A series of new mixed-ligand complexes based on 3,6-bis(imidazol-1-yl)pyridazine: syntheses, structures, and catalytic activities.

Sheng-Bin Zhou[a], Xin-Fang Wang[a], Ceng-Ceng Du[a], Duo-Zhi Wang*[a, b], Dianzeng Jia [b]

[a]*College of Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, P. R. China.*

[b]*Key Laboratory of Energy Materials Chemistry, Ministry of Education, Institute of Applied Chemistry, Xinjiang University, Urumqi, 830046 Xinjiang, P. R. China.*

Table S1. Selected Bond Distances (Å) and Angles (deg) for Complexes **1-7**

		Complex **1**	
N(1)-Ni(1)$^{\#1}$	2.140(3)	N(6)-Ni(1)	2.139(3)
N(7)-Ni(1)	2.088(3)	Ni(1)-N(7)$^{\#2}$	2.088(3)
Ni(1)-N(6)$^{\#2}$	2.139(3)	Ni(1)-N(1)$^{\#3}$	2.140(3)
Ni(1)-N(1)$^{\#4}$	2.140(3)	N(7)-Ni(1)-N(6)	91.31(12)
N(7)$^{\#2}$-Ni(1)-N(6)	88.69(12)	N(7)-Ni(1)-N(6)$^{\#2}$	88.69(12)
N(7)$^{\#2}$-Ni(1)-N(6)$^{\#2}$	91.31(12)	N(7)-Ni(1)-N(1)$^{\#3}$	90.66(12)
N(7)$^{\#2}$-Ni(1)-N(1)$^{\#3}$	89.34(12)	N(6)-Ni(1)-N(1)$^{\#3}$	85.79(11)
N(6)$^{\#2}$-Ni(1)-N(1)$^{\#3}$	94.21(11)	N(7)-Ni(1)-N(1)$^{\#4}$	89.34(12)
N(7)$^{\#2}$-Ni(1)-N(1)$^{\#4}$	90.66(12)	N(6)-Ni(1)-N(1)$^{\#4}$	94.21(11)
N(6)$^{\#2}$-Ni(1)-N(1)$^{\#4}$	85.79(11)		
		Complex **2**	
Cu(1)-N(1)	1.940(3)	Cu(1)-O(2)$^{\#1}$	1.948(3)
Cu(1)-O(9)$^{\#2}$	1.950(3)	Cu(1)-O(8)$^{\#3}$	1.999(3)
Cu(1)-O(3)	2.404(3)	Cu(1)-Cu(2)	2.8793(6)
Cu(1)-Cu(3)$^{\#2}$	3.0034(8)	Cu(2)-O(9)$^{\#2}$	1.938(3)
Cu(2)-O(9)	1.939(3)	Cu(2)-O(3)	1.949(3)
Cu(2)-O(3)$^{\#2}$	1.949(3)	Cu(2)-Cu(1)$^{\#2}$	2.8793(6)
Cu(3)-O(6)	1.917(3)	Cu(3)-O(9)	1.941(3)
Cu(3)-O(4)	1.969(3)	Cu(3)-O(1)$^{\#3}$	1.992(3)
Cu(3)-O(7)$^{\#1}$	2.285(3)	Cu(3)-Cu(1)$^{\#2}$	3.0034(8)
O(1)-Cu(3)$^{\#3}$	1.992(3)	O(2)-Cu(1)$^{\#4}$	1.948(3)
O(9)-Cu(1)$^{\#2}$	1.950(3)	O(7)-Cu(3)$^{\#5}$	2.285(3)
O(8)-Cu(1)$^{\#4}$	2.000(3)	N(1)-Cu(1)-O(2)$^{\#1}$	94.34(13)
O(2)$^{\#1}$-Cu(1)-O(9)$^{\#2}$	91.08(11)	N(1)-Cu(1)-O(8)$^{\#3}$	89.85(13)
O(9)$^{\#2}$-Cu(1)-O(8)$^{\#3}$	86.73(11)	N(1)-Cu(1)-O(3)	96.73(13)
O(2)$^{\#1}$-Cu(1)-O(3)	114.83(12)	O(9)$^{\#2}$-Cu(1)-O(3)	74.61(11)

O(8)$^{\#3}$-Cu(1)-O(3)	79.15(12)	O(9)$^{\#2}$-Cu(1)-Cu(2)	42.07(8)
O(8)$^{\#3}$-Cu(1)-Cu(2)	60.16(9)	O(3)-Cu(1)-Cu(2)	42.11(7)
O(2)$^{\#1}$-Cu(1)-Cu(3)$^{\#2}$	84.75(9)	O(9)$^{\#2}$-Cu(1)-Cu(3)$^{\#2}$	39.36(9)
O(8)$^{\#3}$-Cu(1)-Cu(3)$^{\#2}$	83.98(9)	O(3)-Cu(1)-Cu(3)$^{\#2}$	112.52(7)
Cu(2)-Cu(1)-Cu(3)$^{\#2}$	73.045(17)	O(9)$^{\#2}$-Cu(2)-O(3)	86.48(12)
O(9)-Cu(2)-O(3)	93.52(12)	O(9)$^{\#2}$-Cu(2)-O(3)$^{\#2}$	93.53(12)
O(9)-Cu(2)-O(3)$^{\#2}$	86.47(12)	O(9)$^{\#2}$-Cu(2)-Cu(1)	42.37(8)
O(3)-Cu(2)-Cu(1)	55.80(9)	O(9)-Cu(2)-Cu(1)$^{\#2}$	42.37(8)
O(3)$^{\#2}$-Cu(2)-Cu(1)$^{\#2}$	55.80(9)	O(6)-Cu(3)-O(4)	94.99(13)
O(9)-Cu(3)-O(4)	92.52(13)	O(6)-Cu(3)-O(1)$^{\#3}$	87.96(13)
O(9)-Cu(3)-O(1)$^{\#3}$	86.62(13)	O(6)-Cu(3)-O(7)$^{\#1}$	84.60(12)
O(9)-Cu(3)-O(7)$^{\#1}$	90.66(12)	O(4)-Cu(3)-O(7)$^{\#1}$	98.40(13)
O(1)$^{\#3}$-Cu(3)-O(7)$^{\#1}$	105.12(13)	O(9)-Cu(3)-Cu(1)$^{\#2}$	39.57(8)
O(4)-Cu(3)-Cu(1)$^{\#2}$	119.99(9)	O(1)$^{\#3}$-Cu(3)-Cu(1)$^{\#2}$	72.58(9)
O(7)$^{\#1}$-Cu(3)-Cu(1)$^{\#2}$	60.75(10)		

Complex **3**

Cu(1)-O(4)	1.928(2)	Cu(1)-O(5)$^{\#2}$	1.967(2)
Cu(1)-O(2)	1.977(2)	Cu(1)-N(1)	1.981(3)
Cu(1)-O(3)	2.307(2)	Cu(1)-Cu(2)	3.0285(6)
Cu(2)-O(3)	1.948(2)	Cu(2)-O(3)$^{\#3}$	1.957(2)
Cu(2)-N(3)$^{\#4}$	1.970(3)	Cu(2)-O(1)	1.975(2)
Cu(2)-O(4)	2.310(2)	Cu(2)-Cu(2)$^{\#3}$	2.9653(7)
O(3)-Cu(2)$^{\#3}$	1.957(2)	O(5)-Cu(1)$^{\#5}$	1.967(2)
N(3)-Cu(2)$^{\#6}$	1.970(3)	O(4)-Cu(1)-O(5)$^{\#2}$	94.50(10)
O(4)-Cu(1)-O(2)	90.04(10)	O(5)$^{\#2}$-Cu(1)-N(1)	86.63(11)
O(2)-Cu(1)-N(1)	87.92(11)	O(4)-Cu(1)-O(3)	85.88(9)
O(5)$^{\#2}$-Cu(1)-O(3)	93.60(11)	O(2)-Cu(1)-O(3)	91.26(9)
N(1)-Cu(1)-O(3)	107.09(11)	O(4)-Cu(1)-Cu(2)	49.70(7)
O(5)$^{\#2}$-Cu(1)-Cu(2)	109.83(10)	O(2)-Cu(1)-Cu(2)	76.59(7)
O(3)-Cu(1)-Cu(2)	40.03(6)	O(3)-Cu(2)-O(3)$^{\#3}$	81.19(10)
O(3)$^{\#3}$-Cu(2)-N(3)$^{\#4}$	95.05(11)	O(3)-Cu(2)-O(1)	92.47(10)
N(3)$^{\#4}$-Cu(2)-O(1)	90.54(11)	O(3)-Cu(2)-O(4)	85.35(9)
O(3)$^{\#3}$-Cu(2)-O(4)	101.15(9)	N(3)$^{\#4}$-Cu(2)-O(4)	97.61(10)
O(1)-Cu(2)-O(4)	93.90(9)	O(3)-Cu(2)-Cu(2)$^{\#3}$	40.71(7)
O(3)$^{\#3}$-Cu(2)-Cu(2)$^{\#3}$	40.48(7)	O(4)-Cu(2)-Cu(2)$^{\#3}$	94.27(6)
O(3)-Cu(2)-Cu(1)	49.63(7)	O(3)$^{\#3}$-Cu(2)-Cu(1)	106.69(7)
O(1)-Cu(2)-Cu(1)	80.19(7)	O(4)-Cu(2)-Cu(1)	39.53(6)
Cu(2)$^{\#3}$-Cu(2)-Cu(1)	76.356(17)		

Complex **4**

N(1)-Ni(1)	2.065(4)	N(5)-Ni(1)	2.053(4)
Ni(1)-O(4)	2.031(3)	Ni(1)-O(3)	2.083(4)
Ni(1)-O(1)	2.130(3)	Ni(1)-O(2)	2.178(3)
O(4)-Ni(1)-N(5)	92.94(16)	O(4)-Ni(1)-N(1)	90.97(16)
N(5)-Ni(1)-N(1)	91.26(17)	O(4)-Ni(1)-O(3)	91.12(15)

N(5)-Ni(1)-O(3)	94.03(16)	N(1)-Ni(1)-O(1)	91.56(15)
O(3)-Ni(1)-O(1)	85.32(14)	O(4)-Ni(1)-O(2)	107.51(14)
N(1)-Ni(1)-O(2)	88.39(15)	O(3)-Ni(1)-O(2)	85.82(15)
O(1)-Ni(1)-O(2)	61.11(13)	N(5)-Ni(1)-O(1)	98.47(15)
		Complex **5**	
Co(1)-O(7)$^{\#1}$	2.0981(18)	Co(1)-O(7)	2.0981(18)
Co(1)-N(1)	2.109(2)	Co(1)-N(1)$^{\#1}$	2.109(2)
Co(1)-O(5)	2.1304(16)	Co(1)-O(5)$^{\#1}$	2.1304(16)
Co(2)-N(6)	2.129(2)	Co(2)-N(6)$^{\#2}$	2.129(2)
Co(2)-O(13)$^{\#2}$	2.1398(16)	Co(2)-O(13)	2.1398(16)
Co(2)-O(12)	2.1916(16)	Co(2)-O(12)$^{\#2}$	2.1916(16)
O(7)$^{\#1}$-Co(1)-N(1)	90.15(8)	O(7)-Co(1)-N(1)	89.85(8)
O(7)$^{\#1}$-Co(1)-N(1)$^{\#1}$	89.85(8)	O(7)-Co(1)-N(1)$^{\#1}$	90.15(8)
O(7)$^{\#1}$-Co(1)-O(5)	91.52(7)	O(7)-Co(1)-O(5)	88.48(7)
N(1)-Co(1)-O(5)	90.84(7)	N(1)$^{\#1}$-Co(1)-O(5)	89.16(7)
O(7)$^{\#1}$-Co(1)-O(5)$^{\#1}$	88.48(7)	O(7)-Co(1)-O(5)$^{\#1}$	91.52(7)
N(1)-Co(1)-O(5)$^{\#1}$	89.16(7)	N(1)$^{\#1}$-Co(1)-O(5)$^{\#1}$	90.84(7)
N(6)-Co(2)-O(13)$^{\#2}$	87.58(7)	N(6)$^{\#2}$-Co(2)-O(13)$^{\#2}$	92.41(7)
N(6)-Co(2)-O(13)	92.42(7)	N(6)$^{\#2}$-Co(2)-O(13)	87.59(7)
N(6)-Co(2)-O(12)	92.00(7)	N(6)$^{\#2}$-Co(2)-O(12)	88.00(7)
O(13)$^{\#2}$-Co(2)-O(12)	119.61(6)	O(13)-Co(2)-O(12)	60.40(6)
N(6)-Co(2)-O(12)$^{\#2}$	88.00(7)	N(6)$^{\#2}$-Co(2)-O(12)$^{\#2}$	92.00(7)
O(13)$^{\#2}$-Co(2)-O(12)$^{\#2}$	60.40(6)	O(13)-Co(2)-O(12)$^{\#2}$	119.60(6)
		Complex **6**	
Cu(1)-N(1)	1.908(2)	Cu(1)-N(2)	1.938(2)
Cu(1)-O(2)	2.0303(19)	Cu(1)-O(4)	2.0337(18)
Cu(1)-O(5)	2.340(2)	Cu(2)-N(8)	1.905(2)
Cu(2)-N(7)	1.944(2)	Cu(2)-O(7)	2.0449(18)
Cu(2)-O(9)	2.0489(19)	Cu(2)-O(6)	2.311(2)
N(1)-Cu(1)-O(2)	80.55(8)	N(2)-Cu(1)-O(2)	98.37(8)
N(1)-Cu(1)-O(4)	80.04(8)	N(2)-Cu(1)-O(4)	100.45(8)
N(1)-Cu(1)-O(5)	92.74(9)	N(2)-Cu(1)-O(5)	93.06(9)
O(2)-Cu(1)-O(5)	92.90(8)	O(4)-Cu(1)-O(5)	92.80(8)
N(8)-Cu(2)-O(7)	80.07(8)	N(7)-Cu(2)-O(7)	99.96(8)
N(8)-Cu(2)-O(9)	80.44(8)	N(7)-Cu(2)-O(9)	98.94(9)
N(8)-Cu(2)-O(6)	93.67(8)	N(7)-Cu(2)-O(6)	94.95(9)
O(7)-Cu(2)-O(6)	90.29(8)	O(9)-Cu(2)-O(6)	93.37(9)
		Complex **7**	
Co(1)-O(1)$^{\#1}$	1.926(11)	Co(1)-O(4)	2.011(10)
Co(1)-N(1)$^{\#2}$	2.053(11)	Co(1)-N(4)	2.022(11)
O(1)$^{\#1}$-Co(1)-O(4)	100.8(5)	O(1)$^{\#1}$-Co(1)-N(1)$^{\#2}$	93.4(5)
O(4)-Co(1)-N(1)$^{\#2}$	116.0(4)	O(1)$^{\#1}$-Co(1)-N(4)	119.0(5)
O(4)-Co(1)-N(4)	117.7(4)	N(1)$^{\#2}$-Co(1)-N(4)	107.7(4)

Symmetry codes, **for 1**: #1 -x,y-1/2,-z+1/2, #2 -x+1,-y+1,-z, #3 -x,y+1/2,-z+1/2 , #4 x+1,-y+1/2,

z-1/2; **for 2:** #1 x-1,y,z, #2 -x-1,-y,-z+1, #3 -x,-y,-z+1; **for 3**: #2 x,-y+2,z+1/2, #3 -x+1/2,-y+1/2,-z+1, #4 x+1/2,y-1/2,z, #5 x,-y,z-1/2, #6 x-1/2,y+1/2,z; **for 5:** #1 -x,-y+1,-z,#2 -x+2,-y,-z; **for 7:** #1 -x+1/2,y+1/2,-z+3, #2 x+1/2,-y+3/2,-z;

Table S2 Hydrogen-bonding geometry (Å, °) for **6**

D–H···A	D–H	H···A	D···A	D–H···A
O(6)-H(3W)...O(4)	0.8410(18)	1.950(2)	2.738(3)	163(4)
O(5)-H(1W)...O(7)	0.8418(18)	1.985(2)	2.808(3)	165.6(4)