Supporting Information

Hexanuclear copper-nickel and copper-cobalt complexes for thin film deposition of ceramic oxide composites

Muhammad Sultan,[a] Asif Ali Tahir,[c] Muhammad Mazhar,[b]* Mathias Zeller,[d] K. G. Upul Wijayantha,[c]

[a]Department of Chemistry, Quaid-I-Azam University, Islamabad-45320, Pakistan, [b]Department of Chemistry, Faculty of Science, University of Malaya, Lambah Pantai, Kuala Lumpur 50603, Malaysia, [c]Department of Chemistry, University of Loughborough, Loughborough LE11 3TU, UK. [d]STaRBURSTT-Cyberdiffraction Consortium at YSU and Department of Chemistry, Youngstown State University, 1 University Plaza, Youngstown, Ohio 44555-3663,

Corresponding Author: e-mail: mazhar42pk@yahoo.com

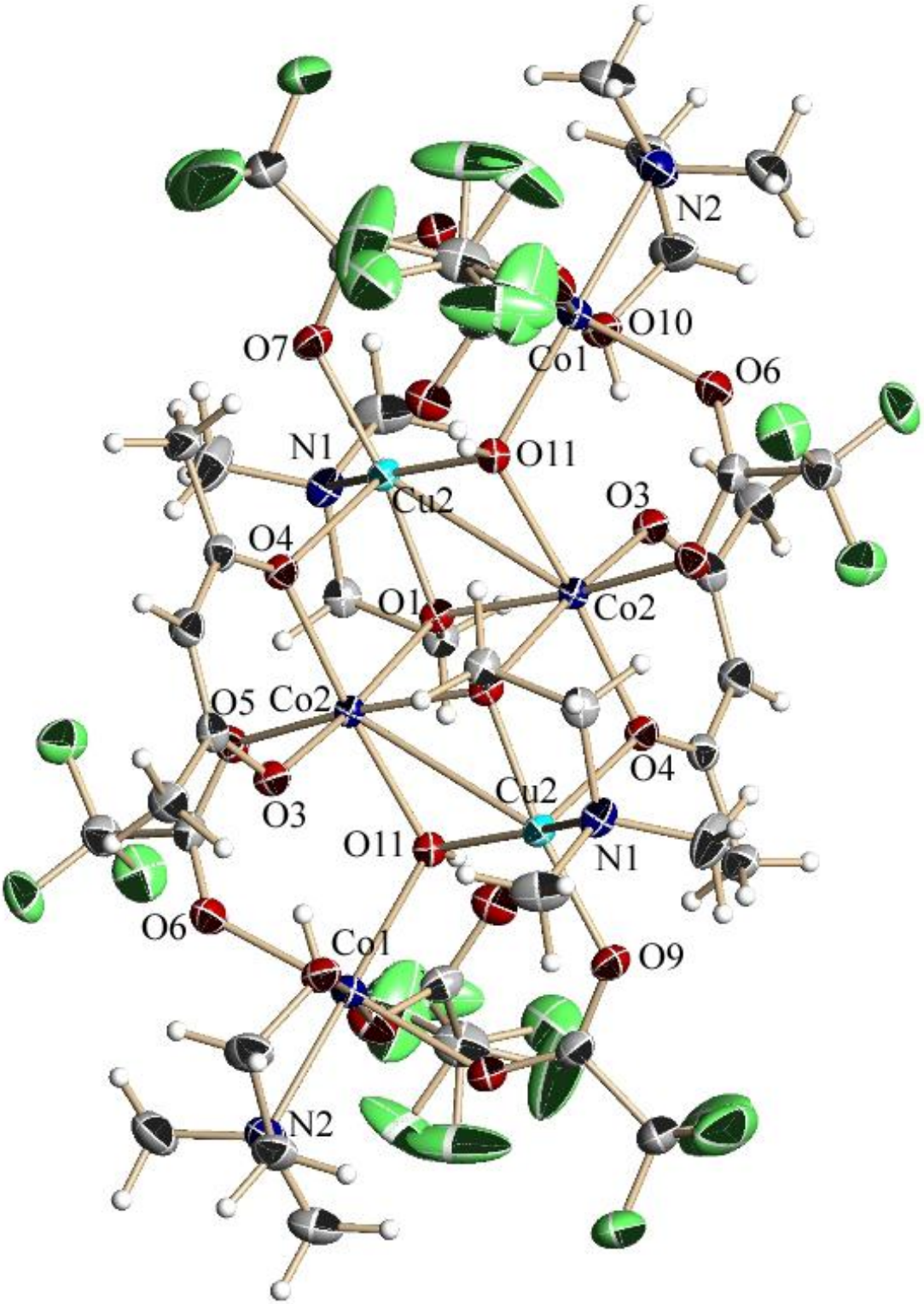

Fig. S1. ORTEP-style drawing showing the molecular structure of $[Cu_2Co_4(acac)_2(dmae)_2\ (dmaeH)_2(OH)_2(TFA)_6]$ (**2**). Thermal ellipsoids are at the 50% probability level.

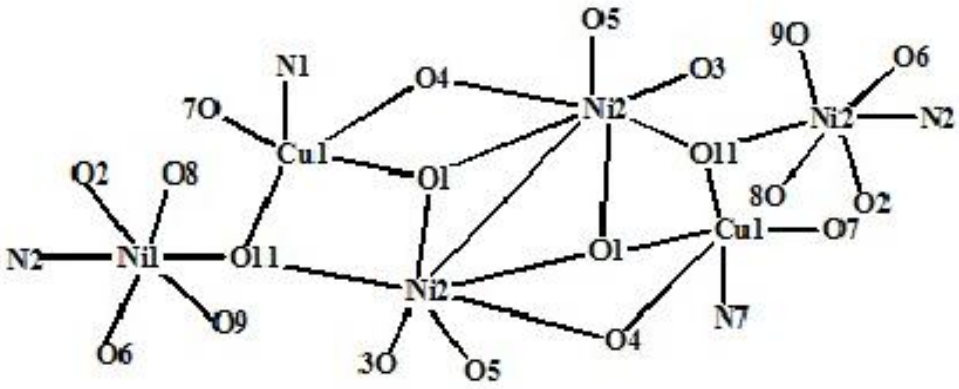

Fig. S2: Chemdraw sketch of M-O central core of $[Cu_2Ni_4(acac)_2(dmae)_2(dmaeH)_2(OH)_2(TFA)_6]$ (**2**).

Table S1: Selected bond distances (Å) for complex (**1**) and (**2**). Symmetry operator (i): $-x+1$, $-y+1$, $-z+1$.

Bond lengths (Å) for complex (**1**)		Bond lengths (Å) for complex (**2**)	
Ni(1)-O(9)	2.0230(19)	Co(1)-O(9)	2.047(2)
Ni(1)-O(11)	2.0658(17)	Co(1)-O(6)	2.099(2)
Ni(1)-O(8)	2.0702(19)	Co(1)-O(11)	2.1011(18)
Ni(1)-O(2)	2.0745(19)	Co(1)-O(8)	2.107(2)
Ni(1)-O(6)	2.0748(19)	Co(1)-O(2)	2.113(2)
Ni(1)-N(2)	2.140(2)	Co(1)-N(2)	2.175(2)
Ni(2)-O(3)	2.0269(17)	Co(2)-O(4)	2.0562(18)
Ni(2)-O(4)	2.0269(17)	Co(2)-O(3)	2.0645(18)
Ni(2)-O(5)	2.0411(17)	Co(2)-O(5)	2.0740(18)
Ni(2)-O(11)	2.0650(17)	Co(2)-O(11)	2.0907(18)
Ni(2)-O(1)	2.0886(16)	Co(2)-O(1)	2.1259(17)
Ni(2)-O(1)^{i}	2.0954(16)	Co(2)-O(1)^{i}	2.1366(17)
Ni(2)-Cu(2)	2.9739(6)	Co(2)-Cu(2)	3.0108(5)

Cu(1)-O(7)	1.9422(18)	Cu(1)-O(7)	1.9460(19)
Cu(1)-O(11)	1.9493(16)	Cu(1)-O(11)	1.9529(17)
Cu(1)-O(1)	1.9608(16)	Cu(1)-O(1)	1.9548(18)
Cu(1)-N(1)	2.034(2)	Cu(1)-N(1)	2.038(2)
Cu(1)-O(4)^{i}	2.3725(17)	Cu(1)-O(4)^{i}	2.3936(18)
O(1)-Ni(2)^{i}	2.0954(16)	O(1)-Co(1)^{i}	2.1366(17)
O(4)-Cu(1)^{i}	2.3724(17)	O(4)-Cu(1)^{i}	2.3936(18)

Table S2: Selected bond angles (°) for complex (**1**). Symmetry operator (i): $-x+1, -y+1, -z+1$.

O(9)-Ni(1)-O(11)	97.09(7)	O(4)-Ni(2)-O(1)^{i}	83.23(7)
O(9)-Ni(1)-O(8)	88.15(8)	O(5)-Ni(2)-O(1)^{i}	95.37(7)
O(11)-Ni(1)-O(8)	91.81(7)	O(11)-Ni(2)-O(1)^{i}	95.20(6)
O(9)-Ni(1)-O(2)	174.26(8)	O(1)-Ni(2)-O(1)^{i}	80.57(6)
O(11)-Ni(1)-O(2)	88.52(7)	O(3)-Ni(2)-Cu(2)	85.96(5)
O(8)-Ni(1)-O(2)	90.49(8)	O(4)-Ni(2)-Cu(2)	136.22(5)
O(9)-Ni(1)-O(6)	88.60(8)	O(5)-Ni(2)-Cu(2)	134.04(5)
O(11)-Ni(1)-O(6)	91.13(7)	O(11)-Ni(2)-Cu(2)	40.72(5)
O(8)-Ni(1)-O(6)	175.87(8)	O(1)-Ni(2)-Cu(2)	41.10(4)
O(2)-Ni(1)-O(6)	92.49(8)	O(1)^{i}-Ni(2)-Cu(2)	93.29(5)

O(9)-Ni(1)-N(2)	91.67(9)	O(7)-Cu(2)-O(11)	99.07(7)
O(11)-Ni(1)-N(2)	171.18(8)	O(7)-Cu(2)-O(1)	172.36(7)
O(8)-Ni(1)-N(2)	87.42(8)	O(11)-Cu(2)-O(1)	87.31(7)
O(2)-Ni(1)-N(2)	82.70(9)	O(7)-Cu(2)-N(1)	89.79(8)
O(6)-Ni(1)-N(2)	90.11(8)	O(11)-Cu(2)-N(1)	155.93(8)
O(3)-Ni(2)-O(4)	89.86(7)	O(1)-Cu(2)-N(1)	85.96(8)
O(3)-Ni(2)-O(5)	92.85(7)	O(7)-Cu(2)-O(4)^{i}	97.92(7)
O(4)-Ni(2)-O(5)	89.66(7)	O(11)-Cu(2)-O(4)^{i}	90.36(7)
O(3)-Ni(2)-O(11)	91.25(7)	O(1)-Cu(2)-O(4)^{i}	77.74(6)
O(4)-Ni(2)-O(11)	176.60(7)	N(1)-Cu(2)-O(4)^{i}	110.66(8)
O(5)-Ni(2)-O(11)	93.49(7)	O(7)-Cu(2)-Ni(2)	142.47(6)
O(3)-Ni(2)-O(1)	91.94(7)	O(11)-Cu(2)-Ni(2)	43.72(5)
O(4)-Ni(2)-O(1)	95.70(7)	O(1)-Cu(2)-Ni(2)	44.44(5)
O(5)-Ni(2)-O(1)	172.82(7)	N(1)-Cu(2)-Ni(2)	122.41(6)
O(11)-Ni(2)-O1	81.06(7)	O(4)^{i}-Cu(2)-Ni(2)	88.63(4)

Table S3: Selected bond angles (°) for complex (**2**). Symmetry operator (i): −*x*+1, −*y*+1, −*z*+1.

O(9)-Co(1)-O(6)	89.50(9)	O(3)-Co(2)-O(1)^{i}	167.52(7)
O(9)-Co(1)-O(11)	96.31(8)	O(5)-Co(2)-O(1)^{i}	95.55(7)
O(6)-Co(1)-O(11)	91.46(7)	O(11)-Co(2)-O(1)^{i}	95.73(7)
O(9)-Co(1)-O(8)	88.30(9)	O(1)-Co(2)-O(1)^{i}	80.52(7)
O(6)-Co(1)-O(8)	176.84(8)	O(4)-Co(2)-Cu(2)	135.73(5)
O(11)-Co(1)-O(8)	91.04(7)	O(3)-Co(2)-Cu(2)	87.11(5)
O(9)-Co(1)-O(2)	174.40(8)	O(5)-Co(2)-Cu(2)	133.19(6)
O(6)-Co(1)-O(2)	92.18(8)	O(11)-Co(2)-Cu(2)	40.15(5)
O(11)-Co(1)-O(2)	88.99(7)	O(1)-Co(2)-Cu(2)	40.30(5)
O(8)-Co(1)-O(2)	89.80(8)	O(1)^{i}-Co(2)-Cu(2)	93.14(5)
O(9)-Co(1)-N(2)	93.50(9)	O(7)-Cu(2)-O(11)	98.82(8)
O(6)-Co(1)-N(2)	90.71(9)	O(7)-Cu(2)-O(1)	172.27(8)
O(11)-Co(1)-N(2)	169.97(9)	O(11)-Cu(2)-O(1)	87.59(7)
O(8)-Co(1)-N(2)	87.16(9)	O(7)-Cu(2)-N(1)	89.94(9)
O(2)-Co(1)-N(2)	81.15(9)	O(11)-Cu(2)-N(1)	155.39(8)
O(4)-Co(2)-O(3)	88.46(7)	O(1)-Cu(2)-N(1)	85.88(8)

O(4)-Co(2)-O(5)	91.03(7)	O(7)-Cu(2)-O(4)^{i}	97.08(7)
O(3)-Co(2)-O(5)	93.35(7)	O(11)-Cu(2)-O(4)^{i}	90.99(7)
O(4)-Co(2)-O(11)	175.64(7)	O(1)-Cu(2)-O(4)^{i}	78.40(7)
O(3)-Co(2)-O(11)	92.50(7)	N(1)-Cu(2)-O(4)^{i}	110.82(8)
O(5)-Co(2)-O(11)	93.16(7)	O(7)-Cu(2)-Co(2)	142.23(6)
O(4)-Co(2)-O(1)	95.94(7)	O(11)-Cu(2)-Co(2)	43.66(5)
O(3)-Co(2)-O(1)	91.76(7)	O(1)-Cu(2)-Co(2)	44.70(5)
O(5)-Co(2)-O(1)	171.47(7)	N(1)-Cu(2)-Co(2)	122.50(7)
O(11)-Co(2)-O(1)	79.79(7)	O(4)^{i}-Cu(2)-Co(2)	89.19(4)

Table S4: Atomic % of element determined by EDX analysis of thin films deposited from complex (**1**) and (**2**) by AACVD

Thin films deposited from complex (**1**)			
Deposition Temperature	Atomic % of elements		
	Copper	Nickel	Oxygen
350 °C	17.33333	33.91667	48.75000
400 °C	16.66667	33.75000	49.58333
450 °C	16.41667	32.95833	50.62500
500 °C	16.79167	33.45833	49.83333
Thin films deposited from complex (**2**)			
Deposition Temperature	Atomic % of elements		

	Copper	Cobalt	Oxygen
350 °C	19.54545	37.72727	42.72727
400 °C	18.63636	37.27273	44.09091
450 °C	17.90909	35.95455	46.13636
500 °C	18.31818	36.50000	45.27273