SUPPORTING INFORMATION

Spectroscopic and Density Functional Studies of the Dinitrosyl Metalloporphyrin Complexes $Fe(P)(NO)_2$ and $Ru(P)(NO)_2$

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Table S-1 Observed ν_{NO} and ν_{CO}, and reduced mass functions for trans-dicarbonyls and trans-dinitrosyls. Asterisks represent degree of isotope incorporation.

Species	ν, ν^*, ν^{**} (cm^{-1})	$(\mu^{**}/\mu)^{-1/2}$ [a]	ν^{**}/ν
$^{14}NO/^{15}NO$			
$Fe(TmTP)(NO)_2$	1694, 1676, 1664	1.0183	1.0180
$Ru(TmTP)(NO)_2$	1641, 1624, 1613	1.0183	1.0174
$^{12}CO/^{13}CO$			
$Ru(TmTP)(CO)_2$	2010, 1983, 1967	1.0227	1.0219

[a] using only N and O, or C and O.

Table S-2 Cartesian coordinates and energies (in hartrees) of $[Ru(NH_3)_5(NO)]^{3+}$ at the B3LYP/3-21g level

$[Ru(NH_3)_5(NO)]^{3+}$ (-4832.5057904)

Ru	-0.093051	-0.000655	0.002182
N	-0.192062	-1.018080	-1.944744
N	-2.278552	0.009604	-0.040840
N	1.715663	0.000211	-0.000153
N	-0.210127	0.995548	1.958455
N	-0.145007	-1.949800	1.020132
N	-0.131462	1.962195	-0.988439
H	-0.895190	-1.776947	-1.950968
H	0.707548	-1.454493	-2.214598
H	-2.693227	0.633322	0.674077
H	-2.691059	-0.926269	0.119731
H	-0.760228	0.447314	2.642126
H	-0.649733	1.930722	1.905114
H	-1.074949	-2.200743	1.396796
H	0.507288	-1.973475	1.824129
H	0.412838	2.665623	-0.458060
H	-1.082382	2.353230	-1.100168
H	0.289730	1.935094	-1.933864
H	0.140883	-2.726917	0.399022
H	-2.647811	0.328228	-0.954332
H	-0.443388	-0.379769	-2.719198
H	0.720213	1.141118	2.389432
O	2.868067	0.004381	-0.018264

Table S-3 Cartesian coordinates and energies (in hartrees) of $[Ru(NH_3)_5(NO)]^{2+}$ at the B3LYP/3-21g level

$[Ru(NH_3)_5(NO)]^{2+}$ (-4833.03713313)

Ru	-0.144905	0.002572	0.006073
N	0.909115	0.073869	-1.909733
N	-2.142975	0.107142	-1.024145
N	1.572769	-0.094153	0.799820
N	-1.067322	-0.072050	2.001756
N	-0.215300	-2.192163	-0.087905
N	-0.063644	2.194466	0.125244
H	0.699599	-0.719120	-2.533854
H	1.922379	0.044965	-1.703315
H	-2.929288	0.095151	-0.358047
H	-2.276939	-0.686715	-1.667442
H	-1.659700	-0.900969	2.157209
H	-1.640407	0.753684	2.230053
H	-1.145202	-2.578161	-0.307498
H	0.070223	-2.577241	0.824843
H	0.071274	2.484619	1.105265
H	-0.906157	2.674352	-0.223604
H	0.742562	2.565372	-0.400055
H	0.446616	-2.569755	-0.782450
H	-2.239458	0.962036	-1.591463
H	0.728749	0.932788	-2.450001
H	-0.296116	-0.112232	2.685939
O	2.729896	-0.075215	0.426493

Table S-4 Cartesian coordinates and energies (in hartrees) of $[Ru(NH_3)_4(NO)_2]^{2+}$ at the B3LYP/3-21g level

$[Ru(NH_3)_4(NO)_2]^{2+}$ (-4905.9275325)

Ru	0.004854	0.188322	0.004987
N	-1.932354	-0.044089	0.022479
N	-0.062150	0.945177	-2.061790
N	0.025711	-0.519709	2.089835
N	1.934346	-0.016801	-0.039287
N	-0.013652	2.262986	0.732828
N	0.007500	-1.881290	-0.690514
H	0.858769	1.300539	-2.362027
H	-0.736727	1.722673	-2.133320
H	-0.127380	-1.537940	2.158062
H	-0.720572	-0.066964	2.640480
H	0.556679	2.877756	0.132049
H	0.365603	2.351105	1.687753
H	0.788240	-2.417341	-0.276442
H	0.112985	-1.958220	-1.714624
H	-0.884186	-2.345075	-0.443804
H	-0.976464	2.635113	0.744923
H	-0.355978	0.235648	-2.750352
H	0.921411	-0.316758	2.560543
O	-2.616493	-1.026172	-0.029421
O	2.650023	-0.972656	-0.075269

Table S-5 Cartesian coordinates and energies (in hartrees) of $[Fe(NH_3)_4(NO)_2]^{2+}$ at the B3LYP/3-21g level

$[Fe(NH_3)_4(NO)_2]^{2+}$ (-1740.6351004)

Fe	0.005059	0.207503	-0.003398
N	-1.728966	0.061548	0.033612
N	-0.063431	1.633287	-1.459123
N	0.022422	-1.236934	1.418552
N	1.724278	0.061305	-0.041935
N	0.043356	1.674349	1.414571
N	-0.022749	-1.304505	-1.352572
H	0.837881	2.128268	-1.561009
H	-0.780425	2.344857	-1.241963
H	-0.785116	-1.877635	1.323691
H	-0.024282	-0.881049	2.387649
H	0.559483	2.506275	1.085205
H	0.513942	1.398237	2.291516
H	0.789866	-1.935628	-1.238687
H	0.005018	-1.000964	-2.340103
H	-0.873036	-1.888525	-1.263631
H	-0.904237	1.995056	1.673409
H	-0.304724	1.282171	-2.399913
H	0.874569	-1.823299	1.375995
O	-2.482748	-0.876749	0.031274
O	2.499642	-0.856525	-0.043216

Table S-6 Cartesian coordinates and energies (in hartrees) of Ru(porphine)$(NO)_2$ at the B3LYP/3-21g level

Ru(porphine)$(NO)_2$ (-5664.3860374)

Ru	0.106880	0.000000	-0.000006
N	1.569415	1.472068	-0.000108
C	1.354494	2.840931	-0.000118
C	2.648914	3.505410	-0.000199
H	2.789761	4.574434	-0.000223
C	3.609665	2.535087	-0.000237
H	4.680008	2.665748	-0.000298
C	2.933443	1.245827	-0.000180
C	0.113012	3.469085	-0.000059
H	0.114953	4.553386	-0.000076
N	-1.350325	1.482005	0.000052
C	-2.710814	1.249022	0.000130
C	-3.388769	2.536443	0.000149
H	-4.459171	2.665736	0.000206
C	-2.428378	3.508546	0.000081
H	-2.570393	4.577339	0.000073
C	-1.133464	2.846022	0.000019
C	-3.328637	-0.000002	0.000184
H	-4.413104	-0.000003	0.000244
N	-1.350323	-1.482006	0.000096
C	-1.133461	-2.846024	0.000106
C	-2.428373	-3.508548	0.000188
H	-2.570388	-4.577342	0.000213
C	-3.388766	-2.536446	0.000227
H	-4.459168	-2.665741	0.000289
C	-2.710812	-1.249025	0.000168
C	0.113016	-3.469085	0.000046
H	0.114959	-4.553386	0.000062
N	1.569416	-1.472067	-0.000064
C	2.933444	-1.245823	-0.000143
C	3.609668	-2.535083	-0.000161
H	4.680011	-2.665742	-0.000218
C	2.648918	-3.505407	-0.000094
H	2.789767	-4.574431	-0.000086
C	1.354498	-2.840930	-0.000032
C	3.555127	0.000002	-0.000195
H	4.639596	0.000003	-0.000255
N	-0.196759	0.000029	1.933002
O	-1.230302	0.000037	2.551568
N	-0.196971	-0.000029	-1.932980
O	-1.230582	-0.000039	-2.551434

Table S-7 Cartesian coordinates and energies (in hartrees) of Fe(porphine)$(NO)_2$ at the B3LYP/3-21g level

Fe(porphine)$_4$(NO)$_2$ (-2499.1067536)

Fe	0.093181	0.000000	-0.000005
N	1.499757	1.419983	-0.000104
C	1.321925	2.800297	-0.000116
C	2.607231	3.467210	-0.000197
H	2.738886	4.537031	-0.000222
C	3.561045	2.497190	-0.000233
H	4.632855	2.611763	-0.000293
C	2.874403	1.221237	-0.000176
C	0.106435	3.451692	-0.000059
H	0.107548	4.534577	-0.000075
N	-1.295489	1.427298	0.000049
C	-2.668086	1.223170	0.000129
C	-3.352332	2.498089	0.000148
H	-4.423918	2.613632	0.000207
C	-2.397419	3.468729	0.000081
H	-2.529643	4.538371	0.000073
C	-1.112500	2.804819	0.000018
C	-3.307278	-0.000011	0.000183
H	-4.390351	-0.000015	0.000245
N	-1.295480	-1.427306	0.000093
C	-1.112482	-2.804827	0.000104
C	-2.397396	-3.468745	0.000186
H	-2.529613	-4.538388	0.000211
C	-3.352316	-2.498111	0.000224
H	-4.423901	-2.613661	0.000287
C	-2.668078	-1.223188	0.000166
C	0.106458	-3.451692	0.000045
H	0.107578	-4.534577	0.000061
N	1.499767	-1.419973	-0.000061
C	2.874411	-1.221218	-0.000139
C	3.561062	-2.497167	-0.000158
H	4.632872	-2.611733	-0.000215
C	2.607254	-3.467193	-0.000093
H	2.738916	-4.537013	-0.000086
C	1.321943	-2.800289	-0.000031
C	3.516300	0.000012	-0.000192
H	4.599502	0.000015	-0.000251
N	-0.121066	0.000027	1.741227
O	-1.086777	0.000036	2.460182
N	-0.121255	-0.000027	-1.741215
O	-1.087043	-0.000041	-2.460066

Figure S-1 Figure showing formation ν(NO) band of $Fe(TPP)(NO)_2$ at 1695 cm^{-1} after after cooling a $CHCl_3$ solution of Fe(TPP)(NO) (2.3 mM) plus NO (8 mM) from room temperature to 213 K.