(15)

Symmetry transformations used to generate equivalent atoms: [#1] -x+1, y+1/2, -z+3/2; [#2] -x, y+1/2, -z+1/2.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Cu(1)-O(3)[#1]	1.964(2)	Cu(1)-N(4)	1.984(3)
Cu(1)-O(1)	2.001(2)	Cu(1)-N(3)[#2]	2.012(3)
O(3)[#1]-Cu(1)-N(4)	89.22(12)	O(3)[#1]-Cu(1)-O(1)	176.60(10)
N(4)-Cu(1)-O(1)	88.25(12)	O(3)[#1]-Cu(1)-N(3)[#2]	88.30(11)
N(4)-Cu(1)-N(3)[#2]	173.98(12)	O(1)-Cu(1)-N(3)[#2]	93.99(11)

Symmetry transformations used to generate equivalent atoms: [#1] x, -y+3/2, z+1/2; [#2] -x, -y+1, -z+1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

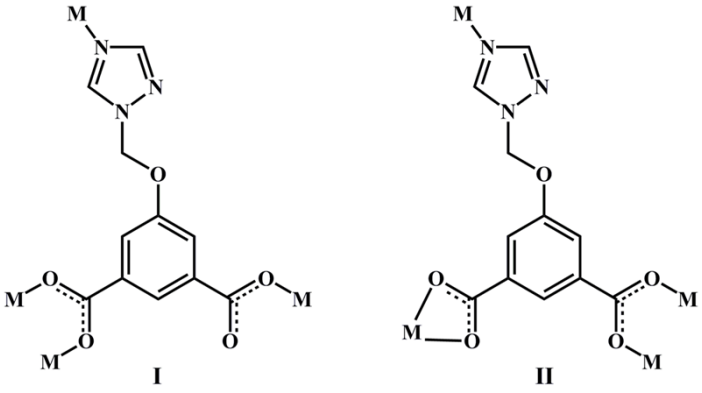
Zn(1)-O(1)	1.960(2)	Zn(1)-O(4)[#1]	1.969(2)
Zn(1)-N(4)	1.990(3)	Zn(1)-N(3)[#2]	2.019(3)
O(1)-Zn(1)-O(4)[#1]	107.63(9)	O(1)-Zn(1)-N(4)	115.33(12)
O(4)[#1]-Zn(1)-N(4)	108.47(11)	O(1)-Zn(1)-N(3)[#2]	105.52(12)
O(4)[#1]-Zn(1)-N(3)[#2]	106.98(12)	N(4)-Zn(1)-N(3)[#2]	112.52(13)

Symmetry transformations used to generate equivalent atoms: [#1] x, y-1, z; [#2] x, y-1, z-1.

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Zn(1)-O(1)	1.977(2)	Zn(1)-O(4)[#1]	1.992(2)
Zn(1)-N(4)	1.994(3)	Zn(1)-N(3)[#2]	2.020(3)
O(1)-Zn(1)-O(4)[#1]	99.08(10)	O(1)-Zn(1)-N(4)	110.18(12)
O(4)[#1]-Zn(1)-N(4)	112.67(11)	O(1)-Zn(1)-N(3)[#2]	110.49(11)
O(4)[#1]-Zn(1)-N(3)[#2]	107.52(12)	N(4)-Zn(1)-N(3)[#2]	115.64(12)

Symmetry transformations used to generate equivalent atoms: #1 x+1/2, -y+1/2, z+1/2; #2 x+1/2, y-1/2, z.



Scheme S1. Coordination modes of L ligands in compounds **1**–**8**.

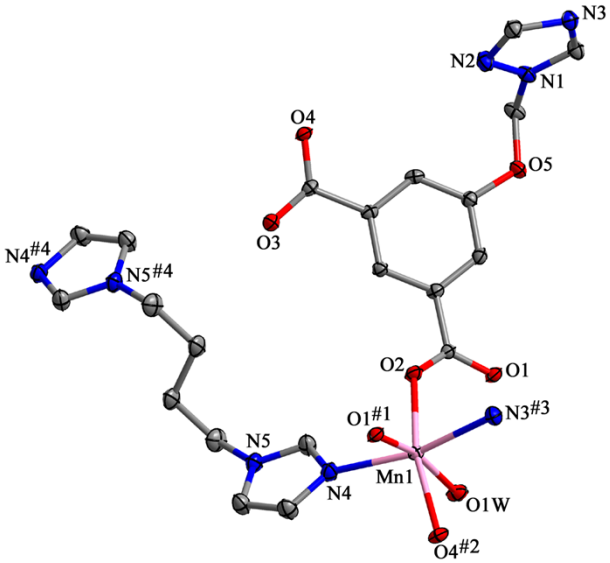


Fig. S1 Crystal structure of $[Mn_2(L)_2(biim\text{-}4)(H_2O)_2]$ (**2**): (a) Coordination environment surrounding Mn1 ion. Symmetry codes: #1 x, y+1, z; #2 x, -y, z-1/2; #3 -x, y+1, -z+3/2; #4 -x+1/2, -y+1/2, -z+2.

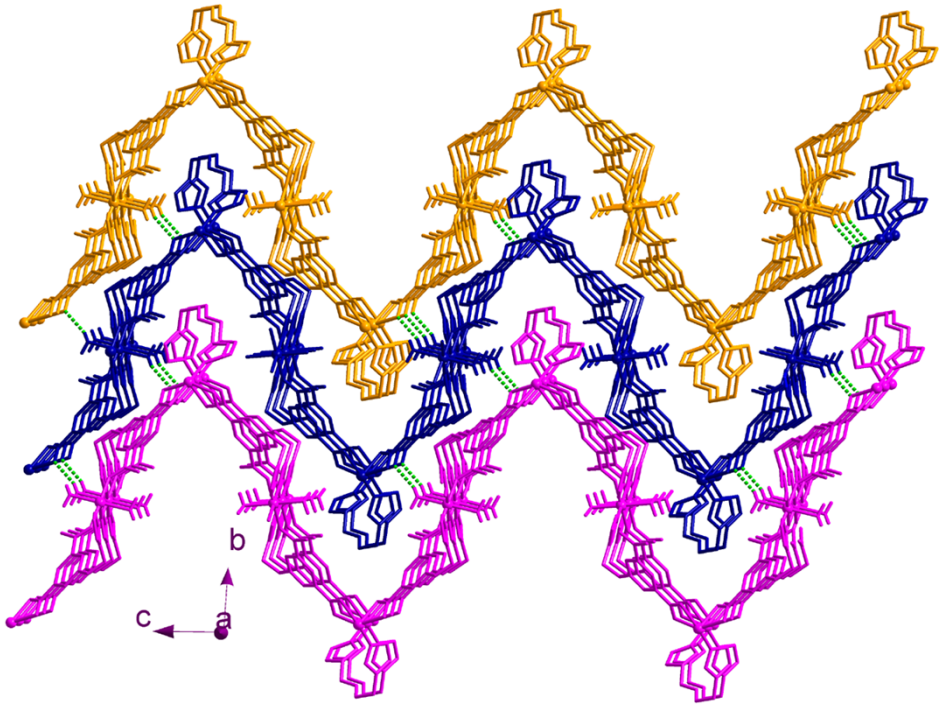


Fig. S2 View of the 3D supramolecular architecture connected by intermolecular hydrogen bonding interactions in **4**.

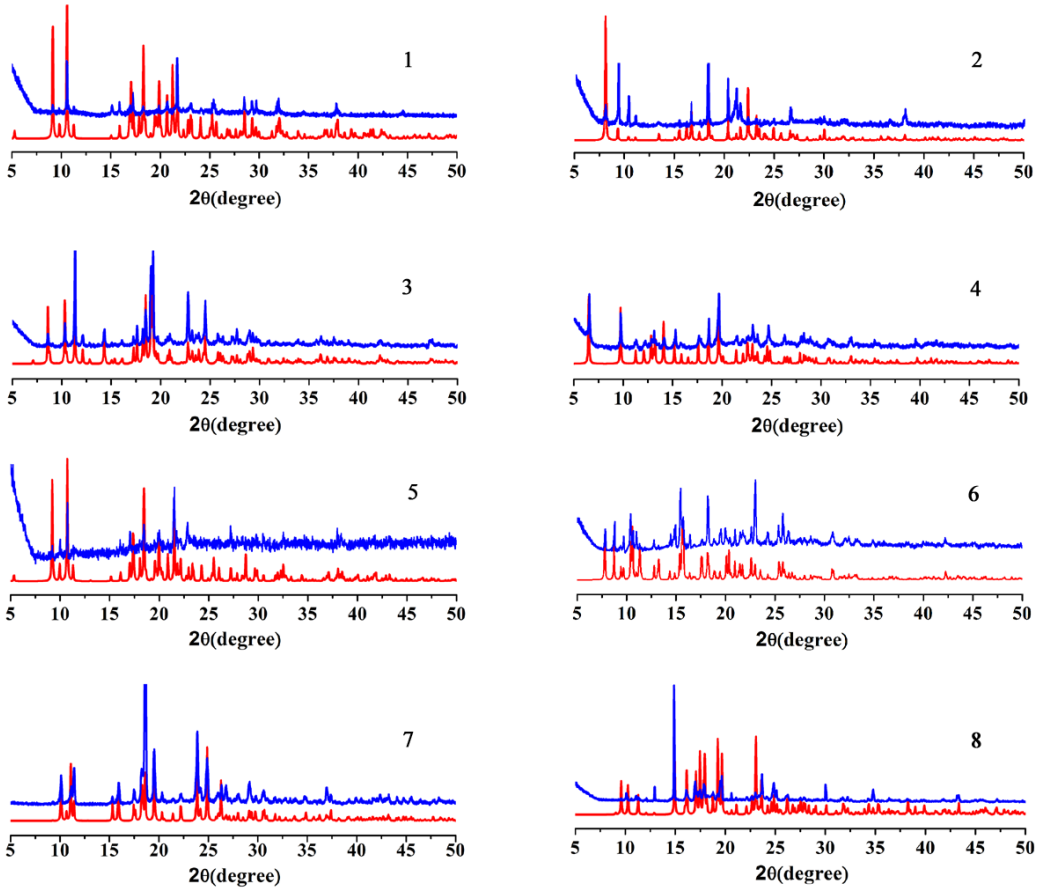


Fig. S3 Simulated (red) and experimental (blue) PXRD patterns of **1**–**8**.

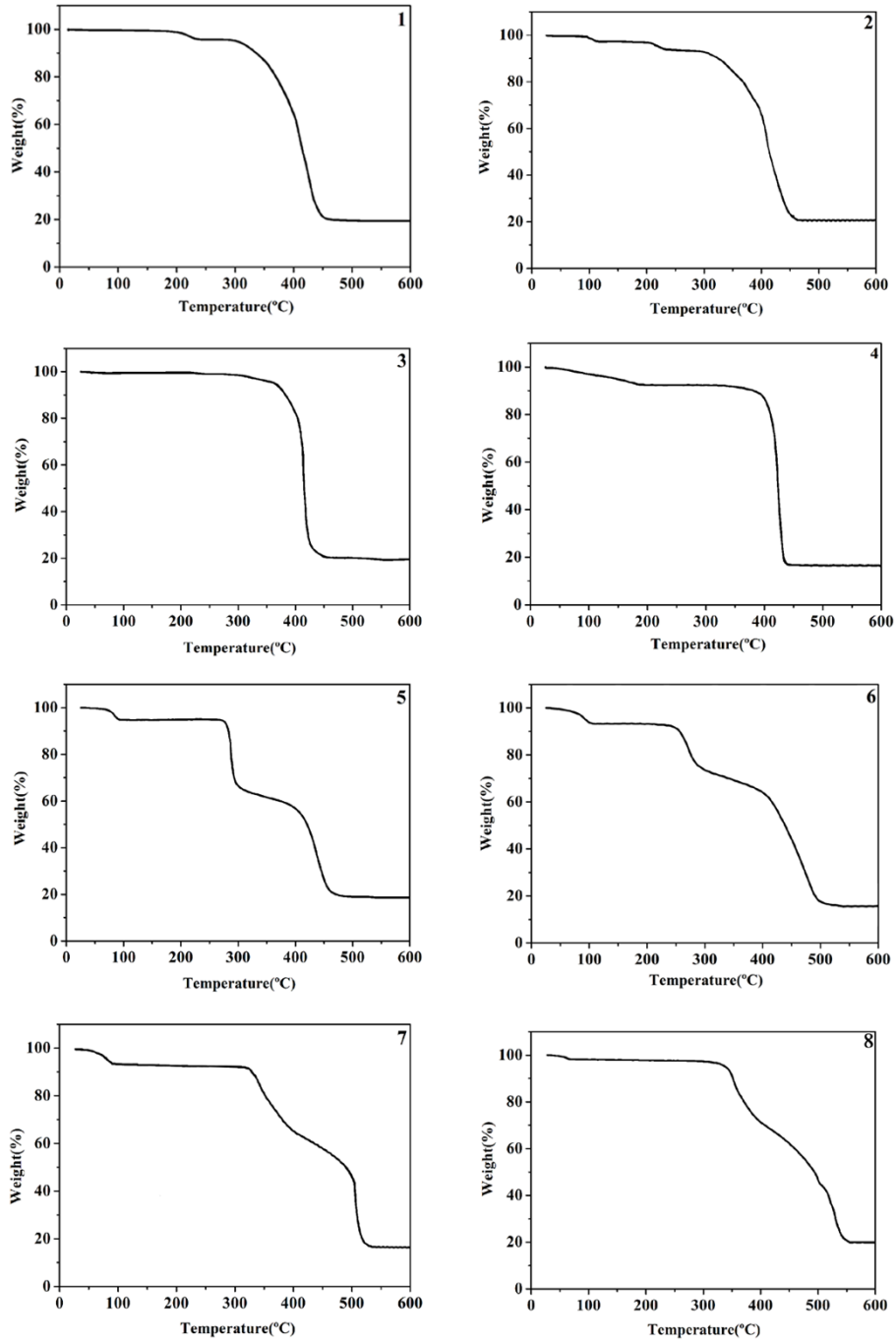


Fig. S4 TGA curves of compounds **1**–**8**.