Supporting Information

Theoretical study on magnetic interaction in pyrazole−bridged dinuclear metal complex: Possibility of intramolecular ferromagnetic interaction by orbital counter−complementarity

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Table S1. Optimized cartesian coordinates (Å) of acetate bridged dinuclear Ni(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Ni	−2.149940	−0.128308	−0.039171	−2.150572	−0.128307	−0.038727
Ni	2.113265	−0.125967	−0.032832	2.113538	−0.126002	−0.032644
C	−0.022402	3.408510	−0.080285	−0.022417	3.408178	−0.080813
H	−0.023251	4.488092	−0.091851	−0.023316	4.487763	−0.092087
N	−0.686915	1.261319	−0.048862	−0.687116	1.260894	−0.050108
C	−1.129198	2.547854	−0.061310	−1.129108	2.547444	−0.062356
C	−2.619839	2.745774	−0.050951	−2.619778	2.745566	−0.051904
O	−3.155510	3.852548	0.110699	−3.155325	3.852361	0.109957
N	−3.244009	1.552936	−0.219831	−3.244116	1.552794	−0.220530
C	−4.668841	1.493725	−0.081420	−4.668849	1.493714	−0.080889
H	−5.212205	2.006703	−0.896384	−5.212846	2.007033	−0.895182
H	−5.031631	1.993595	0.837555	−5.030771	1.993320	0.838596
C	−5.113548	0.039138	−0.053474	−5.113690	0.039179	−0.052905
C	−6.469667	−0.315758	−0.047919	−6.469848	−0.315572	−0.047448
H	−7.223510	0.466268	−0.072570	−7.223619	0.466524	−0.072146
C	−6.832074	−1.657554	−0.011470	−6.832397	−1.657338	−0.011235
H	−7.880542	−1.943664	−0.006777	−7.880896	−1.943338	−0.006755
C	−5.829033	−2.631461	0.017609	−5.829464	−2.631356	0.017692
H	−6.067033	−3.690119	0.046370	−6.067583	−3.689996	0.046081
C	−4.505604	−2.208182	0.007862	−4.505987	−2.208214	0.008235
H	−3.675802	−2.910379	0.031919	−3.676254	−2.910491	0.032265
N	−4.153043	−0.910696	−0.028366	−4.153288	−0.910773	−0.027745
N	0.646383	1.262180	−0.064177	0.646641	1.261818	−0.065234
C	1.085979	2.549732	−0.080214	1.085905	2.549399	−0.080860
C	2.575928	2.751261	−0.091672	2.575932	2.751088	−0.091579
O	3.109276	3.856754	−0.269462	3.109328	3.856598	−0.269043
N	3.202431	1.563085	0.097845	3.202404	1.562973	0.098339
C	4.628400	1.506661	−0.026952	4.628455	1.506686	−0.025430
H	4.997201	1.980516	−0.957352	4.997984	1.981405	−0.955077
H	5.162209	2.046584	0.776824	5.161643	2.045850	0.779294
C	5.079535	0.054101	−0.008671	5.079713	0.054141	−0.008009

C	6.437271	−0.294274	0.006481	6.437531	−0.294024	0.006020
H	7.187232	0.491818	0.014033	7.187374	0.492184	0.013440
C	6.806095	−1.634767	0.012607	6.806594	−1.634457	0.010999
H	7.855839	−1.915929	0.024790	7.856391	−1.915461	0.022178
C	5.807659	−2.613738	0.004450	5.808320	−2.613591	0.002729
H	6.050530	−3.671671	0.008976	6.051351	−3.671491	0.006116
C	4.482333	−2.196542	−0.008854	4.482929	−2.196591	−0.009214
H	3.656348	−2.903455	−0.018550	3.657077	−2.903665	−0.018907
N	4.123259	−0.900362	−0.013379	4.123612	−0.900488	−0.012525
N	−2.160602	−0.075266	2.100711	−2.161857	−0.073407	2.101308
H	−1.611940	−0.846976	2.475645	−1.613796	−0.845342	2.476686
H	−1.710717	0.801418	2.359806	−1.711292	0.803051	2.359977
H	−3.075117	−0.095795	2.548720	−3.076411	−0.092984	2.549255
N	−2.064666	−0.218358	−2.173807	−2.064374	−0.220648	−2.173343
H	−1.113380	−0.161229	−2.530070	−1.112820	−0.164792	−2.529062
H	−2.524017	0.672660	−2.363953	−2.522830	0.670584	−2.364656
H	−2.552909	−0.950327	−2.687293	−2.553066	−0.952663	−2.686334
N	2.026281	−0.157594	2.102386	2.025020	−0.157425	2.102678
H	1.074443	−0.100101	2.457128	1.072832	−0.101091	2.456632
H	2.479063	0.740408	2.274042	2.476894	0.740844	2.275170
H	2.519254	−0.874913	2.631789	2.518282	−0.874580	2.632040
N	2.130479	−0.130286	−2.172637	2.132876	−0.130540	−2.172613
H	1.581082	−0.905834	−2.538579	1.585002	−0.906450	−2.540082
H	1.688266	0.743620	−2.453501	1.689692	0.742996	−2.453143
H	3.048719	−0.164941	−2.612092	3.051642	−0.163386	−2.611091
C	−0.012040	−2.528302	−0.008314	−0.012468	−2.527896	−0.007893
O	1.115621	−1.977655	−0.174433	1.115056	−1.977204	−0.174626
O	−1.134233	−1.964217	0.159471	−1.134425	−1.963858	0.161593
C	−0.040570	−4.060276	−0.027624	−0.041127	−4.059872	−0.028598
H	−0.607468	−4.435957	0.830593	−0.607589	−4.436228	0.829607
H	−0.561110	−4.403804	−0.929812	−0.562144	−4.402640	−0.930811
H	0.966863	−4.482156	−0.018362	0.966301	−4.481780	−0.020205

Table S1. (continued)

acetate bridged dinuclear Co(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Co	−2.162302	−0.158533	−0.019694	−2.164121	−0.159869	−0.023470
Co	2.105520	−0.161540	−0.041147	2.107703	−0.162308	−0.041999
C	−0.025024	3.414103	−0.086080	−0.024558	3.412699	−0.087632
H	−0.024641	4.493708	−0.104535	−0.024161	4.492328	−0.104225
N	−0.690734	1.268020	0.007162	−0.690757	1.266414	0.000687
C	−1.130895	2.554943	0.007076	−1.130577	2.553428	0.001893
C	−2.620220	2.747319	0.058107	−2.619843	2.746684	0.053312
O	−3.160100	3.858778	0.155424	−3.158699	3.858536	0.151636
N	−3.246446	1.540284	−0.011730	−3.247145	1.540254	−0.015785
C	−4.676129	1.506962	0.075483	−4.676652	1.507898	0.074540
H	−5.169583	2.091749	−0.722289	−5.171604	2.091984	−0.722847
H	−5.062258	1.954737	1.011353	−5.060453	1.956929	1.010747
C	−5.170522	0.069919	−0.004256	−5.171705	0.070948	−0.002577
C	−6.540777	−0.228094	−0.002050	−6.542023	−0.226723	0.001886
H	−7.260999	0.583714	0.052074	−7.261980	0.585360	0.055339
C	−6.959618	−1.551786	−0.070519	−6.961314	−1.550418	−0.063803
H	−8.019106	−1.793938	−0.071033	−8.020867	−1.792277	−0.062710
C	−5.998011	−2.565222	−0.139610	−6.000089	−2.564218	−0.132478
H	−6.280140	−3.612060	−0.193577	−6.282567	−3.611070	−0.184294
C	−4.658671	−2.196606	−0.137476	−4.660657	−2.195930	−0.133224
H	−3.861731	−2.935002	−0.184654	−3.864045	−2.934661	−0.180645
N	−4.249930	−0.916243	−0.072071	−4.251468	−0.915580	−0.070423
N	0.639167	1.265525	−0.104267	0.639951	1.264078	−0.107647
C	1.080245	2.551867	−0.149578	1.080825	2.550601	−0.150010
C	2.569363	2.741755	−0.207767	2.570029	2.741368	−0.204520
O	3.109922	3.849932	−0.335544	3.110115	3.850013	−0.330025
N	3.194859	1.536752	−0.106084	3.196131	1.536753	−0.102391
C	4.624910	1.503054	−0.186657	4.626373	1.503814	−0.180005
H	5.014347	1.921032	−1.135079	5.017703	1.924336	−1.126496
H	5.114308	2.115051	0.593067	5.113905	2.113933	0.602370
C	5.122237	0.070568	−0.058364	5.123808	0.071111	−0.054333

C	6.493316	−0.223610	−0.043786	6.494897	−0.222896	−0.038058
H	7.211816	0.587969	−0.119929	7.213412	0.589023	−0.110279
C	6.914989	−1.543306	0.069615	6.916586	−1.542884	0.071878
H	7.975055	−1.782507	0.083901	7.976661	−1.781966	0.087249
C	5.955456	−2.556506	0.166010	5.957059	−2.556531	0.163409
H	6.239850	−3.600311	0.255211	6.241466	−3.600574	0.249716
C	4.615221	−2.191591	0.144618	4.616812	−2.191755	0.141073
H	3.819790	−2.930018	0.211051	3.821376	−2.930461	0.204172
N	4.203706	−0.915158	0.035973	4.205301	−0.915056	0.035657
N	−2.197518	−0.263458	2.191860	−2.197989	−0.264190	2.187555
H	−1.489763	−0.900332	2.553221	−1.489481	−0.901131	2.547300
H	−1.991512	0.678102	2.521406	−1.990894	0.677229	2.516778
H	−3.091599	−0.542682	2.591811	−3.091246	−0.543189	2.589517
N	−1.916940	−0.079784	−2.217976	−1.921514	−0.082442	−2.221647
H	−0.957355	0.217221	−2.380816	−0.963064	0.217462	−2.385859
H	−2.514423	0.711760	−2.453008	−2.521781	0.706966	−2.456818
H	−2.134627	−0.848177	−2.850252	−2.137501	−0.851968	−2.853135
N	1.899143	−0.019593	2.160336	1.897928	−0.019631	2.159570
H	0.965750	0.349639	2.328684	0.964784	0.350856	2.326486
H	2.553660	0.731462	2.374967	2.553083	0.731040	2.373629
H	2.068659	−0.790050	2.804786	2.066050	−0.789258	2.805382
N	2.171990	−0.288676	−2.256847	2.175106	−0.287845	−2.257359
H	1.524609	−0.957542	−2.670705	1.527947	−0.957456	−2.670321
H	1.934360	0.645656	−2.585978	1.934761	0.646261	−2.585127
H	3.101752	−0.509614	−2.608999	3.104523	−0.506671	−2.611712
C	−0.013621	−2.594623	−0.007100	−0.012084	−2.594622	−0.009895
O	1.126197	−2.045456	−0.067646	1.128062	−2.046030	−0.068520
O	−1.145932	−2.029826	0.065686	−1.144180	−2.029139	0.061238
C	−0.041562	−4.125916	−0.035980	−0.040909	−4.125884	−0.038964
H	−0.645572	−4.505119	0.795191	−0.641580	−4.504591	0.794871
H	−0.524312	−4.464233	−0.960602	−0.527846	−4.464128	−0.961401
H	0.964542	−4.547528	0.016205	0.965162	−4.548011	0.009339

Table S1. (continued)

acetate bridged dinuclear Fe(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Fe	−2.214781	−0.263392	−0.072627	−2.214772	−0.262012	−0.076292
Fe	2.179758	−0.256514	0.020987	2.179875	−0.255073	0.024791
C	−0.021519	3.355992	−0.083869	−0.021449	3.357023	−0.084154
H	−0.022368	4.435422	−0.104189	−0.022285	4.436437	−0.104843
N	−0.688305	1.205884	−0.051375	−0.688317	1.206967	−0.053321
C	−1.127324	2.494546	−0.079786	−1.127245	2.495530	−0.082676
C	−2.611572	2.705534	−0.094575	−2.611631	2.706687	−0.097421
O	−3.134533	3.825971	−0.013089	−3.134227	3.827299	−0.016421
N	−3.265416	1.512904	−0.194263	−3.265612	1.514112	−0.196271
C	−4.698808	1.532726	−0.122747	−4.698913	1.533825	−0.122092
H	−5.168275	2.059269	−0.974175	−5.170232	2.060970	−0.972082
H	−5.070101	2.076372	0.765702	−5.068270	2.076818	0.767596
C	−5.233750	0.110777	−0.083583	−5.233829	0.111833	−0.082666
C	−6.609653	−0.152170	−0.077997	−6.609770	−0.150975	−0.079245
H	−7.307816	0.679985	−0.106672	−7.307808	0.681222	−0.109610
C	−7.064421	−1.465804	−0.036612	−7.064758	−1.464552	−0.038006
H	−8.129539	−1.680830	−0.031717	−8.129914	−1.679432	−0.034791
C	−6.126775	−2.503263	−0.002446	−6.127335	−2.502109	−0.001871
H	−6.433088	−3.544197	0.029896	−6.433837	−3.542993	0.030356
C	−4.779089	−2.169902	−0.010843	−4.779574	−2.168856	−0.007463
H	−4.005692	−2.934159	0.015441	−4.006309	−2.933172	0.021112
N	−4.333149	−0.898049	−0.051060	−4.333422	−0.897103	−0.047473
N	0.648894	1.207227	−0.036101	0.649034	1.208394	−0.033460
C	1.085790	2.496904	−0.055933	1.085846	2.497980	−0.053093
C	2.569480	2.711490	−0.054471	2.569676	2.712709	−0.051861
O	3.089054	3.829661	−0.178072	3.088904	3.830951	−0.176020
N	3.227180	1.524706	0.083173	3.227475	1.525971	0.085185
C	4.659959	1.546358	−0.000100	4.660142	1.547401	−0.000562
H	5.022391	2.068151	−0.905088	5.020841	2.068874	−0.906445
H	5.134730	2.095904	0.833722	5.136615	2.097143	0.832137
C	5.198861	0.125389	−0.006392	5.198979	0.126368	−0.007446

C	6.575475	−0.133694	−0.019948	6.575644	−0.132545	−0.019631
H	7.271337	0.700877	−0.021927	7.271418	0.702099	−0.020498
C	7.033782	−1.446679	−0.030277	7.034137	−1.445479	−0.029728
H	8.099445	−1.658784	−0.041200	8.099847	−1.657419	−0.039486
C	6.099050	−2.487301	−0.025444	6.099583	−2.486235	−0.026062
H	6.408223	−3.527866	−0.032473	6.408922	−3.526754	−0.032812
C	4.750491	−2.157615	−0.011754	4.750936	−2.156708	−0.014385
H	3.979202	−2.924357	−0.008982	3.979731	−2.923544	−0.013102
N	4.301157	−0.886435	−0.001748	4.301428	−0.885616	−0.004629
N	−2.140994	−0.226075	2.199638	−2.139444	−0.228731	2.195951
H	−1.434833	−0.871971	2.548197	−1.436912	−0.880966	2.539965
H	−1.829297	0.722354	2.403981	−1.821055	0.716691	2.403805
H	−2.994272	−0.391219	2.731636	−2.992961	−0.390533	2.728554
N	−2.075356	−0.245544	−2.337366	−2.077610	−0.245828	−2.338597
H	−1.128141	−0.086600	−2.675266	−1.130980	−0.089959	−2.679602
H	−2.561695	0.650216	−2.398602	−2.561813	0.651232	−2.398438
H	−2.532063	−0.896844	−2.974719	−2.538149	−0.896307	−2.974020
N	2.045689	−0.170139	2.282346	2.047089	−0.170401	2.283905
H	1.098919	0.011268	2.610093	1.100485	0.008292	2.613660
H	2.542734	0.721034	2.319286	2.542193	0.721914	2.320240
H	2.490821	−0.808201	2.940914	2.495050	−0.807959	2.941037
N	2.098051	−0.282715	−2.252194	2.096754	−0.284676	−2.248284
H	1.406230	−0.948921	−2.591325	1.407578	−0.955717	−2.583191
H	1.771556	0.655186	−2.480815	1.765142	0.650696	−2.479816
H	2.957815	−0.444924	−2.774532	2.956473	−0.444596	−2.771362
C	−0.007693	−2.638039	0.007077	−0.007443	−2.639474	0.006812
O	1.126190	−2.078262	−0.048636	1.126753	−2.079903	−0.044515
O	−1.135676	−2.062900	0.056313	−1.135787	−2.064686	0.051737
C	−0.034224	−4.165337	0.002880	−0.033874	−4.166924	0.002903
H	−0.642410	−4.529664	0.837426	−0.643631	−4.531078	0.836391
H	−0.512420	−4.518338	−0.918301	−0.510391	−4.520148	−0.919055
H	0.972171	−4.583509	0.068195	0.972398	−4.585082	0.070274

Table S1. (continued)

acetate bridged dinuclear Mni(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Mn	2.224138	−0.382723	−0.073014	−2.225103	−0.381360	−0.066820
Mn	2.185981	−0.366983	0.003862	2.185631	−0.366253	0.008185
C	−0.031337	3.284393	−0.070685	−0.031460	3.284796	−0.066748
H	−0.034875	4.363832	−0.078252	−0.034868	4.364221	−0.075621
N	−0.695402	1.135300	−0.068410	−0.695889	1.135755	−0.060753
C	−1.135463	2.421074	−0.087308	−1.135737	2.421636	−0.079988
C	−2.620017	2.651966	−0.106498	−2.620296	2.652866	−0.098163
O	−3.110512	3.790267	−0.043828	−3.110500	3.791152	−0.033169
N	−3.300743	1.477265	−0.185776	−3.301225	1.478520	−0.180383
C	−4.730496	1.570896	−0.134836	−4.730996	1.572183	−0.129872
H	−5.160797	2.111409	−0.999752	−5.160611	2.117072	−0.992273
H	−5.086351	2.152103	0.736850	−5.087296	2.149054	0.744595
C	−5.367965	0.193180	−0.080903	−5.368712	0.194330	−0.082766
C	−6.764919	0.053256	−0.053433	−6.765823	0.054110	−0.067934
H	−7.386752	0.944139	−0.075360	−7.387616	0.944871	−0.095215
C	−7.332955	−1.212999	0.002436	−7.334113	−1.212285	−0.018037
H	−8.413066	−1.331660	0.025440	−8.414369	−1.331162	−0.005231
C	−6.492874	−2.331504	0.028375	−6.494093	−2.330649	0.014990
H	−6.890621	−3.340576	0.071523	−6.892007	−3.339828	0.053864
C	−5.121354	−2.115569	−0.003170	−5.122387	−2.114426	−0.004023
H	−4.421632	−2.948913	0.014734	−4.422713	−2.947673	0.019588
N	−4.565354	−0.890592	−0.056633	−4.566158	−0.889335	−0.052049
N	0.646852	1.139834	−0.041205	0.646562	1.140117	−0.036576
C	1.078507	2.428832	−0.041007	1.078338	2.429141	−0.038749
C	2.561332	2.670620	−0.019661	2.561263	2.670959	−0.022800
O	3.044024	3.811048	−0.101543	3.043634	3.810980	−0.111797
N	3.249825	1.502652	0.086384	3.250133	1.503459	0.085871
C	4.679350	1.605028	0.044131	4.679469	1.605415	0.035957
H	5.038248	2.169438	−0.837380	5.033956	2.166183	−0.849675
H	5.099247	2.167343	0.900139	5.103798	2.171122	0.887502

C	5.326015	0.230509	0.025176	5.325785	0.230682	0.019402
C	6.723935	0.098426	0.019761	6.723634	0.098256	0.008536
H	7.340471	0.993147	0.033794	7.340419	0.992885	0.016024
C	7.299676	−1.165425	−0.004225	7.298998	−1.165830	−0.012165
H	8.380652	−1.278199	−0.009636	8.379919	−1.278876	−0.021572
C	6.466343	−2.289135	−0.020994	6.465370	−2.289412	−0.020266
H	6.870388	−3.296449	−0.039687	6.869130	−3.296893	−0.035876
C	5.093259	−2.080845	−0.012603	5.092370	−2.080780	−0.007351
H	4.398082	−2.918045	−0.024547	4.396947	−2.917838	−0.012816
N	4.530076	−0.858270	0.010299	4.529565	−0.857975	0.012364
N	−2.240670	−0.376388	2.261804	−2.238737	−0.383081	2.267235
H	−1.694895	−1.102352	2.722758	−1.683672	−1.107505	2.719364
H	−1.788251	0.519880	2.438933	−1.793756	0.515933	2.449070
H	−3.156551	−0.344788	2.706131	−3.152691	−0.363867	2.716201
N	−2.381063	−0.401707	−2.416060	−2.379127	−0.401230	−2.409897
H	−1.531275	−0.467621	−2.973016	−1.528025	−0.467798	−2.964762
H	−2.688231	0.572270	−2.427610	−2.685872	0.572859	−2.422795
H	−3.098267	−0.958073	−2.878440	−3.095403	−0.957607	−2.873701
N	2.334001	−0.331862	2.349873	2.337581	−0.326440	2.353864
H	1.485366	−0.389580	2.909505	1.489163	−0.374870	2.914714
H	2.636629	0.643550	2.339759	2.647575	0.646646	2.339074
H	3.054208	−0.874730	2.823500	3.054072	−0.872880	2.829014
N	2.231081	−0.375931	−2.333945	2.226875	−0.378227	−2.330024
H	1.744656	−1.123463	−2.826151	1.739972	−1.127012	−2.819843
H	1.736924	0.496953	−2.516628	1.731761	0.494003	−2.513191
H	3.159160	−0.286326	−2.743621	3.154023	−0.288744	−2.741837
C	0.004345	−2.793611	−0.021634	0.005216	−2.793805	−0.016717
O	1.138863	−2.233538	−0.054348	1.140362	−2.234844	−0.048033
O	−1.122588	−2.217114	0.021161	−1.121230	−2.216464	0.026347
C	−0.023072	−4.321840	−0.047594	−0.023495	−4.322020	−0.044410
H	−0.642420	−4.697841	0.773562	−0.639968	−4.698330	0.778808
H	−0.489813	−4.661260	−0.979796	−0.494259	−4.660073	−0.975053
H	0.982093	−4.742238	0.024374	0.981553	−4.743374	0.023458

Table S1. (continued)

acetate bridged dinuclear Cr(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Cr	−2.143477	−0.165492	−0.043319	−2.144032	−0.165242	−0.044375
Cr	2.106419	−0.161545	−0.019648	2.107008	−0.161258	−0.020719
C	−0.022662	3.371483	−0.079751	−0.022660	3.370643	−0.079566
H	−0.023661	4.450579	−0.095170	−0.023670	4.449745	−0.094347
N	−0.689623	1.224634	−0.053125	−0.689668	1.223434	−0.054120
C	−1.125923	2.511833	−0.074082	−1.125879	2.510937	−0.074580
C	−2.614383	2.698141	−0.085460	−2.614475	2.698105	−0.086166
O	−3.171503	3.797245	−0.103811	−3.170582	3.797752	−0.104485
N	−3.224427	1.475947	−0.072395	−3.225092	1.476434	−0.073083
C	−4.661695	1.406731	−0.078966	−4.662279	1.407289	−0.079676
H	−5.102477	1.899202	−0.962720	−5.103109	1.899512	−0.963566
H	−5.111523	1.921414	0.787419	−5.112124	1.922186	0.786585
C	−5.079999	−0.047758	−0.062717	−5.080730	−0.047188	−0.062978
C	−6.422401	−0.440567	−0.065002	−6.423235	−0.439659	−0.064490
H	−7.197114	0.320154	−0.078460	−7.197753	0.321267	−0.077771
C	−6.746455	−1.792619	−0.050148	−6.747656	−1.791606	−0.048881
H	−7.786181	−2.107548	−0.051802	−7.787466	−2.106260	−0.049759
C	−5.717545	−2.739584	−0.033249	−5.718964	−2.738810	−0.032114
H	−5.926724	−3.804068	−0.021549	−5.928398	−3.803240	−0.019757
C	−4.406795	−2.287316	−0.031623	−4.408098	−2.286867	−0.031377
H	−3.560571	−2.967054	−0.018938	−3.562065	−2.966849	−0.018752
N	−4.089169	−0.975625	−0.045753	−4.090076	−0.975268	−0.046157
N	0.648774	1.225895	−0.045116	0.648857	1.224706	−0.045935
C	1.082256	2.514208	−0.060904	1.082230	2.513332	−0.060901
C	2.569994	2.703916	−0.054767	2.570099	2.703919	−0.054184
O	3.125028	3.804150	−0.067021	3.124112	3.804704	−0.065522
N	3.182795	1.483129	−0.033956	3.183484	1.483649	−0.033968
C	4.620252	1.418837	−0.024881	4.620859	1.419429	−0.024676
H	5.068880	1.916304	−0.901819	5.069661	1.917047	−0.901462
H	5.058628	1.931880	0.848340	5.059122	1.932294	0.848718
C	5.043427	−0.034014	−0.009301	5.044175	−0.033419	−0.009331

C	6.387294	−0.421687	−0.000748	6.388136	−0.420755	0.000177
H	7.159082	0.342104	−0.004619	7.159723	0.343245	−0.002768
C	6.716426	−1.772482	0.011990	6.717629	−1.771454	0.012957
H	7.757305	−2.083512	0.018282	7.758582	−2.082211	0.020213
C	5.690942	−2.723242	0.016198	5.692369	−2.722458	0.016074
H	5.903921	−3.786987	0.025700	5.905598	−3.786157	0.025565
C	4.378563	−2.275852	0.007833	4.379882	−2.275390	0.006826
H	3.535342	−2.959303	0.010453	3.536857	−2.959091	0.008797
N	4.055775	−0.965432	−0.004493	4.056702	−0.965055	−0.005374
C	−0.014119	−2.488602	0.004472	−0.014084	−2.490644	0.003711
O	1.118094	−1.920058	0.000991	1.118226	−1.922637	−0.000020
O	−1.145403	−1.915495	−0.012044	−1.145504	−1.918065	−0.012482
C	−0.035663	−4.008007	0.017686	−0.035624	−4.010156	0.017140
H	−0.674263	−4.362110	0.833411	−0.673074	−4.363845	0.833916
H	−0.473232	−4.371823	−0.919096	−0.474937	−4.373736	−0.918881
H	0.968202	−4.420616	0.129677	0.968336	−4.422923	0.127544

Table S1. (continued)

azide bridged dinuclear Ni(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Ni	−2.261032	−0.151977	−0.029743	−2.257532	−0.138526	−0.035590
Ni	2.226098	−0.154288	−0.024629	2.219012	−0.156576	0.062513
C	−0.009345	3.334764	0.039341	−0.004196	3.339294	−0.014313
H	−0.008238	4.413321	0.081553	0.000465	4.418676	−0.021825
N	−0.685262	1.187210	−0.049337	−0.684888	1.192465	0.023705
C	−1.116279	2.480384	−0.004492	−1.112676	2.485883	0.030844
C	−2.598645	2.732410	0.013339	−2.594270	2.730725	0.073182
O	−3.083973	3.871970	0.090772	−3.093166	3.856159	−0.077415
N	−3.270615	1.562406	−0.052395	−3.258423	1.565135	0.267762
C	−4.700086	1.566270	0.007454	−4.688401	1.565736	0.161872
H	−5.171648	2.090116	−0.845475	−5.049122	2.126125	−0.721941
H	−5.094237	2.094250	0.896566	−5.191064	2.057725	1.014526
C	−5.205850	0.132014	0.028336	−5.190922	0.133287	0.075039
C	−6.574883	−0.166827	0.058175	−6.558910	−0.170425	0.100307
H	−7.295998	0.645773	0.065600	−7.280332	0.636593	0.192898
C	−6.991215	−1.493234	0.078385	−6.974190	−1.493992	0.007030
H	−8.050138	−1.736434	0.102471	−8.032455	−1.740516	0.024731
C	−6.028777	−2.507629	0.066924	−6.011288	−2.501282	−0.107823
H	−6.309200	−3.556031	0.081345	−6.290339	−3.547481	−0.182201
C	−4.689406	−2.139438	0.035985	−4.672821	−2.128901	−0.123415
H	−3.891957	−2.878517	0.025741	−3.876076	−2.863653	−0.210752
N	−4.284385	−0.856709	0.017319	−4.268853	−0.848823	−0.034080
N	0.659140	1.185086	−0.036083	0.657944	1.186345	−0.021392
C	1.094673	2.475149	0.011467	1.096871	2.475769	−0.047088
C	2.577665	2.716274	0.036172	2.580598	2.707104	−0.090405
O	3.071341	3.833596	0.251753	3.088967	3.830004	0.046801
N	3.246464	1.558111	−0.179456	3.235144	1.533294	−0.268043
C	4.671821	1.545816	−0.023555	4.664728	1.523442	−0.156133
H	5.205240	2.088181	−0.825466	5.175238	1.996387	−1.014876
H	5.003673	2.047767	0.905621	5.026321	2.095963	0.719498
C	5.165657	0.107456	−0.009058	5.154788	0.088603	−0.042645

C	6.532008	−0.203767	0.004571	6.520236	−0.226984	−0.057340
H	7.260684	0.601997	−0.004021	7.248818	0.572157	−0.161492
C	6.936369	−1.533902	0.028728	6.923961	−1.552113	0.061219
H	7.993243	−1.786753	0.040237	7.980170	−1.807762	0.052106
C	5.964759	−2.539320	0.036340	5.952170	−2.549102	0.190350
H	6.235678	−3.590157	0.054363	6.222092	−3.596083	0.284673
C	4.628397	−2.159051	0.019290	4.616837	−2.165301	0.193838
H	3.823705	−2.890291	0.025946	3.813486	−2.891564	0.291150
N	4.235484	−0.872857	−0.003564	4.224105	−0.883672	0.080108
N	−2.186501	−0.137633	2.110049	−2.071507	−0.392723	2.075004
H	−1.695732	−0.927040	2.527514	−1.104653	−0.514082	2.369483
H	−1.680568	0.716013	2.340761	−2.384213	0.528575	2.380382
H	−3.103265	−0.074954	2.549143	−2.635172	−1.096257	2.549538
N	−2.236288	−0.209570	−2.161660	−2.326798	0.082925	−2.166154
H	−1.687139	−0.973224	−2.553529	−1.912418	−0.718795	−2.639208
H	−1.810860	0.675171	−2.433833	−1.768928	0.908232	−2.381591
H	−3.162016	−0.244240	−2.585032	−3.254484	0.233039	−2.559123
N	2.229000	−0.062448	2.115926	2.286205	0.099530	2.189609
H	1.747158	−0.856378	2.535039	1.863496	−0.691033	2.673940
H	1.721567	0.787456	2.357595	1.735479	0.933133	2.391034
H	3.151662	0.001331	2.542789	3.214305	0.247163	2.582545
N	2.129162	−0.244750	−2.152833	2.036232	−0.444650	−2.043884
H	2.573594	−1.011200	−2.655500	2.594190	−1.161588	−2.504931
H	1.169039	−0.164969	−2.481362	1.069141	−0.561045	−2.339554
H	2.608474	0.624192	−2.388134	2.359236	0.468311	−2.363303
N	1.164462	−1.997360	0.146240	1.077851	−1.939248	0.451040
N	−0.015529	−2.009330	0.059075	−0.027148	−1.956555	0.027706
N	−1.196350	−2.002074	−0.026621	−1.132033	−1.936913	−0.395767

Table S1. (continued)

azide bridged dinuclear Co(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Co	−2.272090	−0.184763	−0.008027	−2.282297	−0.186215	−0.005614
Co	2.242417	−0.194844	0.031761	2.251703	−0.197093	0.031709
C	−0.006900	3.330700	−0.004288	−0.007072	3.327239	−0.006471
H	−0.004462	4.410215	−0.008264	−0.004495	4.406756	−0.011573
N	−0.682717	1.180766	−0.039455	−0.684298	1.177072	−0.031096
C	−1.112970	2.473718	−0.059319	−1.113683	2.470430	−0.048633
C	−2.593710	2.714979	−0.094055	−2.594081	2.714116	−0.071865
O	−3.090834	3.842885	−0.221450	−3.090281	3.842947	−0.193347
N	−3.267777	1.539324	0.024335	−3.269952	1.539514	0.049443
C	−4.699333	1.559563	−0.055587	−4.702064	1.563628	−0.021356
H	−5.069190	2.039589	−0.981252	−5.075480	2.062126	−0.935475
H	−5.166638	2.147021	0.755383	−5.164047	2.136032	0.803485
C	−5.243703	0.140079	0.003071	−5.249514	0.144622	0.014338
C	−6.622641	−0.111484	0.016321	−6.629114	−0.103573	0.022910
H	−7.315903	0.724732	−0.010258	−7.320147	0.734788	0.008841
C	−7.084669	−1.421794	0.064506	−7.094603	−1.413208	0.049796
H	−8.151530	−1.628405	0.076018	−8.162004	−1.617181	0.056857
C	−6.156904	−2.467808	0.099071	−6.169580	−2.462093	0.068579
H	−6.472932	−3.505512	0.136993	−6.488340	−3.499424	0.089969
C	−4.805865	−2.145154	0.084015	−4.817757	−2.142893	0.059329
H	−4.035631	−2.912377	0.107032	−4.049747	−2.912511	0.070745
N	−4.355414	−0.877809	0.037119	−4.363898	−0.876049	0.032616
N	0.659097	1.178038	0.047048	0.659923	1.174200	0.039226
C	1.095255	2.469150	0.057302	1.095436	2.465612	0.044176
C	2.577056	2.703918	0.091744	2.576926	2.702558	0.067162
O	3.079128	3.830660	0.209788	3.078152	3.830301	0.177869
N	3.245931	1.524170	−0.014454	3.247549	1.523585	−0.039537
C	4.677359	1.538694	0.068615	4.679513	1.541943	0.035781
H	5.149357	2.113862	−0.748487	5.146723	2.103628	−0.793458
H	5.047260	2.028499	0.989085	5.052292	2.048319	0.945854
C	5.215330	0.116120	0.028561	5.220629	0.120195	0.016843

C	6.593134	−0.141977	0.026659	6.599111	−0.134325	0.016321
H	7.290142	0.691245	0.048912	7.293908	0.700996	0.024436
C	7.049225	−1.454861	−0.004655	7.058668	−1.446274	0.004966
H	8.115143	−1.666585	−0.006991	8.125139	−1.655180	0.004343
C	6.116748	−2.496833	−0.034276	6.128915	−2.491066	−0.006631
H	6.428119	−3.536334	−0.059298	6.443002	−3.530001	−0.015865
C	4.767188	−2.167765	−0.031310	4.778546	−2.165650	−0.006204
H	3.993483	−2.931565	−0.051133	4.007069	−2.931844	−0.012601
N	4.322453	−0.897911	−0.000355	4.330402	−0.896551	0.005644
N	−1.971521	−0.179913	2.178457	−1.972650	−0.212926	2.179134
H	−2.211646	−0.974770	2.768333	−2.224174	−1.009570	2.761762
H	−0.993132	0.055244	2.330208	−0.989452	0.002597	2.328765
H	−2.519629	0.625484	2.477457	−2.504862	0.599132	2.488623
N	−2.297864	−0.234613	−2.226507	−2.283718	−0.211677	−2.225353
H	−1.735119	−0.994655	−2.605418	−1.736426	−0.984209	−2.601509
H	−1.914796	0.652776	−2.548419	−1.869544	0.667685	−2.530303
H	−3.233523	−0.324039	−2.619005	−3.214772	−0.269480	−2.634487
N	2.262531	−0.218975	2.251425	2.254241	−0.196502	2.252093
H	1.702479	−0.976054	2.640167	1.705999	−0.963107	2.638895
H	1.874980	0.671298	2.559759	1.841728	0.687454	2.545832
H	3.197785	−0.298288	2.647061	3.185489	−0.250277	2.661323
N	1.945683	−0.213711	−2.154670	1.943565	−0.246688	−2.152363
H	2.165776	−1.024150	−2.730980	2.188521	−1.052653	−2.724886
H	0.972568	0.041585	−2.308023	0.962223	−0.024816	−2.304838
H	2.511257	0.573449	−2.469225	2.482547	0.556917	−2.472064
N	1.155256	−2.067917	0.171123	1.150024	−2.076638	0.201854
N	−0.019327	−2.076311	0.020879	−0.020001	−2.084818	0.023715
N	−1.193867	−2.064199	−0.129522	−1.189992	−2.073514	−0.154178

Table S1. (continued)

azide bridged dinuclear Fe(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Fe	−2.346121	−0.202904	0.011848	−2.358288	−0.202366	0.006588
Fe	2.309386	−0.216911	0.012717	2.321948	−0.216404	0.020370
C	−0.007651	3.281023	−0.010067	−0.007597	3.276380	−0.007881
H	−0.004441	4.360287	−0.015273	−0.004398	4.355628	−0.013591
N	−0.690590	1.131202	−0.010549	−0.691393	1.126121	−0.000322
C	−1.115069	2.426612	−0.022138	−1.114837	2.422165	−0.009555
C	−2.591420	2.713904	−0.034979	−2.590041	2.713941	−0.017217
O	−3.035501	3.871245	−0.051743	−3.030374	3.872704	−0.026967
N	−3.317099	1.565704	−0.023036	−3.320248	1.568426	−0.011192
C	−4.745704	1.681550	−0.026698	−4.748394	1.690799	−0.016055
H	−5.128916	2.232945	−0.905591	−5.127278	2.248515	−0.892874
H	−5.130414	2.257125	0.836071	−5.131716	2.263684	0.848962
C	−5.390834	0.304650	−0.007785	−5.400181	0.317153	−0.005809
C	−6.787102	0.164915	−0.021980	−6.797303	0.185066	−0.008992
H	−7.409571	1.055225	−0.047536	−7.415041	1.078967	−0.018984
C	−7.355018	−1.103162	−0.003335	−7.371940	−1.080009	0.000779
H	−8.435248	−1.222417	−0.014029	−8.452853	−1.193381	−0.001446
C	−6.515694	−2.221696	0.029155	−6.538404	−2.203280	0.013524
H	−6.914771	−3.231048	0.044549	−6.942756	−3.210613	0.021420
C	−5.143275	−2.006551	0.042032	−5.164819	−1.995596	0.016046
H	−4.442368	−2.838056	0.067758	−4.468571	−2.831316	0.026077
N	−4.588055	−0.780684	0.023902	−4.602941	−0.772607	0.006713
N	0.662271	1.127254	0.012023	0.663277	1.122112	0.007781
C	1.094587	2.420145	0.010832	1.094504	2.415617	0.003060
C	2.572626	2.698589	0.023571	2.571439	2.698541	0.008704
O	3.023740	3.853327	0.025462	3.018795	3.854644	0.004169
N	3.291295	1.545936	0.029744	3.294696	1.548650	0.018322
C	4.720560	1.653342	0.035402	4.723552	1.662547	0.022599
H	5.110411	2.217721	−0.832382	5.110588	2.224079	−0.848156
H	5.105273	2.211506	0.909412	5.105457	2.227122	0.893730
C	5.357579	0.272532	0.032278	5.367117	0.284991	0.027237

C	6.752981	0.124672	0.050014	6.763413	0.144480	0.031831
H	7.380717	1.011490	0.066714	7.386572	1.034670	0.031978
C	7.313381	−1.146877	0.046085	7.330393	−1.124081	0.035999
H	8.392870	−1.272388	0.059704	8.410602	−1.243938	0.039448
C	6.467489	−2.260715	0.024587	6.490087	−2.242366	0.035731
H	6.860584	−3.272523	0.020796	6.888336	−3.252154	0.038931
C	5.096390	−2.037571	0.007629	5.117782	−2.026396	0.031062
H	4.390582	−2.865139	−0.009722	4.416477	−2.857939	0.030483
N	4.548442	−0.808325	0.011456	4.563318	−0.800011	0.026852
N	−2.327310	−0.385525	2.247354	−2.337790	−0.418478	2.237877
H	−1.882015	−1.249499	2.551256	−1.918192	−1.298186	2.533113
H	−1.777145	0.401833	2.586761	−1.761030	0.348761	2.579205
H	−3.246237	−0.327558	2.681905	−3.252395	−0.333713	2.677043
N	−2.335201	−0.449905	−2.218432	−2.330479	−0.453698	−2.220884
H	−1.935965	−1.333331	−2.530459	−1.920868	−1.341250	−2.506555
H	−1.749932	0.310934	−2.559726	−1.744075	0.303131	−2.568966
H	−3.253835	−0.343153	−2.644065	−3.243229	−0.362211	−2.662510
N	2.292853	−0.439359	2.245577	2.291605	−0.441770	2.250743
H	1.883358	−1.315990	2.563389	1.873042	−1.322304	2.545014
H	1.715879	0.330503	2.580654	1.712878	0.324359	2.591236
H	3.212107	−0.340047	2.671697	3.205154	−0.355249	2.691735
N	2.296390	−0.426249	−2.220169	2.302800	−0.458441	−2.208122
H	1.853211	−1.293253	−2.518514	1.881225	−1.339855	−2.495358
H	1.746354	0.357514	−2.568004	1.728726	0.306944	−2.558029
H	3.216812	−0.370484	−2.651811	3.218374	−0.380509	−2.646512
N	1.159767	−2.113571	0.002294	1.159446	−2.127131	0.025096
N	−0.024340	−2.124707	0.023327	−0.024040	−2.136898	0.025521
N	−1.208367	−2.106196	0.044863	−1.207449	−2.120159	0.025788

Table S1. (continued)

azide bridged dinuclear Mn(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Mn	−2.360977	−0.359862	−0.006260	−2.371664	−0.358347	−0.010376
Mn	2.321840	−0.367424	0.036539	2.331554	−0.366123	0.037778
C	−0.013717	3.213364	−0.011118	−0.014003	3.210612	−0.009406
H	−0.012042	4.292470	−0.018041	−0.012295	4.289714	−0.014948
N	−0.693507	1.064434	−0.002849	−0.694648	1.061309	−0.005675
C	−1.120003	2.357897	−0.015492	−1.120172	2.355342	−0.017521
C	−2.593815	2.646354	−0.026015	−2.593134	2.647164	−0.030168
O	−3.029465	3.808594	−0.026319	−3.026026	3.810332	−0.030576
N	−3.331184	1.507115	−0.031551	−3.333937	1.509977	−0.037393
C	−4.754849	1.673724	−0.025944	−4.757163	1.681301	−0.032386
H	−5.122622	2.234204	−0.906413	−5.123005	2.239546	−0.915084
H	−5.108200	2.275583	0.832367	−5.108077	2.287686	0.823604
C	−5.465155	0.332415	0.009740	−5.472122	0.342739	0.008132
C	−6.867583	0.266239	0.027844	−6.874758	0.281703	0.028142
H	−7.441611	1.188760	0.016308	−7.445434	1.206277	0.015033
C	−7.501273	−0.969340	0.060524	−7.512882	−0.951460	0.064646
H	−8.586211	−1.031673	0.075071	−8.598016	−1.009835	0.080712
C	−6.721148	−2.130686	0.074894	−6.736934	−2.115574	0.080871
H	−7.171590	−3.117919	0.100677	−7.190896	−3.101113	0.109595
C	−5.339974	−1.987331	0.055408	−5.355299	−1.977261	0.059403
H	−4.686165	−2.857283	0.065722	−4.704846	−2.849694	0.071031
N	−4.720278	−0.792282	0.023269	−4.731257	−0.784549	0.023626
N	0.659218	1.062362	0.008887	0.659661	1.059199	0.009597
C	1.089863	2.354514	0.004753	1.089405	2.351894	0.008099
C	2.564611	2.638339	0.013826	2.563318	2.638964	0.019873
O	3.004098	3.799004	−0.003816	3.000157	3.800572	0.005307
N	3.298180	1.496930	0.040312	3.300257	1.499510	0.044926
C	4.722428	1.658557	0.035321	4.724056	1.665982	0.041294
H	5.079620	2.246850	−0.830793	5.079425	2.258165	−0.822828
H	5.090424	2.230309	0.908409	5.089372	2.236338	0.916391
C	5.428153	0.314392	0.020216	5.434639	0.324585	0.022720

C	6.830405	0.243082	0.011034	6.837156	0.258703	0.013321
H	7.407660	1.163651	0.015306	7.410841	1.181488	0.019579
C	7.459848	−0.995020	−0.003810	7.471357	−0.976901	−0.004187
H	8.544623	−1.061317	−0.011394	8.556374	−1.039026	−0.011917
C	6.675680	−2.153718	−0.009288	6.691609	−2.138561	−0.012181
H	7.122725	−3.142754	−0.021291	7.142425	−3.125859	−0.026236
C	5.294936	−2.005317	0.001073	5.310322	−1.995464	−0.001632
H	4.638034	−2.872985	−0.002540	4.656979	−2.865791	−0.007253
N	4.679378	−0.807797	0.015977	4.690084	−0.800361	0.015886
N	−2.355499	−0.475643	2.313550	−2.348867	−0.490392	2.307763
H	−1.983109	−1.324436	2.736286	−1.981841	−1.348156	2.716761
H	−1.744108	0.299770	2.566437	−1.723053	0.274159	2.558458
H	−3.264421	−0.287539	2.732647	−3.249099	−0.293936	2.741569
N	−2.456545	−0.545951	−2.320584	−2.459696	−0.561424	−2.322960
H	−1.890805	−1.278575	−2.745985	−1.894458	−1.301924	−2.735122
H	−2.110515	0.355314	−2.647515	−2.105548	0.334223	−2.656575
H	−3.407163	−0.645544	−2.672589	−3.407841	−0.659430	−2.682046
N	2.415292	−0.516686	2.354371	2.416691	−0.533293	2.354181
H	1.833668	−1.228143	2.794018	1.834201	−1.251809	2.780941
H	2.089573	0.398301	2.663590	2.085152	0.376977	2.671046
H	3.363507	−0.630735	2.708500	3.362564	−0.647958	2.714360
N	2.321400	−0.506581	−2.282098	2.317824	−0.519828	−2.279139
H	1.942614	−1.354703	−2.700486	1.943422	−1.375872	−2.685062
H	1.718104	0.272750	−2.542301	1.702231	0.250223	−2.538209
H	3.233407	−0.329793	−2.699386	3.222636	−0.336390	−2.709071
N	1.162142	−2.255807	0.045114	1.160958	−2.270158	0.045456
N	−0.021968	−2.263182	0.028307	−0.022296	−2.274449	0.025629
N	−1.206030	−2.252872	0.011109	−1.205505	−2.267365	0.005748

Table S1. (continued)

azide bridged dinuclear Cr(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Cr	−2.249173	−0.160117	0.016347	−2.248943	−0.159360	0.016979
Cr	2.246058	−0.172132	−0.002131	2.245830	−0.171387	−0.001765
C	0.007771	3.307506	0.012060	0.007761	3.307198	0.010270
H	0.010660	4.386467	0.015990	0.010645	4.386160	0.013393
N	−0.674130	1.157858	0.008017	−0.674127	1.157305	0.007945
C	−1.095093	2.453771	0.014211	−1.095067	2.453499	0.013179
C	−2.572242	2.706120	0.023666	−2.572162	2.706631	0.023049
O	−3.070798	3.832745	0.033795	−3.069912	3.833681	0.032124
N	−3.245589	1.520388	0.021096	−3.245744	1.521364	0.022295
C	−4.685113	1.518908	0.035363	−4.685180	1.519730	0.037115
H	−5.112828	2.038619	−0.838688	−5.113266	2.040002	−0.836427
H	−5.094788	2.047864	0.912359	−5.094659	2.047988	0.914659
C	−5.168305	0.084951	0.047142	−5.168285	0.085720	0.048094
C	−6.526282	−0.247613	0.065162	−6.526270	−0.246715	0.066180
H	−7.266526	0.546684	0.070931	−7.266399	0.547688	0.072758
C	−6.909207	−1.584229	0.075907	−6.909378	−1.583284	0.075899
H	−7.961602	−1.853167	0.090397	−7.961801	−1.852111	0.090397
C	−5.923181	−2.575514	0.068050	−5.923453	−2.574640	0.066941
H	−6.178425	−3.629789	0.076078	−6.178804	−3.628897	0.074022
C	−4.593416	−2.182939	0.049727	−4.593633	−2.182199	0.048795
H	−3.782673	−2.904851	0.042938	−3.782982	−2.904208	0.041261
N	−4.218368	−0.885594	0.039521	−4.218376	−0.884883	0.039643
N	0.678111	1.154246	0.001950	0.678096	1.153693	0.001667
C	1.106036	2.447893	0.004273	1.105993	2.447622	0.002891
C	2.584546	2.692330	0.000187	2.584457	2.692834	−0.001218
O	3.089221	3.816264	0.004837	3.088327	3.817192	0.002097
N	3.251461	1.502997	−0.007720	3.251617	1.503961	−0.007306
C	4.691033	1.493774	−0.007301	4.691107	1.494587	−0.006327
H	5.113073	2.010182	−0.886062	5.113553	2.011351	−0.884688
H	5.112021	2.021504	0.865062	5.111869	2.021829	0.866478
C	5.166609	0.057269	0.001463	5.166591	0.058034	0.002075

C	6.522905	−0.282508	0.006803	6.522898	−0.281607	0.007847
H	7.267384	0.507840	0.004425	7.267267	0.508851	0.006153
C	6.898799	−1.621131	0.015598	6.898968	−1.620182	0.016170
H	7.949839	−1.895667	0.020252	7.950036	−1.894600	0.021167
C	5.907478	−2.607149	0.018643	5.907741	−2.606275	0.018220
H	6.157163	−3.662760	0.025627	6.157526	−3.661867	0.024745
C	4.579710	−2.207505	0.012513	4.579917	−2.206773	0.011846
H	3.765123	−2.925108	0.014419	3.765417	−2.924476	0.013061
N	4.211477	−0.908188	0.004105	4.211483	−0.907485	0.004034
N	1.172327	−1.960581	0.005171	1.172038	−1.969740	0.005391
N	−0.006493	−1.955757	0.008690	−0.006464	−1.963303	0.009273
N	−1.185338	−1.954600	0.012193	−1.184995	−1.963652	0.012683

Table S2. Calculated total energies and $\langle S^2 \rangle$ values at AFM structures.

M	X	E^{AFM} (hartree)	E^{FM} (hartree)	$\langle S^2 \rangle^{\mathrm{AFM}}$	$\langle S^2 \rangle^{\mathrm{FM}}$
Ni(II)	N_3^-	−4541.52804019	−4541.52668487	2.0000	6.0087
	$CH_3CO_2^-$	−4605.82605099	−4605.82599187	2.0063	6.0071
Co(II)	N_3^-	−4290.49011569	−4290.48904352	3.0098	12.015
	$CH_3CO_2^-$	−4354.78724480	−4354.78716334	3.0128	12.013
Fe(II)	N_3^-	−4052.42827479	−4052.42732033	4.0112	20.015
	$CH_3CO_2^-$	−4116.72712184	−4116.72704255	4.0503	20.050
Mn(II)	N_3^-	−3827.08978820	−3827.08875452	5.0034	30.008
	$CH_3CO_2^-$	−3891.38951682	−3891.38948746	5.0051	30.006
Cr(II)	N_3^-	−3387.81300372	−3387.81235364	4.0275	20.032
	$CH_3CO_2^-$	−3452.12450379	−3452.12426940	4.0259	20.030

Table S3. Calculated total energies and $\langle S^2 \rangle$ values at FM structures.

M	X	E^{AFM} (hartree)	E^{FM} (hartree)	$\langle S^2 \rangle^{\mathrm{AFM}}$	$\langle S^2 \rangle^{\mathrm{FM}}$
Ni(II)	N_3^-	−4541.52824739	−4541.52764286	2.0051	6.0100
	$CH_3CO_2^-$	−4605.82605078	−4605.82599448	2.0063	6.0071
Co(II)	N_3^-	−4290.49005736	−4290.48911519	3.0103	12.015
	$CH_3CO_2^-$	−4354.78720308	−4354.78720066	3.0127	12.013
Fe(II)	N_3^-	−4052.42821489	−4052.42739028	4.0113	20.015
	$CH_3CO_2^-$	−4116.72711564	−4116.72704255	4.0502	20.050
Mn(II)	N_3^-	−3827.08974048	−3827.08881282	5.0038	30.008
	$CH_3CO_2^-$	−3891.38951657	−3891.38949074	5.0051	30.006
Cr(II)	N_3^-	−3387.81298265	−3387.81237828	4.0277	20.032
	$CH_3CO_2^-$	−3452.12450025	−3452.12427470	4.0259	20.031

Table S4. Calculated total energies and $\langle S^2 \rangle$ values of low−spin Fe(II) (s=0) complexes.

M	X	E (hartree)
Fe(II)	N_3^-	−4052.4132214
	$CH_3CO_2^-$	−4116.7127995

Table S5. Calculated total energies and $\langle S^2 \rangle$ values of low−spin Co(II) (*s*=1/2) complexes.

M	X	E^{AFM} (hartree)	E^{FM} (hartree)	$\langle S^2 \rangle^{\mathrm{AFM}}$	$\langle S^2 \rangle^{\mathrm{FM}}$
Co(II)	N_3^-	−4290.4732999	−4290.473254	1.0318	2.0158
	$CH_3CO_2^-$	−4354.7736010	−4354.773599	1.0147	2.0143

Table S6. Stabilization energy (kJ/mol) [1] for each complex.

M	X	AFM state	FM state
Ni(II)	N_3^-	−6757	−6756
	$CH_3CO_2^-$	−6788	−6788
Co(II)	N_3^-	−6545	−6543
	$CH_3CO_2^-$	−6574	−6574
Fe(II)	N_3^-	−6376	−6373
	$CH_3CO_2^-$	−6409	−6409
Mn(II)	N_3^-	−6119	−6117
	$CH_3CO_2^-$	−6155	−6155
Cr(II)	N_3^-	−7504	−7503
	$CH_3CO_2^-$	−7571	−7570

[1] Stabilization energy was calculated by

(Stabilization energy) = E(complex) – {E(M(II))×2 + E(Pyrazole) + E(azide or acetate)}

using optimized structure of each complex. Negative values indicate that the complex is stable.

Table S7. Metal−metal distances (Å) in each complex.

M	X	AFM state	FM state
Ni(II)	N_3^-	4.487	4.478
	$CH_3CO_2^-$	4.263	4.264
Co(II)	N_3^-	4.515	4.534
	$CH_3CO_2^-$	4.268	4.272
Fe(II)	N_3^-	4.656	4.680
	$CH_3CO_2^-$	4.396	4.396
Mn(II)	N_3^-	4.683	4.703
	$CH_3CO_2^-$	4.411	4.411
Cr(II)	N_3^-	4.495	4.495
	$CH_3CO_2^-$	4.250	4.251

Table S8. Optimized cartesian coordinates (Å) of end−on azide bridged dinuclear Cu(II) complex

Atoms	AFM state			FM state		
	x	*y*	*z*	*x*	*y*	*z*
Cu	1.724019	0.281447	0.778216	1.722352	0.282686	0.777730
Cu	−1.723548	0.280305	0.775325	−1.721889	0.281697	0.774635
C	0.000113	3.749423	0.233833	0.000067	3.749843	0.233399
H	0.000634	4.707651	−0.263535	0.000507	4.707841	−0.264429
N	−0.665849	1.817474	1.154681	−0.666025	1.818530	1.156122
C	−1.107583	2.956931	0.576535	−1.107605	2.957833	0.576786
C	−2.577772	2.912545	0.247325	−2.577653	2.913369	0.247691
O	−3.303359	3.888815	0.069074	−3.303752	3.889388	0.070342
N	−2.949904	1.598387	0.153929	−2.949080	1.598901	0.153503
C	−4.336154	1.235551	0.071097	−4.335280	1.235506	0.071746
H	−4.757519	1.403156	−0.934618	−4.757622	1.403605	−0.933463
H	−4.966042	1.828549	0.755392	−4.964838	1.827747	0.757012
C	−4.471221	−0.235125	0.412979	−4.469260	−0.235397	0.412972
C	−5.701856	−0.896205	0.358537	−5.699472	−0.897249	0.358534
H	−6.585813	−0.343590	0.054900	−6.583817	−0.345076	0.055220
C	−5.778429	−2.242876	0.693420	−5.775157	−2.244079	0.692958
H	−6.730454	−2.764663	0.657395	−6.726857	−2.766457	0.656915
C	−4.613766	−2.914376	1.075165	−4.610008	−2.914920	1.074348
H	−4.623945	−3.965633	1.341856	−4.619438	−3.966266	1.340713
C	−3.422678	−2.204825	1.105025	−3.419359	−2.204639	1.104248
H	−2.492340	−2.686976	1.385370	−2.488777	−2.686301	1.384488
N	−3.346612	−0.895551	0.786859	−3.344106	−0.895205	0.786487
N	0.664438	1.817945	1.157164	0.664823	1.818989	1.158283
C	1.107198	2.957988	0.580736	1.107256	2.958771	0.580418
C	2.578551	2.915106	0.256575	2.578276	2.915502	0.255581
O	3.303931	3.892052	0.081240	3.304157	3.892038	0.080179
N	2.951783	1.601348	0.163545	2.950675	1.601349	0.161979
C	4.338208	1.239058	0.082478	4.337062	1.238547	0.081861
H	4.762321	1.412263	−0.921117	4.761836	1.411621	−0.921453
H	4.966341	1.828112	0.771816	4.965021	1.827358	0.771589
C	4.472134	−0.233474	0.416568	4.470101	−0.233975	0.416237

C	5.702250	−0.895208	0.358466	5.699851	−0.896389	0.358441
H	6.586683	−0.341540	0.058150	6.584586	−0.343256	0.058032
C	5.777560	−2.244051	0.684740	5.774480	−2.245122	0.685324
H	6.729049	−2.766560	0.645180	6.725723	−2.768104	0.646136
C	4.612251	−2.916846	1.062194	4.608803	−2.917117	1.063030
H	4.621369	−3.969843	1.321967	4.617349	−3.969984	1.323345
C	3.421852	−2.206349	1.096713	3.418750	−2.206019	1.097122
H	2.491183	−2.689402	1.374297	2.487894	−2.688492	1.374981
N	3.346907	−0.895091	0.786493	3.344444	−0.894829	0.786410
N	0.000660	−0.863021	0.718357	0.000529	−0.861687	0.722051
N	0.000170	−2.081696	0.789342	0.000130	−2.080281	0.789271
N	−0.000445	−3.232490	0.855033	−0.000361	−3.231564	0.851921

Table S9. Calculated total energies and $\langle S^2 \rangle$ values at AFM structures for dinuclear Cu(II) complex with side−on and end−on type azide bridges.

X	E^{AFM} (hartree)	E^{FM} (hartree)	$\langle S^2 \rangle^{\mathrm{AFM}}$	$\langle S^2 \rangle^{\mathrm{FM}}$
side−on	−4579.51635091	−4579.51436140	0.9753	2.0070
end−on	−4579.49453436	−4579.49487450	1.0071	2.0087

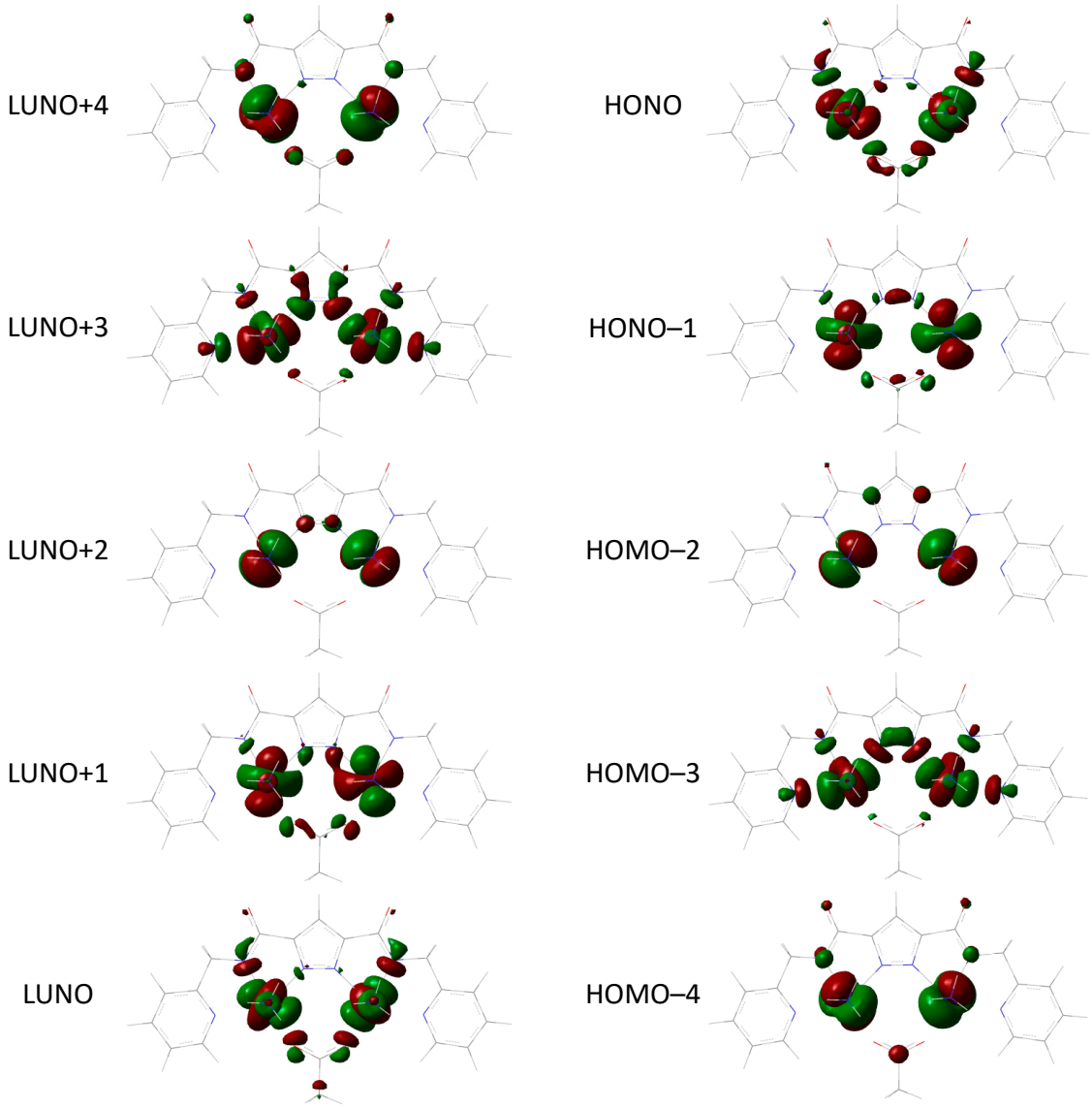

Figure S1. Calculated natural orbitals of magnetic orbitals for acetate−bridged Mn(II) complex.

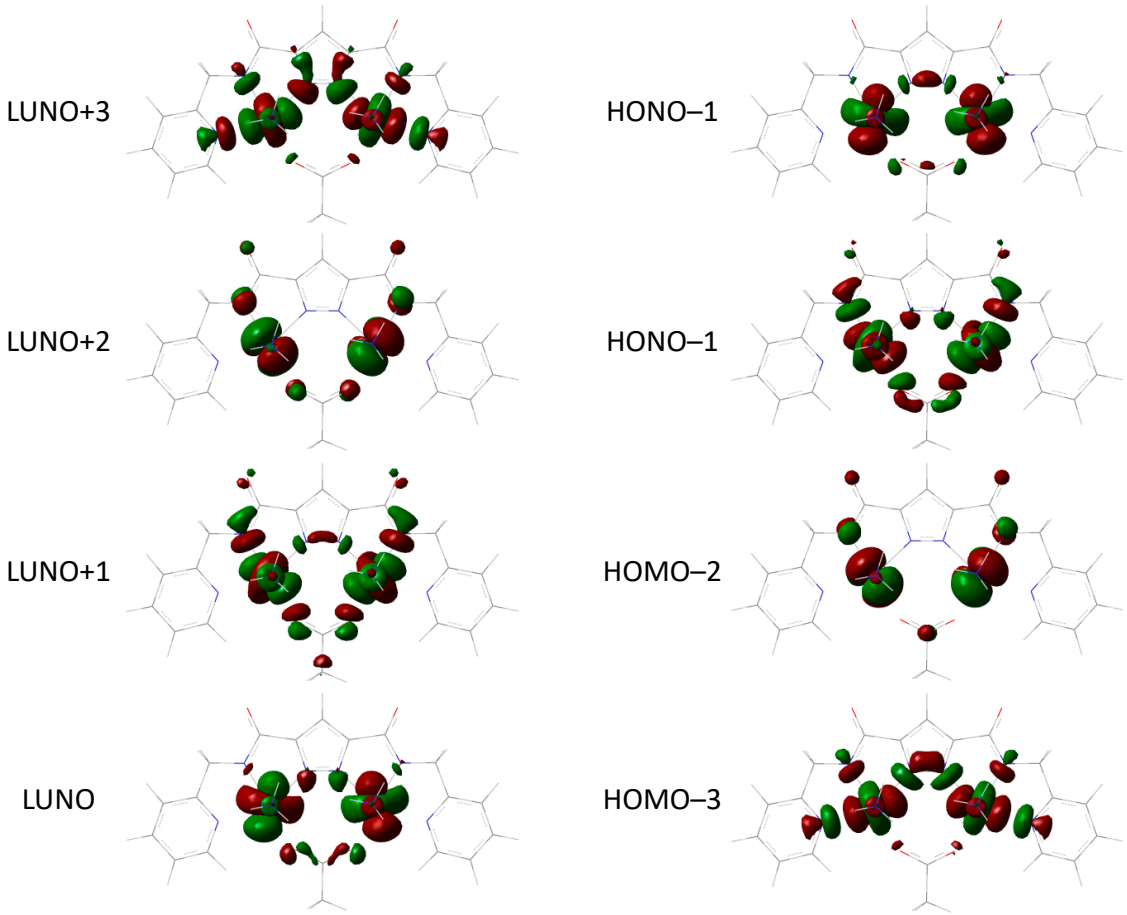

Figure S2. Calculated natural orbitals of magnetic orbitals for acetate−bridged Fe(II) complex.

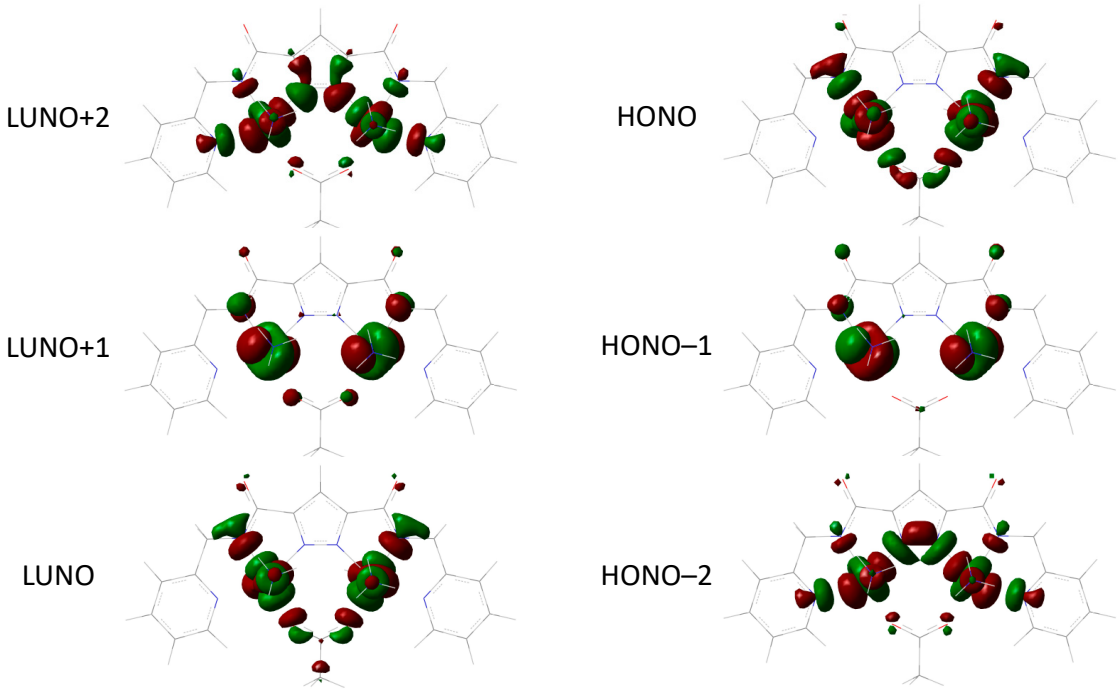

Figure S3. Calculated natural orbitals of magnetic orbitals for acetate−bridged Co(II) complex.

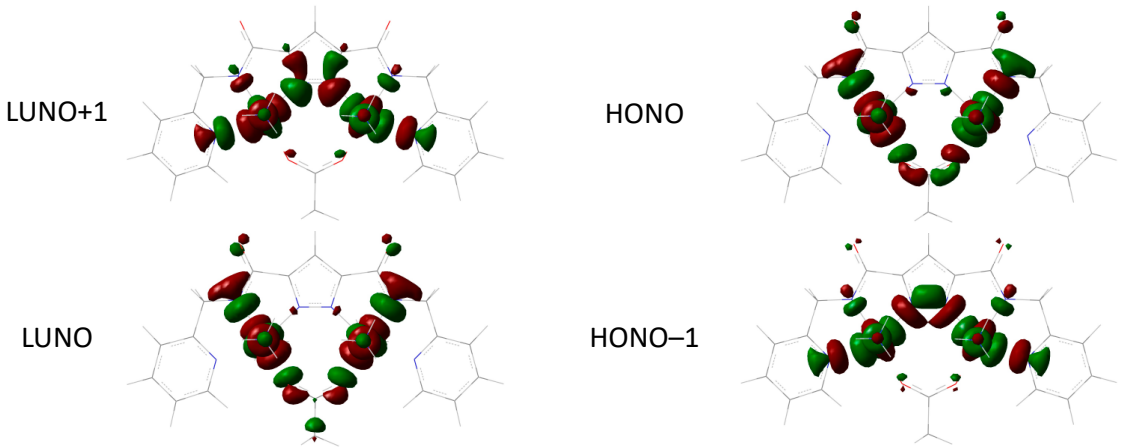

Figure S4. Calculated natural orbitals of magnetic orbitals for acetate−bridged Ni(II) complex.

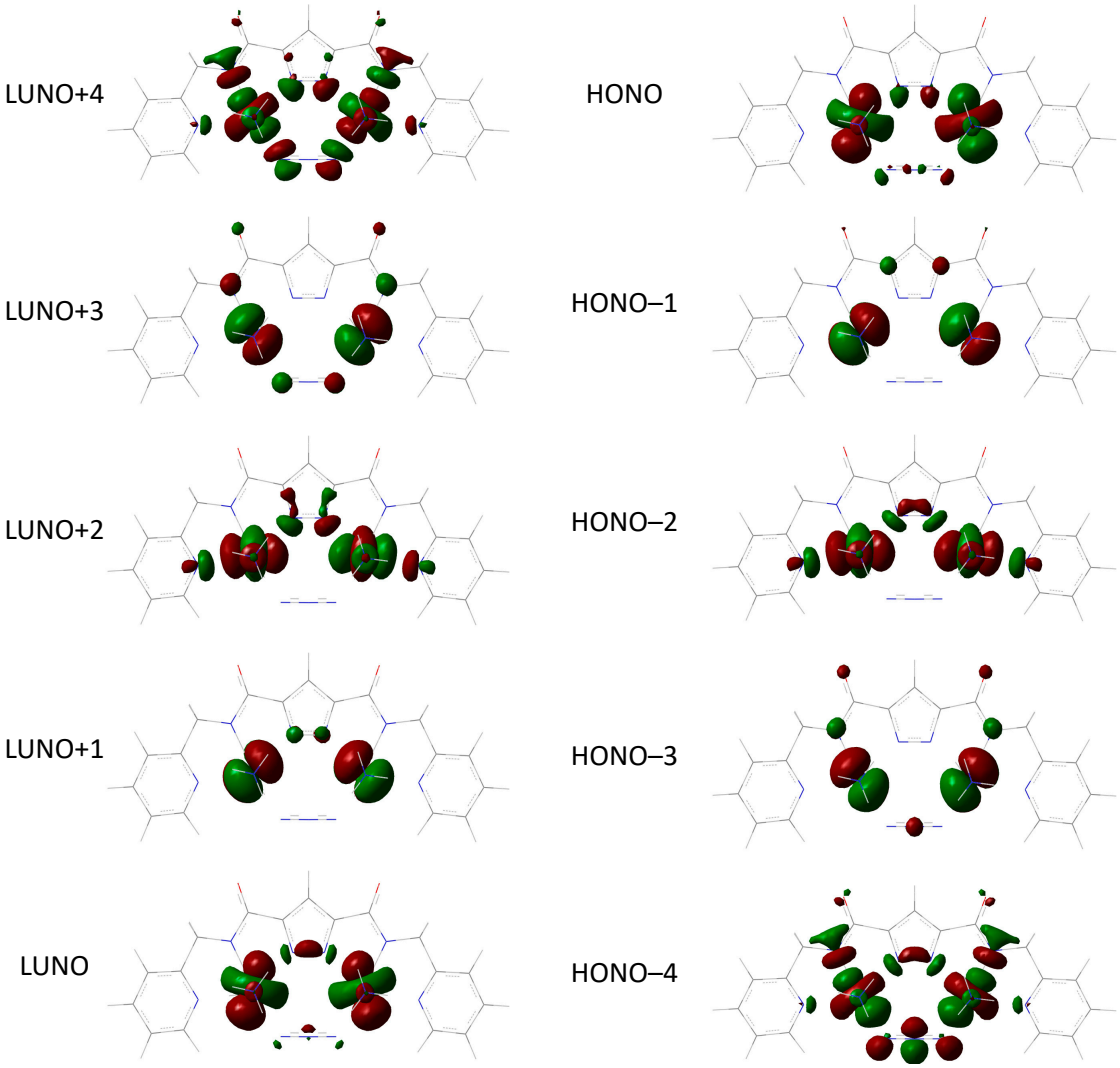

Figure S5. Calculated natural orbitals of magnetic orbitals for azide−bridged Mn(II) complex.

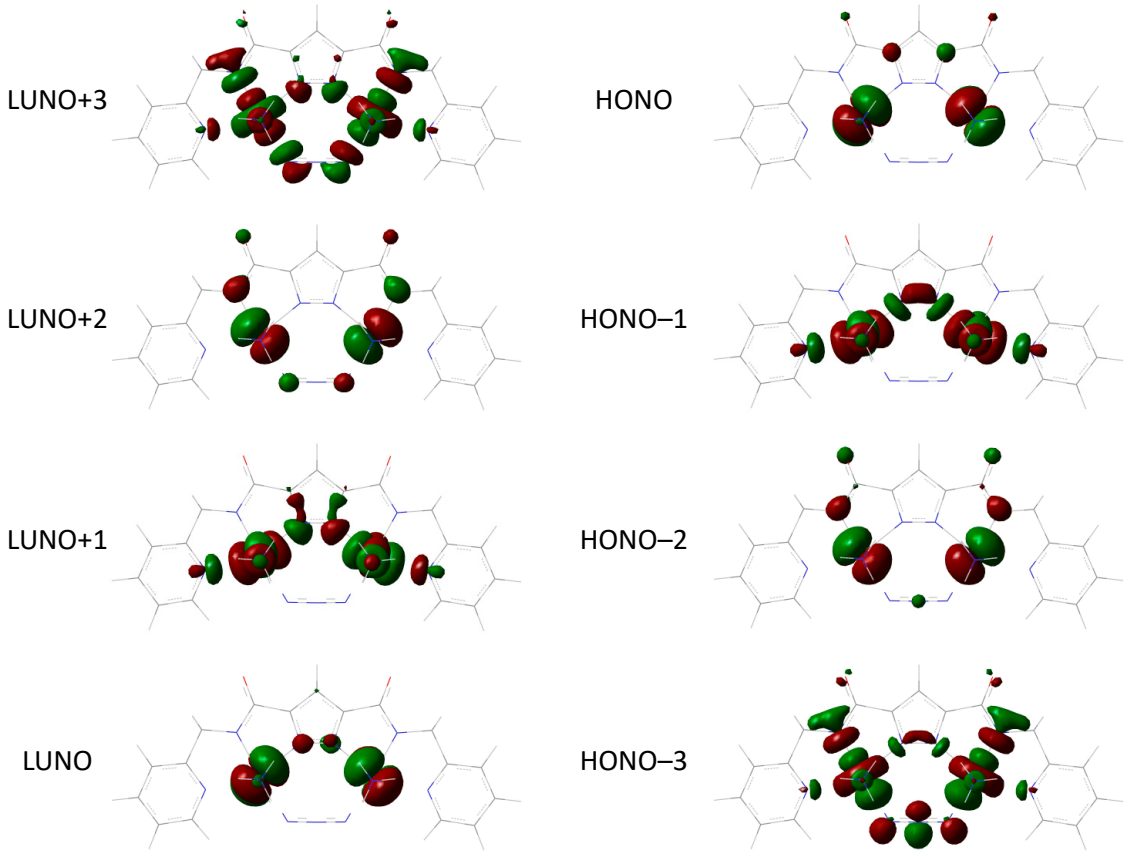

Figure S6. Calculated natural orbitals of magnetic orbitals for azide−bridged Fe(II) complex.

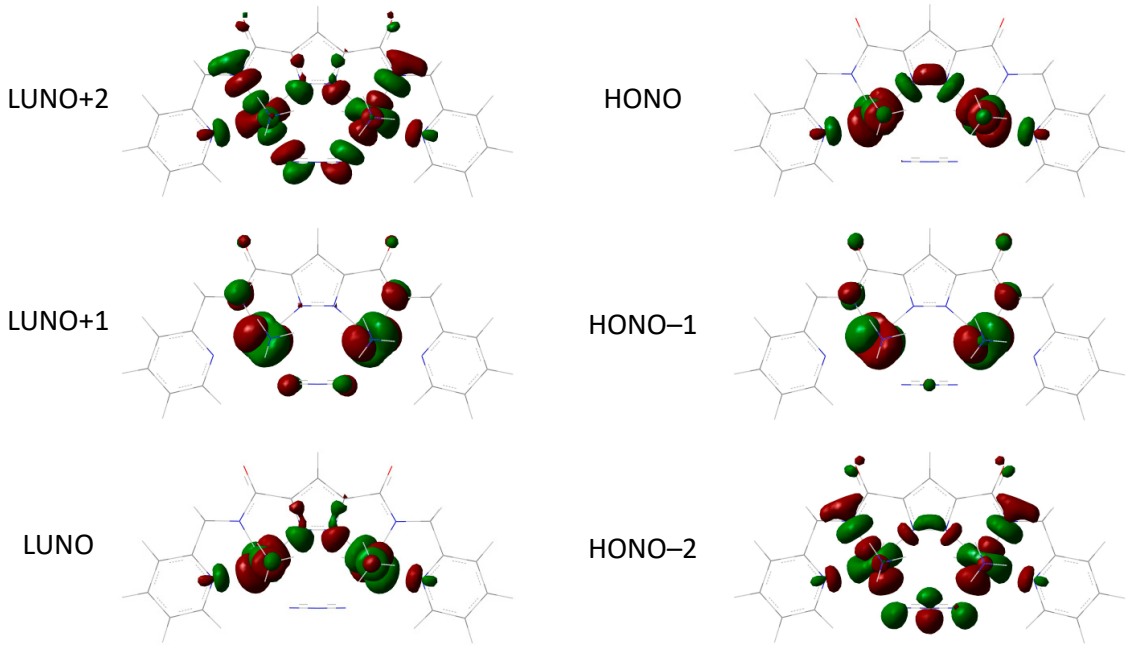

Figure S7. Calculated natural orbitals of magnetic orbitals for azide−bridged Co(II) complex.

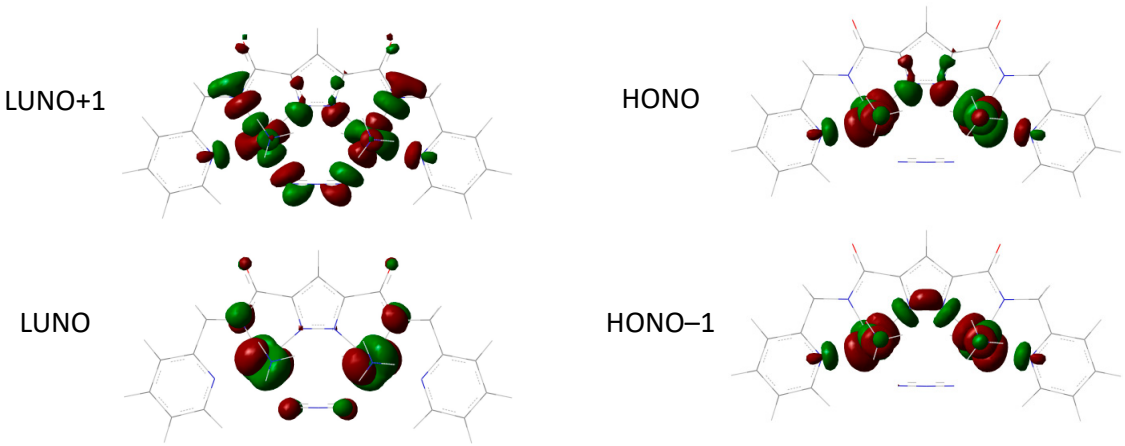

Figure S8. Calculated natural orbitals of magnetic orbitals for azide−bridged Ni(II) complex.