Supporting Information: DFT and TDDFT Calculations

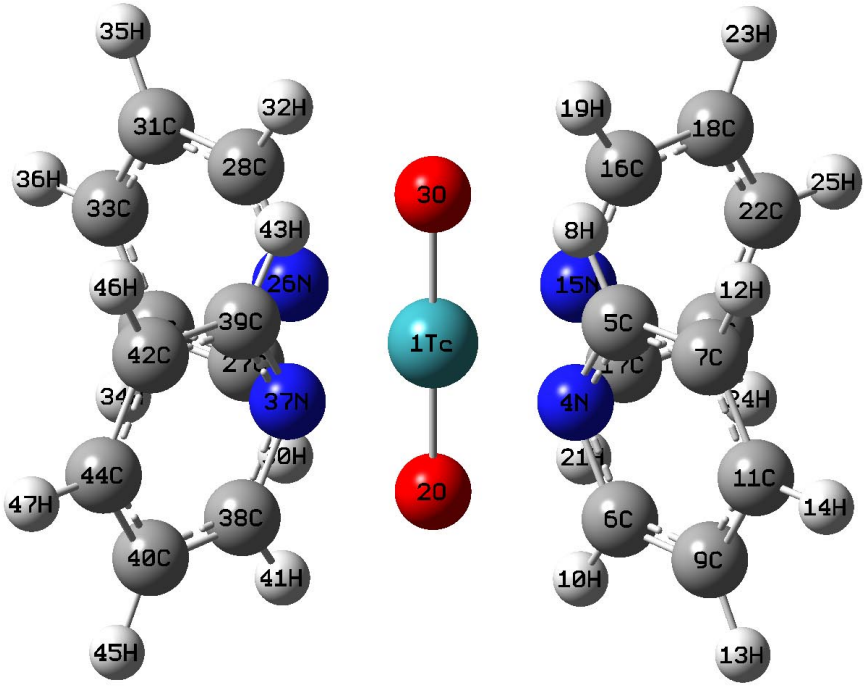

Figure S-1: Gas-phase ball and bond type model of $Tc(C_5H_5N)_4(O)_2^+$ as determined with Gaussian 03. The atom label (*i.e.*, 1, 2, etc..) is followed by the atom symbol (*i.e.*, Tc = technetium, C = carbon, H = hydrogen, O = oxygen, N = nitrogen)

Table S-1: Optimized geometry of $Tc(C_5H_5N)_4(O)_2^+$ in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1223.52709197 au

Tc	0.00000000	0.00000300	0.00000300
O	-1.75796800	0.00031000	-0.00009900
O	1.75796800	-0.00031300	0.00009600
N	-0.00013300	0.00000200	2.20382300
C	1.16104700	-0.00023600	2.88978100
C	-1.16140400	0.00023100	2.88963200
C	1.19909000	-0.00024800	4.27982100
H	2.06330300	-0.00041700	2.28252600

C	-1.19962800	0.00023700	4.27966600
H	-2.06357900	0.00041300	2.28225800
C	-0.00031400	-0.00000200	4.99182600
H	2.16040900	-0.00045000	4.78899400
H	-2.16101200	0.00042700	4.78871500
H	-0.00038300	-0.00000200	6.08064600
N	-0.00039900	-2.20382000	0.00000200
C	1.16069900	-2.88991800	0.00017500
C	-1.16175200	-2.88948900	-0.00018100
C	1.19857600	-4.27996200	0.00017900
H	2.06302900	-2.28277200	0.00032600
C	-1.20014200	-4.27951900	-0.00019100
H	-2.06385200	-2.28200400	-0.00033000
C	-0.00091500	-4.99182300	-0.00000200
H	2.15983300	-4.78925100	0.00032000
H	-2.16158800	-4.78845000	-0.00034500
H	-0.00111500	-6.08064300	-0.00000200
N	0.00013300	0.00000200	-2.20382000
C	-1.16104800	0.00021600	-2.88977800
C	1.16140300	-0.00022100	-2.88962900
C	-1.19909100	0.00022000	-4.27981800
H	-2.06330300	0.00039100	-2.28252200
C	1.19962800	-0.00023000	-4.27966300
H	2.06357800	-0.00039500	-2.28225300
C	0.00031500	-0.00000200	-4.99182300
H	-2.16040800	0.00039300	-4.78899100
H	2.16101200	-0.00041800	-4.78871100
H	0.00038300	-0.00000200	-6.08064300
N	0.00039800	2.20382300	0.00000200
C	-1.16070000	2.88992100	-0.00020200
C	1.16175100	2.88949200	0.00019600
C	-1.19857600	4.27996600	-0.00021700
H	-2.06302900	2.28277600	-0.00036000
C	1.20014200	4.27952200	0.00020500
H	2.06385200	2.28200700	0.00035600
C	0.00091500	4.99182600	-0.00000200
H	-2.15983200	4.78925500	-0.00039400
H	2.16158800	4.78845300	0.00037100
H	0.00111500	6.08064600	-0.00000200

Table S-2: Selected bond lengths[1] of $Tc(C_5H_5N)_4(O)_2^+$based on the calculated singlet ground state.

Tc(1)-O(30)	Tc(1)-O(20)	Tc(1)-N(4)	Tc(1)-N(15)	Tc(1)-N(26)	Tc(1)-N(37)
1.75797	1.75797	2.20382	2.20382	2.20382	2.20382

[1] All bond lengths are reported in units of Å

Table S-3: Calculated singlet excited-states of $Tc(C_5H_5N)_4(O)_2^+$. The excited state number is followed by the spin multiplicity, symmetry, excitation energy, and oscillator strength *f*. The excitation from occupied to virtual orbitals are listed on the next line, followed by the wavefunction coefficients.

Singlet Excited States of $Tc(C^5H_5N)_4(O)_2^+$ (Gas Phase)

```
Excited State   1:   Singlet-A      2.5822 eV  480.16 nm  f=0.0000
      99 ->100         0.60042
      99 ->101        -0.28209
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -1223.43219910
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:   Singlet-A      2.5822 eV  480.16 nm  f=0.0000
      99 ->100         0.28209
      99 ->101         0.60042

 Excited State   3:   Singlet-A      3.3358 eV  371.68 nm  f=0.0000
      86 ->106         0.10524
      99 ->106         0.69318

 Excited State   4:   Singlet-A      3.6027 eV  344.14 nm  f=0.0000
      95 ->101        -0.46303
      96 ->100         0.46303

 Excited State   5:   Singlet-A      3.6257 eV  341.96 nm  f=0.0029
      98 ->101         0.68486

 Excited State   6:   Singlet-A      3.6257 eV  341.96 nm  f=0.0029
      98 ->100         0.68486

 Excited State   7:   Singlet-A      3.9587 eV  313.20 nm  f=0.0000
      95 ->100         0.33157
      95 ->101         0.39045
      96 ->100         0.39045
      96 ->101        -0.33157

 Excited State   8:   Singlet-A      3.9605 eV  313.05 nm  f=0.0000
      95 ->100        -0.39008
      95 ->101         0.33125
      96 ->100         0.33125
      96 ->101         0.39008

 Excited State   9:   Singlet-A      4.2617 eV  290.93 nm  f=0.1875
      99 ->102         0.64371
      99 ->103        -0.25561

 Excited State  10:   Singlet-A      4.2617 eV  290.92 nm  f=0.1877
      99 ->102         0.25562
      99 ->103         0.64374

 Excited State  11:   Singlet-A      4.4554 eV  278.28 nm  f=0.0000
      99 ->105         0.69638

 Excited State  12:   Singlet-A      4.6635 eV  265.86 nm  f=0.0000
      97 ->100         0.70428
```

Table S-4: Calculated triplet excited-states of $Tc(C_5H_5N)_4(O)_2^+$. The excited state number is followed by the spin multiplicity, symmetry, excitation energy, and oscillator strength *f*. The excitation from occupied to virtual orbitals are listed on the next line, followed by the wavefunction coefficients.

Triplet Excited States of $Tc(C^5H_5N)_4(O)_2^+$ (Gas Phase):

```
Excited State   1:   Triplet-A      1.9218 eV  645.15 nm  f=0.0000
      86 ->100         0.13155
      99 ->100         0.74483
      99 ->101         0.16127
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -1223.45646758
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:   Triplet-A      1.9218 eV  645.15 nm  f=0.0000
      86 ->101         0.13155
      99 ->100        -0.16127
      99 ->101         0.74483

 Excited State   3:   Triplet-A      2.3853 eV  519.78 nm  f=0.0000
      95 ->100         0.65335
      96 ->101         0.65335

 Excited State   4:   Triplet-A      2.8469 eV  435.51 nm  f=0.0000
      86 ->106         0.14003
      99 ->106         0.74510

 Excited State   5:   Triplet-A      2.9372 eV  422.11 nm  f=0.0000
      95 ->100        -0.45113
      95 ->101         0.38309
      96 ->100         0.38309
      96 ->101         0.45113

 Excited State   6:   Triplet-A      2.9394 eV  421.80 nm  f=0.0000
      95 ->100         0.38294
      95 ->101         0.45094
      96 ->100         0.45094
      96 ->101        -0.38294

 Excited State   7:   Triplet-A      3.0562 eV  405.68 nm  f=0.0000
      98 ->100         0.64955
      98 ->101        -0.36910

 Excited State   8:   Triplet-A      3.0562 eV  405.68 nm  f=0.0000
      98 ->100         0.36910
      98 ->101         0.64955

 Excited State   9:   Triplet-A      3.6027 eV  344.14 nm  f=0.0000
      95 ->101        -0.46303
      96 ->100         0.46303

 Excited State  10:   Triplet-A      3.6709 eV  337.75 nm  f=0.0000
      86 ->103        -0.12957
      90 ->104        -0.18057
      90 ->105        -0.17340
      91 ->103         0.23138
```

```
     92 ->108         0.16016
     92 ->109         0.11626
     94 ->107         0.21412
     94 ->110        -0.18994
     97 ->108        -0.18526
     99 ->103         0.55753

 Excited State  11:   Triplet-A      3.6709 eV  337.75 nm  f=0.0000
     86 ->102        -0.12955
     89 ->104        -0.18047
     89 ->105         0.17354
     91 ->102        -0.23136
     92 ->108         0.11624
     92 ->109        -0.16013
     93 ->107        -0.21394
     93 ->110        -0.18999
     97 ->109        -0.18522
     99 ->102         0.55756

 Excited State  12:   Triplet-A      3.6979 eV  335.28 nm  f=0.0000
     86 ->104        -0.11197
     89 ->102        -0.18868
     90 ->103        -0.18868
     91 ->105         0.22446
     92 ->107         0.21164
     93 ->108        -0.12788
     93 ->109         0.16110
     94 ->108         0.16110
     94 ->109         0.12788
     97 ->110         0.20061
     99 ->104         0.56216
```

Table S-5. Selected energies and compositions of $TcO_2(py)_4^+$ molecular orbitals

---
-
Fragment 1 is (Tc s-contribution) Basis functions: 1 - 3
Fragment 2 is (Tc p-contribution) Basis functions: 4 - 12
Fragment 3 is (Tc d-contribution) Basis functions: 13 - 22
Fragment 4 is (Oxygen p-contributions) Basis functions: 25 - 27 29 - 31 39 - 41 43 - 45
Fragment 5 is (Oxygen d-contributions) Basis functions: 32 - 36 46 - 50
Fragment 6 is (Total pyridine contribution) Basis functions: 51 - 426 ; 45 atoms.
Fragment 7 is (Oxygen s-contribution) Basis functions: 23 - 24 28 37 - 38 42

MO#		E(eV)		MO Compositions (%)						
			Fragment:	1	2	3	4	5	6	7
110	10	-3.09	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
109	9	-3.28	a	0.0	0.0	0.4	0.1	0.0	99.5	0.0
108	8	-3.28	a	0.0	0.0	0.4	0.1	0.0	99.5	0.0
107	7	-3.48	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
106	6	-3.51	a	0.0	0.0	66.2	0.0	0.0	33.8	0.0
105	5	-3.83	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
104	4	-3.84	a	0.0	0.0	5.1	0.0	0.0	94.9	0.0
103	3	-4.05	a	0.0	2.1	0.0	0.0	0.0	97.9	0.0
102	2	-4.05	a	0.0	2.1	0.0	0.0	0.0	97.9	0.0
101	1	-4.73	a	0.0	0.0	55.6	40.4	0.2	3.7	0.0
100	0	-4.73	a	0.0	0.0	55.6	40.4	0.2	3.7	0.0
--- occupied - unoccupied orbital gap ---						4.270 eV				
99	0	-8.99	a	0.0	0.0	73.3	0.0	0.0	26.7	0.0
98	-1	-10.07	a	0.0	1.9	0.0	96.8	-0.1	1.8	-0.5
97	-2	-10.13	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
96	-3	-10.16	a	0.0	2.6	0.0	88.6	0.1	8.8	0.0
95	-4	-10.16	a	0.0	2.6	0.0	88.6	0.1	8.8	0.0
94	-5	-10.20	a	0.0	0.0	0.1	0.2	0.0	99.7	0.0
93	-6	-10.20	a	0.0	0.0	0.1	0.2	0.0	99.7	0.0
92	-7	-10.28	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
91	-8	-10.87	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
90	-9	-10.95	a	0.0	0.0	0.0	0.1	0.0	99.9	0.0
89	-10	-10.95	a	0.0	0.0	0.0	0.1	0.0	99.9	0.0
88	-11	-11.41	a	0.0	3.6	0.0	1.6	0.0	94.7	0.0
87	-12	-11.41	a	0.0	3.6	0.0	1.6	0.0	94.7	0.0
86	-13	-11.56	a	0.0	0.0	15.3	0.0	0.0	84.7	0.0
85	-14	-12.29	a	4.3	0.0	2.4	4.8	0.0	88.5	0.0
84	-15	-12.37	a	0.0	0.0	15.5	0.0	0.0	84.5	0.0

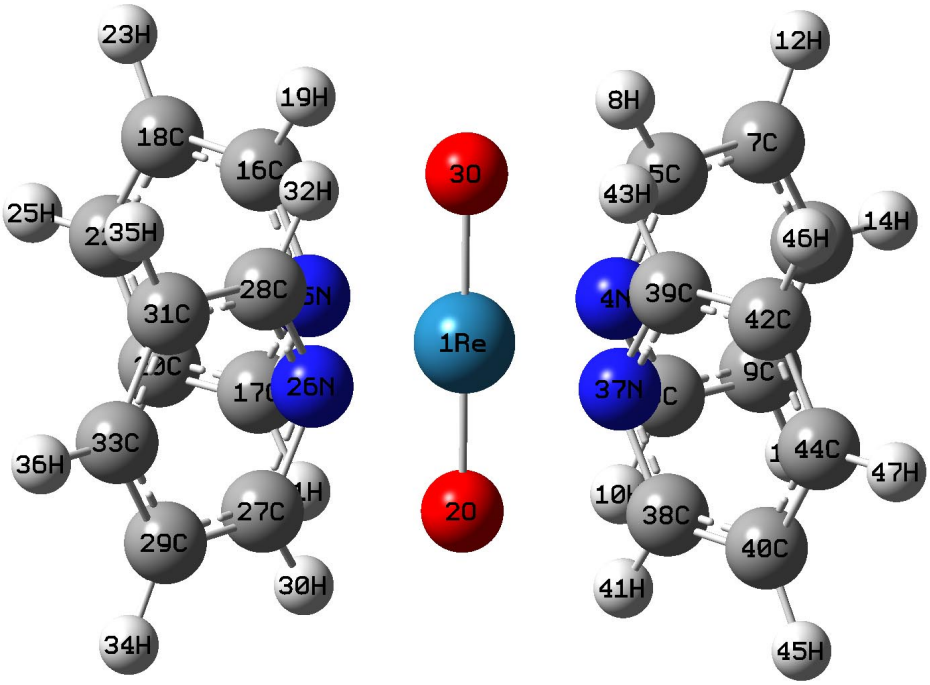

Figure S-2: Gas-phase ball and bond type model of $Re(C_5H_5N)_4(O)_2^+$ as determined with Gaussian 03. The atom label (*i.e.*, 1, 2, etc..) is followed by the atom symbol (*i.e.*, Re = rhenium, C = carbon, H = hydrogen, O = oxygen, N = nitrogen)

Table S-6: Optimized geometry of $Re(C_5H_5N)_4(O)_2^+$ in the singlet ground state in the gas phase with E(RB+HF-LYP) = -1222.59750278 au

Re	0.00000000	0.00000200	0.00000200
O	-1.76568100	-0.00003400	-0.00012300
O	1.76568100	0.00003100	0.00012100
N	-0.00015800	0.00000000	2.18170400
C	1.16235600	-0.00002500	2.87210700
C	-1.16277900	0.00002100	2.87192800
C	1.19807700	-0.00003000	4.26113400
H	2.06411900	-0.00004800	2.26507300
C	-1.19871600	0.00002300	4.26094800
H	-2.06444800	0.00004600	2.26475100
C	-0.00037500	-0.00000100	4.97458400
H	2.15989600	-0.00005500	4.76930100
H	-2.16061500	0.00004000	4.76896700
H	-0.00045800	-0.00000500	6.06327000
N	0.00003300	-2.18170200	0.00000000

C	1.16261100	-2.87199900	0.00004800
C	-1.16252400	-2.87203300	-0.00005300
C	1.19845900	-4.26102300	0.00004800
H	2.06431800	-2.26488300	0.00008700
C	-1.19833400	-4.26105600	-0.00005600
H	-2.06424700	-2.26493700	-0.00008900
C	0.00007300	-4.97458200	-0.00000100
H	2.16032500	-4.76910300	0.00008400
H	-2.16018500	-4.76916400	-0.00010000
H	0.00008800	-6.06326900	-0.00000500
N	0.00015800	0.00000000	-2.18170200
C	-1.16235600	0.00001300	-2.87210500
C	1.16277900	-0.00001700	-2.87192600
C	-1.19807700	0.00001200	-4.26113200
H	-2.06411800	0.00003100	-2.26507100
C	1.19871600	-0.00001800	-4.26094700
H	2.06444700	-0.00003300	-2.26474900
C	0.00037500	-0.00000100	-4.97458200
H	-2.15989600	0.00002100	-4.76930100
H	2.16061500	-0.00003500	-4.76896600
H	0.00045800	-0.00000500	-6.06326900
N	-0.00003300	2.18170300	0.00000000
C	-1.16261100	2.87200000	-0.00009100
C	1.16252400	2.87203400	0.00008700
C	-1.19845900	4.26102400	-0.00009900
H	-2.06431900	2.26488500	-0.00016000
C	1.19833400	4.26105800	0.00009200
H	2.06424800	2.26493900	0.00015800
C	-0.00007300	4.97458300	-0.00000100
H	-2.16032500	4.76910400	-0.00018000
H	2.16018500	4.76916500	0.00016400
H	-0.00008800	6.06327000	-0.00000500

Table S-7: Selected bond lengths[1] of $Re(C_5H_5N)_4(O)_2^+$based on the calculated singlet ground state.

Re(1)-O(30)	Re(1)-O(20)	Re(1)-N(4)	Re(1)-N(15)	Re(1)-N(26)	Re(1)-N(37)
1.76568	1.76568	2.18170	2.18170	2.18170	2.18170

[1] All bond lengths are reported in units of Å

Table S-8: Calculated singlet excited-states of $Re(C_5H_5N)_4(O)_2^+$. The excited state number is followed by the spin multiplicity, symmetry, excitation energy, and oscillator strength *f*. The excitation from occupied to virtual orbitals are listed on the next line, followed by the wavefunction coefficients.

Singlet Excited States of $Re(C^5H_5N)_4(O)_2^+$ (Gas Phase):

```
Excited State   1:   Singlet-A      2.9207 eV  424.50 nm  f=0.0000
      99 ->102        -0.42366
      99 ->103         0.52360
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -1222.49016936
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:   Singlet-A      2.9207 eV  424.50 nm  f=0.0000
      99 ->102         0.52360
      99 ->103         0.42366

 Excited State   3:   Singlet-A      3.6906 eV  335.95 nm  f=0.2745
      99 ->100         0.68193

 Excited State   4:   Singlet-A      3.6906 eV  335.95 nm  f=0.2745
      99 ->101         0.68193

 Excited State   5:   Singlet-A      3.8777 eV  319.74 nm  f=0.0000
      99 ->104         0.69176

 Excited State   6:   Singlet-A      4.1163 eV  301.20 nm  f=0.0000
      99 ->110         0.69808

 Excited State   7:   Singlet-A      4.2103 eV  294.48 nm  f=0.0037
      99 ->106         0.69577

 Excited State   8:   Singlet-A      4.3652 eV  284.03 nm  f=0.0000
      96 ->102        -0.40719
      96 ->103         0.23668
      97 ->102         0.23668
      97 ->103         0.40719

 Excited State   9:   Singlet-A      4.4036 eV  281.55 nm  f=0.0000
      99 ->107         0.69262

 Excited State  10:   Singlet-A      4.4036 eV  281.55 nm  f=0.0000
      99 ->108         0.69261

 Excited State  11:   Singlet-A      4.4631 eV  277.80 nm  f=0.0112
      98 ->102         0.50205
      98 ->103         0.47244

 Excited State  12:   Singlet-A      4.4631 eV  277.80 nm  f=0.0112
      98 ->102        -0.47244
      98 ->103         0.50205
```

Table S-9: Calculated triplet excited-states of $Re(C_5H_5N)_4(O)_2^+$. The excited state number is followed by the spin multiplicity, symmetry, excitation energy, and oscillator strength *f*. The excitation from occupied to virtual orbitals are listed on the next line, followed by the wavefunction coefficients.

Triplet Excited States of $Re(C^5H_5N)_4(O)_2^+$ (Gas Phase):

```
Excited State   1:   Triplet-A      2.3316 eV  531.76 nm  f=0.0000
      99 ->102        -0.47496
      99 ->103         0.57946
 This state for optimization and/or second-order correction.
 Total Energy, E(RPA) =  -1222.51181806
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:   Triplet-A      2.3316 eV  531.76 nm  f=0.0000
      99 ->102         0.57946
      99 ->103         0.47496

 Excited State   3:   Triplet-A      3.2030 eV  387.09 nm  f=0.0000
      89 ->105        -0.12488
      91 ->100         0.10558
      91 ->101        -0.10911
      92 ->107        -0.10224
      93 ->106        -0.11716
      95 ->108         0.10929
      99 ->100         0.68053

 Excited State   4:   Triplet-A      3.2030 eV  387.09 nm  f=0.0000
      90 ->105        -0.12488
      91 ->100        -0.10911
      91 ->101        -0.10559
      92 ->108         0.10224
      94 ->106         0.11716
      95 ->107        -0.10929
      99 ->101         0.68053

 Excited State   5:   Triplet-A      3.2868 eV  377.22 nm  f=0.0000
      96 ->102         0.30304
      96 ->103         0.52136
      97 ->102         0.52136
      97 ->103        -0.30304

 Excited State   6:   Triplet-A      3.3383 eV  371.40 nm  f=0.0000
      89 ->100        -0.14179
      90 ->101        -0.14179
      91 ->104         0.15289
      92 ->106        -0.12542
      93 ->107        -0.11889
      94 ->108        -0.11889
      95 ->109        -0.11972
      99 ->105         0.69034

 Excited State   7:   Triplet-A      3.4059 eV  364.02 nm  f=0.0000
      89 ->100        -0.11447
      89 ->101         0.11001
      90 ->100         0.11001
      90 ->101         0.11447
```

```
     91 ->105         0.16197
     92 ->109         0.13213
     93 ->108        -0.13871
     94 ->107        -0.13871
     95 ->106         0.15117
     99 ->104         0.65040

 Excited State   8:   Triplet-A      3.7091 eV  334.27 nm  f=0.0000
     86 ->110         0.10199
     99 ->110         0.73150

 Excited State   9:   Triplet-A      3.7599 eV  329.75 nm  f=0.0000
     96 ->102         0.16966
     96 ->103        -0.54049
     97 ->102         0.54049
     97 ->103         0.16966

 Excited State  10:   Triplet-A      3.7621 eV  329.56 nm  f=0.0000
     96 ->102         0.54031
     96 ->103         0.16960
     97 ->102        -0.16960
     97 ->103         0.54031

 Excited State  11:   Triplet-A      3.9284 eV  315.61 nm  f=0.0000
     98 ->102         0.70336
     98 ->103        -0.21421

 Excited State  12:   Triplet-A      3.9284 eV  315.61 nm  f=0.0000
     98 ->102         0.21421
     98 ->103         0.70336
```

Table S-10. Selected energies and compositions of $ReO_2(py)_4^+$ molecular orbitals

---

```
Fragment 1 is (Re s-contribution) Basis functions:  1 - 3
Fragment 2 is (Re p-contribution) Basis functions:  4 - 12
Fragment 3 is (Re d-contribution) Basis functions:  13 - 22
Fragment 4 is (Oxygen p-contributions) Basis functions:  25 - 27  29 - 31
39 - 41  43 - 45
Fragment 5 is (Oxygen d-contributions) Basis functions:  32 - 36  46 - 50
Fragment 6 is (Total pyridine contribution) Basis functions:  51 - 426 ; 45
atoms.
Fragment 7 is (Leftovers) Basis functions:  23 - 24  28  37 - 38  42
```

MO#		E(eV)		MO Compositions (%) Fragment: 1	2	3	4	5	6	7
110	10	-2.39	a	0.0	0.0	64.9	0.0	0.1	35.0	0.0
109	9	-3.10	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
108	8	-3.30	a	0.0	0.0	0.6	0.0	0.0	99.4	0.0
107	7	-3.30	a	0.0	0.0	0.6	0.0	0.0	99.4	0.0
106	6	-3.50	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
105	5	-3.75	a	0.0	0.0	8.7	0.0	0.0	91.3	0.0
104	4	-3.90	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
103	3	-3.98	a	0.0	0.0	56.6	38.3	0.3	4.8	0.0
102	2	-3.98	a	0.0	0.0	56.6	38.3	0.3	4.8	0.0
101	1	-4.14	a	0.0	2.1	0.0	0.0	0.0	97.9	0.0
100	0	-4.14	a	0.0	2.1	0.0	0.0	0.0	97.9	0.0
--- occupied - unoccupied orbital gap --- 4.300 eV										
99	0	-8.44	a	0.0	0.0	71.0	0.0	0.0	29.0	0.0
98	-1	-10.12	a	0.0	1.9	0.0	96.6	-0.1	2.0	-0.3
97	-2	-10.14	a	0.0	3.0	0.0	88.7	0.1	8.3	0.0
96	-3	-10.14	a	0.0	3.0	0.0	88.7	0.1	8.3	0.0
95	-4	-10.15	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
94	-5	-10.22	a	0.0	0.0	0.1	0.2	0.0	99.7	0.0
93	-6	-10.22	a	0.0	0.0	0.1	0.2	0.0	99.7	0.0
92	-7	-10.30	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
91	-8	-10.91	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
90	-9	-11.03	a	0.0	0.2	0.0	0.4	0.0	99.4	0.0
89	-10	-11.03	a	0.0	0.2	0.0	0.4	0.0	99.4	0.0
88	-11	-11.60	a	0.0	3.0	0.0	0.8	0.0	96.2	0.0
87	-12	-11.60	a	0.0	3.0	0.0	0.8	0.0	96.2	0.0
86	-13	-11.61	a	0.0	0.0	12.6	0.0	0.0	87.4	0.0
85	-14	-12.45	a	0.0	0.0	33.9	43.2	0.4	22.6	0.0
84	-15	-12.45	a	0.0	0.0	33.9	43.2	0.4	22.6	0.0
83	-16	-12.52	a	0.0	0.0	12.1	0.0	0.0	87.9	0.0
82	-17	-12.60	a	4.1	0.0	2.7	1.2	0.0	92.0	0.0
81	-18	-12.91	a	0.0	0.0	0.0	0.0	0.0	100.0	0.0
80	-19	-12.97	a	0.0	0.3	0.0	0.6	0.0	99.1	0.0

Supporting Information: Full Author List for References 14 and 16

14. Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.;

Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

16. Stephenson, K. A.; Banerjee, S. R.; Besanger, T.; Sogbein, O. O.; Levadala, M. K.; McFarlane, N.; Lemon, J. A.; Boreham, D. R.; Maresca, K. P.; Brennan, J. D.; Babich, J. W.; Zubieta, J.; Valliant, J. F. *J. Am. Chem. Soc.* **2004,** *126*, 8598-8599.