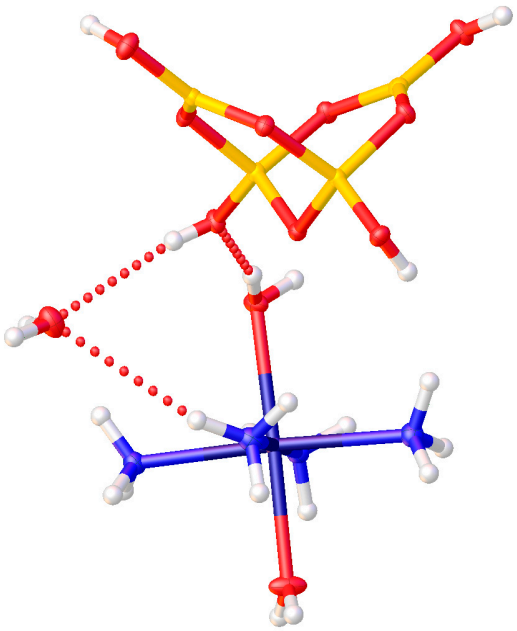
Supplementary X-Ray Crystallographic data

Compound **1**



Crystal Data. $B_4H_{22}N_4NiO_{12}$, M_r = 372.16, monoclinic, $P2_1/c$ (No. 14), a = 8.27730(10) Å, b = 20.5277(3) Å, c = 8.01330(10) Å, β = 91.2830(10)°, α = γ = 90°, V = 1361.23(3) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(Mo K$_\alpha$) = 1.492, 15477 reflections measured, 3128 unique (R_{int} = 0.0329) which were used in all calculations. The final wR_2 was 0.0528 (all data) and R_1 was 0.0216 (I≥2 σ(I)).

Compound	**MAB1**
Formula	$B_4H_{22}N_4NiO_{12}$
$D_{calc.}$/ g cm^{-3}	1.816
μ/mm^{-1}	1.492
Formula Weight	372.16
Colour	blue
Shape	block-shaped
Size/mm^3	0.16×0.12×0.06
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	8.27730(10)
b/Å	20.5277(3)
c/Å	8.01330(10)
α/°	90
β/°	91.2830(10)
γ/°	90
V/Å^3	1361.23(3)
Z	4
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/°	2.461
Θ_{max}/°	27.481
Measured Refl's.	15477
Indep't Refl's	3128
Refl's I≥2 σ(I)	3021
R_{int}	0.0329
Parameters	278
Restraints	0
Largest Peak	0.340
Deepest Hole	-0.295
GooF	1.027
wR_2 (all data)	0.0528
wR_2	0.0523
R_1 (all data)	0.0224
R_1	0.0216

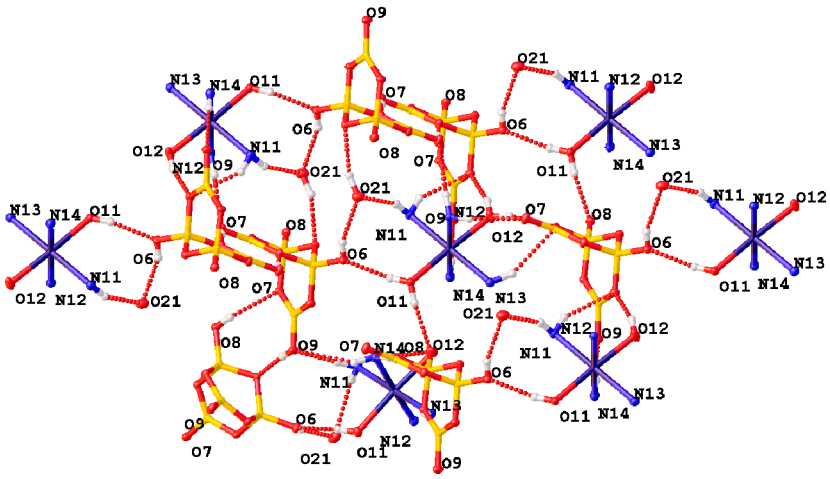


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in **MAB1**: N11–O9_*1: 3.417 Å, O8–O5*_1: 3.166 Å, N12–O7_*2: 2.96 Å, N14–O8*_3: 3.023 Å, O6–O21: 2.843 Å, N14–O9_*1: 3.12 Å, N14–O9*_4: 3.187 Å, O12–O4_*4: 2.704 Å, N13–O5*_3: 3.332 Å, O12–O2_*2: 2.781 Å, N12–O7*_5: 3.053 Å, O21–O3_*5: 2.849 Å, O9–O3*_6: 2.681 Å, O11–O6: 2.684 Å, N13–O21_*7: 3.173 Å, O11–O8*_8: 2.725 Å, N13–O2_*2: 3.233 Å, O7–O1*_9: 2.659 Å, N11–O4_*4: 3.384 Å, N11–O21: 3.414 Å, O21–O11*_7: 2.964 Å.

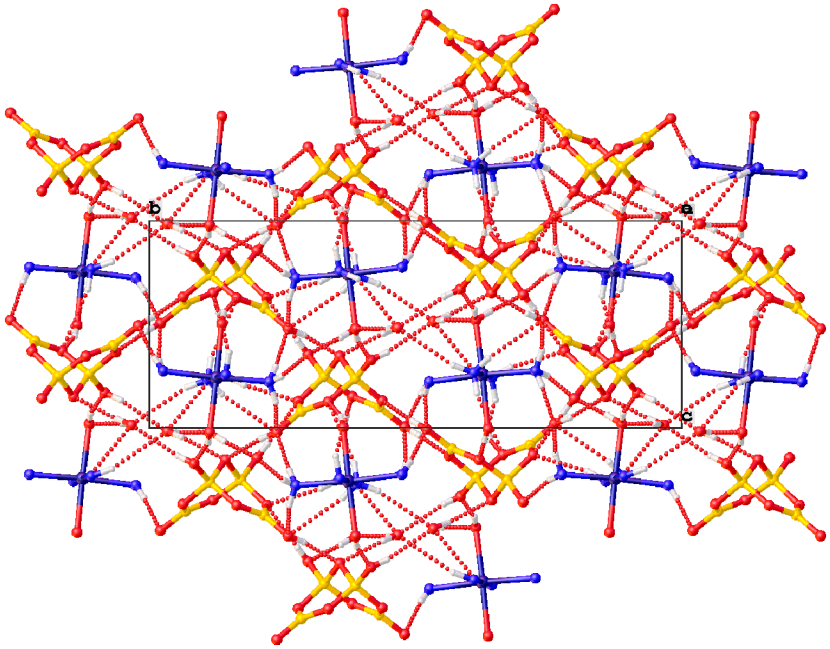


Figure S2: Packing diagram of MAB1.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O1	4873.0(11)	4370.1(4)	1330.1(11)	10.51(18)
O2	7413.3(11)	3808.0(4)	1525.8(11)	9.40(18)
O3	5318.4(11)	3572.2(4)	3480.3(11)	8.52(17)
O4	3368.4(11)	3361.6(4)	1278.2(11)	10.24(18)
O5	5911.6(11)	2795.3(4)	1289.3(11)	9.66(18)
O6	2768.2(11)	4158.6(5)	3291.1(12)	11.29(19)
O7	7206.2(11)	4792.2(5)	56.6(12)	13.12(19)
O8	7840.2(11)	2981.0(5)	3561.3(12)	10.34(18)

Atom	x	y	z	U_{eq}
O9	3577.4(11)	2392.7(5)	-200.5(12)	12.76(19)
B1	4073.4(17)	3866.5(7)	2391.0(17)	8.9(3)
B2	6478.5(17)	4322.4(7)	996.0(17)	9.6(3)
B3	6604.6(16)	3285.1(7)	2494.0(17)	8.7(3)
B4	4318.7(17)	2848.7(7)	804.6(17)	9.7(3)
Ni1	272.0(2)	3742.2(2)	7428.7(2)	8.82(6)
O11	-2.6(12)	3869.7(5)	4803.2(12)	11.83(19)
O12	386.3(13)	3642.1(6)	10033.2(13)	18.0(2)
N11	2808.4(14)	3907.5(7)	7322.8(16)	13.6(2)
N12	-46.3(14)	4741.8(6)	7759.0(15)	11.8(2)
N13	-2265.0(14)	3570.3(6)	7558.8(15)	12.2(2)
N14	712.5(15)	2749.8(6)	7238.2(16)	13.4(2)
O21	2991.3(13)	5335.7(5)	5152.6(13)	18.7(2)

Table S2: Anisotropic Displacement Parameters (×10^4) for **MAB1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	8.9(4)	9.7(4)	12.9(4)	3.1(3)	1.0(3)	1.1(3)
O2	7.8(4)	9.5(5)	11.0(4)	0.9(3)	1.2(3)	0.3(3)
O3	9.1(4)	8.1(4)	8.4(4)	0.0(3)	0.1(3)	0.3(3)
O4	8.9(4)	10.1(4)	11.7(4)	-1.4(3)	-1.7(3)	0.5(3)
O5	8.6(4)	9.4(4)	10.9(4)	-2.7(3)	-0.8(3)	0.6(3)
O6	10.8(4)	9.2(5)	14.0(4)	-2.3(4)	2.3(4)	0.4(4)
O7	9.5(4)	12.4(5)	17.5(5)	5.2(4)	1.8(4)	1.6(4)
O8	9.9(4)	10.3(5)	10.7(4)	1.9(4)	-1.1(4)	0.2(4)
O9	9.3(4)	13.2(5)	15.8(5)	-5.9(4)	-0.7(4)	0.5(4)
B1	8.5(6)	8.7(6)	9.6(6)	0.5(5)	0.3(5)	0.1(5)
B2	11.0(6)	9.0(7)	8.8(6)	-1.6(5)	-0.4(5)	-0.2(5)
B3	8.4(6)	8.4(7)	9.3(6)	-0.3(5)	-0.7(5)	-0.2(5)
B4	10.2(6)	10.0(7)	8.8(6)	1.3(5)	0.7(5)	-0.6(5)
Ni1	7.75(9)	9.84(10)	8.85(9)	-0.32(6)	0.05(6)	0.30(6)
O11	11.0(4)	14.4(5)	10.1(4)	-1.7(4)	1.0(4)	-2.3(4)
O12	9.6(5)	34.4(6)	9.9(5)	1.2(4)	0.3(4)	5.6(4)
N11	11.1(5)	15.6(6)	14.2(6)	-1.5(5)	0.6(4)	0.6(5)
N12	10.0(5)	12.2(6)	13.1(5)	-1.7(4)	0.0(4)	0.6(4)
N13	10.9(5)	12.4(6)	13.3(5)	-0.9(5)	0.1(4)	-0.2(4)
N14	12.2(5)	13.0(6)	14.9(6)	-0.3(5)	2.5(5)	0.6(5)
O21	16.1(5)	16.2(5)	23.7(5)	-5.7(4)	-3.3(4)	1.5(4)

Table S3: Bond Lengths in Å for **MAB1**.

Atom	Atom	Length/Å
O1	B1	1.5015(17)
O1	B2	1.3651(17)
O2	B2	1.3709(17)
O2	B3	1.4917(16)
O3	B1	1.4658(16)
O3	B3	1.4640(16)
O4	B1	1.4787(16)
O4	B4	1.3729(17)
O5	B3	1.4991(16)
O5	B4	1.3705(16)
O6	B1	1.4428(17)
O7	B2	1.3710(17)
O8	B3	1.4588(16)
O9	B4	1.3708(17)
Ni1	O11	2.1272(10)
Ni1	O12	2.0972(10)
Ni1	N11	2.1303(12)
Ni1	N12	2.0864(12)
Ni1	N13	2.1342(12)
Ni1	N14	2.0759(12)

Table S4: Bond Angles in ° for **MAB1**.

Atom	Atom	Atom	Angle/°
B2	O1	B1	120.34(10)
B2	O2	B3	117.29(10)
B3	O3	B1	110.76(9)
B4	O4	B1	118.92(10)
B4	O5	B3	118.73(10)
O3	B1	O1	107.94(10)
O3	B1	O4	109.44(11)
O4	B1	O1	108.30(10)
O6	B1	O1	109.96(11)
O6	B1	O3	113.45(10)
O6	B1	O4	107.64(10)
O1	B2	O2	122.67(12)
O1	B2	O7	119.92(12)
O2	B2	O7	117.39(12)
O2	B3	O5	108.51(10)
O3	B3	O2	109.35(10)
O3	B3	O5	110.20(10)
O8	B3	O2	107.22(10)
O8	B3	O3	111.38(10)
O8	B3	O5	110.10(10)
O5	B4	O4	122.45(12)
O5	B4	O9	121.80(12)
O9	B4	O4	115.75(11)
O11	Ni1	N11	91.41(4)
O11	Ni1	N13	89.15(4)
O12	Ni1	O11	176.16(4)
O12	Ni1	N11	91.87(5)
O12	Ni1	N13	87.57(5)
N11	Ni1	N13	179.37(5)
N12	Ni1	O11	89.63(4)
N12	Ni1	O12	88.46(5)
N12	Ni1	N11	88.61(5)
N12	Ni1	N13	91.68(5)
N14	Ni1	O11	93.61(4)
N14	Ni1	O12	88.45(5)
N14	Ni1	N11	88.77(5)
N14	Ni1	N12	175.88(5)
N14	Ni1	N13	90.91(5)

Table S5: Torsion Angles in ° for **MAB1**.

Atom	Atom	Atom	Atom	Angle/°
B1	O1	B2	O2	3.28(18)
B1	O1	B2	O7	-178.56(11)
B1	O3	B3	O2	62.60(13)
B1	O3	B3	O5	-56.59(13)
B1	O3	B3	O8	-179.08(10)
B1	O4	B4	O5	-1.75(18)
B1	O4	B4	O9	178.77(11)
B2	O1	B1	O3	25.21(15)
B2	O1	B1	O4	-93.19(13)
B2	O1	B1	O6	149.45(11)
B2	O2	B3	O3	-32.51(14)
B2	O2	B3	O5	87.72(13)
B2	O2	B3	O8	-153.39(10)
B3	O2	B2	O1	0.41(18)
B3	O2	B2	O7	-177.79(11)
B3	O3	B1	O1	-57.89(13)
B3	O3	B1	O4	59.78(13)
B3	O3	B1	O6	180.00(10)
B3	O5	B4	O4	5.17(18)
B3	O5	B4	O9	-175.38(11)
B4	O4	B1	O1	87.04(13)
B4	O4	B1	O3	-30.40(15)
B4	O4	B1	O6	-154.11(11)
B4	O5	B3	O2	-95.70(13)
B4	O5	B3	O3	24.01(15)
B4	O5	B3	O8	147.25(11)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H6	3040(20)	4461(9)	3650(20)	10(4)
H7	6550(30)	5061(11)	-340(30)	35(6)

Atom	x	y	z	U_{eq}
H8	7450(20)	2784(9)	4220(20)	17(5)
H9	4180(30)	2100(10)	-510(20)	30(5)
H11A	820(30)	3896(10)	4290(20)	25(5)
H11B	-570(30)	3597(10)	4370(30)	29(5)
H12A	1230(30)	3601(10)	10560(30)	33(6)
H12B	-320(30)	3702(9)	10600(30)	21(5)
H11C	3270(20)	3641(10)	6640(30)	25(5)
H11D	3270(30)	3846(10)	8310(30)	33(6)
H11E	3110(30)	4293(11)	6970(30)	34(6)
H12C	-900(30)	4819(10)	8260(20)	28(5)
H12D	760(20)	4897(9)	8350(20)	24(5)
H12E	-70(30)	4985(12)	6890(30)	46(6)
H13A	-2670(30)	3222(11)	7080(30)	35(6)
H13B	-2850(30)	3912(11)	7200(30)	33(5)
H13C	-2540(20)	3502(10)	8640(30)	31(5)
H14A	-140(20)	2526(10)	7480(20)	19(5)
H14B	990(20)	2626(9)	6260(30)	25(5)
H14C	1500(30)	2630(10)	7950(20)	29(5)
H21A	3740(30)	5606(11)	5430(30)	44(6)
H21B	2040(30)	5508(12)	5220(30)	50(7)

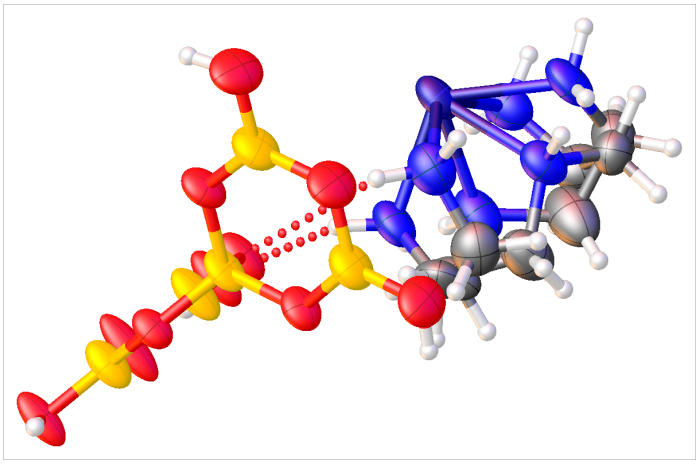
Table S7: Hydrogen Bond information for **MAB1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O6	H6	O21	0.719(18)	2.161(18)	2.8434(15)	158.9(18)
O7	H7	O1[1]	0.83(2)	1.83(2)	2.6585(13)	177(2)
O8	H8	O5[2]	0.743(19)	2.43(2)	3.1658(13)	173.6(19)
O9	H9	O3[3]	0.82(2)	1.87(2)	2.6807(13)	171(2)
O11	H11A	O6	0.81(2)	1.89(2)	2.6841(14)	167(2)
O11	H11B	O8[4]	0.81(2)	1.92(2)	2.7253(14)	171(2)
O12	H12A	O4[5]	0.81(2)	1.92(2)	2.7036(14)	164(2)
O12	H12B	O2[6]	0.76(2)	2.04(2)	2.7810(14)	164(2)
N11	H11C	O9[2]	0.87(2)	2.60(2)	3.4170(16)	157.4(17)
N11	H11D	O4[5]	0.87(2)	2.58(2)	3.3839(16)	153.0(18)
N11	H11E	O21	0.88(2)	2.59(2)	3.4137(18)	156.7(18)
N12	H12C	O7[6]	0.83(2)	2.15(2)	2.9597(15)	162.5(19)
N12	H12D	O7[7]	0.87(2)	2.18(2)	3.0531(15)	175.3(17)
N13	H13A	O5[8]	0.87(2)	2.47(2)	3.3320(15)	167.7(19)
N13	H13B	O21[9]	0.89(2)	2.44(2)	3.1729(16)	139.7(18)
N13	H13C	O2[6]	0.91(2)	2.40(2)	3.2329(15)	152.3(18)
N14	H14A	O8[8]	0.87(2)	2.17(2)	3.0232(16)	169.6(16)
N14	H14B	O9[2]	0.86(2)	2.47(2)	3.1201(16)	133.5(16)
N14	H14C	O9[5]	0.89(2)	2.30(2)	3.1868(15)	176.3(18)
O21	H21A	O3[7]	0.86(2)	2.04(2)	2.8487(14)	155(2)
O21	H21B	O11[9]	0.86(3)	2.12(3)	2.9641(15)	166(2)

––––

[1]1-x,1-y,-z; [2]+x,1/2-y,1/2+z; [3]+x,1/2-y,-1/2+z; [4]-1+x,+y,+z; [5]+x,+y,1+z; [6]-1+x,+y,1+z; [7]1-x,1-y,1-z; [8]-1+x,1/2-y,1/2+z; [9]-x,1-y,1-z

Compound **2**



Crystal Data. $C_8H_{34}B_{10}N_6NiO_{20}$, M_r = 701.22, triclinic, *P*-1 (No. 2), a = 8.5763(5) Å, b = 9.2902(6) Å, c = 9.3493(6) Å, α = 78.098(5)°, β = 89.108(5)°, γ = 89.110(5)°, V = 728.75(8) Å^3, T = 100(2) K, Z = 1, Z' = 0.5, μ(Synchrotron) = 0.699, 6342 reflections measured, 3152 unique (R_{int} = 0.0476) which were used in all calculations. The final wR_2 was 0.2109 (all data) and R_1 was 0.0767 (I≥2 σ(I)).

Compound	**MAB2**
Formula	$C_8H_{34}B_{10}N_6NiO_{20}$
$D_{calc.}$/ g cm^{-3}	1.598
μ/mm^{-1}	0.699
Formula Weight	701.22
Colour	orange
Shape	blade-shaped
Size/mm^3	0.02×0.02×0.01
T/K	100(2)
Crystal System	triclinic
Space Group	*P*-1
a/Å	8.5763(5)
b/Å	9.2902(6)
c/Å	9.3493(6)
α/°	78.098(5)
β/°	89.108(5)
γ/°	89.110(5)
V/Å^3	728.75(8)
Z	1
Z'	0.5
Wavelength/Å	0.6889
Radiation type	Synchrotron
Θ_{min}/°	2.728
Θ_{max}/°	26.572
Measured Refl's.	6342
Indep't Refl's	3152
Refl's I≥2 σ(I)	2526
R_{int}	0.0476
Parameters	273
Restraints	0
Largest Peak	1.314
Deepest Hole	-0.953
GooF	1.077
wR_2 (all data)	0.2109
wR_2	0.2025
R_1 (all data)	0.0882
R_1	0.0767

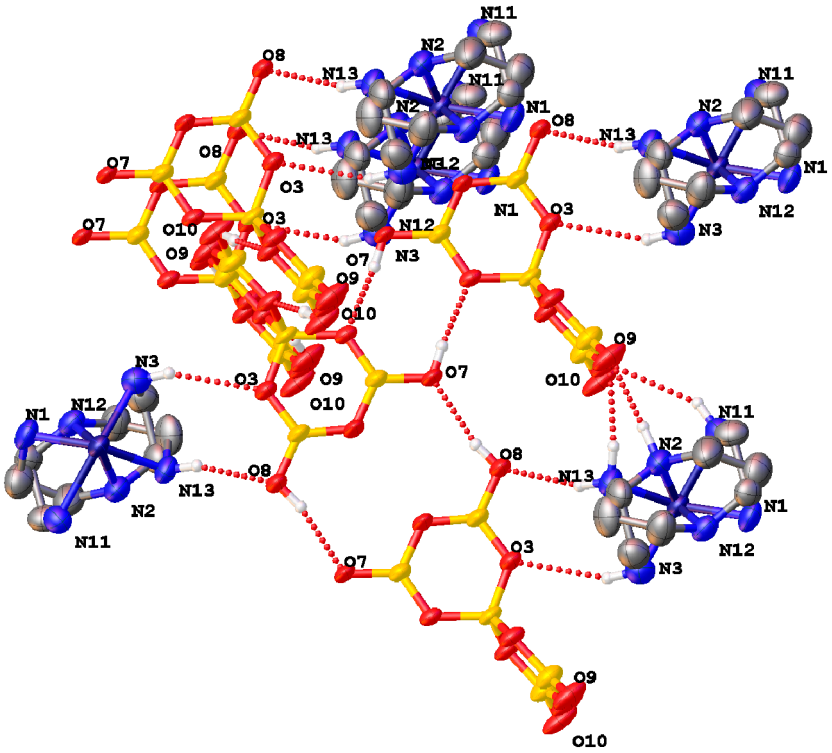


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ˚ are present in **MAB2**: N1–O8_*5: 2.969 Å, N1–O10*_7: 3.208 Å, N2–O9_*6: 2.916 Å, N3–O3: 3.296 Å, N3–O5*_7: 3.382 Å, O7–O1_*1: 2.689 Å, O8–O7*_2: 2.826 Å, O9–O4_*3: 2.727 Å, O10–O6*_4: 2.735 Å, N11–O3_*5: 3.303 Å, N11–O5*_6: 3.372 Å, N12–O5_*7: 3.517 Å, N13–O8: 2.935 Å, N13–O9*_6: 3.216 Å.

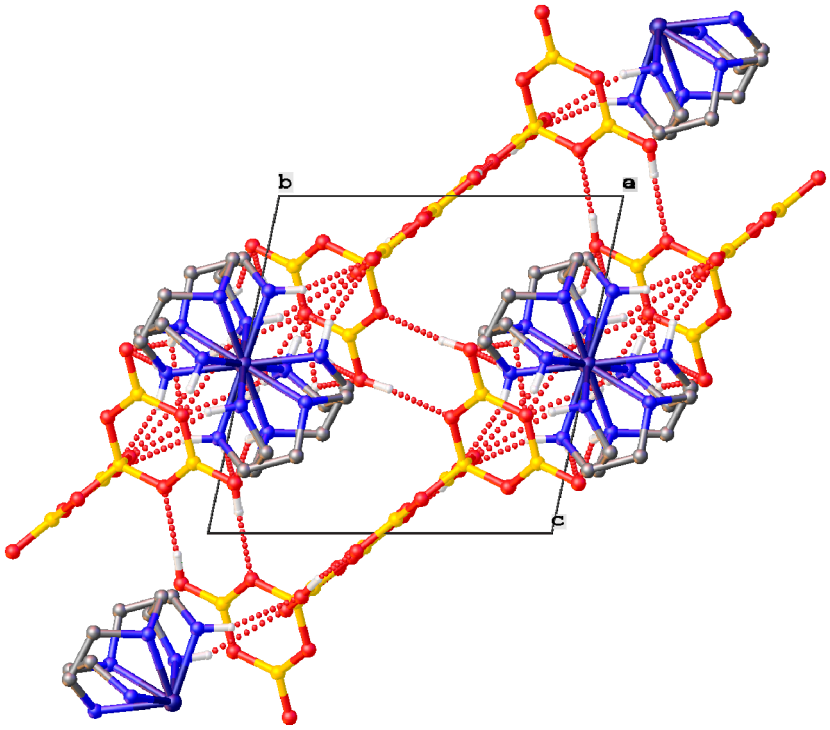


Figure S2: Packing diagram of MAB2.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ni1	0	0	5000	45.2(3)
N1	294(9)	-2188(8)	4741(8)	61.9(19)
N2	-906(8)	-1114(8)	7007(8)	60.9(18)
N3	2141(8)	-165(8)	6228(8)	61.9(19)
C1	-890(20)	-3132(17)	5681(18)	75(4)
C2	-1199(16)	-2718(13)	7050(16)	87(4)
C3	210(15)	-955(16)	8116(14)	62(3)
C4	1898(12)	-1193(12)	7606(12)	69(2)
O1	3989(3)	3999(3)	8983(3)	36.5(5)
O2	1264(3)	4330(5)	9307(5)	76.8(12)
O3	2122(3)	2740(3)	7742(3)	47.9(7)
O4	4536(3)	1554(3)	8634(3)	43.4(6)
O5	6078(4)	1478(3)	6502(3)	61.8(9)
O6	4538(3)	3633(3)	6559(3)	43.8(6)
O7	2990(3)	5561(3)	10535(3)	53.9(8)
O8	-554(3)	3098(4)	8118(4)	58.9(8)
O9	6248(4)	-466(4)	8514(4)	65.4(9)
O10	6255(4)	3497(4)	4556(4)	65.9(9)
B1	3779(4)	2982(5)	7972(5)	40.2(9)
B2	2784(5)	4619(5)	9592(5)	47.2(10)
B3	957(5)	3392(6)	8388(6)	53.9(12)
B4	5587(6)	854(6)	7911(6)	51.5(11)
B5	5597(6)	2893(6)	5873(5)	52.2(11)
N11	-2137(10)	-1232(10)	5163(10)	59(2)
N12	891(10)	-2040(9)	6124(9)	53(2)
N13	-310(10)	277(9)	7177(9)	55(2)
C11	-1907(14)	-2623(14)	6189(14)	61(3)
C12	-197(17)	-3166(17)	5947(18)	51(3)
C13	1168(19)	-2087(16)	7710(14)	77(4)
C14	890(30)	-665(19)	8131(18)	71(5)

Table S2: Anisotropic Displacement Parameters (×10⁴) for **MAB2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	35.3(4)	57.9(5)	50.9(4)	-31.5(3)	7.1(3)	3.0(3)
N1	62(4)	74(4)	62(4)	-43(4)	2(3)	13(3)
N2	48(4)	73(4)	72(4)	-39(4)	13(3)	-4(3)
N3	48(4)	68(4)	75(5)	-26(4)	1(3)	0(3)
C1	90(12)	57(6)	80(9)	-22(6)	8(8)	-3(8)
C2	82(8)	92(7)	98(9)	-44(7)	33(7)	-25(6)
C3	64(7)	76(7)	51(5)	-27(5)	1(5)	-9(5)
C4	61(6)	67(5)	79(6)	-17(5)	-9(5)	3(5)
O1	22.1(11)	49.6(13)	42.9(12)	-22.4(11)	7.4(9)	4.3(9)
O2	20.2(13)	123(3)	120(3)	-101(3)	4.7(15)	5.6(15)
O3	25.4(12)	68.5(16)	62.5(16)	-43.8(14)	5.9(10)	4.5(11)
O4	31.7(13)	49.8(13)	53.5(15)	-23.9(12)	14.1(10)	6.5(10)
O5	58(2)	67.9(19)	60.4(18)	-19.8(15)	25.8(15)	22.4(15)
O6	32.1(13)	60.1(15)	45.0(14)	-25.8(12)	8.7(10)	12.9(11)
O7	19.8(12)	81.7(19)	78.8(19)	-60.2(17)	5.9(12)	5.4(12)
O8	24.3(13)	89(2)	83(2)	-65.7(18)	4.4(12)	4.2(13)
O9	63(2)	62.3(18)	71(2)	-18.1(16)	28.0(17)	24.4(15)
O10	61(2)	78(2)	57.6(18)	-16.8(16)	26.2(15)	28.2(17)
B1	23.7(18)	54(2)	50(2)	-28.9(18)	9.6(15)	8.0(15)
B2	23.3(18)	68(3)	62(3)	-41(2)	6.4(16)	3.7(17)
B3	23.3(19)	81(3)	73(3)	-54(3)	6.3(18)	5.9(19)
B4	41(2)	60(3)	59(3)	-27(2)	11.4(19)	10(2)
B5	41(2)	67(3)	53(2)	-25(2)	12.5(19)	11(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N11	51(5)	73(5)	59(5)	-25(4)	2(4)	-8(4)
N12	46(4)	66(5)	54(4)	-26(4)	2(3)	11(4)
N13	55(5)	59(5)	58(5)	-33(4)	14(4)	-2(4)
C11	51(6)	72(7)	55(6)	-4(5)	11(5)	-4(5)
C12	54(8)	43(5)	56(7)	-10(4)	-1(6)	3(6)
C13	83(9)	85(9)	70(8)	-32(7)	-17(6)	19(8)
C14	106(16)	68(9)	42(6)	-14(6)	-19(9)	1(10)

Table S3: Bond Lengths in Å for **MAB2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	N1	2.107(7)	O2	B3	1.375(5)
Ni1	N1[1]	2.107(7)	O3	B1	1.469(5)
Ni1	N2	2.092(8)	O3	B3	1.358(5)
Ni1	N2[1]	2.092(8)	O4	B1	1.488(5)
Ni1	N3	2.167(7)	O4	B4	1.355(5)
Ni1	N3[1]	2.167(7)	O5	B4	1.387(6)
Ni1	N11	2.163(8)	O5	B5	1.384(6)
Ni1	N11[1]	2.162(8)	O6	B1	1.480(5)
Ni1	N12	2.107(8)	O6	B5	1.362(5)
Ni1	N12[1]	2.107(8)	O7	B2	1.379(5)
Ni1	N13[1]	2.115(8)	O8	B3	1.367(5)
Ni1	N13	2.115(8)	O9	B4	1.358(6)
N1	C1	1.503(17)	O10	B5	1.361(6)
N2	C2	1.507(13)	N11	C11	1.455(15)
N2	C3	1.453(14)	N12	C12	1.449(17)
N3	C4	1.451(13)	N12	C13	1.496(14)
C1	C2	1.43(2)	N13	C14	1.52(2)
C3	C4	1.544(17)	C11	C12	1.572(18)
O1	B1	1.482(4)	C13	C14	1.47(2)
O1	B2	1.349(5)	––––		
O2	B2	1.376(5)	[1]-x,-y,1-z		

Table S4: Bond Angles in ° for **MAB2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ni1	N3	90.5(3)	N12	Ni1	N13[1]	99.5(3)
N1[1]	Ni1	N3	89.5(3)	N12	Ni1	N13	80.5(3)
N1	Ni1	N13[1]	64.3(3)	N12[1]	Ni1	N13[1]	80.5(3)
N1[1]	Ni1	N13[1]	115.7(3)	N12[1]	Ni1	N13	99.5(3)
N2[1]	Ni1	N1	99.8(3)	N13	Ni1	N3[1]	114.0(3)
N2	Ni1	N1	80.2(3)	N13[1]	Ni1	N3[1]	66.0(3)
N2[1]	Ni1	N3	97.5(3)	N13[1]	Ni1	N11[1]	90.4(3)
N2	Ni1	N3	82.5(3)	N13	Ni1	N11[1]	89.6(3)
N2	Ni1	N13[1]	140.1(3)	N13[1]	Ni1	N11	89.6(3)
N2[1]	Ni1	N13[1]	39.9(3)	N13	Ni1	N11	90.4(3)
N3[1]	Ni1	N3	180.0	N13[1]	Ni1	N13	180.0
N11	Ni1	N3[1]	44.4(3)	C1	N1	Ni1	108.9(7)
N11[1]	Ni1	N3[1]	135.6(3)	C2	N2	Ni1	113.2(6)
N11[1]	Ni1	N11	180.0	C3	N2	Ni1	106.9(6)
N12[1]	Ni1	N1[1]	39.7(3)	C3	N2	C2	110.4(10)
N12	Ni1	N1[1]	140.3(3)	C4	N3	Ni1	108.2(6)
N12	Ni1	N3[1]	121.8(3)	C2	C1	N1	113.8(11)
N12[1]	Ni1	N3[1]	58.2(3)	C1	C2	N2	113.1(11)
N12	Ni1	N11	82.0(3)	N2	C3	C4	111.2(10)
N12[1]	Ni1	N11[1]	82.0(3)	N3	C4	C3	107.2(9)
N12	Ni1	N11[1]	98.0(3)	B2	O1	B1	123.1(3)
N12[1]	Ni1	N11	98.0(3)	B3	O2	B2	119.7(3)
N12[1]	Ni1	N12	180.0(3)	B3	O3	B1	122.7(3)

Atom	Atom	Atom	Angle/°
B4	O4	B1	123.4(3)
B5	O5	B4	119.5(3)
B5	O6	B1	123.3(3)
O1	B1	O4	107.8(3)
O3	B1	O1	111.6(3)
O3	B1	O4	109.1(3)
O3	B1	O6	109.6(3)
O6	B1	O1	108.2(3)
O6	B1	O4	110.5(3)
O1	B2	O2	121.3(3)
O1	B2	O7	122.7(3)
O2	B2	O7	116.0(3)
O3	B3	O2	121.6(4)
O3	B3	O8	118.8(4)
O8	B3	O2	119.5(4)
O4	B4	O5	121.0(4)
O4	B4	O9	123.0(4)
O9	B4	O5	116.0(4)
O6	B5	O5	121.1(4)
O10	B5	O5	116.4(4)
O10	B5	O6	122.5(4)
C11	N11	Ni1	108.6(7)
C12	N12	Ni1	107.8(7)
C12	N12	C13	110.6(11)
C13	N12	Ni1	113.3(7)
C14	N13	Ni1	108.8(9)
N11	C11	C12	107.2(9)
N12	C12	C11	109.3(12)
C14	C13	N12	113.3(11)
C13	C14	N13	112.4(12)

––––

[1]-x,-y,1-z

Table S5: Torsion Angles in ° for **MAB2**.

Atom	Atom	Atom	Atom	Angle/°
Ni1	N1	C1	C2	-36.8(16)
Ni1	N2	C2	C1	-3.8(16)
Ni1	N2	C3	C4	-43.5(11)
Ni1	N3	C4	C3	-37.3(10)
Ni1	N11	C11	C12	-37.9(12)
Ni1	N12	C12	C11	-44.4(12)
Ni1	N12	C13	C14	-5.0(18)
Ni1	N13	C14	C13	-38.0(18)
N1	C1	C2	N2	27(2)
N2	C3	C4	N3	55.8(13)
C2	N2	C3	C4	80.0(11)
C3	N2	C2	C1	-123.6(14)
B1	O1	B2	O2	0.3(7)
B1	O1	B2	O7	179.8(4)
B1	O3	B3	O2	0.0(8)
B1	O3	B3	O8	-179.6(4)
B1	O4	B4	O5	3.0(6)
B1	O4	B4	O9	-178.6(4)
B1	O6	B5	O5	-2.6(6)
B1	O6	B5	O10	178.4(4)
B2	O1	B1	O3	-0.4(5)
B2	O1	B1	O4	-120.3(4)
B2	O1	B1	O6	120.2(4)
B2	O2	B3	O3	-0.3(9)
B2	O2	B3	O8	179.4(5)
B3	O2	B2	O1	0.1(8)
B3	O2	B2	O7	-179.5(5)
B3	O3	B1	O1	0.3(6)
B3	O3	B1	O4	119.3(4)
B3	O3	B1	O6	-119.5(4)
B4	O4	B1	O1	-128.3(4)
B4	O4	B1	O3	110.4(4)
B4	O4	B1	O6	-10.3(5)
B4	O5	B5	O6	-6.0(7)
B4	O5	B5	O10	173.0(4)
B5	O5	B4	O4	5.8(7)
B5	O5	B4	O9	-172.7(4)
B5	O6	B1	O1	127.9(4)
B5	O6	B1	O3	-110.3(4)
B5	O6	B1	O4	10.0(5)
N11	C11	C12	N12	56.4(14)

Atom	Atom	Atom	Atom	Angle/°
N12	C13	C14	N13	28(2)
C12	N12	C13	C14	-126.2(16)
C13	N12	C12	C11	80.0(12)

Table S6: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **MAB2**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	166.37	-2235.45	3787.68	74
H1B	1272.3	-2517.94	5009.95	74
H2	-1911.53	-629.31	7208.87	73
H3A	2934.97	-488.91	5713.58	74
H3B	2396.43	733.17	6393.8	74
H1C	-1881.23	-3076.5	5136.96	90
H1D	-522.14	-4166.93	5868.94	90
H2A	-530.37	-3321.24	7805.05	105
H2B	-2299.26	-2935.25	7340.25	105
H3C	-18.19	-1680.56	9027.41	74
H3D	102.69	41.24	8332.22	74
H4A	2647.93	-1008.4	8340.18	82
H4B	2049.39	-2216.06	7474.08	82
H7	3946.72	5641.79	10675.38	81
H8	-1154.79	3498.7	8642.66	88
H9	5881.3	-761.47	9360.36	98
H10	5932.1	4367.82	4286.54	99
H11A	-2930.74	-710.88	5479.9	71
H11B	-2389.54	-1399.86	4270.02	71
H12	1906.48	-2235.4	5654.96	64
H13A	-190.95	1239.58	7216.69	66
H13B	-1288.29	2.5	7502.41	66
H11C	-2668.24	-3353.87	6010.17	73
H11D	-2050.89	-2485.65	7205.54	73
H12A	29.03	-4086.32	6664.38	61
H12B	-84.29	-3372.71	4953.01	61
H13C	473.24	-2828.4	8301.8	92
H13D	2257.81	-2408.45	7939.29	92
H14A	1886.41	-126.28	8058.71	85
H14B	530.68	-840.17	9162.61	85

Table S7: Hydrogen Bond information for **MAB2**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1A	O8^1	0.91	2.12	2.970(7)	155.2
N1	H1B	O10^2	0.91	2.30	3.208(8)	172.8
N2	H2	O9^3	1.00	2.00	2.916(7)	150.6
N3	H3A	O5^2	0.91	2.56	3.382(8)	150.4
N3	H3B	O3	0.91	2.46	3.295(8)	152.2
O7	H7	O1^4	0.84	1.85	2.689(3)	174.4
O8	H8	O7^5	0.84	2.01	2.826(3)	164.7
O9	H9	O4^6	0.84	1.90	2.727(4)	168.7
O10	H10	O6^7	0.84	1.90	2.734(4)	170.7
N11	H11A	O5^3	0.91	2.55	3.372(10)	150.8
N11	H11B	O3^1	0.91	2.47	3.302(9)	152.8
N12	H12	O5^2	1.00	2.63	3.517(9)	148.5
N13	H13A	O8	0.91	2.09	2.936(8)	154.2
N13	H13B	O9^3	0.91	2.31	3.216(9)	172.5

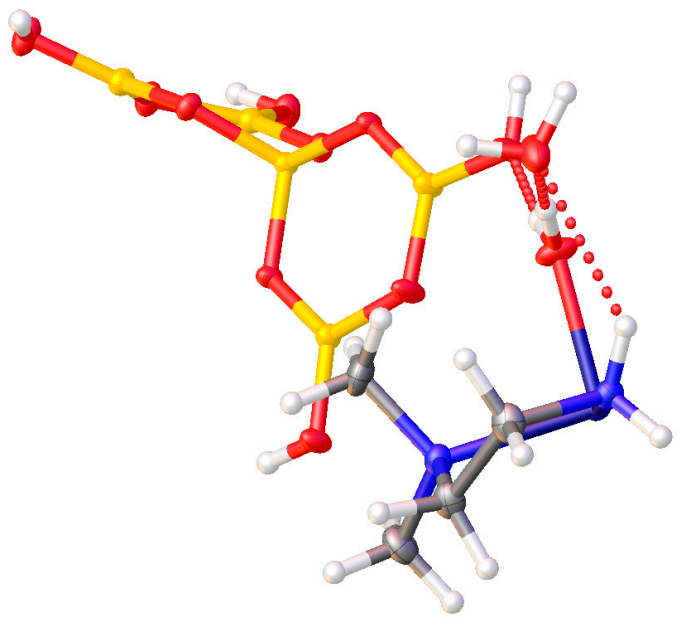
––––

^{1}-x,-y,1-z; ^{2}1-x,-y,1-z; ^{3}-1+x,+y,+z; ^{4}1-x,1-y,2-z; ^{5}-x,1-y,2-z; ^{6}1-x,-y,2-z; ^{7}1-x,1-y,1-z

Table S8: Atomic Occupancies for all atoms that are not fully occupied in **MAB2**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
N1	0.560(6)	H1D	0.560(6)	N11	0.440(6)	H11D	0.440(6)
H1A	0.560(6)	C2	0.560(6)	H11A	0.440(6)	C12	0.440(6)
H1B	0.560(6)	H2A	0.560(6)	H11B	0.440(6)	H12A	0.440(6)
N2	0.560(6)	H2B	0.560(6)	N12	0.440(6)	H12B	0.440(6)
H2	0.560(6)	C3	0.560(6)	H12	0.440(6)	C13	0.440(6)
N3	0.560(6)	H3C	0.560(6)	N13	0.440(6)	H13C	0.440(6)
H3A	0.560(6)	H3D	0.560(6)	H13A	0.440(6)	H13D	0.440(6)
H3B	0.560(6)	C4	0.560(6)	H13B	0.440(6)	C14	0.440(6)
C1	0.560(6)	H4A	0.560(6)	C11	0.440(6)	H14A	0.440(6)
H1C	0.560(6)	H4B	0.560(6)	H11C	0.440(6)	H14B	0.440(6)

Compound **3**



Crystal Data. $C_8H_{40}B_{10}N_4NiO_{24}$, M_r = 743.25, triclinic, *P*-1 (No. 2), a = 8.6570(3) Å, b = 9.7443(3) Å, c = 10.2101(3) Å, α = 107.087(3)°, β = 102.747(3)°, γ = 95.002(3)°, V = 792.23(5) Å^3, T = 100(2) K, Z = 1, Z' = 0.5, μ(Mo K$_\alpha$) = 0.708, 12978 reflections measured, 3628 unique (R_{int} = 0.0163) which were used in all calculations. The final wR_2 was 0.0731 (all data) and R_1 was 0.0270 (I≥2 σ(I)).

Compound	**MAB3**
Formula	$C_8H_{40}B_{10}N_4NiO_{24}$
$D_{calc.}$/ g cm^{-3}	1.558
μ/mm^{-1}	0.708
Formula Weight	743.25
Colour	blue
Shape	block-shaped
Size/mm^3	0.23×0.21×0.08
T/K	100(2)
Crystal System	triclinic
Space Group	*P*-1
a/Å	8.6570(3)
b/Å	9.7443(3)
c/Å	10.2101(3)
α/°	107.087(3)
β/°	102.747(3)
γ/°	95.002(3)
V/Å^3	792.23(5)
Z	1
Z'	0.5
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/°	2.216
Θ_{max}/°	27.481
Measured Refl's.	12978
Indep't Refl's	3628
Refl's I≥2 σ(I)	3568
R_{int}	0.0163
Parameters	225
Restraints	0
Largest Peak	0.719
Deepest Hole	-0.510
GooF	1.088
wR_2 (all data)	0.0731
wR_2	0.0730
R_1 (all data)	0.0272
R_1	0.0270

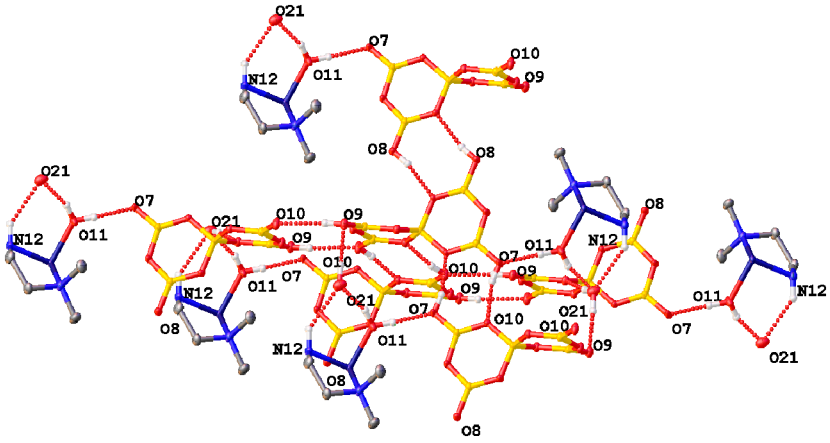


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in **MAB3**: O11–O21: 2.675 Å, O11–O7: 2.686 Å, N12–O2_*6: 2.987 Å, N12–021: 3.217 Å, 07–01*_1: 2.64 Å, O8–O3_*2: 2.692 Å, 09–010*_3: 2.837 Å, O10–O6_*4: 2.735 Å, 021–04*_5: 2.753 Å, O21–O9_*1: 2.884 Å.*

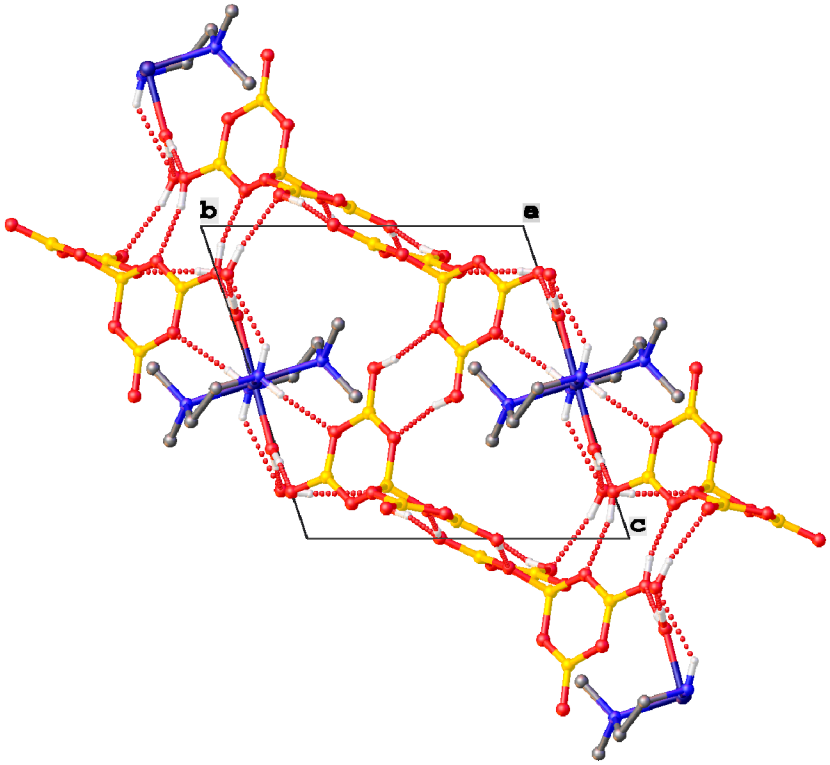


Figure S2: Packing diagram of MAB3.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ni1	10000	0	5000	10.62(9)
O11	9342.1(11)	-151.9(11)	2877.1(10)	20.0(2)
N11	10941.2(13)	2336.8(11)	5700.1(12)	15.5(2)
N12	12321.6(12)	-200.8(11)	4807.4(11)	14.6(2)
C11	12684.8(15)	2379.6(14)	6249.3(15)	19.1(3)
C12	13308.9(15)	1254.7(14)	5200.1(15)	20.2(3)
C13	10661.9(17)	2995.7(15)	4551.1(16)	23.3(3)

Atom	x	y	z	U_{eq}
C14	10316.6(17)	3221.3(15)	6853.5(16)	23.0(3)
O1	4680.3(10)	1750.3(9)	1139.3(9)	11.41(17)
O2	6351.7(11)	1981.9(10)	3411.1(9)	17.8(2)
O3	4659.1(10)	3746.5(9)	3219.7(9)	12.21(17)
O4	2201.0(10)	2496.4(9)	1469.3(9)	12.74(18)
O5	1449.0(10)	4542.4(10)	812.4(10)	15.17(19)
O6	4118.8(10)	4048.9(9)	915.3(9)	12.08(17)
O7	6367.3(12)	1.3(11)	1505.6(10)	22.3(2)
O8	6425.6(11)	3867.1(10)	5437.1(9)	16.15(19)
O9	-514.7(10)	2781.2(10)	983.9(10)	16.12(19)
O10	3121.2(11)	5872.9(10)	-33.6(10)	17.65(19)
B1	3909.2(15)	3018.1(14)	1686.3(13)	10.5(2)
B2	5768.2(16)	1245.3(15)	1977.5(14)	14.2(3)
B3	5787.3(15)	3239.6(14)	4026.6(14)	12.0(2)
B4	1049.8(16)	3285.2(14)	1101.4(14)	12.9(2)
B5	2935.8(16)	4822.3(14)	579.1(14)	13.1(2)
O21	11696.3(13)	-301.6(11)	1552.8(11)	23.3(2)

Table S2: Anisotropic Displacement Parameters (×10⁴) for **MAB3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	8.91(12)	13.52(13)	10.88(12)	5.87(8)	2.12(8)	3.65(8)
O11	14.0(4)	35.7(5)	14.4(4)	13.3(4)	3.4(3)	8.5(4)
N11	13.5(5)	15.2(5)	18.6(5)	6.1(4)	4.2(4)	4.0(4)
N12	12.0(5)	16.9(5)	16.0(5)	6.5(4)	3.4(4)	4.4(4)
C11	12.4(6)	18.2(6)	24.1(6)	5.7(5)	1.6(5)	1.0(4)
C12	11.9(5)	20.4(6)	29.1(7)	8.1(5)	7.1(5)	2.1(5)
C13	23.5(7)	20.3(6)	30.8(7)	15.7(6)	5.6(6)	5.4(5)
C14	21.2(6)	18.2(6)	26.0(7)	0.2(5)	7.3(5)	5.3(5)
O1	12.8(4)	11.5(4)	9.0(4)	2.0(3)	1.3(3)	5.8(3)
O2	21.3(5)	17.5(4)	10.4(4)	0.0(3)	-1.9(3)	12.1(4)
O3	14.5(4)	11.9(4)	9.1(4)	2.0(3)	0.9(3)	6.3(3)
O4	11.2(4)	12.5(4)	15.5(4)	5.6(3)	3.2(3)	3.7(3)
O5	12.6(4)	16.3(4)	21.4(4)	10.7(3)	5.9(3)	7.0(3)
O6	11.2(4)	13.7(4)	13.7(4)	7.0(3)	3.3(3)	5.0(3)
O7	25.9(5)	21.5(5)	11.5(4)	-2.7(4)	-5.1(4)	16.5(4)
O8	19.0(4)	15.2(4)	10.9(4)	0.3(3)	-0.2(3)	9.4(3)
O9	12.3(4)	15.9(4)	22.7(5)	9.1(4)	4.6(3)	5.7(3)
O10	13.8(4)	20.8(4)	26.3(5)	15.7(4)	8.1(4)	8.2(3)
B1	10.9(6)	10.5(5)	9.8(5)	2.9(4)	1.9(4)	4.2(4)
B2	14.3(6)	14.5(6)	11.8(6)	2.1(5)	0.5(5)	6.5(5)
B3	11.7(6)	11.4(6)	12.3(6)	3.5(5)	1.8(5)	3.8(4)
B4	13.6(6)	13.5(6)	11.5(6)	3.4(5)	3.1(5)	4.8(5)
B5	12.9(6)	13.7(6)	13.7(6)	5.4(5)	2.9(5)	5.3(5)
O21	31.0(5)	16.4(4)	25.1(5)	5.9(4)	13.9(4)	2.6(4)

Table S3: Bond Lengths in Å for **MAB3**.

Atom	Atom	Length/Å
Ni1	O11[1]	2.0727(9)
Ni1	O11	2.0727(9)
Ni1	N11[1]	2.1961(11)
Ni1	N11	2.1961(11)
Ni1	N12[1]	2.0824(10)
Ni1	N12	2.0824(10)
N11	C11	1.4820(16)
N11	C13	1.4804(17)
N11	C14	1.4792(17)
N12	C12	1.4852(16)
C11	C12	1.5198(18)
O1	B1	1.4787(14)
O1	B2	1.3542(16)
O2	B2	1.3806(15)
O2	B3	1.3867(15)
O3	B1	1.4814(14)
O3	B3	1.3582(15)
O4	B1	1.4671(15)
O4	B4	1.3650(15)
O5	B4	1.3751(16)
O5	B5	1.3784(16)
O6	B1	1.4689(15)
O6	B5	1.3660(15)
O7	B2	1.3591(16)
O8	B3	1.3511(15)
O9	B4	1.3666(16)
O10	B5	1.3628(16)

––––

[1]2-x,-y,1-z

Table S4: Bond Angles in ˚ for **MAB3**.

Atom	Atom	Atom	Angle/˚
O11[1]	Ni1	O11	180.000(14)
O11	Ni1	N11[1]	86.65(4)
O11[1]	Ni1	N11	86.65(4)
O11[1]	Ni1	N11[1]	93.35(4)
O11	Ni1	N11	93.35(4)
O11[1]	Ni1	N12	91.73(4)
O11	Ni1	N12[1]	91.72(4)
O11	Ni1	N12	88.27(4)
O11[1]	Ni1	N12[1]	88.27(4)
N11	Ni1	N11[1]	180.0
N12[1]	Ni1	N11[1]	83.00(4)
N12	Ni1	N11[1]	97.00(4)
N12[1]	Ni1	N11	97.00(4)
N12	Ni1	N11	83.00(4)
N12	Ni1	N12[1]	180.0
C11	N11	Ni1	102.42(7)
C13	N11	Ni1	114.11(8)
C13	N11	C11	110.00(10)
C14	N11	Ni1	113.87(8)
C14	N11	C11	108.98(10)
C14	N11	C13	107.30(11)
C12	N12	Ni1	110.67(8)
N11	C11	C12	110.67(11)
N12	C12	C11	110.15(10)
B2	O1	B1	123.62(9)
B2	O2	B3	120.01(10)
B3	O3	B1	124.54(9)
B4	O4	B1	121.42(10)
B4	O5	B5	118.86(10)
B5	O6	B1	120.90(9)
O1	B1	O3	110.16(9)
O4	B1	O1	108.23(9)
O4	B1	O3	109.48(9)
O4	B1	O6	110.86(9)
O6	B1	O1	108.85(9)
O6	B1	O3	109.26(9)
O1	B2	O2	121.23(11)
O1	B2	O7	124.09(11)
O7	B2	O2	114.68(11)
O3	B3	O2	120.02(11)
O8	B3	O2	115.23(11)
O8	B3	O3	124.75(11)
O4	B4	O5	120.65(11)
O4	B4	O9	118.84(11)
O9	B4	O5	120.48(11)
O6	B5	O5	120.91(11)
O10	B5	O5	116.02(11)
O10	B5	O6	123.05(11)

––––

[1]2-x,-y,1-z

Table S5: Torsion Angles in ° for **MAB3**.

Atom	Atom	Atom	Atom	Angle/°
Ni1	N11	C11	C12	47.76(11)
Ni1	N12	C12	C11	27.28(13)
N11	C11	C12	N12	-52.60(14)
C13	N11	C11	C12	-73.93(13)
C14	N11	C11	C12	168.69(11)
B1	O1	B2	O2	-6.39(19)
B1	O1	B2	O7	173.33(12)
B1	O3	B3	O2	2.18(18)
B1	O3	B3	O8	-177.09(11)
B1	O4	B4	O5	5.22(17)
B1	O4	B4	O9	-176.71(10)
B1	O6	B5	O5	-7.24(17)
B1	O6	B5	O10	174.64(11)
B2	O1	B1	O3	7.66(15)
B2	O1	B1	O4	-112.00(12)
B2	O1	B1	O6	127.43(12)
B2	O2	B3	O3	0.07(18)
B2	O2	B3	O8	179.40(11)
B3	O2	B2	O1	2.01(19)
B3	O2	B2	O7	-177.73(12)
B3	O3	B1	O1	-5.61(15)
B3	O3	B1	O4	113.29(12)
B3	O3	B1	O6	-125.14(11)
B4	O4	B1	O1	-142.95(10)
B4	O4	B1	O3	96.95(12)
B4	O4	B1	O6	-23.65(14)
B4	O5	B5	O6	-13.70(17)
B4	O5	B5	O10	164.55(11)
B5	O5	B4	O4	14.72(17)
B5	O5	B4	O9	-163.32(11)
B5	O6	B1	O1	143.50(10)
B5	O6	B1	O3	-96.16(12)
B5	O6	B1	O4	24.57(14)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB3**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H11A	9963.13	-203.67	2304.13	30
H11B	8382.52	-63.39	2451.62	30
H12A	12781.76	-692.52	5382.22	18
H12B	12284.25	-720.28	3897.44	18
H11C	12885.34	2183.81	7165.2	23
H11D	13266.99	3361.58	6417.76	23
H12C	13268.19	1536.57	4338.7	24
H12D	14440.68	1216.03	5629.12	24
H13A	9505.57	2939.22	4176.71	35
H13B	11116.19	2466.95	3788.95	35
H13C	11179.11	4017.14	4926.93	35
H14A	10444.29	2791.79	7618.94	35
H14B	9176.61	3242.99	6484.8	35
H14C	10914.99	4215.3	7220.9	35
H7	5932.79	-405.51	636.78	33
H8	5994.01	4595.5	5735.34	24
H9	-1100.02	3355.23	742.63	24
H10	4007.75	5887.86	-240.94	26
H21A	11861.96	548.62	1447.08	35
H21B	11452.37	-974.08	727.68	35

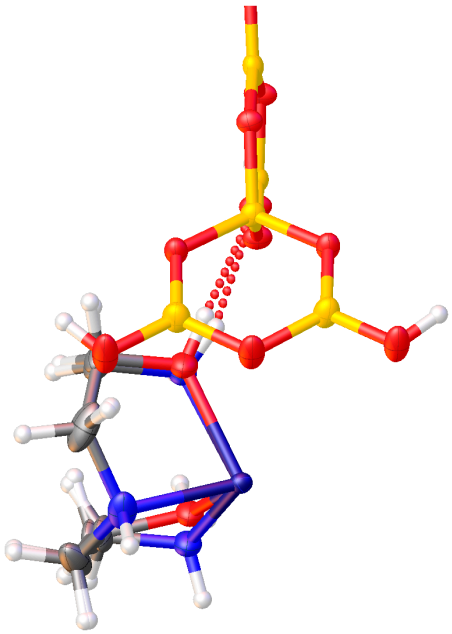
Table S7: Hydrogen Bond information for **MAB3**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O11	H11A	O21	0.87	1.83	2.6749(14)	163.6
O11	H11B	O7	0.87	1.81	2.6859(13)	176.5
N12	H12A	O2[1]	0.91	2.08	2.9867(14)	174.4
N12	H12B	O21	0.91	2.50	3.2172(15)	136.5
O7	H7	O1[2]	0.84	1.83	2.6399(12)	161.8
O8	H8	O3[3]	0.84	1.87	2.6917(12)	167.4
O9	H9	O10[4]	0.84	2.04	2.8373(12)	159.5
O10	H10	O6[5]	0.84	1.90	2.7354(12)	173.2
O21	H21A	O4[6]	0.87	1.89	2.7526(13)	172.3
O21	H21B	O9[2]	0.87	2.03	2.8836(14)	165.8

––––

[1]2-x,-y,1-z; [2]1-x,-y,-z; [3]1-x,1-y,1-z; [4]-x,1-y,-z; [5]1-x,1-y,-z; [6]1+x,+y,+z

Compound **4**



Crystal Data. $C_8H_{32}B_{10}N_4NiO_{22}$, M_r = 703.18, monoclinic, $P2_1/c$ (No. 14), a = 8.3891(2) Å, b = 11.6666(3) Å, c = 14.3092(4) Å, β = 90.035(2)˚, $\alpha = \gamma$ = 90˚, V = 1400.47(6) Å^3, T = 100(2) K, Z = 2, Z' = 0.5, μ(Mo K$_\alpha$) = 0.791, 6239 reflections measured, 6239 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1124 (all data) and R_1 was 0.0499 (I≥2 σ(I)).

Compound	**MAB4**
Formula	$C_8H_{32}B_{10}N_4NiO_{22}$
$D_{calc.}$/ g cm^{-3}	1.668
μ/mm^{-1}	0.791
Formula Weight	703.18
Colour	Lilac
Shape	rod-shaped
Size/mm^3	0.34×0.05×0.04
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	8.3891(2)
b/Å	11.6666(3)
c/Å	14.3092(4)
α/˚	90
β/˚	90.035(2)
γ/˚	90
V/Å^3	1400.47(6)
Z	2
Z'	0.5
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/˚	2.252
Θ_{max}/˚	27.496
Measured Refl's.	6239
Indep't Refl's	6239
Refl's I≥2 σ(I)	5795
R_{int}	.
Parameters	223
Restraints	13
Largest Peak	0.961
Deepest Hole	-0.466
GooF	1.126
wR_2 (all data)	0.1124
wR_2	0.1103
R_1 (all data)	0.0542
R_1	0.0499

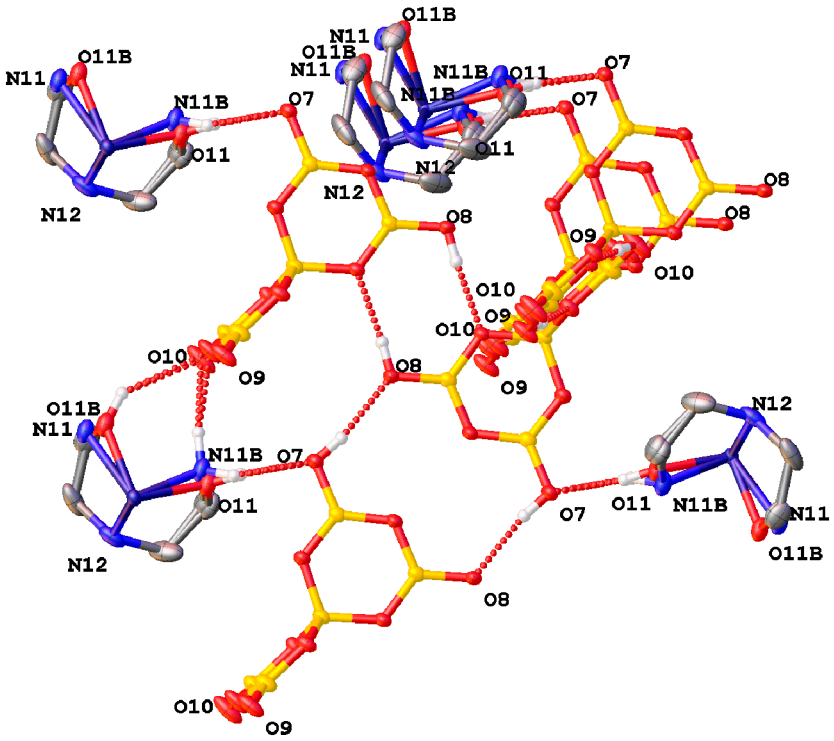


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in **MAB4**: O7–O8_*1: 2.804 Å, O8–O3*_2: 2.678 Å, O9–O6_*3: 2.74 Å, O10–O4*_4: 2.726 Å, N12–O9_*6: 2.973 Å, N11–O1*_7: 2.975 Å, O11–O7: 2.77 Å, N11B–O7: 2.867 Å, N11B–O5_*5: 2.981 Å, N11B–O10*_5: 3 Å, O11B–O5_*5: 3.125 Å, O11B–O10*_5: 3.22 Å.

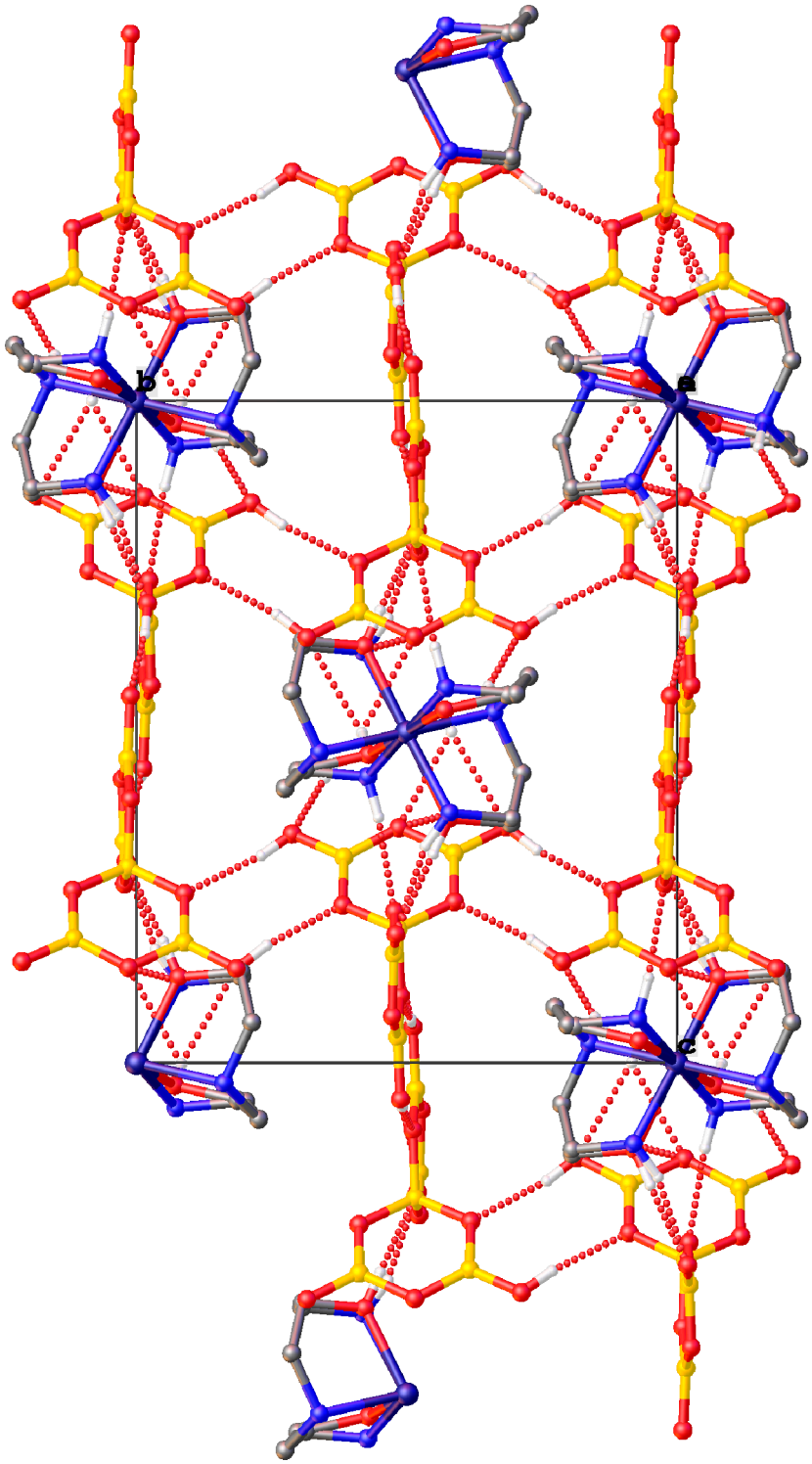


Figure S2: Packing diagram of MAB4.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
O1	2069(2)	4775.4(16)	2290.8(12)	17.5(4)
O2	1197(2)	4735.0(16)	707.2(12)	19.1(4)
O3	3970(2)	4881.8(15)	1011.7(12)	15.6(4)
O4	4592(2)	3814.3(14)	2387.3(12)	17.2(4)

Atom	x	y	z	U_{eq}
O5	6001(3)	4853.2(17)	3555.7(15)	28.1(5)
O6	4459(2)	5882.9(15)	2438.3(13)	18.4(4)
O7	-660(2)	4801.1(17)	1948.2(13)	19.6(4)
O8	2956(2)	4885.7(17)	-546.1(12)	19.6(4)
O9	6318(3)	2877.4(17)	3464.2(15)	28.2(5)
O10	6038(3)	6847.3(18)	3571.9(17)	36.9(6)
B1	3756(3)	4839(2)	2033(2)	16.0(5)
B2	888(3)	4770(2)	1651(2)	15.1(5)
B3	2737(3)	4833(2)	397(2)	14.8(5)
B4	5617(4)	3837(3)	3117(2)	22.2(6)
B5	5474(4)	5878(3)	3172(2)	23.8(6)
Ni1	0	5000	5000	14.33(13)
N12	920(3)	6614(2)	5300.4(19)	29.9(6)
C12	-259(5)	7258(3)	5845(2)	41.7(9)
C13	1397(4)	7131(3)	4383(3)	43.1(9)
C11	-1975(15)	7020(20)	5580(40)	30.3(17)
C14	210(40)	6930(30)	3620(20)	31(3)
N11	-2045(9)	5727(4)	5671(6)	24.6(5)
O11	-306(7)	5780(5)	3700(6)	24.6(5)
C11B	-1910(20)	6870(30)	5560(60)	30.3(17)
C14B	80(70)	6940(40)	3690(40)	31(3)
N11B	-718(14)	5795(9)	3780(12)	24.6(5)
O11B	-2196(11)	5700(5)	5338(6)	24.6(5)

Table S2: Anisotropic Displacement Parameters ($\times 10^4$) for **MAB4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	13.5(9)	23.9(9)	15.1(8)	0.9(7)	-2.7(6)	1.4(7)
O2	12.0(9)	29.9(10)	15.3(9)	-1.5(7)	-3.0(6)	-2.3(7)
O3	11.8(8)	19.0(9)	15.9(8)	0.2(7)	-2.9(6)	-0.7(7)
O4	15.8(9)	15.7(8)	20.0(9)	0.5(7)	-7.0(7)	0.2(7)
O5	34.5(12)	19.2(10)	30.7(11)	1.0(8)	-22.4(9)	0.0(8)
O6	20.9(9)	15.1(8)	19.1(9)	-0.6(7)	-7.7(7)	0.6(7)
O7	14.0(9)	29.2(10)	15.4(8)	0.8(7)	-2.8(7)	-0.1(7)
O8	10.6(8)	32.0(10)	16.3(9)	-1.2(8)	-1.7(7)	0.3(8)
O9	31.7(11)	17.9(9)	35.0(12)	2.0(8)	-22.0(9)	-0.9(8)
O10	50.0(15)	18.7(10)	41.8(13)	-0.4(9)	-32.7(11)	-0.7(10)
B1	13.2(13)	16.9(13)	17.8(13)	1.2(10)	-4.4(10)	0.6(10)
B2	15.3(13)	12.8(12)	17.1(13)	0.4(10)	-2.3(10)	-0.3(10)
B3	14.3(13)	12.3(12)	17.7(13)	-1.0(10)	-2.4(10)	1.4(10)
B4	20.5(15)	19.6(14)	26.3(16)	3.0(11)	-9.1(12)	-1.2(11)
B5	24.4(16)	21.8(15)	25.1(16)	-0.8(12)	-10.0(12)	-0.8(12)
Ni1	16.0(2)	14.7(2)	12.2(2)	0.52(17)	-1.39(15)	1.14(17)
N12	29.0(14)	23.6(12)	37.2(14)	1.9(10)	-19.7(11)	-0.6(10)
C12	64(2)	30.6(16)	30.2(17)	-10.3(13)	-24.2(16)	16.1(16)
C13	28.8(17)	32.5(17)	68(3)	23.0(17)	-9.2(16)	-10.1(14)
C11	40(2)	14(6)	37(3)	1(6)	12(3)	11(2)
C14	40(5)	25.0(16)	28(5)	9(2)	11(5)	3(3)
N11	32.9(18)	22.2(8)	18.7(17)	-0.4(9)	6(2)	1.1(10)
O11	32.9(18)	22.2(8)	18.7(17)	-0.4(9)	6(2)	1.1(10)
C11B	40(2)	14(6)	37(3)	1(6)	12(3)	11(2)
C14B	40(5)	25.0(16)	28(5)	9(2)	11(5)	3(3)
N11B	32.9(18)	22.2(8)	18.7(17)	-0.4(9)	6(2)	1.1(10)
O11B	32.9(18)	22.2(8)	18.7(17)	-0.4(9)	6(2)	1.1(10)

Table S3: Bond Lengths in Å for **MAB4**.

Atom	Atom	Length/Å
O1	B1	1.465(3)
O1	B2	1.348(3)
O2	B2	1.377(3)
O2	B3	1.371(3)
O3	B1	1.473(3)
O3	B3	1.359(3)
O4	B1	1.475(3)
O4	B4	1.352(3)
O5	B4	1.380(4)
O5	B5	1.388(4)
O6	B1	1.472(3)
O6	B5	1.351(4)
O7	B2	1.366(3)
O8	B3	1.364(3)
O9	B4	1.359(4)
O10	B5	1.353(4)
Ni1	N12[1]	2.079(2)
Ni1	N12	2.079(2)
Ni1	N11	2.142(7)
Ni1	N11[1]	2.142(7)
Ni1	O11[1]	2.087(8)
Ni1	O11	2.087(8)
Ni1	N11B[1]	2.066(16)
Ni1	N11B	2.066(16)
Ni1	O11B	2.072(9)
Ni1	O11B[1]	2.072(9)
N12	C12	1.467(5)
N12	C13	1.500(4)
C12	C11	1.513(8)
C12	C11B	1.512(10)
C13	C14	1.493(8)
C13	C14B	1.496(10)
C11	N11	1.51(3)
C14	O11	1.41(2)
C11B	O11B	1.42(3)
C14B	N11B	1.50(3)

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[1]-x,1-y,1-z

Table S4: Bond Angles in ° for **MAB4**.

Atom	Atom	Atom	Angle/°
B2	O1	B1	122.6(2)
B3	O2	B2	119.6(2)
B3	O3	B1	123.2(2)
B4	O4	B1	123.5(2)
B4	O5	B5	119.1(2)
B5	O6	B1	123.7(2)
O1	B1	O3	111.7(2)
O1	B1	O4	109.4(2)
O1	B1	O6	109.2(2)
O3	B1	O4	108.1(2)
O6	B1	O3	108.3(2)
O6	B1	O4	110.2(2)
O1	B2	O2	121.8(2)
O1	B2	O7	119.1(2)
O7	B2	O2	119.0(2)
O3	B3	O2	120.7(2)
O3	B3	O8	122.4(2)
O8	B3	O2	116.8(2)
O4	B4	O5	121.1(2)
O4	B4	O9	122.8(3)
O9	B4	O5	116.1(2)
O6	B5	O5	120.8(3)
O6	B5	O10	123.0(3)
O10	B5	O5	116.2(3)
N12	Ni1	N12[1]	180.0
N12	Ni1	N11	81.13(17)
N12[1]	Ni1	N11[1]	81.13(17)
N12[1]	Ni1	N11	98.87(17)
N12	Ni1	N11[1]	98.87(17)
N12	Ni1	O11	80.52(19)
N12	Ni1	O11[1]	99.49(19)
N12[1]	Ni1	O11[1]	80.51(19)
N12[1]	Ni1	O11	99.49(19)
N11	Ni1	N11[1]	180.0
O11[1]	Ni1	N11	82.6(3)
O11	Ni1	N11	97.4(3)
O11	Ni1	N11[1]	82.6(3)
O11[1]	Ni1	N11[1]	97.4(3)
O11	Ni1	O11[1]	180.0(3)
N11B	Ni1	N12	82.9(4)
N11B[1]	Ni1	N12	97.1(4)
N11B[1]	Ni1	N11B	180.0
N11B	Ni1	O11B[1]	103.8(5)
N11B[1]	Ni1	O11B	103.8(5)
N11B	Ni1	O11B	76.2(5)
N11B[1]	Ni1	O11B[1]	76.2(5)
O11B[1]	Ni1	N12	94.3(2)
O11B	Ni1	N12	85.7(2)
O11B	Ni1	O11B[1]	180.0
C12	N12	Ni1	108.9(2)
C12	N12	C13	116.0(3)
C13	N12	Ni1	106.4(2)
N12	C12	C11	114.5(12)
N12	C12	C11B	108.9(19)
C14	C13	N12	113.3(14)
C14B	C13	N12	109(2)
N11	C11	C12	101.7(14)
O11	C14	C13	107.4(14)
C11	N11	Ni1	109.1(13)
C14	O11	Ni1	116.5(10)
O11B	C11B	C12	120.1(19)
C13	C14B	N11B	114(2)
C14B	N11B	Ni1	109.9(13)
C11B	O11B	Ni1	106.3(13)

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[1]-x,1-y,1-z

Table S5: Torsion Angles in ° for **MAB4**.

Atom	Atom	Atom	Atom	Angle/°
B1	O1	B2	O2	5.0(4)
B1	O1	B2	O7	-174.8(2)
B1	O3	B3	O2	-0.2(4)
B1	O3	B3	O8	179.3(2)
B1	O4	B4	O5	-2.9(4)
B1	O4	B4	O9	176.7(3)
B1	O6	B5	O5	4.2(5)
B1	O6	B5	O10	-176.0(3)
B2	O1	B1	O3	-0.6(3)
B2	O1	B1	O4	-120.2(2)
B2	O1	B1	O6	119.2(2)
B2	O2	B3	O3	4.7(3)
B2	O2	B3	O8	-174.8(2)
B3	O2	B2	O1	-7.1(4)
B3	O2	B2	O7	172.7(2)
B3	O3	B1	O1	-1.8(3)
B3	O3	B1	O4	118.5(2)
B3	O3	B1	O6	-122.2(2)
B4	O4	B1	O1	-107.6(3)
B4	O4	B1	O3	130.6(3)
B4	O4	B1	O6	12.5(4)
B4	O5	B5	O6	7.1(5)
B4	O5	B5	O10	-172.7(3)
B5	O5	B4	O4	-7.7(4)
B5	O5	B4	O9	172.7(3)
B5	O6	B1	O1	107.0(3)
B5	O6	B1	O3	-131.2(3)
B5	O6	B1	O4	-13.2(4)
Ni1	N12	C12	C11	-35(2)
Ni1	N12	C12	C11B	-31(3)
Ni1	N12	C13	C14	42.0(19)
Ni1	N12	C13	C14B	46(3)
N12	C12	C11	N11	54(3)
N12	C12	C11B	O11B	36(7)
N12	C13	C14	O11	-42(4)
N12	C13	C14B	N11B	-38(6)
C12	N12	C13	C14	-79.3(19)
C12	N12	C13	C14B	-76(3)
C12	C11	N11	Ni1	-46(3)
C12	C11B	O11B	Ni1	-21(7)
C13	N12	C12	C11	85(2)
C13	N12	C12	C11B	89(3)
C13	C14	O11	Ni1	21(4)
C13	C14B	N11B	Ni1	11(6)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H7	-1269.14	4840.12	1483.28	29
H8	3935.21	4922.36	-664.07	29
H9	6056.3	2309.38	3137.68	42
H10	5851.76	7408.45	3220.66	55
H12	1899.41	6515.16	5690.99	36
H12A	-53.19	8087.06	5761.67	50
H12B	-108.32	7076.99	6514.8	50

Atom	x	y	z	U_{eq}
H12C	-139.03	8088.82	5723.93	50
H12D	-91.91	7120.57	6520.31	50
H13A	1537.01	7967.82	4465.4	52
H13B	2436.97	6807.4	4191.12	52
H13C	1592.93	7962.7	4460.43	52
H13D	2391.23	6769.7	4155.76	52
H11A	-2723.68	7391.81	6021.96	36
H11B	-2213.12	7267.64	4938.83	36
H14A	-703.21	7456.73	3688.41	37
H14B	709.14	7057	3003.76	37
H11C	-2950.7	5459.01	5398.11	30
H11D	-2058.29	5523.87	6285.11	30
H11	-500(70)	5490(30)	3159(14)	37
H11E	-2642	7074.64	6079.87	36
H11F	-2233.06	7331.85	5015.12	36
H14C	526.31	7016.24	3052.25	37
H14D	-725.73	7552.22	3771.67	37
H11G	-459.16	5348.29	3280.68	30
H11H	-1794.3	5889.1	3784.24	30
H11I	-3060(50)	5830(80)	5010(30)	37

Table S7: Hydrogen Bond information for **MAB4**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O7	H7	O8[1]	0.84	1.97	2.804(2)	169.1
O8	H8	O3[2]	0.84	1.84	2.678(3)	174.1
O9	H9	O6[3]	0.84	1.91	2.740(3)	171.2
O10	H10	O4[4]	0.84	1.89	2.726(3)	170.6
N12	H12	O9[5]	1.00	2.05	2.973(3)	152.8
N11	H11D	O1[6]	0.91	2.07	2.975(8)	174.6
O11	H11	O7	0.861(13)	1.913(18)	2.770(9)	173(6)
N11B	H11G	O7	0.91	2.02	2.866(17)	154.5
N11B	H11H	O5[7]	0.91	2.23	2.981(13)	139.1
N11B	H11H	O10[7]	0.91	2.16	3.001(12)	154.0
O11B	H11I	O5[7]	0.878(14)	2.50(5)	3.125(9)	128(5)
O11B	H11I	O10[7]	0.878(14)	2.49(6)	3.220(9)	141(7)

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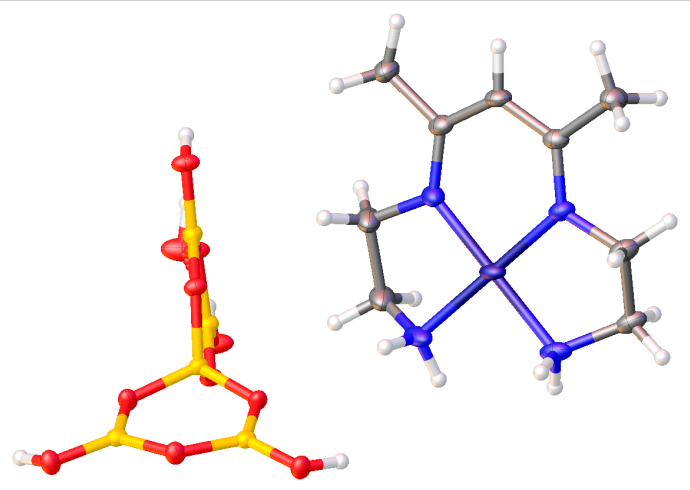
[1]-x,1-y,-z; [2]1-x,1-y,-z; [3]1-x,-1/2+y,1/2-z; [4]1-x,1/2+y,1/2-z; [5]1-x,1-y,1-z; [6]-x,1-y,1-z; [7]-1+x,+y,+z

Table S8: Atomic Occupancies for all atoms that are not fully occupied in **MAB4**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
H12A	0.603(11)	C11	0.603(11)	H11D	0.603(11)	H14D	0.397(11)
H12B	0.603(11)	H11A	0.603(11)	O11	0.603(11)	N11B	0.397(11)
H12C	0.397(11)	H11B	0.603(11)	H11	0.603(11)	H11G	0.397(11)
H12D	0.397(11)	C14	0.603(11)	C11B	0.397(11)	H11H	0.397(11)
H13A	0.603(11)	H14A	0.603(11)	H11E	0.397(11)	O11B	0.397(11)
H13B	0.603(11)	H14B	0.603(11)	H11F	0.397(11)	H11I	0.397(11)
H13C	0.397(11)	N11	0.603(11)	C14B	0.397(11)		
H13D	0.397(11)	H11C	0.603(11)	H14C	0.397(11)		

Compound **5**



Crystal Data. $C_9H_{25}B_5N_4NiO_{11}$, M_r = 478.09, triclinic, *P*-1 (No. 2), a = 8.5386(2) Å, b = 11.3328(3) Å, c = 11.8717(3) Å, α = 115.914(3)°, β = 101.626(2)°, γ = 99.670(2)°, V = 968.39(5) Å^3, T = 100(2) K, Z = 2, Z' = 1, μ(Mo K$_\alpha$) = 1.065, 16639 reflections measured, 4433 unique (R_{int} = 0.0216) which were used in all calculations. The final wR_2 was 0.0765 (all data) and R_1 was 0.0278 (I≥2 σ(I)).

Compound	**MAB5**
Formula	$C_9H_{25}B_5N_4NiO_{11}$
$D_{calc.}$/ g cm^{-3}	1.640
μ/mm^{-1}	1.065
Formula Weight	478.09
Colour	pink
Shape	block-shaped
Size/mm^3	0.05×0.04×0.04
T/K	100(2)
Crystal System	triclinic
Space Group	*P*-1
a/Å	8.5386(2)
b/Å	11.3328(3)
c/Å	11.8717(3)
α/°	115.914(3)
β/°	101.626(2)
γ/°	99.670(2)
V/Å^3	968.39(5)
Z	2
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/°	2.545
Θ_{max}/°	27.481
Measured Refl's.	16639
Indep't Refl's	4433
Refl's I≥2 σ(I)	4042
R_{int}	0.0216
Parameters	280
Restraints	0
Largest Peak	0.459
Deepest Hole	-0.318
GooF	1.036
wR_2 (all data)	0.0765
wR_2	0.0745
R_1 (all data)	0.0314
R_1	0.0278

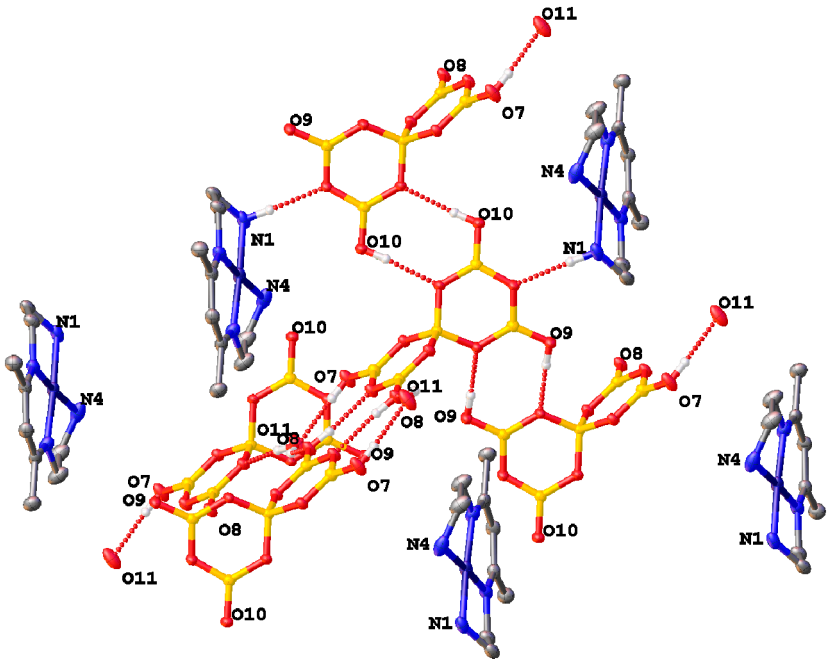


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ˚ are present in **MAB5**: N1–O5_*1: 2.958 Å, N1–O1*_2: 3.375 Å, N4–O1_*2: 2.952 Å, O7–O11: 2.654 Å, O8–O2*_3: 2.793 Å, O9–O4_*4: 2.696 Å, O10–O6*_1: 2.756 Å, O11–O3_*5: 2.739 Å, O11–O8*_3: 2.781 Å.

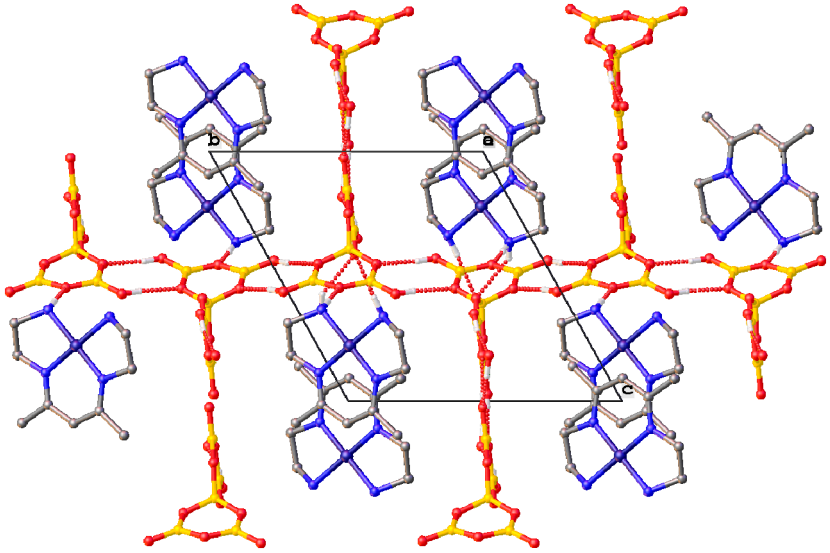


Figure S2: Packing diagram of MAB5.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB5**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
C1	3718(2)	-615.8(19)	3117.5(16)	24.8(3)
C2	4111(2)	-1153.5(19)	1832.7(16)	24.3(3)
C3	3105.3(19)	-1054.7(17)	-163.1(15)	19.8(3)
C4	2414(2)	-487.7(17)	-901.6(15)	21.6(3)
C5	1919(2)	696.8(17)	-412.6(15)	20.6(3)

Atom	x	y	z	U_{eq}
C6	1662(3)	2744.9(19)	1287.1(18)	32.4(4)
C7	1635(3)	3230(2)	2683.9(18)	34.5(4)
C8	3524(2)	-2366.9(18)	-884.5(17)	26.3(4)
C9	1096(2)	1097.8(19)	-1384.5(16)	26.7(4)
B1	8857.0(19)	6855.1(17)	3903.0(15)	12.9(3)
B2	5765(2)	6324.8(18)	3147.5(16)	16.0(3)
B3	7216(2)	5750.7(17)	1543.0(16)	13.9(3)
B4	11416(2)	8830.2(17)	5173.6(15)	14.0(3)
B5	11425(2)	6739.7(17)	5206.7(16)	13.8(3)
N1	4033.2(17)	876.5(16)	3642.7(13)	23.8(3)
N2	3364.8(16)	-499.1(15)	1122.6(13)	19.6(3)
N3	2143.2(17)	1470.7(14)	858.6(13)	21.0(3)
N4	3080(2)	2989.5(15)	3369.7(14)	30.4(3)
O1	7224.0(12)	6748.4(11)	4103.5(10)	14.2(2)
O2	5727.1(12)	5829.4(11)	1831.6(10)	16.0(2)
O3	8673.6(12)	6180.6(11)	2483.7(10)	14.1(2)
O4	9759.8(12)	8310.4(11)	4501.1(10)	15.1(2)
O5	12284.9(12)	8019.2(11)	5456.7(10)	15.5(2)
O6	9768.7(12)	6193.7(10)	4512.4(10)	14.5(2)
O7	4370.0(14)	6376.3(14)	3497.9(11)	26.2(3)
O8	7211.7(13)	5216.0(12)	264.7(10)	17.7(2)
O9	12279.7(12)	10144.6(11)	5622.5(11)	16.8(2)
O10	12297.0(13)	6097.2(11)	5710.6(11)	17.1(2)
O11	1554.4(14)	6058.4(15)	1815.2(12)	32.6(3)
Ni1	3143.8(2)	1183.3(2)	2210.1(2)	19.48(7)

Table S2: Anisotropic Displacement Parameters (×10⁴) for **MAB5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	19.4(7)	38.2(10)	18.4(7)	16.6(7)	4.4(6)	6.0(7)
C2	21.6(8)	35.4(10)	19.7(8)	15.7(7)	6.8(6)	10.3(7)
C3	18.3(7)	23.2(8)	15.3(7)	7.5(6)	6.5(6)	3.3(6)
C4	24.7(8)	24.4(8)	12.5(7)	7.1(6)	6.3(6)	4.3(6)
C5	21.6(7)	23.0(8)	15.5(7)	9.6(6)	6.5(6)	1.5(6)
C6	56.8(12)	22.1(9)	23.7(9)	11.4(7)	20.7(8)	14.1(8)
C7	60.5(13)	23.6(9)	24.2(9)	10.6(8)	22.7(9)	15.1(9)
C8	31.6(9)	27.1(9)	20.2(8)	10.0(7)	9.6(7)	10.9(7)
C9	36.1(9)	27.2(9)	19.6(8)	12.9(7)	10.1(7)	10.0(7)
B1	12.8(7)	14.5(8)	11.5(7)	6.8(6)	2.5(5)	4.7(6)
B2	15.3(7)	18.7(8)	13.4(7)	7.2(6)	5.0(6)	5.0(6)
B3	14.3(7)	15.1(8)	13.8(7)	7.7(6)	5.1(6)	5.3(6)
B4	14.2(7)	16.5(8)	12.1(7)	6.7(6)	4.8(6)	6.2(6)
B5	14.7(7)	15.5(8)	12.2(7)	6.6(6)	5.0(6)	6.5(6)
N1	16.1(6)	34.7(8)	13.5(6)	8.7(6)	3.3(5)	0.8(6)
N2	17.4(6)	25.8(7)	14.7(6)	10.0(6)	4.8(5)	4.3(5)
N3	27.6(7)	18.2(7)	16.7(6)	7.3(5)	10.4(5)	4.6(5)
N4	43.0(9)	23.4(7)	15.7(7)	4.8(6)	13.2(6)	-3.3(6)
O1	12.9(5)	18.5(5)	11.1(5)	7.0(4)	3.6(4)	4.8(4)
O2	11.9(5)	23.5(6)	10.8(5)	6.9(4)	3.0(4)	5.6(4)
O3	11.8(5)	19.2(5)	12.0(5)	7.6(4)	3.9(4)	5.7(4)
O4	12.7(5)	13.8(5)	16.9(5)	7.7(4)	0.6(4)	3.8(4)
O5	12.2(5)	15.6(5)	18.7(5)	8.8(4)	2.7(4)	5.1(4)
O6	14.1(5)	14.7(5)	14.4(5)	8.4(4)	0.9(4)	3.5(4)
O7	14.3(5)	44.1(8)	14.7(5)	9.9(5)	4.9(4)	7.6(5)
O8	12.5(5)	27.1(6)	11.7(5)	8.0(4)	3.5(4)	6.0(4)
O9	12.8(5)	14.8(5)	22.0(5)	8.8(4)	3.2(4)	4.9(4)
O10	15.4(5)	16.7(5)	19.7(5)	10.6(4)	2.0(4)	5.0(4)
O11	15.9(6)	52.2(9)	19.4(6)	7.5(6)	6.9(5)	11.5(6)
Ni1	20.08(11)	22.15(12)	10.75(10)	5.25(8)	5.44(8)	0.18(8)

Table S3: Bond Lengths in Å for **MAB5**.

Atom	Atom	Length/Å
C1	C2	1.508(2)
C1	N1	1.476(2)
C2	N2	1.468(2)
C3	C4	1.393(2)
C3	C8	1.504(2)
C3	N2	1.324(2)
C4	C5	1.388(2)
C5	C9	1.507(2)
C5	N3	1.324(2)
C6	C7	1.508(2)
C6	N3	1.468(2)
C7	N4	1.470(3)
B1	O1	1.4553(18)
B1	O3	1.4750(18)
B1	O4	1.4653(19)
B1	O6	1.4609(18)
B2	O1	1.3501(19)
B2	O2	1.4011(18)
B2	O7	1.3409(19)
B3	O2	1.3885(18)
B3	O3	1.3395(19)
B3	O8	1.3651(19)
B4	O4	1.3560(19)
B4	O5	1.3807(19)
B4	O9	1.351(2)
B5	O5	1.3814(19)
B5	O6	1.3610(19)
B5	O10	1.3513(19)
N1	Ni1	1.9171(14)
N2	Ni1	1.8453(14)
N3	Ni1	1.8461(14)
N4	Ni1	1.9218(15)

Table S4: Bond Angles in ° for **MAB5**.

Atom	Atom	Atom	Angle/°
N1	C1	C2	106.32(13)
N2	C2	C1	106.92(14)
C4	C3	C8	117.56(14)
N2	C3	C4	122.57(15)
N2	C3	C8	119.86(15)
C5	C4	C3	125.66(14)
C4	C5	C9	117.74(14)
N3	C5	C4	122.59(15)
N3	C5	C9	119.68(15)
N3	C6	C7	107.40(15)
N4	C7	C6	107.03(16)
O1	B1	O3	110.39(11)
O1	B1	O4	108.45(12)
O1	B1	O6	109.23(11)
O4	B1	O3	108.89(11)
O6	B1	O3	109.26(12)
O6	B1	O4	110.62(12)
O1	B2	O2	120.40(13)
O7	B2	O1	117.93(13)
O7	B2	O2	121.66(14)
O3	B3	O2	122.05(13)
O3	B3	O8	118.30(13)
O8	B3	O2	119.64(13)
O4	B4	O5	120.14(14)
O9	B4	O4	122.76(13)
O9	B4	O5	117.08(13)
O6	B5	O5	120.36(13)
O10	B5	O5	116.77(13)
O10	B5	O6	122.85(14)
C1	N1	Ni1	107.98(10)
C2	N2	Ni1	113.75(10)
C3	N2	C2	119.27(14)
C3	N2	Ni1	126.46(12)
C5	N3	C6	118.50(14)
C5	N3	Ni1	126.73(12)
C6	N3	Ni1	114.64(11)
C7	N4	Ni1	107.08(11)
B2	O1	B1	124.66(11)
B3	O2	B2	118.09(12)
B3	O3	B1	123.37(11)
B4	O4	B1	122.78(12)
B4	O5	B5	119.65(12)
B5	O6	B1	122.53(12)
N1	Ni1	N4	92.81(7)
N2	Ni1	N1	86.46(6)
N2	Ni1	N3	95.21(6)
N2	Ni1	N4	175.96(6)
N3	Ni1	N1	175.85(6)
N3	Ni1	N4	85.79(6)

Table S5: Torsion Angles in ° for **MAB5**.

Atom	Atom	Atom	Atom	Angle/°
C1	C2	N2	C3	-161.06(14)
C1	C2	N2	Ni1	26.63(16)
C2	C1	N1	Ni1	42.62(14)
C2	N2	Ni1	N1	-2.27(11)
C2	N2	Ni1	N3	-178.45(11)
C3	C4	C5	C9	-176.21(15)
C3	C4	C5	N3	3.8(3)
C3	N2	Ni1	N1	-173.92(14)

Atom	Atom	Atom	Atom	Angle/°
C3	N2	Ni1	N3	9.90(14)
C4	C3	N2	C2	-179.52(14)
C4	C3	N2	Ni1	-8.3(2)
C4	C5	N3	C6	176.61(15)
C4	C5	N3	Ni1	0.9(2)
C5	N3	Ni1	N2	-6.27(14)
C5	N3	Ni1	N4	169.80(14)
C6	C7	N4	Ni1	-44.71(16)
C6	N3	Ni1	N2	177.91(12)
C6	N3	Ni1	N4	-6.02(12)
C7	C6	N3	C5	166.08(16)
C7	C6	N3	Ni1	-17.7(2)
C8	C3	C4	C5	178.57(15)
C8	C3	N2	C2	2.0(2)
C8	C3	N2	Ni1	173.22(11)
C9	C5	N3	C6	-3.4(2)
C9	C5	N3	Ni1	-179.07(11)
N1	C1	C2	N2	-44.11(17)
N2	C3	C4	C5	0.0(3)
N3	C6	C7	N4	40.1(2)
O1	B1	O3	B3	10.50(19)
O1	B1	O4	B4	140.31(13)
O1	B1	O6	B5	-138.62(13)
O1	B2	O2	B3	1.9(2)
O2	B2	O1	B1	5.9(2)
O2	B3	O3	B1	-4.2(2)
O3	B1	O1	B2	-11.38(19)
O3	B1	O4	B4	-99.54(14)
O3	B1	O6	B5	100.54(15)
O3	B3	O2	B2	-2.6(2)
O4	B1	O1	B2	107.83(15)
O4	B1	O3	B3	-108.45(15)
O4	B1	O6	B5	-19.32(18)
O4	B4	O5	B5	-8.4(2)
O5	B4	O4	B1	-7.8(2)
O5	B5	O6	B1	5.5(2)
O6	B1	O1	B2	-131.54(14)
O6	B1	O3	B3	130.64(14)
O6	B1	O4	B4	20.54(18)
O6	B5	O5	B4	9.6(2)
O7	B2	O1	B1	-175.11(14)
O7	B2	O2	B3	-177.08(15)
O8	B3	O2	B2	177.10(13)
O8	B3	O3	B1	176.02(13)
O9	B4	O4	B1	173.87(13)
O9	B4	O5	B5	169.97(12)
O10	B5	O5	B4	-168.78(13)
O10	B5	O6	B1	-176.21(13)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB5**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1A	2537.22	-1054.32	2971.42	30
H1B	4443.53	-807.18	3741.69	30
H2A	5335.39	-923.25	1997.97	29
H2B	3633.42	-2162.45	1309.58	29
H4	2269.56	-952.06	-1819.63	26
H6A	544.53	2576.71	707.69	39
H6B	2477.76	3446.84	1247.06	39
H7A	1713.39	4218.27	3121.76	41

Atom	x	y	z	U_{eq}
H7B	583.9	2714.82	2692.75	41
H8A	4672.07	-2272.55	-437.31	40
H8B	3419.06	-2563.28	-1790.8	40
H8C	2751.99	-3120.04	-895.68	40
H9A	-68.69	1033.13	-1403.77	40
H9B	1130.82	479.22	-2263.03	40
H9C	1692.03	2041.87	-1118.72	40
H1C	5150.25	1307.1	4010.1	29
H1D	3528.87	1215.82	4273.56	29
H4A	2968.69	3046.4	4136.83	36
H4B	4039.16	3626.46	3559	36
H7	3559.85	6152.26	2837.85	39
H8	6228.08	4956.84	-232.21	27
H9	11610.34	10587.97	5540.14	25
H10	11640.38	5388.28	5602.16	26
H11A	586.45	5981.91	1945.8	49
H11B	1423.16	5556.29	984.41	49

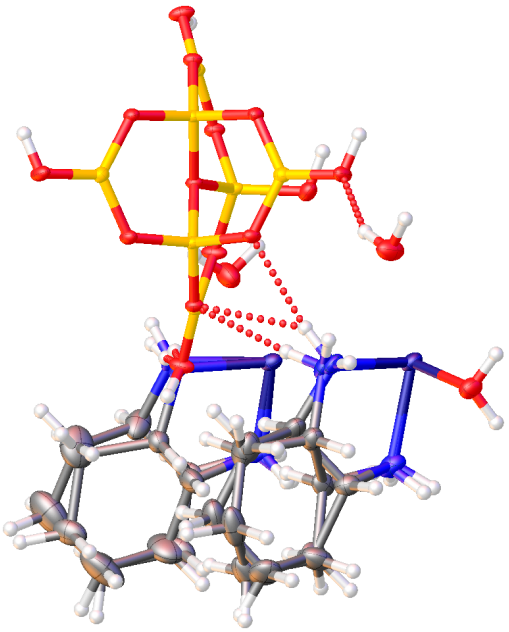
Table S7: Hydrogen Bond information for **MAB5**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1C	O5[1]	0.91	2.06	2.9576(17)	169.4
N1	H1D	O1[2]	0.91	2.56	3.3749(18)	149.1
N4	H4A	O1[2]	0.91	2.04	2.9520(17)	177.8
O7	H7	O11	0.84	1.85	2.6542(17)	161.1
O8	H8	O2[3]	0.84	1.98	2.7930(15)	161.9
O9	H9	O4[4]	0.84	1.86	2.6955(14)	175.1
O10	H10	O6[1]	0.84	1.92	2.7558(15)	175.7
O11	H11A	O3[5]	0.87	1.88	2.7395(15)	168.7
O11	H11B	O8[3]	0.87	2.06	2.7813(16)	140.5

––––

[1]2-x,1-y,1-z; [2]1-x,1-y,1-z; [3]1-x,1-y,-z; [4]2-x,2-y,1-z; [5]-1+x,+y,+z

Compound **6**



Crystal Data. $C_{12}H_{39}B_7N_4NiO_{17}$, M_r = 645.85, monoclinic, $C2/c$ (No. 15), a = 22.3539(4) Å, b = 11.0192(2) Å, c = 22.8834(4) Å, β = 107.630(2)°, α = γ = 90°, V = 5371.94(18) Å^3, T = 100(2) K, Z = 8, Z' = 1, μ(Mo K$_\alpha$) = 0.806, 33628 reflections measured, 6154 unique (R_{int} = 0.0281) which were used in all calculations. The final wR_2 was 0.1087 (all data) and R_1 was 0.0384 (I≥2 σ(I)).

Compound	**MAB6**
Formula	$C_{12}H_{39}B_7N_4NiO_{17}$
$D_{calc.}$/ g cm^{-3}	1.597
μ/mm^{-1}	0.806
Formula Weight	645.85
Colour	orange
Shape	prism-shaped
Size/mm^3	0.15×0.15×0.09
T/K	100(2)
Crystal System	monoclinic
Space Group	$C2/c$
a/Å	22.3539(4)
b/Å	11.0192(2)
c/Å	22.8834(4)
α/°	90
β/°	107.630(2)
γ/°	90
V/Å^3	5371.94(18)
Z	8
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/°	2.159
Θ_{max}/°	27.483
Measured Refl's.	33628
Indep't Refl's	6154
Refl's I≥2 σ(I)	5759
R_{int}	0.0281
Parameters	519
Restraints	1247
Largest Peak	0.842
Deepest Hole	-0.714
GooF	1.051
wR_2 (all data)	0.1087
wR_2	0.1072
R_1 (all data)	0.0408
R_1	0.0384

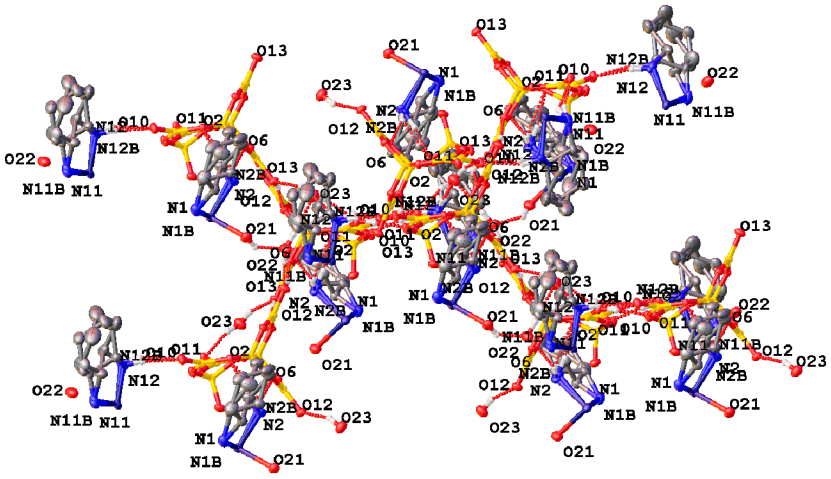


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ˚ are present in **MAB6**: O21–O22_*1: 2.697 Å, O21–O3*_6: 3.213 Å, O21–O14_*6: 2.981 Å, N1–O22*_7: 3.251 Å, N1–O14_*6: 3.199 Å, N2–O2: 3.101 Å, N2–O6: 2.938 Å, N1B–O22*_7: 3.268 Å, N1B–O14_*6: 3.191 Å, N2B–O2: 3.288 Å, N2B–O6: 2.986 Å, N11–O3*_7: 2.963 Å, N11–O11_*9: 3.001 Å, N12–O10: 2.821 Å, N12–O23*_10: 3.114 Å, N11B–O3_*7: 3.017 Å, N11B–O11*_9: 3.077 Å, N12B–O10: 2.986 Å, N12B–O23_*10: 2.868 Å, O10–O8*_8: 2.694 Å, O11–O5_*2: 2.71 Å, O12–O9*_3: 2.77 Å, O13–O7_*4: 2.69 Å, O22–O23*_10: 2.837 Å, O22–O13_*5: 2.809 Å, O23–O12: 2.796 Å, O23–O11*_3: 2.811 Å.

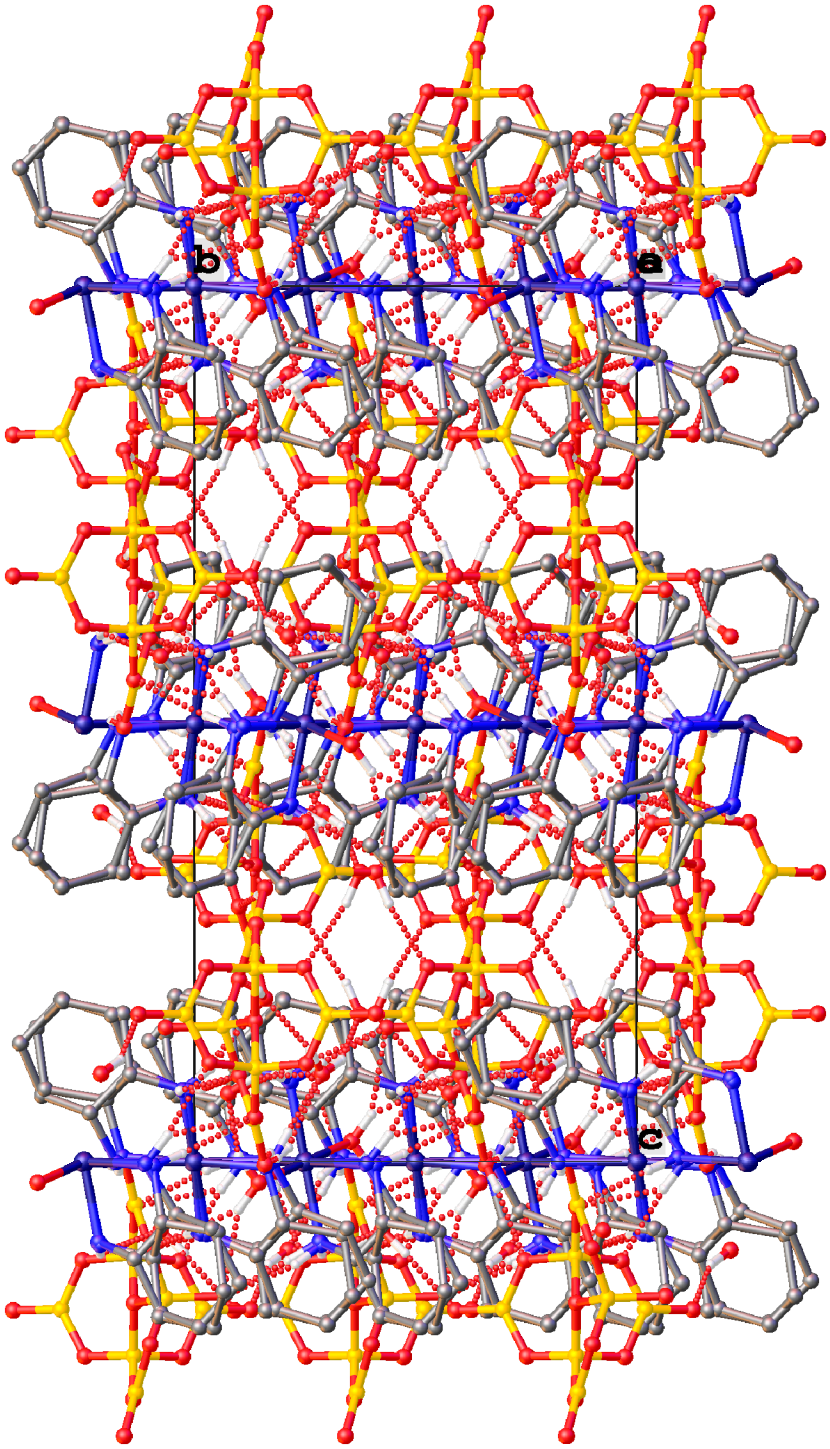


Figure S2: Packing diagram of MAB6.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB6**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ni1	7500	2500	5000	17.99(10)
O21	8346.5(7)	1451.2(14)	5235.0(7)	23.4(3)
N1	7700(7)	2875(13)	5949(7)	22.3(13)
N2	8055(6)	4073(10)	5045(3)	20.1(13)
C1	8014(2)	4074(4)	6097.1(17)	22.8(9)
C2	8438(2)	4263(4)	5690.8(19)	23.8(9)

Atom	x	y	z	U_{eq}
C3	8750(6)	5514(10)	5803(3)	34.0(15)
C4	9136(2)	5660(5)	6477(3)	42.0(13)
C5	8733(3)	5432(6)	6889(3)	44.3(17)
C6	8399(6)	4200(10)	6767(3)	39(3)
N1B	7690(11)	2830(20)	5915(10)	21.4(18)
N2B	8096(10)	3898(16)	5023(5)	21(2)
C1B	8244(3)	3644(6)	6107(2)	23.3(14)
C2B	8182(4)	4588(6)	5600(3)	27.1(15)
C3B	8770(8)	5393(16)	5764(5)	30.9(19)
C4B	8864(5)	6017(7)	6382(3)	39.7(18)
C5B	8910(5)	5107(9)	6889(4)	45(3)
C6B	8349(7)	4234(12)	6730(4)	25(3)
Ni2	5000	5000	5000	16.09(10)
N11	4948(8)	5151(7)	5814(5)	20.6(11)
N12	5275(4)	6634(7)	5058(2)	16.8(11)
C11	5002.4(19)	6453(4)	5998.8(18)	21.5(8)
C12	5472.6(18)	7004(3)	5711.6(15)	22.8(8)
C13	5534(4)	8377(5)	5832(2)	28.0(12)
C14	5753(2)	8574(5)	6530(2)	36.1(11)
C15	5313(2)	7983(4)	6836(2)	36.7(10)
C16	5243(3)	6620(6)	6693(2)	30.6(13)
N11B	4948(16)	5272(16)	5821(11)	21(2)
N12B	5184(11)	6766(18)	4994(5)	16.8(11)
C11B	5285(6)	6410(7)	6066(4)	33(2)
C12B	5139(5)	7362(7)	5561(4)	36(2)
C13B	5591(12)	8449(16)	5761(8)	53(4)
C14B	5507(7)	8939(11)	6355(6)	66(3)
C15B	5632(7)	8004(11)	6856(5)	67(3)
C16B	5228(12)	6857(15)	6677(7)	56(5)
O1	6846.4(6)	6368.3(11)	3390.3(5)	9.8(2)
O2	7285.0(6)	6363.2(12)	4491.7(5)	11.8(3)
O3	6182.8(6)	6011.7(13)	4015.6(6)	16.6(3)
O4	6422.6(6)	6393.6(12)	2286.0(6)	11.8(2)
O5	5755.1(6)	6005.5(12)	2915.9(6)	13.0(3)
O6	7826.7(6)	5344.8(12)	3869.1(6)	12.3(2)
O7	7361.4(6)	5271.0(11)	2774.9(6)	11.5(2)
O8	7763.3(6)	7533.3(11)	3879.4(6)	12.3(3)
O9	7361.8(6)	7480.5(11)	2783.6(6)	11.2(2)
O10	6528.4(6)	6588.4(13)	5032.4(6)	17.0(3)
O11	5337.7(6)	6590.5(13)	1870.3(6)	16.7(3)
O12	8064.5(7)	3733.4(12)	3314.1(6)	16.1(3)
O13	8018.1(7)	9099.1(12)	3306.0(6)	17.0(3)
O14	6396.4(7)	4349.1(12)	3467.9(6)	18.7(3)
B1	6285.2(9)	5656.2(19)	3445.3(9)	12.5(4)
B2	7444.4(9)	6389.4(18)	3926.8(9)	10.9(4)
B3	6994.7(9)	6377.3(18)	2790.6(9)	10.0(4)
B4	6682.1(10)	6338.5(19)	4510.8(9)	13.0(4)
B5	5847.4(10)	6328.8(18)	2370.8(9)	12.4(4)
B6	7746.6(9)	4803.9(19)	3316.5(9)	12.0(4)
B7	7710.0(9)	8021.3(18)	3318.5(9)	12.2(4)
O22	3632.6(6)	5764.8(15)	4220.3(8)	30.7(4)
O23	9249.1(6)	2883.2(15)	3994.0(7)	27.2(3)

Table S2: Anisotropic Displacement Parameters (×10^4) for **MAB6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	18.70(19)	18.77(19)	15.43(18)	5.65(13)	3.57(14)	0.20(13)
O21	26.4(8)	22.7(7)	19.5(7)	4.2(6)	4.7(6)	4.8(6)
N1	22(2)	28(2)	16(2)	5(2)	4.1(19)	0.7(19)
N2	22(2)	15(3)	22.0(18)	7.0(15)	4.3(15)	1(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	19(2)	22(2)	24.9(18)	-2.7(15)	2.6(15)	8.4(15)
C2	24(2)	21(2)	22.5(19)	1.9(15)	1.0(17)	-0.6(16)
C3	32(2)	20(3)	46(2)	2(2)	5(2)	-4(2)
C4	25(2)	25(2)	66(3)	-9(2)	-3(2)	3.2(19)
C5	36(3)	40(3)	44(3)	-17(3)	-7(2)	5(2)
C6	39(5)	48(5)	23(3)	-7(3)	0(3)	1(4)
N1B	20(3)	27(3)	17(3)	4(3)	6(3)	-1(3)
N2B	24(3)	18(4)	19(2)	8(2)	3(2)	3(3)
C1B	22(3)	28(3)	19(2)	2(2)	5(2)	-1(2)
C2B	30(4)	23(3)	21(3)	5(2)	-1(3)	0(3)
C3B	29(3)	21(3)	39(3)	2(3)	4(3)	4(3)
C4B	40(5)	24(3)	48(4)	-5(3)	5(3)	-2(3)
C5B	46(6)	46(6)	28(4)	3(4)	-9(4)	-6(4)
C6B	23(5)	27(5)	27(5)	-4(4)	11(4)	13(3)
Ni2	14.41(18)	20.47(19)	12.87(17)	3.02(13)	3.35(13)	-2.94(13)
N11	18.1(17)	26(2)	16.1(17)	0.4(17)	3.0(15)	-5.4(17)
N12	13(3)	18(2)	18.1(13)	7.5(14)	2.3(16)	2.8(16)
C11	14.4(18)	29.6(18)	21.1(16)	-4.4(13)	6.3(15)	-7.8(15)
C12	25.8(18)	20.5(16)	23.0(16)	-1.1(12)	8.8(13)	-1.1(14)
C13	27(3)	25(2)	31(2)	0.9(17)	8.0(19)	0.0(18)
C14	31(2)	47(3)	30(2)	-9.2(19)	9.2(18)	-16(2)
C15	33(2)	42(2)	35(2)	-14.8(17)	11.1(19)	-4.1(19)
C16	23(2)	40(3)	29(2)	-10.1(19)	8.8(19)	-11.9(18)
N11B	19(3)	29(3)	15(3)	4(3)	5(3)	-5(3)
N12B	13(3)	18(2)	18.1(13)	7.5(14)	2.3(16)	2.8(16)
C11B	43(6)	28(4)	27(4)	-8(3)	10(4)	-12(4)
C12B	48(5)	29(4)	40(4)	6(3)	30(4)	8(3)
C13B	47(7)	49(7)	76(8)	-4(6)	38(7)	6(5)
C14B	57(8)	65(7)	81(8)	-35(5)	26(6)	-25(6)
C15B	52(7)	81(7)	62(6)	-43(5)	8(6)	-11(6)
C16B	80(10)	62(8)	38(6)	-11(5)	34(7)	-10(7)
O1	10.1(6)	12.6(6)	6.3(5)	0.3(4)	2.0(4)	-1.0(4)
O2	12.9(6)	15.2(6)	7.2(5)	0.4(5)	2.6(5)	-0.2(5)
O3	13.9(6)	27.8(7)	8.4(6)	-1.1(5)	3.7(5)	-6.0(5)
O4	11.2(6)	15.7(6)	7.6(5)	0.3(5)	1.7(5)	0.3(5)
O5	11.3(6)	18.2(6)	8.5(6)	0.7(5)	1.5(5)	-1.1(5)
O6	12.9(6)	14.4(6)	8.5(6)	0.0(5)	1.5(5)	2.4(5)
O7	14.7(6)	11.0(6)	8.3(6)	-0.3(5)	3.0(5)	1.9(5)
O8	13.3(6)	13.4(6)	8.8(6)	0.4(5)	1.2(5)	-3.1(5)
O9	13.9(6)	11.3(6)	8.0(6)	0.7(4)	2.6(5)	-1.3(5)
O10	14.8(6)	26.5(7)	9.9(6)	-3.5(5)	4.2(5)	-4.4(5)
O11	10.9(6)	27.9(7)	9.9(6)	4.3(5)	1.2(5)	-0.3(5)
O12	20.4(7)	14.9(6)	10.8(6)	-1.1(5)	1.5(5)	5.3(5)
O13	21.8(7)	16.5(7)	10.1(6)	2.1(5)	0.7(5)	-7.1(5)
O14	22.1(7)	14.6(6)	16.2(7)	3.1(5)	1.0(5)	-2.6(5)
B1	12.1(9)	16.9(9)	7.3(8)	1.3(7)	1.2(7)	-2.5(7)
B2	12.1(9)	12.9(9)	7.1(8)	0.3(7)	2.1(7)	0.0(7)
B3	11.8(9)	11.3(9)	6.9(8)	-0.2(7)	2.7(7)	0.3(7)
B4	15.5(9)	14.0(9)	9.4(8)	0.4(7)	3.8(7)	-1.7(7)
B5	13.7(9)	13.1(9)	9.5(8)	-1.0(7)	2.2(7)	-1.2(7)
B6	12.4(9)	13.3(9)	10.5(9)	0.1(7)	3.5(7)	-1.0(7)
B7	13.6(9)	11.2(9)	11.4(9)	0.7(7)	3.1(7)	0.2(7)
O22	41.4(10)	25.5(8)	27.2(8)	-6.7(7)	13.5(7)	-9.5(7)
O23	28.3(8)	32.2(8)	19.1(7)	-1.7(6)	4.4(6)	9.8(7)

Table S3: Bond Lengths in Å for **MAB6**.

Atom	Atom	Length/Å
Ni1	O21	2.1422(15)
Ni1	O21[1]	2.1421(15)
Ni1	N1	2.121(15)
Ni1	N1[1]	2.121(15)
Ni1	N2	2.116(13)
Ni1	N2[1]	2.116(13)

Atom	Atom	Length/Å
Ni1	N1B	2.04(2)
Ni1	N2B	2.03(2)
Ni1	N2B[1]	2.03(2)
N1	C1	1.487(7)
N2	C2	1.482(6)
C1	C2	1.529(5)
C1	C6	1.520(6)
C2	C3	1.531(7)
C3	C4	1.530(7)
C4	C5	1.510(7)
C5	C6	1.534(7)
N1B	C1B	1.486(8)
N2B	C2B	1.486(7)
C1B	C2B	1.533(6)
C1B	C6B	1.520(7)
C2B	C3B	1.534(8)
C3B	C4B	1.530(8)
C4B	C5B	1.513(7)
C5B	C6B	1.535(8)
Ni2	N11	1.908(12)
Ni2	N11[2]	1.908(12)
Ni2	N12	1.894(9)
Ni2	N12[2]	1.894(9)
Ni2	N11B[2]	1.94(2)
Ni2	N11B	1.94(2)
Ni2	N12B	1.99(2)
Ni2	N12B[2]	1.99(2)
N11	C11	1.490(6)
N12	C12	1.483(5)
C11	C12	1.524(4)
C11	C16	1.527(5)
C12	C13	1.536(6)
C13	C14	1.536(5)
C14	C15	1.515(5)
C15	C16	1.535(6)
N11B	C11B	1.482(8)
N12B	C12B	1.484(7)
C11B	C12B	1.522(7)
C11B	C16B	1.522(8)
C12B	C13B	1.544(9)
C13B	C14B	1.526(9)
C14B	C15B	1.503(9)
C15B	C16B	1.535(9)
O1	B1	1.517(2)
O1	B2	1.517(2)
O1	B3	1.506(2)
O2	B2	1.441(2)
O2	B4	1.362(2)
O3	B1	1.445(2)
O3	B4	1.376(2)
O4	B3	1.440(2)
O4	B5	1.359(2)
O5	B1	1.466(2)
O5	B5	1.372(2)
O6	B2	1.463(2)
O6	B6	1.360(2)
O7	B3	1.475(2)
O7	B6	1.377(2)
O8	B2	1.468(2)
O8	B7	1.363(2)
O9	B3	1.469(2)
O9	B7	1.372(2)
O10	B4	1.366(2)
O11	B5	1.379(2)
O12	B6	1.378(2)
O13	B7	1.378(2)
O14	B1	1.460(3)

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[1]3/2-x,1/2-y,1-z; [2]1-x,1-y,1-z

Table S4: Bond Angles in ° for **MAB6**.

Atom	Atom	Atom	Angle/°
O21[1]	Ni1	O21	180.0
N1[1]	Ni1	O21[1]	87.2(6)
N1[1]	Ni1	O21	92.8(6)
N1	Ni1	O21	87.2(6)
N1	Ni1	O21[1]	92.8(6)
N1[1]	Ni1	N1	180.0
N2	Ni1	O21[1]	91.7(4)
N2	Ni1	O21	88.3(4)
N2[1]	Ni1	O21	91.7(4)
N2[1]	Ni1	O21[1]	88.3(4)
N2	Ni1	N1[1]	98.5(2)
N2	Ni1	N1	81.5(2)
N2[1]	Ni1	N1	98.5(2)
N2[1]	Ni1	N1[1]	81.5(2)
N2	Ni1	N2[1]	180.0
N1B	Ni1	O21	86.8(9)
N2B[1]	Ni1	O21	96.9(6)
N2B	Ni1	O21	83.1(6)
N2B[1]	Ni1	N1B	95.3(3)
N2B	Ni1	N1B	84.7(3)
C1	N1	Ni1	110.2(7)
C2	N2	Ni1	108.5(6)
N1	C1	C2	108.7(7)
N1	C1	C6	113.2(7)
C6	C1	C2	109.6(6)
N2	C2	C1	108.0(6)
N2	C2	C3	113.0(6)
C1	C2	C3	110.8(5)
C4	C3	C2	110.7(7)
C5	C4	C3	110.4(6)
C4	C5	C6	112.6(6)
C1	C6	C5	111.0(7)
C1B	N1B	Ni1	107.8(12)
C2B	N2B	Ni1	108.6(11)
N1B	C1B	C2B	108.1(10)
N1B	C1B	C6B	114.4(11)
C6B	C1B	C2B	111.9(7)
N2B	C2B	C1B	106.4(9)
N2B	C2B	C3B	112.5(10)
C1B	C2B	C3B	109.4(8)
C4B	C3B	C2B	110.7(8)
C5B	C4B	C3B	111.7(9)
C4B	C5B	C6B	111.8(9)
C1B	C6B	C5B	111.9(8)

Atom	Atom	Atom	Angle/°
N11[2]	Ni2	N11	180.0(4)
N11[2]	Ni2	N11B[2]	3.9(7)
N11	Ni2	N11B[2]	176.1(7)
N11	Ni2	N12B[2]	90.3(4)
N11[2]	Ni2	N12B[2]	89.7(4)
N12	Ni2	N11[2]	92.1(2)
N12[2]	Ni2	N11	92.1(2)
N12[2]	Ni2	N11[2]	87.9(2)
N12	Ni2	N11	87.9(2)
N12	Ni2	N12[2]	180.0
N12	Ni2	N11B[2]	95.8(4)
N12[2]	Ni2	N11B[2]	84.2(4)
N12	Ni2	N12B[2]	173.0(8)
N12[2]	Ni2	N12B[2]	7.0(8)
N11B[2]	Ni2	N11B	180.0
N11B	Ni2	N12B[2]	94.1(5)
N11B	Ni2	N12B	85.9(5)
N11B[2]	Ni2	N12B[2]	85.9(5)
N11B[2]	Ni2	N12B	94.1(5)
N12B	Ni2	N12B[2]	180.0
C11	N11	Ni2	109.7(6)
C12	N12	Ni2	108.8(5)
N11	C11	C12	105.6(6)
N11	C11	C16	112.6(6)
C12	C11	C16	109.3(4)
N12	C12	C11	107.0(5)
N12	C12	C13	115.8(4)
C11	C12	C13	110.5(4)
C14	C13	C12	108.0(4)
C15	C14	C13	111.9(4)
C14	C15	C16	111.2(4)
C11	C16	C15	108.7(5)
C11B	N11B	Ni2	109.0(13)
C12B	N12B	Ni2	111.0(11)
N11B	C11B	C12B	109.1(11)
N11B	C11B	C16B	116.6(12)
C12B	C11B	C16B	114.6(10)
N12B	C12B	C11B	107.6(9)
N12B	C12B	C13B	113.0(11)
C11B	C12B	C13B	109.8(11)
C14B	C13B	C12B	107.0(10)
C15B	C14B	C13B	113.1(12)
C14B	C15B	C16B	113.8(11)
C11B	C16B	C15B	107.8(9)

Atom	Atom	Atom	Angle/°
B1	O1	B2	119.27(13)
B3	O1	B1	119.66(13)
B3	O1	B2	110.75(13)
B4	O2	B2	123.03(14)
B4	O3	B1	120.24(15)
B5	O4	B3	122.25(14)
B5	O5	B1	120.87(15)
B6	O6	B2	120.84(14)
B6	O7	B3	119.18(14)
B7	O8	B2	120.15(14)
B7	O9	B3	121.16(14)
O3	B1	O1	107.21(14)
O3	B1	O5	111.44(15)
O3	B1	O14	107.89(15)
O5	B1	O1	106.10(14)
O14	B1	O1	112.15(15)
O14	B1	O5	112.00(15)
O2	B2	O1	109.20(14)
O2	B2	O6	112.02(15)
O2	B2	O8	109.93(14)
O6	B2	O1	108.09(14)
O6	B2	O8	111.03(15)
O8	B2	O1	106.37(14)
O4	B3	O1	110.09(14)
O4	B3	O7	110.83(14)
O4	B3	O9	110.13(14)
O7	B3	O1	107.09(14)
O9	B3	O1	107.05(14)
O9	B3	O7	111.53(14)
O2	B4	O3	122.85(17)
O2	B4	O10	122.49(17)
O10	B4	O3	114.61(17)
O4	B5	O5	123.57(17)
O4	B5	O11	116.73(16)
O5	B5	O11	119.70(17)
O6	B6	O7	122.92(17)
O6	B6	O12	117.13(16)
O7	B6	O12	119.94(16)
O8	B7	O9	122.20(17)
O8	B7	O13	117.25(16)
O9	B7	O13	120.54(16)

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[1]3/2-x,1/2-y,1-z; [2]1-x,1-y,1-z

Table S5: Torsion Angles in ° for **MAB6**.

Atom	Atom	Atom	Atom	Angle/°
Ni1	N1	C1	C2	-35.0(12)
Ni1	N1	C1	C6	-157.0(8)
Ni1	N2	C2	C1	-44.6(8)
Ni1	N2	C2	C3	-167.5(7)
Ni1	N1B	C1B	C2B	39.8(18)
Ni1	N1B	C1B	C6B	165.2(11)
Ni1	N2B	C2B	C1B	41.8(13)
Ni1	N2B	C2B	C3B	161.6(11)
N1	C1	C2	N2	53.0(10)
N1	C1	C2	C3	177.3(10)
N1	C1	C6	C5	177.8(10)
N2	C2	C3	C4	179.7(9)
C1	C2	C3	C4	58.3(12)

Atom	Atom	Atom	Atom	Angle/°
C2	C1	C6	C5	56.3(11)
C2	C3	C4	C5	-55.5(12)
C3	C4	C5	C6	54.2(10)
C4	C5	C6	C1	-55.3(12)
C6	C1	C2	N2	177.2(7)
C6	C1	C2	C3	-58.5(9)
N1B	C1B	C2B	N2B	-54.3(17)
N1B	C1B	C2B	C3B	-176.1(15)
N1B	C1B	C6B	C5B	-177.6(15)
N2B	C2B	C3B	C4B	-176.0(13)
C1B	C2B	C3B	C4B	-58.0(17)
C2B	C1B	C6B	C5B	-54.2(14)
C2B	C3B	C4B	C5B	57.1(18)
C3B	C4B	C5B	C6B	-53.6(15)
C4B	C5B	C6B	C1B	52.0(16)
C6B	C1B	C2B	N2B	178.8(11)
C6B	C1B	C2B	C3B	57.0(12)
Ni2	N11	C11	C12	-36.3(10)
Ni2	N11	C11	C16	-155.5(6)
Ni2	N12	C12	C11	-40.0(5)
Ni2	N12	C12	C13	-163.6(5)
Ni2	N11B	C11B	C12B	41(2)
Ni2	N11B	C11B	C16B	172.8(16)
Ni2	N12B	C12B	C11B	27.3(15)
Ni2	N12B	C12B	C13B	148.7(14)
N11	Ni2	N12	C12	16.0(6)
N11[1]	Ni2	N12	C12	-164.0(6)
N11	C11	C12	N12	49.1(7)
N11	C11	C12	C13	175.9(7)
N11	C11	C16	C15	177.2(8)
N12	C12	C13	C14	-179.0(6)
C11	C12	C13	C14	59.2(7)
C12	C11	C16	C15	60.2(6)
C12	C13	C14	C15	-56.2(8)
C13	C14	C15	C16	56.8(7)
C14	C15	C16	C11	-57.6(7)
C16	C11	C12	N12	170.4(5)
C16	C11	C12	C13	-62.7(6)
N11B	C11B	C12B	N12B	-44.3(19)
N11B	C11B	C12B	C13B	-167.7(17)
N11B	C11B	C16B	C15B	177.6(19)
N12B	C12B	C13B	C14B	-178.2(15)
C11B	C12B	C13B	C14B	-58.0(19)
C12B	C11B	C16B	C15B	-53(2)
C12B	C13B	C14B	C15B	58(2)
C13B	C14B	C15B	C16B	-56.4(19)
C14B	C15B	C16B	C11B	51(2)
C16B	C11B	C12B	N12B	-177.1(14)
C16B	C11B	C12B	C13B	59.4(15)
B1	O1	B2	O2	-34.2(2)
B1	O1	B2	O6	87.86(18)
B1	O1	B2	O8	-152.84(14)
B1	O1	B3	O4	36.9(2)
B1	O1	B3	O7	-83.69(18)
B1	O1	B3	O9	156.58(14)
B1	O3	B4	O2	1.0(3)
B1	O3	B4	O10	-176.44(16)
B1	O5	B5	O4	-2.5(3)
B1	O5	B5	O11	176.53(16)
B2	O1	B1	O3	49.8(2)
B2	O1	B1	O5	168.98(14)
B2	O1	B1	O14	-68.45(19)

Atom	Atom	Atom	Atom	Angle/°
B2	O1	B3	O4	-178.30(14)
B2	O1	B3	O7	61.13(17)
B2	O1	B3	O9	-58.60(17)
B2	O2	B4	O3	18.0(3)
B2	O2	B4	O10	-164.80(17)
B2	O6	B6	O7	7.5(3)
B2	O6	B6	O12	-171.63(16)
B2	O8	B7	O9	0.2(3)
B2	O8	B7	O13	179.68(16)
B3	O1	B1	O3	-168.35(14)
B3	O1	B1	O5	-49.2(2)
B3	O1	B1	O14	73.41(19)
B3	O1	B2	O2	-179.21(14)
B3	O1	B2	O6	-57.11(17)
B3	O1	B2	O8	62.19(17)
B3	O4	B5	O5	-13.4(3)
B3	O4	B5	O11	167.63(16)
B3	O7	B6	O6	-2.8(3)
B3	O7	B6	O12	176.28(16)
B3	O9	B7	O8	3.8(3)
B3	O9	B7	O13	-175.64(16)
B4	O2	B2	O1	-0.7(2)
B4	O2	B2	O6	-120.42(18)
B4	O2	B2	O8	115.63(18)
B4	O3	B1	O1	-31.9(2)
B4	O3	B1	O5	-147.54(16)
B4	O3	B1	O14	89.12(19)
B5	O4	B3	O1	-3.9(2)
B5	O4	B3	O7	114.43(18)
B5	O4	B3	O9	-121.68(17)
B5	O5	B1	O1	30.8(2)
B5	O5	B1	O3	147.20(16)
B5	O5	B1	O14	-91.83(19)
B6	O6	B2	O1	22.5(2)
B6	O6	B2	O2	142.83(16)
B6	O6	B2	O8	-93.84(19)
B6	O7	B3	O1	-31.0(2)
B6	O7	B3	O4	-151.07(15)
B6	O7	B3	O9	85.84(18)
B7	O8	B2	O1	-32.2(2)
B7	O8	B2	O2	-150.32(16)
B7	O8	B2	O6	85.16(19)
B7	O9	B3	O1	25.3(2)
B7	O9	B3	O4	144.96(16)
B7	O9	B3	O7	-91.55(18)

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[1]1-x,1-y,1-z

Table S6: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **MAB6**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H21A	8349.09	1002.86	4930.42	35
H21B	8364.06	999.19	5544.41	35
H1A	7337.05	2877.01	6051.43	27
H1B	7953.74	2284.99	6171.55	27
H2A	8308.81	3979.7	4803.79	24
H2B	7803.25	4728.53	4907.9	24
H1	7684.66	4719.87	5998.42	27
H2	8775.21	3632.21	5799.04	29
H3A	9026.44	5613.32	5540.83	41

Atom	x	y	z	U_{eq}
H3B	8423.4	6152.43	5690.85	41
H4A	9491.09	5080.12	6577.89	50
H4B	9311.21	6491.88	6546.7	50
H5A	8414.52	6083.98	6825.42	53
H5B	8998.82	5466.3	7321.67	53
H6A	8714.26	3541.38	6877.82	47
H6B	8119.29	4118.09	7027.77	47
H1BA	7354.13	3184.09	5990.94	26
H1BB	7773.88	2118.08	6128.64	26
H2BA	8472.36	3608.9	5007.51	25
H2BB	7935.42	4391.49	4693.88	25
H1BC	8623.59	3141.83	6130.91	28
H2BC	7803.2	5102.84	5560.99	32
H3BA	9141.89	4890.47	5781.68	37
H3BB	8725.71	6014.6	5440.93	37
H4BA	9252.36	6509	6484.76	48
H4BB	8507.37	6571.67	6352.04	48
H5BA	8930.01	5545.31	7272.24	54
H5BB	9302.81	4634.29	6962.25	54
H6BA	8422.33	3594.94	7048.07	30
H6BB	7966.14	4685.72	6730.81	30
H11A	4574.45	4849.32	5830.67	25
H11B	5261.54	4717.3	6077.1	25
H12A	5602.26	6708.99	4902.11	20
H12B	4957.58	7121.72	4837.7	20
H11	4586.13	6862.44	5831.15	26
H12	5891.08	6627.34	5914.3	27
H13A	5843.29	8727.37	5648.15	34
H13B	5124.79	8780.19	5646.74	34
H14A	6179.2	8232.11	6704.08	43
H14B	5775.56	9455.87	6616.95	43
H15A	4896.54	8377.38	6690.31	44
H15B	5479.24	8102.05	7284.82	44
H16A	5652.75	6209.14	6861.31	37
H16B	4942.81	6257.28	6885.3	37
H11C	4539.33	5331.35	5810.25	25
H11D	5124.64	4637.5	6067.12	25
H12C	5577.42	6871.58	4963.67	20
H12D	4907.16	7117.73	4661.54	20
H11E	5740.06	6215.71	6147.85	39
H12E	4699.23	7654.62	5488.36	43
H13C	6030.34	8184.98	5828.67	64
H13D	5489.72	9085.27	5440.15	64
H14C	5795.97	9632.66	6498.31	80
H14D	5072.85	9243.35	6270.99	80
H15C	5553.98	8372.19	7220.3	81
H15D	6080.4	7769.5	6971.58	81
H16C	5376.84	6224.14	6995.07	67
H16D	4784.69	7043.98	6637.91	67
H10	6847.37	6842.54	5304.56	25
H11F	5005	6447.84	1956.5	25
H12F	7950.21	3434.16	2959.91	24
H13	7895.49	9392.56	2950.73	26
H14	6339.02	4084.83	3110.83	28
H22A	3736.34	6360.23	4033.62	46
H22B	3436.44	5237.63	3959.84	46
H23A	8929.92	3328.72	3832.16	41
H23B	9395.22	2616.81	3716.06	41

Table S7: Hydrogen Bond information for **MAB6**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O21	H21A	O22[1]	0.86	1.93	2.697(2)	148.0
O21	H21B	O3[2]	0.86	2.52	3.213(2)	139.0
O21	H21B	O14[2]	0.86	2.19	2.981(2)	152.8
N1	H1A	O22[3]	0.91	2.55	3.25(2)	134.2
N1	H1B	O14[2]	0.91	2.30	3.20(2)	167.7
N2	H2B	O2	0.91	2.20	3.100(12)	171.6
N2	H2B	O6	0.91	2.49	2.938(10)	110.9
N1B	H1BA	O22[3]	0.91	2.41	3.27(3)	158.3
N1B	H1BB	O14[2]	0.91	2.42	3.19(3)	141.9
N2B	H2BB	O2	0.91	2.58	3.288(19)	135.4
N2B	H2BB	O6	0.91	2.11	2.985(16)	161.4
N11	H11A	O3[3]	0.91	2.06	2.963(13)	170.6
N11	H11B	O11[4]	0.91	2.28	3.002(12)	135.7
N12	H12A	O10	0.91	2.00	2.821(9)	148.6
N12	H12B	O23[5]	0.91	2.26	3.11(2)	157.0
N11B	H11C	O3[3]	0.91	2.31	3.02(3)	134.3
N11B	H11D	O11[4]	0.91	2.21	3.08(3)	158.1
N12B	H12C	O10	0.91	2.11	2.99(2)	162.1
N12B	H12D	O23[5]	0.91	1.96	2.87(3)	174.1
O10	H10	O8[6]	0.84	1.93	2.6937(18)	150.2
O11	H11F	O5[7]	0.84	1.87	2.7105(19)	174.0
O12	H12F	O9[8]	0.84	1.94	2.7702(18)	169.1
O13	H13	O7[9]	0.84	1.86	2.6896(18)	171.2
O22	H22A	O23[5]	0.85	2.05	2.837	153.2
O22	H22B	O13[10]	0.85	1.96	2.809(2)	174.7
O23	H23A	O12	0.85	1.99	2.7955(19)	157.3
O23	H23B	O11[8]	0.85	1.98	2.8107(19)	165.2

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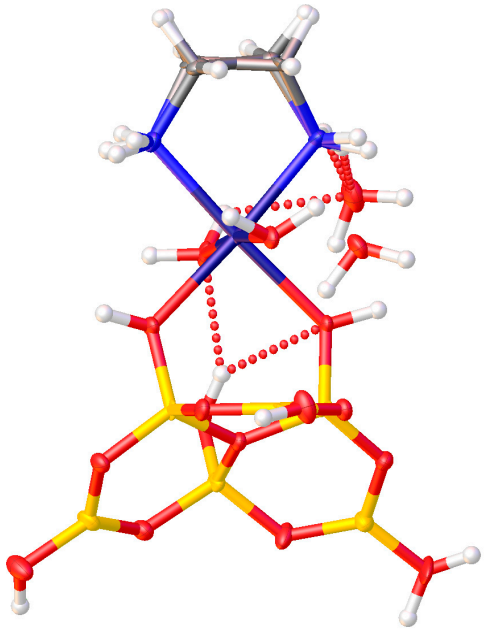
[1]1/2+x,-1/2+y,+z; [2]3/2-x,1/2-y,1-z; [3]1-x,1-y,1-z; [4]+x,1-y,1/2+z; [5]-1/2+x,1/2+y,+z; [6]3/2-x,3/2-y,1-z; [7]1-x,+y,1/2-z; [8]3/2-x,-1/2+y,1/2-z; [9]3/2-x,1/2+y,1/2-z; [10]-1/2+x,-1/2+y,+z

Table S8: Atomic Occupancies for all atoms that are not fully occupied in **MAB6**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
N1	0.602(8)	N1B	0.398(8)	N11	0.680(7)	N11B	0.320(7)
H1A	0.602(8)	H1BA	0.398(8)	H11A	0.680(7)	H11C	0.320(7)
H1B	0.602(8)	H1BB	0.398(8)	H11B	0.680(7)	H11D	0.320(7)
N2	0.602(8)	N2B	0.398(8)	N12	0.680(7)	N12B	0.320(7)
H2A	0.602(8)	H2BA	0.398(8)	H12A	0.680(7)	H12C	0.320(7)
H2B	0.602(8)	H2BB	0.398(8)	H12B	0.680(7)	H12D	0.320(7)
C1	0.602(8)	C1B	0.398(8)	C11	0.680(7)	C11B	0.320(7)
H1	0.602(8)	H1BC	0.398(8)	H11	0.680(7)	H11E	0.320(7)
C2	0.602(8)	C2B	0.398(8)	C12	0.680(7)	C12B	0.320(7)
H2	0.602(8)	H2BC	0.398(8)	H12	0.680(7)	H12E	0.320(7)
C3	0.602(8)	C3B	0.398(8)	C13	0.680(7)	C13B	0.320(7)
H3A	0.602(8)	H3BA	0.398(8)	H13A	0.680(7)	H13C	0.320(7)
H3B	0.602(8)	H3BB	0.398(8)	H13B	0.680(7)	H13D	0.320(7)
C4	0.602(8)	C4B	0.398(8)	C14	0.680(7)	C14B	0.320(7)
H4A	0.602(8)	H4BA	0.398(8)	H14A	0.680(7)	H14C	0.320(7)
H4B	0.602(8)	H4BB	0.398(8)	H14B	0.680(7)	H14D	0.320(7)
C5	0.602(8)	C5B	0.398(8)	C15	0.680(7)	C15B	0.320(7)
H5A	0.602(8)	H5BA	0.398(8)	H15A	0.680(7)	H15C	0.320(7)
H5B	0.602(8)	H5BB	0.398(8)	H15B	0.680(7)	H15D	0.320(7)
C6	0.602(8)	C6B	0.398(8)	C16	0.680(7)	C16B	0.320(7)
H6A	0.602(8)	H6BA	0.398(8)	H16A	0.680(7)	H16C	0.320(7)
H6B	0.602(8)	H6BB	0.398(8)	H16B	0.680(7)	H16D	0.320(7)

Compound **7**



Crystal Data. $C_2H_{20}B_6N_2NiO_{16}$, M_r = 451.77, triclinic, *P*-1 (No. 2), a = 8.5116(7) Å, b = 9.7946(5) Å, c = 9.8073(8) Å, α = 89.873(5)˚, β = 82.901(7)˚, γ = 74.372(6)˚, V = 780.94(10) Å^3, T = 100(2) K, Z = 2, Z' = 1, μ(Mo K$_\alpha$) = 1.333, 5883 reflections measured, 5883 unique (R_{int} = .) which were used in all calculations. The final wR_2 was 0.1902 (all data) and R_1 was 0.0682 (I≥2 σ(I)).

Compound	**MAB7**
Formula	$C_2H_{20}B_6N_2NiO_{16}$
$D_{calc.}$/ g cm^{-3}	1.921
μ/mm^{-1}	1.333
Formula Weight	451.77
Colour	light blue
Shape	blade-shaped
Size/mm^3	0.13×0.03×0.01
T/K	100(2)
Crystal System	triclinic
Space Group	*P*-1
a/Å	8.5116(7)
b/Å	9.7946(5)
c/Å	9.8073(8)
α/˚	89.873(5)
β/˚	82.901(7)
γ/˚	74.372(6)
V/Å^3	780.94(10)
Z	2
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/˚	2.094
Θ_{max}/˚	27.573
Measured Refl's.	5883
Indep't Refl's	5883
Refl's I≥2 σ(I)	5320
R_{int}	.
Parameters	291
Restraints	277
Largest Peak	1.859
Deepest Hole	-0.863
GooF	1.022
wR_2 (all data)	0.1902
wR_2	0.1834
R_1 (all data)	0.0744
R_1	0.0682

.

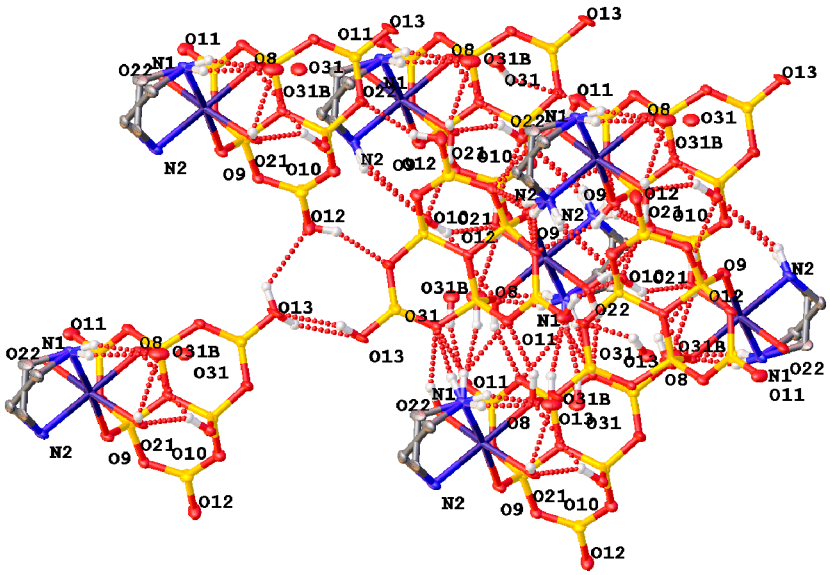


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ˚ are present in **MAB7**: O8–O2_*1: 2.786 Å, O9–O3*_2: 2.831 Å, O10–O8: 3.227 Å, O10–O21: 2.704 Å, O11–O10_*3: 2.805 Å, O12–O6*_4: 2.798 Å, O13–O12_*5: 2.96 Å, O13–O13*_9: 2.684 Å, O21–O31: 2.872 Å, O21–O31B: 2.842 Å, O21–O5_*7: 3.087 Å, O21–O10*_7: 2.806 Å, O22–O4_*2: 2.725 Å, O22–O7*_1: 2.745 Å, N1–O2_*1: 3.017 Å, N1–O7*_1: 3.172 Å, N1–O31B: 2.993 Å, N2–O10_*7: 3.28 Å, N2–O3*_2: 2.997 Å, N2–O4_*2: 3.189 Å, O31–O11*_1: 2.715 Å, O31–O31_*6: 3.013 Å, O31–O11*_8: 2.993 Å, O31B–O11_*1: 2.812 Å.*

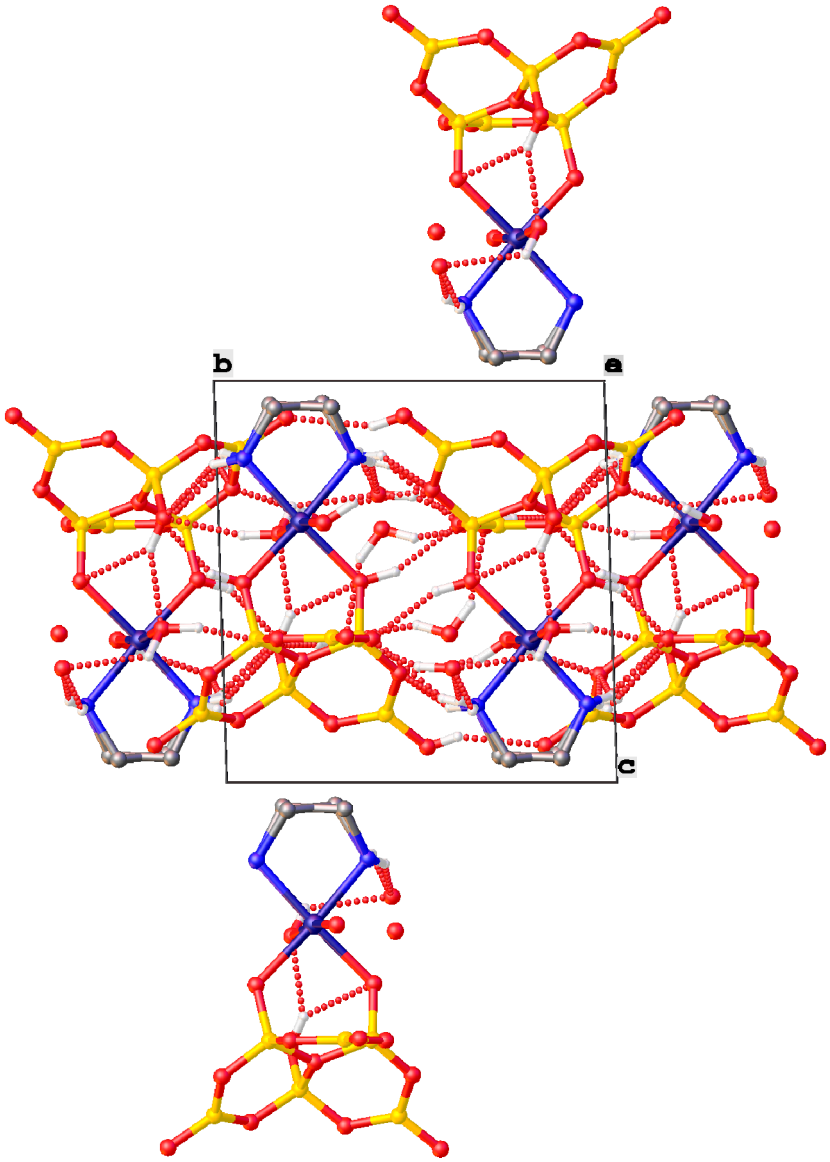


Figure S2: Packing diagram of MAB7.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB7**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ni1	3411.1(7)	7892.1(6)	3529.8(5)	11.8(2)
O1	2858(4)	7982(4)	6965(3)	12.4(6)
O2	5418(4)	6162(3)	6430(4)	13.5(7)
O3	5433(4)	8592(3)	6432(4)	14.0(7)
O4	3060(4)	10371(4)	7323(3)	13.8(7)
O5	760(5)	9677(4)	8449(4)	16.2(7)
O6	829(5)	7254(4)	8545(4)	20.6(8)
O7	3018(4)	5494(4)	7286(3)	13.9(6)
O8	3228(4)	6420(3)	5009(4)	13.1(7)
O9	3203(5)	9420(3)	5040(4)	13.7(7)
O10	-32(4)	8606(4)	6579(3)	15.5(6)
O11	7914(4)	6824(4)	6384(4)	21.2(7)
O12	1395(5)	11810(4)	9081(4)	23.1(8)
O13	1381(6)	4835(4)	9119(5)	30.7(10)
O21	833(4)	8462(4)	3825(3)	15.3(6)

Atom	x	y	z	U_{eq}
O22	5949(4)	7314(4)	3546(3)	15.0(6)
N1	3625(6)	6458(4)	1904(4)	15.1(8)
N2	3511(6)	9299(4)	1943(4)	15.7(8)
B1	3632(7)	6496(5)	6414(5)	12.0(10)
B2	3651(7)	9124(5)	6432(6)	12.4(10)
B3	1058(6)	8388(6)	7638(5)	14.2(9)
B4	6292(6)	7176(6)	6406(4)	13.6(9)
B5	1709(7)	10597(6)	8288(6)	16.3(10)
B6	1732(7)	5877(6)	8302(5)	16.7(10)
C1	4350(30)	7017(15)	668(13)	19(4)
C2	3520(30)	8593(12)	607(12)	15(4)
C1B	3570(30)	7243(14)	567(12)	17(3)
C2B	4320(30)	8477(12)	694(11)	15(3)
O31	-9(14)	5820(9)	3698(14)	21(3)
O31B	387(11)	5884(8)	2838(14)	26(3)

Table S2: Anisotropic Displacement Parameters (×10^4) for **MAB7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$\$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	21.4(3)	6.3(3)	9.1(3)	1.3(3)	-3.0(2)	-5.8(3)
O1	19.1(15)	7.9(13)	10.9(14)	1.0(14)	-2.0(11)	-4.5(13)
O2	18.7(17)	8.8(15)	14.2(17)	-0.8(13)	-2.2(13)	-5.6(12)
O3	22.1(17)	7.5(14)	14.2(17)	1.3(13)	-3.9(13)	-6.4(12)
O4	20.5(16)	10.6(15)	11.8(15)	-2.2(14)	-0.2(12)	-7.3(13)
O5	23.8(18)	13.1(15)	12.2(17)	-1.9(13)	-0.8(14)	-6.8(14)
O6	26(2)	10.2(15)	21(2)	4.7(14)	6.9(15)	-1.7(14)
O7	20.2(16)	9.5(15)	11.2(15)	1.3(15)	0.1(12)	-3.5(14)
O8	21.8(17)	6.6(14)	11.6(16)	0.3(13)	-3.0(13)	-4.8(12)
O9	23.3(17)	8.3(15)	11.2(16)	-0.5(13)	-3.1(13)	-6.9(13)
O10	21.6(16)	11.7(15)	13.3(15)	2.3(16)	-2.4(12)	-4.3(15)
O11	18.2(16)	14.0(15)	32.7(19)	-5.4(17)	-4.1(14)	-6.1(15)
O12	32(2)	19.9(18)	19(2)	-6.2(16)	7.3(16)	-13.9(16)
O13	56(3)	6.8(16)	24(2)	4.6(16)	9(2)	-6.0(17)
O21	21.6(16)	6.6(14)	19.9(16)	3.5(15)	-6.8(12)	-5.6(13)
O22	22.7(16)	8.1(14)	15.2(15)	-0.4(15)	0.1(12)	-6.9(14)
N1	27(2)	10.4(18)	9.4(19)	2.1(15)	-5.6(16)	-5.6(16)
N2	26(2)	9.4(18)	13(2)	2.1(15)	-4.3(17)	-6.8(16)
B1	21(2)	8(2)	8(2)	3.7(18)	-0.6(18)	-5.9(18)
B2	22(3)	4(2)	13(2)	0.2(19)	-2.8(19)	-7.1(18)
B3	23(2)	9(2)	12(2)	0(2)	1.2(17)	-7(2)
B4	21(2)	18(2)	3.1(19)	-5(2)	1.9(16)	-8(2)
B5	23(3)	15(2)	12(2)	-5(2)	-2.2(19)	-7(2)
B6	24(2)	11(2)	13(2)	-1(2)	2.5(18)	-4(2)
C1	36(10)	12(5)	8(5)	-6(4)	-2(5)	-5(6)
C2	27(10)	14(5)	5(4)	5(3)	1(5)	-7(5)
C1B	29(8)	15(5)	8(4)	2(4)	-3(5)	-6(5)
C2B	19(8)	16(5)	9(5)	3(3)	0(4)	-6(4)
O31	32(5)	13(4)	18(7)	-6(3)	-1(4)	-6(4)
O31B	31(4)	15(4)	34(8)	-6(3)	-11(4)	-5(3)

Table S3: Bond Lengths in Å for **MAB7**.

Atom	Atom	Length/Å
Ni1	O8	2.065(3)
Ni1	O9	2.065(3)
Ni1	O21	2.096(3)
Ni1	O22	2.082(3)
Ni1	N1	2.086(4)
Ni1	N2	2.085(4)
O1	B1	1.498(6)
O1	B2	1.515(6)
O1	B3	1.538(6)
O2	B1	1.468(7)
O2	B4	1.391(7)
O3	B2	1.465(7)
O3	B4	1.382(7)
O4	B2	1.441(6)
O4	B5	1.365(6)
O5	B3	1.439(6)
O5	B5	1.360(7)
O6	B3	1.461(6)
O6	B6	1.365(7)
O7	B1	1.460(6)
O7	B6	1.358(6)
O8	B1	1.468(6)
O9	B2	1.470(6)
O10	B3	1.455(6)
O11	B4	1.327(6)
O12	B5	1.367(7)
O13	B6	1.369(7)
N1	C1	1.463(14)
N1	C1B	1.517(13)
N2	C2	1.481(13)
N2	C2B	1.456(12)
C1	C2	1.52(2)
C1B	C2B	1.53(2)

Table S4: Bond Angles in ° for **MAB7**.

Atom	Atom	Atom	Angle/°
O8	Ni1	O9	90.48(12)
O8	Ni1	O21	84.85(14)
O8	Ni1	O22	89.04(14)
O8	Ni1	N1	93.51(14)
O8	Ni1	N2	175.70(15)
O9	Ni1	O21	85.55(14)
O9	Ni1	O22	88.86(14)
O9	Ni1	N1	176.01(14)
O9	Ni1	N2	93.21(14)
O22	Ni1	O21	171.67(12)
O22	Ni1	N1	91.39(16)
O22	Ni1	N2	93.24(16)
N1	Ni1	O21	94.61(16)
N2	Ni1	O21	93.23(16)
N2	Ni1	N1	82.80(14)
B1	O1	B2	117.7(3)
B1	O1	B3	119.1(4)
B2	O1	B3	120.1(4)
B4	O2	B1	124.1(4)
B4	O3	B2	124.9(4)
B5	O4	B2	123.6(4)
B5	O5	B3	124.4(4)
B6	O6	B3	122.3(4)
B6	O7	B1	124.1(4)
B1	O8	Ni1	124.8(3)
B2	O9	Ni1	124.8(3)
C1	N1	Ni1	107.6(5)
C1B	N1	Ni1	109.2(5)
C2	N2	Ni1	110.0(5)
C2B	N2	Ni1	108.2(5)
O2	B1	O1	108.9(4)
O7	B1	O1	110.2(4)
O7	B1	O2	107.8(4)
O7	B1	O8	111.0(4)
O8	B1	O1	107.6(4)
O8	B1	O2	111.2(4)
O3	B2	O1	108.6(4)
O3	B2	O9	112.2(4)
O4	B2	O1	110.0(4)
O4	B2	O3	108.4(4)
O4	B2	O9	111.4(4)
O9	B2	O1	106.3(4)
O5	B3	O1	108.4(4)
O5	B3	O6	109.0(4)
O5	B3	O10	109.9(4)
O6	B3	O1	108.1(4)
O10	B3	O1	109.7(3)
O10	B3	O6	111.7(4)
O3	B4	O2	118.6(4)
O11	B4	O2	122.1(5)
O11	B4	O3	119.3(5)
O4	B5	O12	114.8(5)
O5	B5	O4	122.3(5)
O5	B5	O12	122.9(5)
O6	B6	O13	120.1(4)
O7	B6	O6	122.1(5)
O7	B6	O13	117.8(5)
N1	C1	C2	109.3(14)
N2	C2	C1	109.6(14)
N1	C1B	C2B	108.8(12)
N2	C2B	C1B	108.0(13)

Table S5: Torsion Angles in ° for **MAB7**.

Atom	Atom	Atom	Atom	Angle/°
Ni1	O8	B1	O1	46.1(5)
Ni1	O8	B1	O2	-73.1(4)
Ni1	O8	B1	O7	166.8(3)
Ni1	O9	B2	O1	-48.5(5)
Ni1	O9	B2	O3	70.0(4)
Ni1	O9	B2	O4	-168.3(3)
Ni1	N1	C1	C2	-44(2)
Ni1	N1	C1B	C2B	31.5(19)
Ni1	N2	C2	C1	-30(2)
Ni1	N2	C2B	C1B	46.6(19)
N1	C1	C2	N2	50(3)
N1	C1B	C2B	N2	-52(2)
B1	O1	B2	O3	-45.4(5)
B1	O1	B2	O4	-163.9(4)
B1	O1	B2	O9	75.4(5)
B1	O1	B3	O5	162.2(4)
B1	O1	B3	O6	44.3(5)
B1	O1	B3	O10	-77.8(5)
B1	O2	B4	O3	3.1(6)
B1	O2	B4	O11	-178.1(4)
B1	O7	B6	O6	3.9(8)
B1	O7	B6	O13	-174.3(5)
B2	O1	B1	O2	46.2(5)
B2	O1	B1	O7	164.4(4)
B2	O1	B1	O8	-74.4(5)
B2	O1	B3	O5	-38.2(5)
B2	O1	B3	O6	-156.2(4)
B2	O1	B3	O10	81.8(5)
B2	O3	B4	O2	-2.4(6)
B2	O3	B4	O11	178.8(4)
B2	O4	B5	O5	-2.9(8)
B2	O4	B5	O12	176.8(5)
B3	O1	B1	O2	-153.7(4)
B3	O1	B1	O7	-35.6(5)
B3	O1	B1	O8	85.6(4)
B3	O1	B2	O3	154.7(4)
B3	O1	B2	O4	36.3(6)
B3	O1	B2	O9	-84.4(5)
B3	O5	B5	O4	0.0(8)
B3	O5	B5	O12	-179.7(5)
B3	O6	B6	O7	7.1(8)
B3	O6	B6	O13	-174.7(5)
B4	O2	B1	O1	-24.1(6)
B4	O2	B1	O7	-143.7(4)
B4	O2	B1	O8	94.3(5)
B4	O3	B2	O1	22.5(6)
B4	O3	B2	O4	141.9(4)
B4	O3	B2	O9	-94.7(5)
B5	O4	B2	O1	-14.7(6)
B5	O4	B2	O3	-133.2(4)
B5	O4	B2	O9	102.9(5)
B5	O5	B3	O1	19.3(6)
B5	O5	B3	O6	136.7(5)
B5	O5	B3	O10	-100.6(5)
B6	O6	B3	O1	-29.0(6)
B6	O6	B3	O5	-146.6(5)
B6	O6	B3	O10	91.7(6)
B6	O7	B1	O1	10.4(6)

Atom	Atom	Atom	Atom	Angle/°
B6	O7	B1	O2	129.2(5)
B6	O7	B1	O8	-108.7(5)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB7**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H8	3450(60)	5520(15)	4760(30)	20
H9	3430(60)	10220(30)	4820(30)	20
H10	500.99	8235.68	5830.87	23
H11	8212.17	7547.03	6563.35	32
H12	627.41	11825.27	9712.59	35
H13A	2048.19	4051.2	8863.3	46
H13	988.5	5176.86	9912.49	46
H21A	458.36	8106.87	3147.18	23
H21B	442.36	9392.88	3850.46	23
H22A	6367.33	7994.79	3202.79	23
H22B	6410.15	6528.1	3042.57	23
H1AA	4281.52	5593.38	2082.44	18
H1AB	2618.27	6358.03	1783.81	18
H1BC	4592.52	5768.91	1870.49	18
H1BD	2788.07	6037.86	2029.63	18
H2AA	2624.77	10071.03	2087.7	19
H2AB	4436.34	9598.26	1929.12	19
H2BC	2476.75	9807.81	1819.31	19
H2BD	4084.52	9913.97	2154.09	19
H1A	4187.9	6516.05	-159.32	23
H1B	5540.91	6859.68	686.72	23
H2A	4123.18	9010.91	-134.67	18
H2B	2378.18	8739	401.92	18
H1BA	2413.39	7603.57	379.93	21
H1BB	4189.85	6592.28	-203.6	21
H2BA	5516.69	8114.18	740.11	18
H2BB	4161.06	9079.94	-116.47	18
H31A	607.81	5007.07	3915.31	32
H31B	-292.5	6391.42	4417.51	32
H31C	952.75	5004.4	2879.84	40
H31D	-105.31	6197.24	3652.65	40

Table S7: Hydrogen Bond information for **MAB7**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O8	H8	O2[1]	0.879(12)	1.97(2)	2.786(5)	154(4)
O9	H9	O3[2]	0.881(12)	2.02(2)	2.831(5)	152(4)
O10	H10	O8	0.84	2.55	3.227(5)	137.9
O10	H10	O21	0.84	1.97	2.704(5)	144.9
O11	H11	O10[3]	0.84	2.04	2.805(5)	151.7
O12	H12	O6[4]	0.84	2.04	2.798(6)	150.3
O13	H13A	O12[5]	0.84	2.41	2.960(5)	123.9
O13	H13	O13[6]	0.84	2.12	2.684(9)	123.9
O21	H21A	O31	0.88	2.43	2.872(9)	111.7
O21	H21A	O31B	0.88	2.22	2.841(8)	127.5
O21	H21B	O5[7]	0.88	2.65	3.087(5)	111.8
O21	H21B	O10[7]	0.88	1.95	2.807(5)	163.3
O22	H22A	O4[2]	0.88	1.85	2.724(5)	170.0
O22	H22B	O7[1]	0.88	1.93	2.744(5)	153.4
N1	H1AA	O2[1]	0.91	2.23	3.017(5)	143.8
N1	H1BC	O7[1]	0.91	2.32	3.171(5)	154.7
N1	H1BD	O31B	0.91	2.14	2.993(12)	155.2
N2	H2AA	O10[7]	0.91	2.45	3.281(6)	151.4
N2	H2AB	O4[2]	0.91	2.34	3.188(6)	154.1
N2	H2BD	O3[2]	0.91	2.17	2.997(5)	150.9
O31	H31A	O11[1]	0.87	1.89	2.715(10)	157.1
O31	H31A	O31[8]	0.87	2.51	3.01(3)	117.4
O31	H31B	O11[9]	0.87	2.27	2.993(13)	140.4
O31B	H31C	O11[1]	0.87	1.97	2.812(9)	161.4

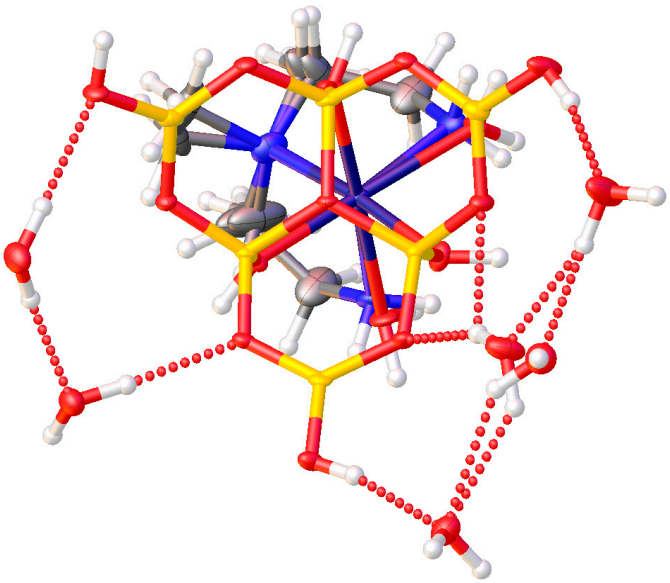
––––

[1]1-x,1-y,1-z; [2]1-x,2-y,1-z; [3]1+x,+y,+z; [4]-x,2-y,2-z; [5]+x,-1+y,+z; [6]-x,1-y,2-z; [7]-x,2-y,1-z; [8]-x,1-y,1-z; [9]-1+x,+y,+z

Table S8: Atomic Occupancies for all atoms that are not fully occupied in **MAB7**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
H13A	0.5	H2AB	0.48(3)	H2A	0.48(3)	H2BB	0.52(3)
H13	0.5	H2BC	0.52(3)	H2B	0.48(3)	O31	0.47(2)
H1AA	0.48(3)	H2BD	0.52(3)	C1B	0.52(3)	H31A	0.47(2)
H1AB	0.48(3)	C1	0.48(3)	H1BA	0.52(3)	H31B	0.47(2)
H1BC	0.52(3)	H1A	0.48(3)	H1BB	0.52(3)	O31B	0.53(2)
H1BD	0.52(3)	H1B	0.48(3)	C2B	0.52(3)	H31C	0.53(2)
H2AA	0.48(3)	C2	0.48(3)	H2BA	0.52(3)	H31D	0.53(2)

Compound 8



Crystal Data. $C_4H_{30}B_6N_2NiO_{19}$, M_r = 533.87, triclinic, *P*-1 (No. 2), a = 9.1508(4) Å, b = 9.8599(4) Å, c = 13.5971(4) Å, α = 88.525(3)˚, β = 70.627(3)˚, γ = 65.245(4)˚, V = 1041.79(8) Å^3, T = 100(2) K, Z = 2, Z' = 1, μ(Mo Kα) = 1.023, 15537 reflections measured, 4713 unique (R_{int} = 0.0461) which were used in all calculations. The final wR_2 was 0.1048 (all data) and R_1 was 0.0403 (I≥2 σ(I)).

Compound	**MAB8**
Formula	$C_4H_{30}B_6N_2NiO_{19}$
$D_{calc.}$/ g cm^{-3}	1.702
μ/mm^{-1}	1.023
Formula Weight	533.87
Colour	bluish green
Shape	plate-shaped
Size/mm^3	0.12×0.04×0.01
T/K	100(2)
Crystal System	triclinic
Space Group	*P*-1
a/Å	9.1508(4)
b/Å	9.8599(4)
c/Å	13.5971(4)
α/˚	88.525(3)
β/˚	70.627(3)
γ/˚	65.245(4)
V/Å^3	1041.79(8)
Z	2
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo Kα
Θ_{min}/˚	2.620
Θ_{max}/˚	27.483
Measured Refl's.	15537
Indep't Refl's	4713
Refl's I≥2 σ(I)	3882
R_{int}	0.0461
Parameters	376
Restraints	375
Largest Peak	1.334
Deepest Hole	-0.806
GooF	1.064
wR_2 (all data)	0.1048
wR_2	0.1005
R_1 (all data)	0.0535
R_1	0.0403

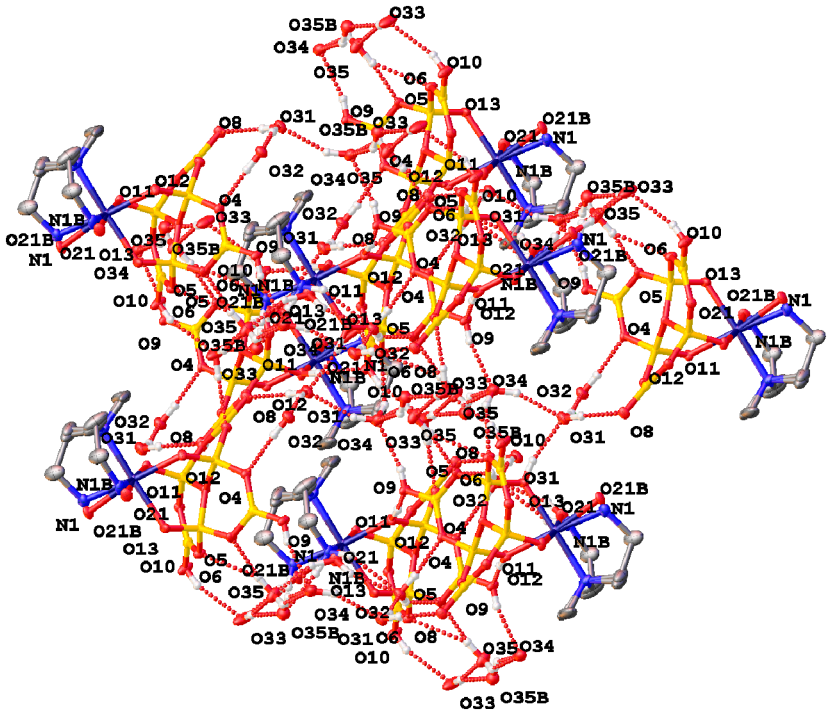


Figure S1: The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in **MAB8**: O8–O2_*1: 2.716 Å, O9–O34: 2.714 Å, O10–O33: 2.808 Å, O11–O10*_9: 2.842 Å, O12–O9_*10: 2.704 Å, O13–O31*_2: 2.743 Å, O21–O32_*10: 2.746 Å, O21–O35*_3: 2.867 Å, N1–O10_*9: 3.12 Å, N1–O33*_3: 3.033 Å, O21B–O33_*3: 2.978 Å, O21B–O10*_9: 3.138 Å, N1B–O35B_*3: 2.992 Å, N1B–O32*_10: 3.1 Å, O34–O6_*4: 2.841 Å, O34–O31*_5: 2.766 Å, O35B–O34: 3.007 Å, O35B–N1B_*6: 2.992 Å, O31–O8: 2.842 Å, O31–O32: 2.791 Å, O35–O34: 2.831 Å, O35–O5: 2.881 Å, O35–O6: 3.143 Å, O32–O4: 2.729 Å, O32–O5*_10: 3.204 Å, O32–O35B_*7: 2.824 Å, O33–O35B: 2.65 Å, O33–O35: 2.809 Å, O33–O3*_8: 2.833 Å.

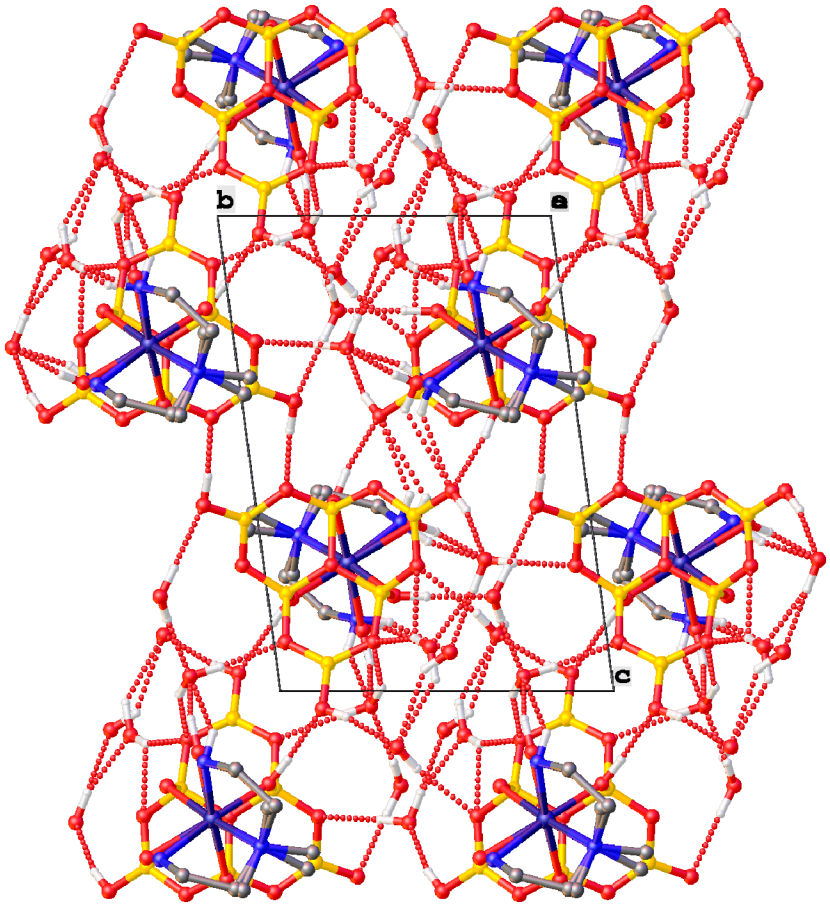


Figure S2: Packing diagram of MAB8.

Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **MAB8**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Ni1	233.5(3)	7452.8(3)	7301.7(2)	10.54(10)
O1	3182.4(19)	7965.7(18)	7354.1(11)	9.0(3)
O2	3923(2)	9019.0(19)	5768.0(11)	11.5(3)
O3	1850(2)	10637.4(18)	7355.6(12)	11.4(3)
O4	1794.3(19)	9655.6(19)	8971.7(11)	11.5(3)
O5	3387(2)	7018.3(19)	8969.5(12)	14.0(3)
O6	5114(2)	5401.8(19)	7367.9(12)	13.8(3)
O7	5206(2)	6355.6(19)	5718.6(11)	12.0(3)
O8	3452(2)	11569.8(19)	6090.7(12)	14.2(3)
O9	2708(2)	8810(2)	10374.7(13)	14.8(4)
O10	7407(2)	4063(2)	5788.1(14)	22.7(4)
O11	2166(2)	7639(2)	6025.8(12)	12.5(3)
O12	128.7(19)	9282.1(19)	8044.6(12)	12.1(3)
O13	2040(2)	6216.6(19)	7994.7(13)	15.1(3)
B1	3645(3)	7717(3)	6169.0(19)	11.4(5)
B2	1689(3)	9428(3)	7946.2(18)	9.9(5)
B3	3438(3)	6602(3)	7933.8(19)	9.7(5)
B4	3090(3)	10374(3)	6386.9(19)	11.3(5)
B5	2645(3)	8471(3)	9420.0(19)	11.0(5)
B6	5870(3)	5295(3)	6300(2)	13.2(5)
O21	-1578(14)	7300(15)	8714(7)	17.0(17)
N1	340(10)	5727(10)	6453(9)	18.5(17)
N2	-1750(50)	8830(40)	6740(40)	20.7(9)

Atom	x	y	z	U_{eq}
C1	-1180(7)	6334(8)	6114(5)	35.8(11)
C2	-1560(50)	7860(30)	5830(20)	35.8(17)
C3	-3340(30)	9170(30)	7540(20)	52(2)
C4	-1480(20)	10097(15)	6251(10)	42(3)
O21B	868(9)	5325(8)	6481(6)	15.4(13)
N1B	-1758(18)	7430(20)	8501(9)	17(2)
N2B	-1760(50)	8790(40)	6720(50)	20.7(9)
C1B	-3383(7)	8338(8)	8346(5)	35.8(11)
C2B	-3550(40)	9370(30)	7580(20)	52(2)
C3B	-1660(50)	8080(30)	5810(20)	35.8(17)
C4B	-1860(20)	10323(15)	6600(9)	31(3)
O34	4905(2)	6723(2)	11182.4(14)	21.2(4)
O35B	7594(13)	4761(10)	9182(5)	23(2)
O31	2708(2)	13234(2)	8010.3(14)	20.6(4)
O35	6763(4)	5335(4)	9072(2)	24.0(10)
O32	387(2)	12648(2)	9687.4(14)	19.8(4)
O33	9123(3)	3338(3)	7235.0(15)	34.8(5)

Table S2: Anisotropic Displacement Parameters (×10⁴) for **MAB8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	9.90(16)	14.51(18)	9.00(16)	1.96(11)	-3.11(12)	-7.14(12)
O1	9.7(7)	12.0(8)	4.5(7)	0.8(6)	-1.1(6)	-5.2(6)
O2	12.4(7)	15.1(9)	6.5(7)	2.0(6)	-1.0(6)	-7.4(7)
O3	12.4(7)	11.5(8)	8.4(7)	1.3(6)	-1.0(6)	-5.4(7)
O4	10.9(7)	13.0(8)	6.7(7)	-1.0(6)	-1.2(6)	-3.1(7)
O5	20.9(8)	14.1(9)	7.3(7)	1.6(6)	-5.6(7)	-7.5(7)
O6	11.2(7)	14.9(9)	8.3(7)	1.1(6)	-1.0(6)	-1.3(7)
O7	12.1(8)	13.7(9)	7.0(7)	-0.1(6)	-0.5(6)	-4.8(7)
O8	15.6(8)	16.5(9)	8.2(7)	0.8(6)	1.1(7)	-9.1(7)
O9	13.9(8)	16.0(9)	9.2(8)	-1.0(7)	-4.6(7)	-0.9(7)
O10	14.9(9)	28.4(11)	10.3(8)	-3.7(8)	-4.6(7)	4.3(8)
O11	11.9(8)	20.2(9)	5.4(7)	-1.2(6)	-0.2(6)	-9.0(7)
O12	7.6(7)	12.8(8)	11.7(8)	-2.2(6)	0.4(6)	-3.4(7)
O13	14.2(8)	13.0(9)	21.9(9)	6.4(7)	-8.1(7)	-8.2(7)
B1	11.4(11)	17.8(14)	5.7(11)	2.9(10)	-1.7(9)	-8.1(10)
B2	9.2(11)	12.7(13)	6.0(10)	0.4(9)	-0.5(9)	-4.6(10)
B3	8.8(11)	11.2(13)	7.6(11)	1.5(9)	-2.0(9)	-3.6(10)
B4	9.8(11)	17.0(13)	8.0(11)	2.6(10)	-3.7(9)	-6.1(10)
B5	9.3(11)	14.9(13)	6.3(11)	0.4(9)	0.8(9)	-5.7(10)
B6	10.3(11)	16.9(14)	10.7(11)	-1.7(10)	-2.0(10)	-5.6(10)
O21	21(3)	23(3)	7(3)	4(3)	0(2)	-14(3)
N1	21(4)	22(4)	15(3)	4(3)	-4(3)	-14(3)
N2	15.6(10)	29.4(17)	21.2(19)	7.7(18)	-10.5(10)	-10.9(12)
C1	16.3(18)	45(3)	38(2)	15(2)	-2.5(18)	-11.5(19)
C2	30(3)	30(5)	37.8(19)	-11(3)	-20.4(18)	3(4)
C3	22(5)	86(6)	26(2)	16(3)	-8(3)	-4(5)
C4	48(8)	39(7)	62(9)	35(6)	-38(7)	-26(7)
O21B	22(4)	15(3)	9(2)	-3(2)	-1(3)	-11(3)
N1B	21(3)	28(5)	8(4)	1(3)	-4(3)	-15(3)
N2B	15.6(10)	29.4(17)	21.2(19)	7.7(18)	-10.5(10)	-10.9(12)
C1B	16.3(18)	45(3)	38(2)	15(2)	-2.5(18)	-11.5(19)
C2B	22(5)	86(6)	26(2)	16(3)	-8(3)	-4(5)
C3B	30(3)	30(5)	37.8(19)	-11(3)	-20.4(18)	3(4)
C4B	40(7)	17(3)	36(6)	-7(4)	-30(5)	2(4)
O34	22.1(9)	22.1(10)	22.5(9)	8.0(8)	-10.1(8)	-11.0(8)
O31	22.3(9)	17.2(10)	23.1(9)	0.4(8)	-4.4(8)	-11.9(8)
O35	16.5(18)	36(2)	13.5(13)	-3.8(12)	-4.8(11)	-5.2(16)
O32	24.0(9)	15.6(9)	18.4(9)	-0.1(7)	-5.0(8)	-9.0(8)
O33	28.0(11)	31.5(12)	21.9(10)	-5.9(9)	-12.4(9)	11.4(9)

Table S3: Bond Lengths in Å for **MAB8**.

Atom	Atom	Length/Å
Ni1	O11	2.0956(15)
Ni1	O12	2.0415(17)
Ni1	O13	2.0958(17)
Ni1	O21	2.131(11)
Ni1	N1	2.031(11)
Ni1	N2	2.13(2)
Ni1	O21B	2.158(8)
Ni1	N1B	2.009(15)
Ni1	N2B	2.14(2)
O1	B1	1.522(3)
O1	B2	1.508(3)
O1	B3	1.513(3)
O2	B1	1.468(3)
O2	B4	1.362(3)
O3	B2	1.452(3)
O3	B4	1.367(3)
O4	B2	1.458(3)
O4	B5	1.363(3)
O5	B3	1.457(3)
O5	B5	1.358(3)

Atom	Atom	Length/Å
O6	B3	1.445(3)
O6	B6	1.371(3)
O7	B1	1.440(3)
O7	B6	1.353(3)
O8	B4	1.369(3)
O9	B5	1.374(3)
O10	B6	1.379(3)
O11	B1	1.462(3)
O12	B2	1.457(3)
O13	B3	1.458(3)
N1	C1	1.490(9)
N2	C2	1.50(6)
N2	C3	1.40(6)
N2	C4	1.475(14)
C1	C2	1.46(2)
N1B	C1B	1.463(12)
N2B	C2B	1.54(6)
N2B	C3B	1.39(6)
N2B	C4B	1.488(16)
C1B	C2B	1.44(2)

Table S4: Bond Angles in ° for **MAB8**.

Atom	Atom	Atom	Angle/°
O11	Ni1	O13	90.66(6)
O11	Ni1	O21	173.2(3)
O11	Ni1	N2	93.1(13)
O11	Ni1	O21B	87.9(2)
O11	Ni1	N2B	93.2(13)
O12	Ni1	O11	85.85(6)
O12	Ni1	O13	84.26(7)
O12	Ni1	O21	89.3(4)
O12	Ni1	N2	92.2(11)
O12	Ni1	O21B	168.81(18)
O12	Ni1	N2B	93.7(11)
O13	Ni1	O21	84.0(2)
O13	Ni1	N2	174.6(17)
O13	Ni1	O21B	86.56(18)
O13	Ni1	N2B	175.5(16)
O21	Ni1	N2	91.9(14)
N1	Ni1	O11	90.7(3)
N1	Ni1	O12	175.1(3)
N1	Ni1	O13	99.3(2)
N1	Ni1	O21	94.4(5)
N1	Ni1	N2	84.5(12)
N1B	Ni1	O11	175.3(4)
N1B	Ni1	O12	92.5(6)
N1B	Ni1	O13	93.6(3)
N1B	Ni1	O21B	94.5(6)
N1B	Ni1	N2B	82.5(13)
N2B	Ni1	O21B	95.9(12)
B2	O1	B1	117.35(17)
B2	O1	B3	116.19(16)
B3	O1	B1	117.62(18)
B4	O2	B1	120.47(17)
B4	O3	B2	122.42(19)

Atom	Atom	Atom	Angle/°
B5	O4	B2	121.21(19)
B5	O5	B3	122.74(19)
B6	O6	B3	121.12(19)
B6	O7	B1	123.00(18)
B1	O11	Ni1	120.69(13)
B2	O12	Ni1	121.19(14)
B3	O13	Ni1	120.50(13)
O2	B1	O1	105.86(19)
O7	B1	O1	109.89(18)
O7	B1	O2	109.70(17)
O7	B1	O11	112.5(2)
O11	B1	O1	105.27(16)
O11	B1	O2	113.32(19)
O3	B2	O1	108.00(16)
O3	B2	O4	109.17(19)
O3	B2	O12	112.73(19)
O4	B2	O1	108.41(18)
O12	B2	O1	106.72(18)
O12	B2	O4	111.65(17)
O5	B3	O1	107.70(19)
O5	B3	O13	112.22(17)
O6	B3	O1	108.90(17)
O6	B3	O5	108.77(18)
O6	B3	O13	112.7(2)
O13	B3	O1	106.36(17)
O2	B4	O3	122.6(2)
O2	B4	O8	122.4(2)
O3	B4	O8	115.0(2)
O4	B5	O9	116.6(2)
O5	B5	O4	122.8(2)
O5	B5	O9	120.5(2)
O6	B6	O10	118.7(2)

Atom	Atom	Atom	Angle/°
O7	B6	O6	123.4(2)
O7	B6	O10	117.9(2)
C1	N1	Ni1	107.6(5)
C2	N2	Ni1	105(2)
C3	N2	Ni1	108(2)
C3	N2	C2	109.1(15)
C3	N2	C4	118(3)
C4	N2	Ni1	112.9(14)
C4	N2	C2	103(3)
C2	C1	N1	111.7(16)

Atom	Atom	Atom	Angle/°
C1	C2	N2	108.2(18)
C1B	N1B	Ni1	110.7(7)
C2B	N2B	Ni1	112(3)
C3B	N2B	Ni1	113(3)
C3B	N2B	C2B	113.1(16)
C3B	N2B	C4B	113(3)
C4B	N2B	Ni1	111.3(14)
C4B	N2B	C2B	93(3)
C2B	C1B	N1B	123.5(13)
C1B	C2B	N2B	105.7(16)

Table S5: Torsion Angles in ° for **MAB8**.

Atom	Atom	Atom	Atom	Angle/°
Ni1	O11	B1	O1	-11.5(2)
Ni1	O11	B1	O2	-126.76(16)
Ni1	O11	B1	O7	108.10(17)
Ni1	O12	B2	O1	-6.7(2)
Ni1	O12	B2	O3	111.70(18)
Ni1	O12	B2	O4	-124.99(16)
Ni1	O13	B3	O1	1.8(2)
Ni1	O13	B3	O5	119.33(17)
Ni1	O13	B3	O6	-117.45(17)
Ni1	N1	C1	C2	38.2(14)
Ni1	N2	C2	C1	41(3)
Ni1	N1B	C1B	C2B	-14(2)
Ni1	N2B	C2B	C1B	-24(3)
B1	O1	B2	O3	-44.2(2)
B1	O1	B2	O4	-162.38(16)
B1	O1	B2	O12	77.2(2)
B1	O1	B3	O5	164.34(16)
B1	O1	B3	O6	46.5(2)
B1	O1	B3	O13	-75.2(2)
B1	O2	B4	O3	-6.5(3)
B1	O2	B4	O8	172.5(2)
B1	O7	B6	O6	0.9(3)
B1	O7	B6	O10	-177.6(2)
B2	O1	B1	O2	55.1(2)
B2	O1	B1	O7	173.48(17)
B2	O1	B1	O11	-65.2(2)
B2	O1	B3	O5	-49.0(2)
B2	O1	B3	O6	-166.83(17)
B2	O1	B3	O13	71.5(2)
B2	O3	B4	O2	20.0(3)
B2	O3	B4	O8	-159.1(2)
B2	O4	B5	O5	-2.5(3)
B2	O4	B5	O9	178.31(18)
B3	O1	B1	O2	-158.67(17)
B3	O1	B1	O7	-40.3(2)
B3	O1	B1	O11	81.1(2)
B3	O1	B2	O3	169.06(17)
B3	O1	B2	O4	50.9(2)
B3	O1	B2	O12	-69.5(2)
B3	O5	B5	O4	4.2(3)
B3	O5	B5	O9	-176.58(19)
B3	O6	B6	O7	6.5(3)
B3	O6	B6	O10	-174.9(2)
B4	O2	B1	O1	-28.3(3)
B4	O2	B1	O7	-146.8(2)
B4	O2	B1	O11	86.6(2)
B4	O3	B2	O1	5.6(3)

Atom	Atom	Atom	Atom	Angle/°
B4	O3	B2	O4	123.3(2)
B4	O3	B2	O12	-112.1(2)
B5	O4	B2	O1	-23.9(2)
B5	O4	B2	O3	-141.34(19)
B5	O4	B2	O12	93.4(2)
B5	O5	B3	O1	20.7(3)
B5	O5	B3	O6	138.6(2)
B5	O5	B3	O13	-96.0(2)
B6	O6	B3	O1	-28.8(3)
B6	O6	B3	O5	-145.9(2)
B6	O6	B3	O13	89.0(2)
B6	O7	B1	O1	15.6(3)
B6	O7	B1	O2	131.6(2)
B6	O7	B1	O11	-101.3(2)
N1	C1	C2	N2	-54(3)
C3	N2	C2	C1	-75(2)
C4	N2	C2	C1	160(2)
N1B	C1B	C2B	N2B	26(3)
C3B	N2B	C2B	C1B	105(2)
C4B	N2B	C2B	C1B	-139(2)

Table S6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MAB8**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H8	4212.07	11327.16	5487.84	21
H9	3310(40)	8120(40)	10540(20)	21(8)
H10	7830(40)	3710(40)	6190(30)	27(9)
H11	2500(30)	7170(30)	5394(9)	19
H12	-726(18)	9940(20)	8553(16)	18
H13	2420(30)	5243(12)	8010(20)	23
H21A	-1593.01	7197.5	9402.43	25
H21B	-2152.71	6758.6	8620.13	25
H1A	1329.93	5345.82	5881.36	22
H1B	316.94	4976.92	6852.71	22
H1C	-956.29	5657.71	5501.87	43
H1D	-2193.99	6355	6692.21	43
H2A	-2635.25	8267.8	5670.27	43
H2B	-613.41	7829.38	5195.07	43
H3A	-3534.13	8258.59	7617.45	78
H3B	-4263	9951.57	7349.81	78
H3C	-3332.82	9526.14	8198.82	78
H4A	-1527.26	10781.12	6784.12	63
H4B	-2375.57	10643.22	5957.08	63
H4C	-347.77	9709.37	5688.17	63
H21C	364.69	4708.83	6655.3	23
H21D	1839.39	4870.63	5936.6	23
H1BA	-1620.68	6467.79	8549.35	21
H1BB	-1782.1	7807.52	9114.07	21
H1BC	-3800.5	7619.65	8190.02	43
H1BD	-4209.3	8929.62	9035.57	43
H2BA	-3911.55	10402.09	7902.13	63
H2BB	-4414.9	9390.63	7286.88	63
H3BA	-633.52	7995.54	5225.35	54
H3BB	-2687.06	8672.95	5635.9	54
H3BC	-1584.34	7070.24	5922.51	54
H4BA	-2308.75	10892.64	7298.35	47
H4BB	-2630.68	10842.36	6215.45	47
H4BC	-711.2	10248.27	6211.8	47
H34A	4497.33	6212.31	11631.37	32
H34B	5562.64	6977.09	11397.44	32

Atom	x	y	z	U_{eq}
H35A	6703.32	5580.01	9535.55	35
H35B	8526.61	4800.69	9179.94	35
H31A	2990.77	12704.57	7418.77	31
H31B	1883.2	13109.15	8488.87	31
H35C	6440.41	5308.2	9747.96	36
H35D	5859.74	5754.81	8892.39	36
H32A	738.81	11699.36	9487.11	30
H32B	-702.11	13041.47	10069.67	30
H33A	8404.09	3797.38	7858.29	52
H33B	9918.02	2492.57	7293.24	52

Table S7: Hydrogen Bond information for **MAB8**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O8	H8	O2[1]	0.84	1.89	2.716(2)	169.7
O9	H9	O34	0.76(3)	1.97(3)	2.714(3)	165(3)
O10	H10	O33	0.76(3)	2.07(4)	2.808(3)	163(3)
O11	H11	O10[2]	0.878(9)	2.001(11)	2.842(2)	160.1(17)
O12	H12	O9[3]	0.864(9)	1.845(9)	2.704(2)	172.5(18)
O13	H13	O31[4]	0.876(9)	1.885(10)	2.743(2)	165.8(17)
O21	H21A	O32[3]	0.94	1.96	2.746(10)	140.8
O21	H21B	O35[5]	0.93	2.01	2.867(15)	152.4
N1	H1A	O10[2]	0.91	2.36	3.120(11)	140.6
N1	H1B	O33[5]	0.91	2.27	3.033(11)	141.8
O21B	H21C	O33[5]	0.89	2.09	2.978(9)	173.8
O21B	H21D	O10[2]	0.89	2.55	3.138(9)	124.7
N1B	H1BA	O35B[5]	0.91	2.15	3.00(2)	154.3
N1B	H1BB	O32[3]	0.91	2.31	3.099(11)	144.4
O34	H34A	O6[6]	0.87	2.06	2.841(2)	148.9
O34	H34B	O31[7]	0.87	1.94	2.766(3)	158.3
O35B	H35A	O34	0.87	2.26	3.007(8)	143.3
O35B	H35B	N1B[8]	0.87	2.67	3.00(2)	103.5
O31	H31A	O8	0.87	1.97	2.841(2)	175.8
O31	H31B	O32	0.87	1.93	2.791(2)	168.5
O35	H35C	O34	0.87	2.10	2.831(3)	141.3
O35	H35D	O5	0.87	2.04	2.881(4)	161.5
O35	H35D	O6	0.87	2.46	3.143(4)	135.7
O32	H32A	O4	0.87	1.87	2.729(2)	172.1
O32	H32B	O5[3]	0.87	2.39	3.203(2)	154.9
O32	H32B	O35B[9]	0.87	2.39	2.824(11)	111.6
O33	H33A	O35B	0.87	1.82	2.650(7)	159.5
O33	H33A	O35	0.87	1.96	2.810(4)	163.9
O33	H33B	O3[10]	0.87	1.97	2.833(3)	175.4

––––

[1]1-x,2-y,1-z; [2]1-x,1-y,1-z; [3]-x,2-y,2-z; [4]+x,-1+y,+z; [5]-1+x,+y,+z; [6]1-x,1-y,2-z; [7]1-x,2-y,2-z; [8]1+x,+y,+z; [9]-1+x,1+y,+z; [10]1+x,-1+y,+z

Table S8: Atomic Occupancies for all atoms that are not fully occupied in **MAB8**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
O21	0.504(5)	H1D	0.504(5)	H4A	0.504(5)	N2B	0.496(5)
H21A	0.504(5)	C2	0.504(5)	H4B	0.504(5)	C1B	0.496(5)
H21B	0.504(5)	H2A	0.504(5)	H4C	0.504(5)	H1BC	0.496(5)
N1	0.504(5)	H2B	0.504(5)	O21B	0.496(5)	H1BD	0.496(5)
H1A	0.504(5)	C3	0.504(5)	H21C	0.496(5)	C2B	0.496(5)
H1B	0.504(5)	H3A	0.504(5)	H21D	0.496(5)	H2BA	0.496(5)
N2	0.504(5)	H3B	0.504(5)	N1B	0.496(5)	H2BB	0.496(5)
C1	0.504(5)	H3C	0.504(5)	H1BA	0.496(5)	C3B	0.496(5)
H1C	0.504(5)	C4	0.504(5)	H1BB	0.496(5)	H3BA	0.496(5)

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
H3BB	0.496(5)	H4BA	0.496(5)	O35B	0.294(10)	O35	0.706(10)
H3BC	0.496(5)	H4BB	0.496(5)	H35A	0.294(10)	H35C	0.706(10)
C4B	0.496(5)	H4BC	0.496(5)	H35B	0.294(10)	H35D	0.706(10)