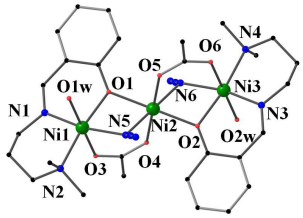
Supporting Information

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

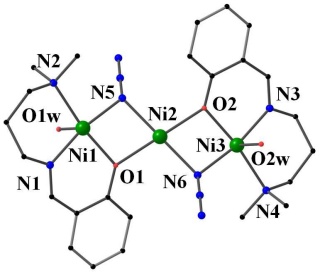
Table S1. Atomic spin densities (in au) of all the model systems in all of their spin states of complex **1**.

Model 1(a)



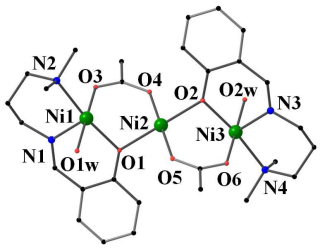
Atoms	Septet	Quintet	Triplet	Singlet
Ni1	1.643318	1.654699	1.656108	0.022713
Ni2	1.655109	1.649531	-1.680054	-1.670470
Ni3	1.651257	0.015017	1.691516	1.665638
N1	0.083589	0.072021	0.075016	-0.062723
N2	0.065743	0.063393	0.064965	0.064431
N3	0.070730	-0.057031	0.069283	0.072155
N4	0.064124	0.066385	0.059069	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)

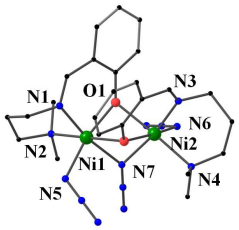


Atoms	Septet	Quintet	Triplet	Singlet
Ni1	1.658622	1.630421	1.663736	1.668938
Ni2	1.629719	0.432936	-0.003656	0.000110
Ni3	1.657433	1.654588	0.053346	-1.668961
N1	0.144134	0.121310	0.131462	0.131089
N2	0.077897	0.079499	0.078072	0.077755
N3	0.144982	0.103317	-0.106230	-0.131090

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

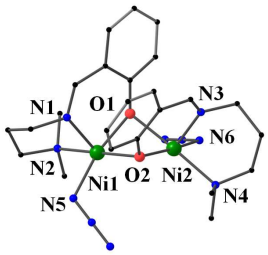
Table S2. Atomic spin densities (in au) of all the model systems in all of their spin states of complex **2**.

Model 2(a)



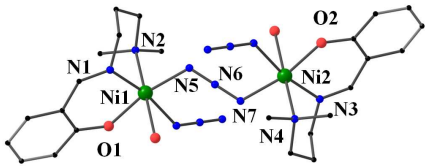
Atoms	Quintet	Triplet	Singlet
Ni1	1.604052	1.612218	0.000509
Ni2	1.605334	-0.047470	0.000505
N1	0.082794	0.067342	-0.078678
N2	0.082054	0.082547	0.000837
N3	0.083941	0.027526	0.078925
N4	0.081416	-0.096346	-0.000577
N5	0.019208	0.018928	0.020088
N6	0.018615	0.016182	-0.020537
N7	0.047509	0.032443	0.000459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