

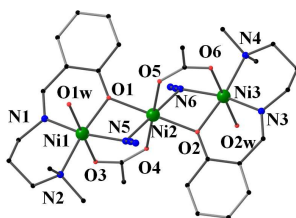
## Supporting Information

A rare phenoxido/acetato/azido bridged tri-nuclear and an unprecedented phenoxido/azido bridged 1D polynuclear nickel(II) complexes: Synthesis, crystal structure and magnetic properties with theoretical investigations on the exchange mechanism.

Rituparna Biswas, Sandip Mukherjee, Paramita Kar and Ashutosh Ghosh

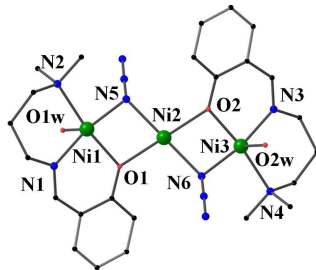
**Table S1.** Atomic spin densities (in au) of all the model systems in all of their spin states of complex 1.

**Model 1(a)**



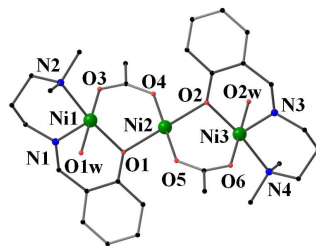
Atoms	Septet	Quintet	Triplet	Singlet
Ni1	1.643318	1.654699	1.656108	0.022713
Ni2	1.655109	1.649531	-1.680054	-1.670470
Ni3	1.651257	0.015017	1.691516	1.665638
N1	0.083589	0.072021	0.075016	-0.062723
N2	0.065743	0.063393	0.064965	0.064431
N3	0.070730	-0.057031	0.069283	0.072155
N4	0.064124	0.066385	0.059069	0.062864
N5	0.064208	0.050738	0.005497	-0.053383
N6	0.055762	-0.004596	-0.000870	0.025178
O1	0.104158	0.103346	0.017909	0.014747
O2	0.103139	0.102680	0.010374	0.015233
O3	0.060120	0.058739	0.061760	-0.001287
O4	0.049519	0.051240	-0.048908	-0.050874
O5	0.049333	0.051828	-0.049535	-0.049825
O6	0.059184	-0.012897	0.055128	0.059670
O1w	0.025659	0.025381	0.025721	-0.002573
O2w	0.025409	-0.006316	0.023859	0.025178

**Model 1(b)**



Atoms	Septet	Quintet	Triplet	Singlet
Ni1	1.665042	1.667247	0.027738	0.002989
Ni2	1.561346	0.009986	1.606783	-0.006738
Ni3	1.658214	1.667349	0.028557	-0.000601
N1	0.090932	0.084605	0.002144	0.000426
N2	0.082629	0.083529	0.001827	-0.001991
N3	0.091269	0.084553	0.004617	-0.004380
N4	0.084557	0.083483	-0.014854	0.005482
N5	0.075456	0.031952	0.029481	-0.001853
N6	0.075199	0.032486	0.035878	0.002788
O1	0.147838	0.040359	0.085067	-0.000238
O2	0.147026	0.040173	0.077745	0.003048
O1w	0.039774	0.039803	-0.000822	0.000085
O2w	0.040231	0.039814	0.000366	-0.000260

**Model 1(c)**

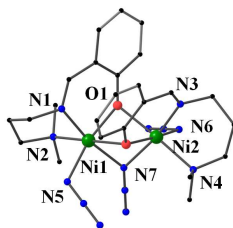


Atoms	Septet	Quintet	Triplet	Singlet
Ni1	1.658622	1.630421	1.663736	1.668938
Ni2	1.629719	0.432936	-0.003656	0.000110
Ni3	1.657433	1.654588	0.053346	-1.668961
N1	0.144134	0.121310	0.131462	0.131089
N2	0.077897	0.079499	0.078072	0.077755
N3	0.144982	0.103317	-0.106230	-0.131090

N4	0.078169	0.080324	-0.014469	-0.077747
O1	0.127096	-0.023118	0.046398	0.051038
O2	0.126546	-0.041986	0.078072	-0.051083
O3	0.060023	0.060549	0.053652	0.054250
O4	0.079464	-0.012999	0.003107	0.002283
O5	0.080043	-0.018478	-0.003100	-0.002338
O6	0.059699	0.056689	0.058490	-0.054244
O1w	0.029642	0.028794	0.029552	0.029681
O2w	0.029587	0.027954	0.030196	-0.029679

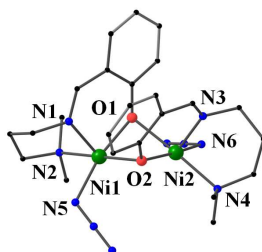
**Table S2.** Atomic spin densities (in au) of all the model systems in all of their spin states of complex **2**.

**Model 2(a)**



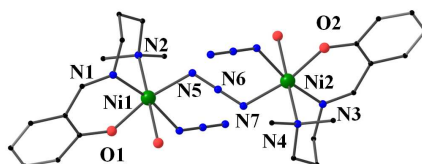
Atoms	Quintet	Triplet	Singlet
Ni1	1.604052	1.612218	0.000509
Ni2	1.605334	-0.047470	0.000505
N1	0.082794	0.067342	-0.078678
N2	0.082054	0.082547	0.000837
N3	0.083941	0.027526	0.078925
N4	0.081416	-0.096346	-0.000577
N5	0.019208	0.018928	0.020088
N6	0.018615	0.016182	-0.020537
N7	0.047509	0.032443	0.000459
O1	0.079133	0.027486	0.043572
O2	0.078895	0.078692	-0.043861

**Model 2(b)**



Atoms	Quintet	Triplet	Singlet
Ni1	1.596008	1.608782	0.014964
Ni2	1.601565	0.015876	0.000936
N1	0.138536	0.118183	-0.037583
N2	0.095713	0.094070	0.059153
N3	0.133126	0.023249	-0.034821
N4	0.094555	-0.098861	0.060380
N5	0.022218	0.021502	-0.010806
N6	0.021881	0.003143	-0.007124
O1	0.091965	0.029772	-0.013331
O2	0.091726	0.091290	-0.015276

**Model 2(c)**



Atoms	Quintet	Triplet	Singlet
Ni1	1.526619	1.520139	1.509699
Ni2	1.529127	1.666764	-1.509734
N1	-0.205897	-0.210752	0.363144
N2	0.035358	0.035461	0.039379
N3	-0.204897	-0.213065	-0.363137
N4	0.035342	0.039059	-0.039370
N5	0.049812	0.050532	-0.060886
N6	0.020213	0.020902	-0.000040
N7	0.048122	0.048249	0.060937
O1	0.043204	0.044750	0.088999
O2	0.043209	0.040963	-0.088990