Supporting Information

for

Cooperation between metal and ligand in oxygen atom transport by N-confused porphyrin oxorhenium(V) complexes

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General

All the reactions were performed in oven-dried reaction vessels under Ar or N_2. Commercially available solvents and reagents were used without further purification unless otherwise mentioned. CH_2Cl_2 was dried by passing through a pad of alumina. Thin-layer chromatography (TLC) was carried out on aluminum sheets coated with silica gel 60 F_{254} (MERCK). Preparative separation was performed by silica gel flash column chromatography (KANTO Silica Gel 60 N, spherical, neutral, 40–50 μm) or silica gel gravity column chromatography (KANTO Silica Gel 60 N, spherical, neutral, 63–210 μm). ^{1}H NMR spectra were recorded in $CDCl_3$ solution on a JNM-AL SERIES FT-NMR spectrometer (JEOL) at 300 MHz, and chemical shifts were reported relative to a residual proton of a deuterated solvent, $CHCl_3$ (δ = 7.26) in ppm. ^{13}C NMR spectra were recorded in $CDCl_3$ solution on the same instrument at 75 MHz, and chemical shifts were reported relative to $CDCl_3$ (δ = 77.00) in ppm. UV-Vis absorption spectra were recorded on a UV-3150PC spectrometer (Shimadzu). Mass spectra were recorded on a Bruker Daltonics autoflex MALDI-TOF MS spectrometer and a JEOL JMS-T100CS (ESI mode). IR absorptions were recorded on FT/IR-4200 (JASCO).

Synthesis

2-Methyl-3,21-dioxo-NCTPP oxorhenium complex (5) and 2-methyl-3-oxo-NCTPP oxorhenium complex (6)

To a solution of Re(2-methyl-NCTPP)$(CO)_3$ (**4**) (20.0 mg, 0.0223 mmol) in 2 mL of $C_6H_4Cl_2$, TEMPO (17.5 mg, 0.112 mmol, 5.0 equiv) was added and the reaction mixture was stirred for 64.5 h at 140 °C. The resulting solution was concentrated to dryness in vacuo. The crude residue was separated by silica gel column chromatography with CH_2Cl_2. The second brown and third red fraction were collected and concentrated to dryness to give **5** and **6** in 48% yield and 2% yield, respectively.

5: IR (powder, cm^{-1}) 961 (Re=O); ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 2.90 (s, 3H), 7.87–7.92 (m, 12H), 7.98 (d, J = 6.7 Hz, 1H), 8.05 (d, J = 6.7 Hz, 1H), 8.10 (d, J = 7.0 Hz, 1H), 8.19–8.26 (m, 3H), 8.39 (d, J = 4.9 Hz, 1H), 8.49 (d, J = 7.9 Hz, 1H), 8.61 (d, J = 4.9 Hz, 1H), 8.65 (d, J = 5.2 Hz, 1H), 8.72 (d, J = 4.9 Hz, 1H), 8.79 (d, J = 5.2 Hz, 1H), 8.90 (d, J = 4.9 Hz, 1H), 8.97 (d, J = 4.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 Hz, ppm): δ 31.84, 117.23, 122.73, 124.28, 122.45, 127.50, 127.55, 127.60, 127.85, 128.54, 128.59, 128.66, 128.86, 129.25, 129.72, 130.53, 131.27, 132.49, 132.77, 133.11, 133.58, 133.72, 134.17, 136.14, 138.47, 140.17, 140.84, 141.16, 142.55, 146.82, 148.27, 149.69, 150.62, 150.68, 152.78, 164.96; MS (MALDI, positive) *m/z* 860.39 (M^+); HRMS (ESI$^+$) Found: *m/z* 859.18795, Calcd for $C_{45}H_{30}N_4O_3{}^{185}Re$ ($[M+H]^+$): *m/z* 859.18475; UV-vis (CH_2Cl_2, λ_{max}/nm, (log ε)) 384 (4.46), 508 (4.61); UV-vis (Pyridine, λ_{max}/nm, (log ε)) 385 (4.44), 511 (4.60).

6: IR (powder, cm^{-1}) 1000.9 (Re=O); ^{1}H NMR ($CDCl_3$, 300 MHz, ppm): δ 3.44 (s, 3H), 7.72–7.81 (m, 12H), 7.92–8.14 (m, 6H), 8.27–8.28 (m, 2H), 8.94–8.96 (m, 3H), 9.05–9.09 (m, 3H); ^{13}C NMR

($CDCl_3$, 75 Hz): δ 31.53, 118.41, 124.818, 124.98, 127.47, 127.51, 127.61, 128.42, 128.58, 129.41, 129.97, 130.01, 130.09, 130.20, 130.34, 133.16, 133.38, 133.41, 133.56, 137.16, 140.41, 140.68, 140.74, 141.06, 145.21, 145.56, 146.10, 146.94, 148.74, 151.46, 154.01; MS (MALDI, positive) *m/z* 844.1 (M^+); HRMS (ESI^+) Found: *m/z* 842.18131, Calcd for $C_{45}H_{29}N_4O_2{}^{185}Re$ (M^+): *m/z* 842.18201; UV-vis (CH_2Cl_2, λ_{max}/nm, (log ε)) 331 (4.45), 484 (4.83), 557 (3.94), 673 (3.59); UV-vis (Pyridine, λ_{max} /nm, (log ε)) 327 (4.61), 356 (4.63), 539 (4.59), 681 (3.75).

ReO(COR)

To a solution of triphenylcorrole (40 mg, 0.076 mmol) in 4 mL of $C_6H_4Cl_2$, $Re(CO)_5Br$ (24 mg, 0.033 mmol) was added and the reaction mixture was stirred for 18 h at 140 °C. The resulting solution was concentrated to dryness in vacuo. The crude residue was separated by silica gel column chromatography with CH_2Cl_2. The first fraction was collected and concentrated to dryness to give **ReO(COR)** in 43% yield. IR (powder, cm^{-1}) 986 (Re=O); ^1H NMR ($CDCl_3$, 300 MHz, ppm): δ 7.71–7.92 (m, 10H, phenyl), 8.09 (br-s, 2H, phenyl), 8.54 (d, *J* = 7.8 Hz, 1H , phenyl), 8.61 (br-s, 2H, phenyl), 9.12 (d, *J* = 4.8 Hz, 2H), 9.31–9.34 (m, 4H), 9.62 (d, *J* = 4.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 117.42, 118.64, 121.61,126.68, 127.00, 127.54, 127.59, 127.86, 127.92, 128.00, 128.30, 133.80, 134.12, 137.00, 140.14, 140.84, 143.69, 144.98; MS (MALDI, positive) *m/z* 726.1 (M^+); HRMS (ESI^+) Found: *m/z* 724.14378, Calcd for $C_{37}H_{23}N_4O^{185}Re$ (M^+): *m/z* 724.14014.

Catalytic oxygen atom transfer reaction with 1 mol% catalyst

Triphenylphosphine (122 mg, 0.468 mmol, 1.0 equiv) was added to a solution of 4-phenylpyridine *N*-oxide (80 mg, 0.468 mmol, 1.0 equiv) and catalyst (1 mol%) in 4 mL of toluene. After stirring at 80 °C for 24 h, the resulting solution was poured onto a silica gel column. Column chromatography was performed with $MeOH/CH_2Cl_2$ = 1/200–1/100 (v/v) to give 4-phenylpyridine. All the yields were based on the amounts of isolated products.

Catalytic oxygen atom transfer reaction with 0.01 mol% catalyst

Triphenylphosphine (122 mg, 0.468 mmol, 1.0 equiv) was added to a solution of 4-phenylpyridine *N*-oxide (80 mg, 0.468 mmol, 1.0 equiv) and catalyst (0.01 mol%, 0.0395 mg, 4.68 μmol) in 4 mL of toluene. Reaction temperature was gradually raised from 80 to 110 °C for 49 h and the resulting solution was poured onto a silica gel column. Column chromatography was performed with $MeOH/CH_2Cl_2$ = 1/200–1/100 (v/v) to give 4-phenylpyridine in 55% yield (39.6 mg, 0.256 mmol).

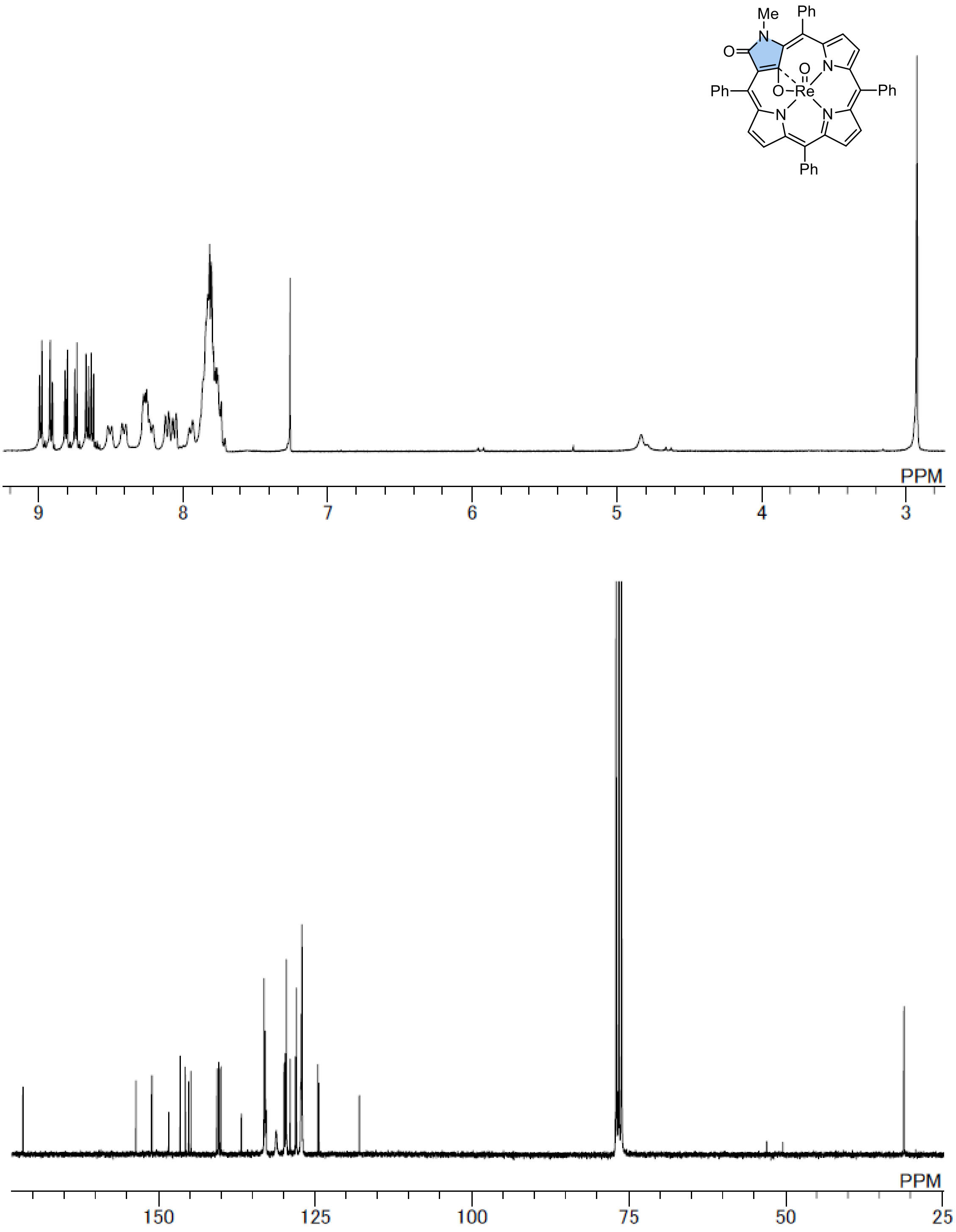


Fig. S1 ^{1}H and ^{13}C NMR spectra of **5** in $CDCl_3$.

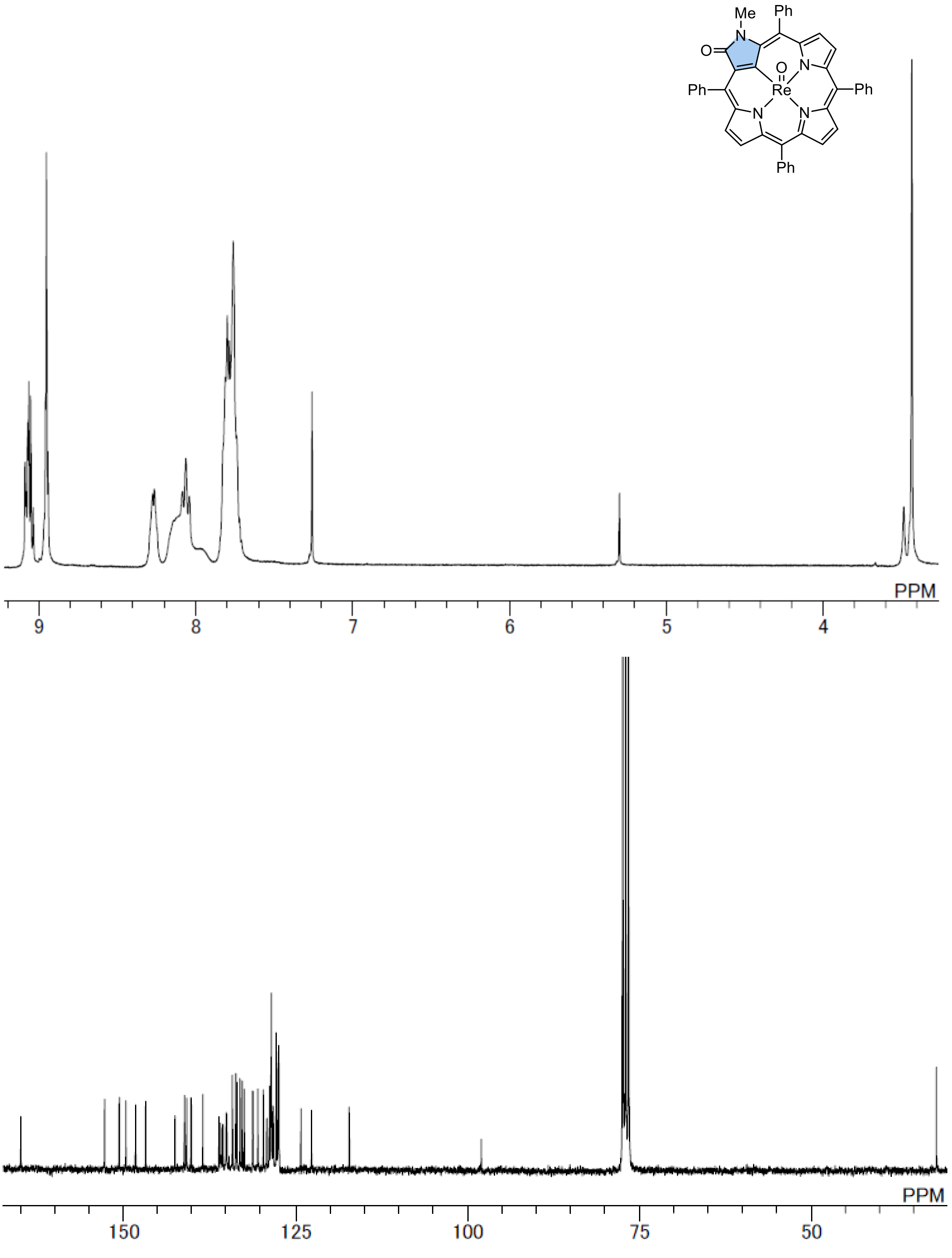


Fig. S2 ^{1}H and ^{13}C NMR spectra of **6** in $CDCl_3$.

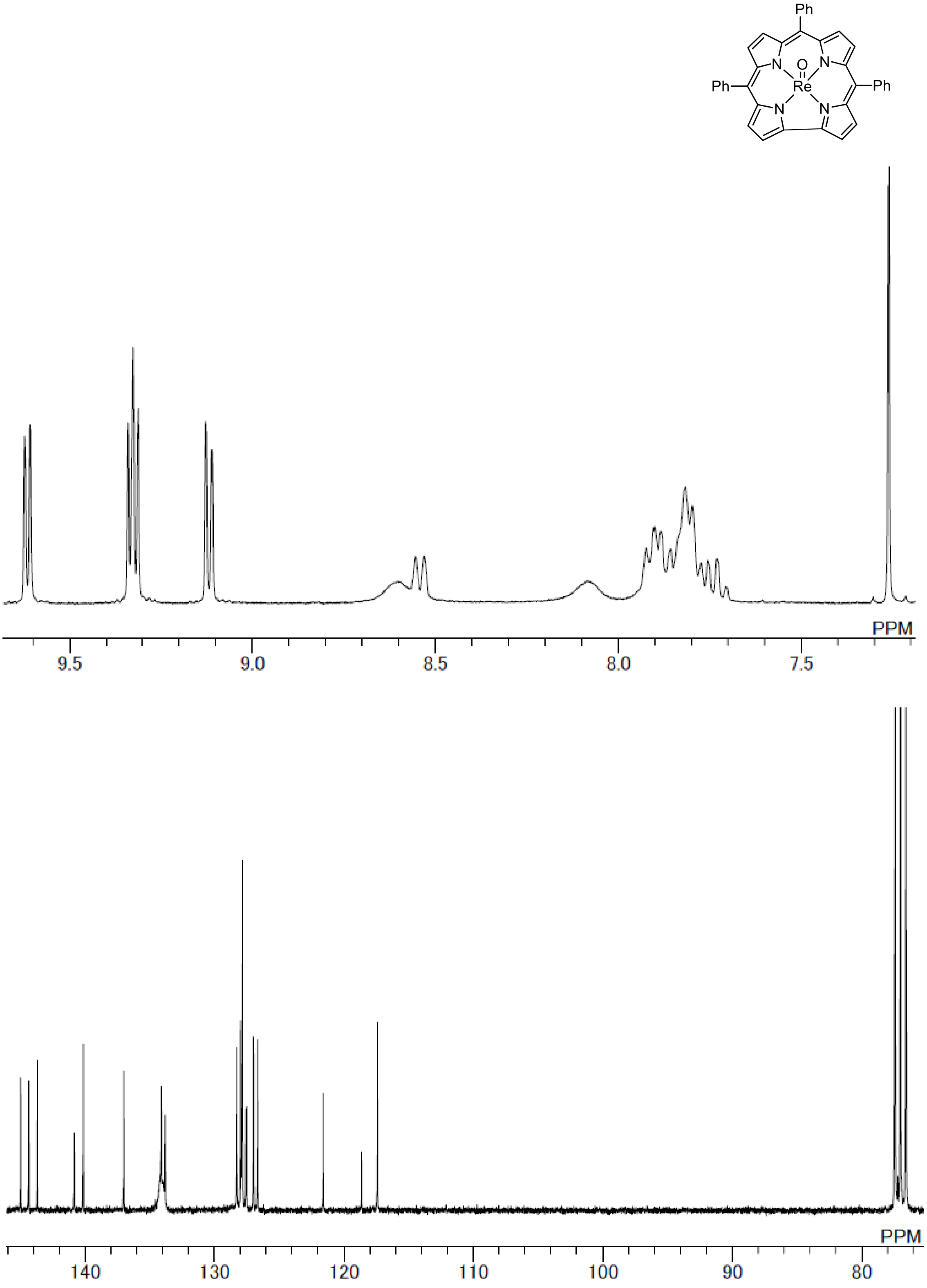


Fig. S3 ^{1}H and ^{13}C NMR spectra of **ReO(COR)** in $CDCl_3$.

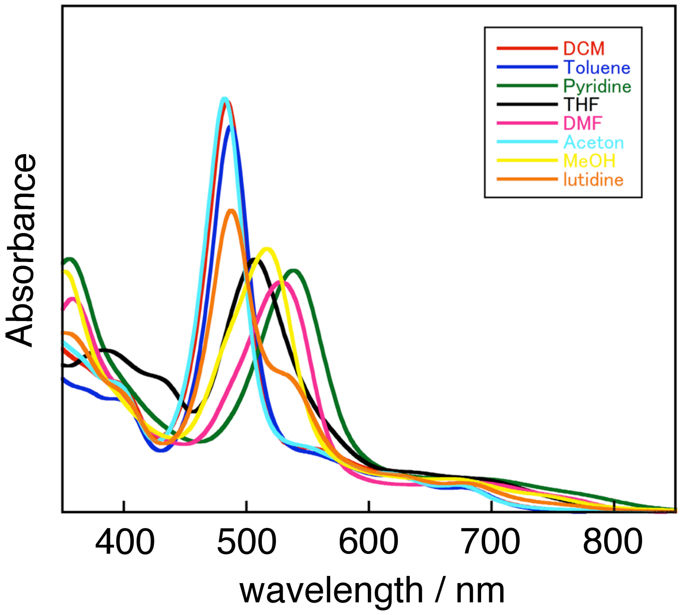


Fig. S4 Absorption spectra of **6** in various solvents.

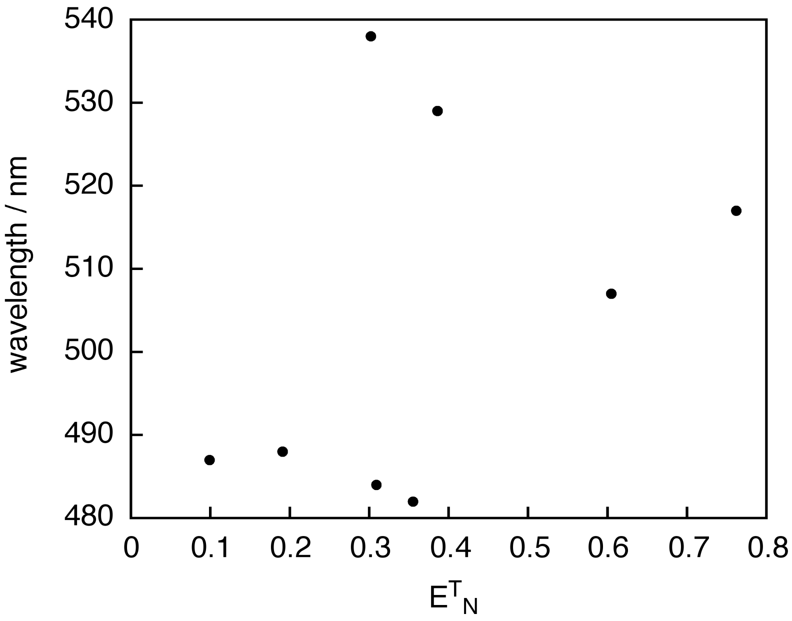


Fig. S5 Relationship between absorption maxima (λ_{max}) of **6** and solvent polarity ($E^T{}_N$).

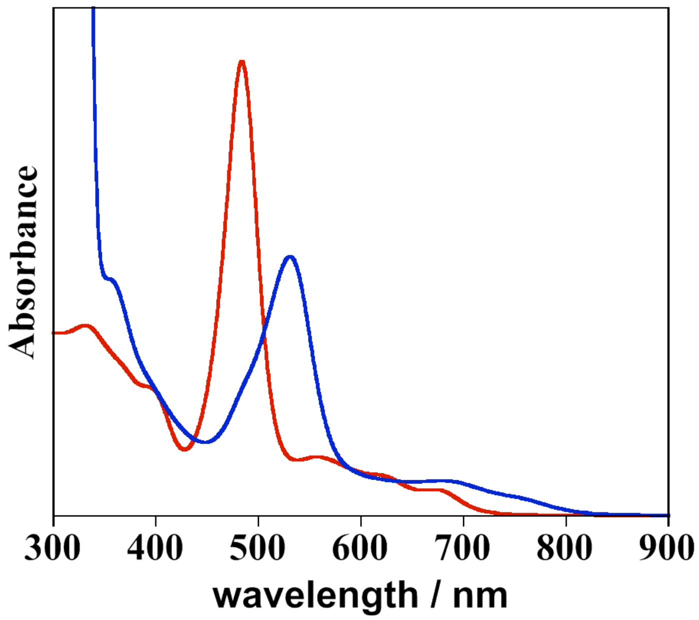


Fig. S6 Absorption spectra of **6** with (— blue line) and without (— red line) excess pyridine *N*-oxide in CH_2Cl_2.

Calculation details

All density functional theory[1] calculations were achieved with a Gaussian09 program package.[2] The basis sets implemented in the program were used. The B3LYP density functional method[3] was used with a 631LAN basis set for structural optimizations and frequency calculation. The 631LAN bases set is composed of 6-31G** for C, H, N, O and LANL2DZ for Re. Initial structures were based on the X-ray structures or arbitrary constracted and equilibrium geometries were fully optimized and verified by the frequency calculations, where no imaginary frequency was found.

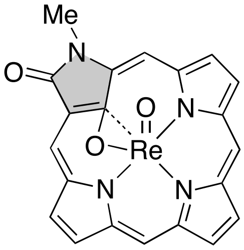
1) (a) P. Hohenberg, W. Kohn, *Phys. Rev.,* 1964, **136**, B864. (b) W. Kohn, L. J. Sham, *Phys. Rev.,* 1965, **140,** A1133.

2) Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

3) (a) A. D. Becke, *J. Phys. Chem.* 1993, **98**, 5648. (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785. (c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.,* 1980, **58**, 1200. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.,* 1994, **98**, 11623.

Cartesian coordinates and vibrational frequencies for the optimized structures

ReO(oxo-NCPO)



E(RB3LYP) = -1331.93825971 A.U.

Stoichiometry C21H13N4O3Re
Framework group C1[X(C21H13N4O3Re)]
Deg. of freedom 120
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

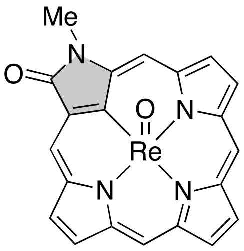
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	75	0	0.001341	–0.000629	–0.001540
2	8	0	0.000179	–0.001276	1.694972
3	8	0	1.283999	–0.000414	–1.534149
4	8	0	5.150714	1.281675	0.961783
5	6	0	4.231871	0.651646	0.464088
6	6	0	2.971595	1.142803	–0.153673
7	6	0	2.251868	0.000167	–0.582159
8	6	0	2.950297	–1.175516	–0.143753
9	7	0	4.152343	–0.755503	0.423810
10	6	0	5.104411	–1.599275	1.119234
11	1	0	5.856017	–0.939524	1.554978
12	1	0	4.613189	–2.170444	1.914699
13	1	0	5.595114	–2.294492	0.429812
14	7	0	0.103894	2.074304	–0.348677
15	6	0	–0.985209	2.905741	–0.499938
16	6	0	–0.542551	4.269586	–0.572757
17	1	0	–1.193966	5.125434	–0.689319
18	6	0	0.821371	4.252855	–0.483038
19	1	0	1.500548	5.094597	–0.511708
20	6	0	1.234192	2.882109	–0.359986
21	6	0	2.561915	2.464257	–0.187913
22	6	0	2.510434	–2.486267	–0.222625
23	7	0	0.054893	–2.061647	–0.384011
24	6	0	1.172806	–2.875494	–0.420642
25	6	0	0.748106	–4.235817	–0.603734
26	1	0	1.417550	–5.083938	–0.661481
27	6	0	–0.616681	–4.235622	–0.702570
28	1	0	–1.274266	–5.080665	–0.857262
29	6	0	–1.046981	–2.873109	–0.581240
30	6	0	–2.355538	–2.416226	–0.690813
31	7	0	–1.930685	0.023353	–0.601149
32	6	0	–2.771534	–1.087196	–0.694923
33	6	0	–4.119347	–0.634436	–0.821298
34	1	0	–4.978256	–1.286146	–0.912160
35	6	0	–4.105100	0.736946	–0.804722
36	1	0	–4.950303	1.409002	–0.871537
37	6	0	–2.747659	1.156576	–0.665758
38	6	0	–2.304954	2.473672	–0.616390
39	1	0	–3.064945	3.242914	–0.710149
40	1	0	–3.129950	–3.166937	–0.812726
41	1	0	3.218296	–3.289143	–0.040896
42	1	0	3.301994	3.232659	0.017869

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	50.6233	70.1150	73.1873
Red. masses --	6.0287	6.0363	5.4793
Frc consts --	0.0091	0.0175	0.0173
IR Inten --	0.2006	3.0464	0.5559

ReO(NCPO)



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E(RB3LYP) =    -1256.73925337         A.U.

Stoichiometry                         C21H13N4O2Re
Framework group                       C1[X(C21H13N4O2Re)]
Deg. of freedom                       117
Full point group                                    C1
Largest Abelian subgroup                            C1         NOp    1
Largest concise Abelian subgroup                    C1         NOp    1
                                   Standard orientation:
---------------------------------------------------------------------
 Center      Atomic        Atomic                Coordinates (Angstroms)
 Number        Number         Type                X               Y              Z
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      1           6              0          –0.000521     0.003020    –0.000232
      2           6              0          –0.000673     0.001791     1.491605
      3           6              0           1.327074    –0.000735     1.966558
      4           6              0           2.144993     0.000241     0.793920
      5           6              0           3.525439     0.012208     0.755855
      6           6              0           4.307982    –0.067197     1.909077
      7           6              0           5.734996    –0.162749     1.904711
      8           6              0           6.142063    –0.318838     3.201205
      9           6              0           4.968707    –0.321539     4.015327
     10           6              0           4.951862    –0.541709     5.378627
     11           6              0           3.811232    –0.640845     6.167551
     12           6              0           3.805634    –0.906989     7.570470
     13           6              0           2.498337    –0.915680     7.977300
     14           6              0           1.695463    –0.652216     6.825988
     15           6              0           0.309581    –0.558184     6.825633
     16           6              0          –0.484769    –0.332698     5.716241
     17           6              0          –1.915334    –0.338408     5.726455
     18           6              0          –2.329774    –0.173121     4.435320
     19           6              0          –1.160743    –0.065735     3.617531
     20           6              0          –1.167000     0.012282     2.228772
     21           6              0           1.803078     0.000644    –1.727865
     22           1              0           6.345933    –0.135131     1.012172
     23           1              0           7.149263    –0.442869     3.576202
     24           1              0           4.692964    –1.066802     8.168519
     25           1              0           2.108661    –1.078942     8.973249
     26           1              0          –2.520864    –0.473873     6.612757
     27           1              0          –3.342237    –0.147925     4.054923
     28           1              0           2.395547     0.894629    –1.952448
     29           1              0           2.403807    –0.889076    –1.947235
     30           1              0           0.911101    –0.004468    –2.356530
     31           7              0           1.349386     0.002315    –0.353463
     32           7              0           3.837679    –0.131946     3.212692
     33           7              0           2.508412    –0.492287     5.709787
     34           7              0          –0.019886    –0.131774     4.415358
     35           8              0          –0.940789     0.002459    –0.780586
     36           8              0           1.967913     2.088180     4.018398
     37          75              0           1.938258     0.411275     3.895578
     38           1              0           4.048630     0.041567    –0.193912
     39           1              0          –2.119765     0.038191     1.708931
     40           1              0          –0.195653    –0.702540     7.775087
     41           1              0           5.908810    –0.675829     5.872375
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 Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
 activities (A**4/AMU), depolarization ratios for plane and unpolarized
 incident light, reduced masses (AMU), force constants (mDyne/A),
 and normal coordinates:
                                1                          2                           3
                                A                          A                           A
 Frequencies --          45.7959                    59.3817                    79.3531
 Red. masses --          5.8370                     5.2043                     6.3728
 Frc consts   --         0.0072                     0.0108                     0.0236
 IR Inten      --        0.0150                     1.3313                     1.9600
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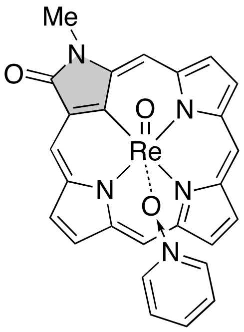
Re(NCPO)(pyridine *N*-oxide)



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E(RB3LYP) =    -1580.19668991         A.U.

Stoichiometry            C26H18N5O3Re
Framework group          C1[X(C26H18N5O3Re)]
Deg. of freedom          153
Full point group                                   C1        NOp    1
Largest Abelian subgroup                           C1        NOp    1
Largest concise Abelian subgroup                   C1        NOp    1
                              Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic              Coordinates (Angstroms)
Number      Number       Type              X           Y           Z
---------------------------------------------------------------------
     1         75           0        0.128152    0.740125   –0.143813
     2          7           0       –0.064989   –0.414418    4.008213
     3          7           0        2.134741    0.431566    0.307388
     4          7           0        0.617205    0.484719   –2.182063
     5          7           0       –1.829477    0.188988   –0.641500
     6          8           0       –0.025665    2.402134    0.046797
     7          8           0       –2.293804   –0.812972    4.560248
     8          6           0       –1.431598   –0.529573    3.740286
     9          6           0       –1.560764   –0.244192    2.278442
    10          6           0       –0.291015    0.023461    1.750512
    11          6           0        0.626868   –0.099592    2.830541
    12          6           0        2.001614    0.053305    2.759493
    13          6           0        2.694793    0.281988    1.561707
    14          6           0        4.121748    0.331578    1.448278
    15          6           0        4.425587    0.477077    0.120259
    16          6           0        3.187770    0.521964   –0.597449
    17          6           0        3.068675    0.611084   –1.979333
    18          6           0        1.885176    0.595643   –2.719225
    19          6           0        1.782404    0.694357   –4.145347
    20          6           0        0.448455    0.649120   –4.462380
    21          6           0       –0.277034    0.519363   –3.232860
    22          6           0       –1.664139    0.427221   –3.102959
    23          6           0       –2.375163    0.261334   –1.919802
    24          6           0       –3.797085    0.096233   –1.835154
    25          6           0       –4.110602   –0.093595   –0.517050
    26          6           0       –2.889755   –0.046235    0.232222
    27          6           0       –2.777495   –0.255857    1.606126
    28          1           0        4.806808    0.245576    2.281558
    29          1           0        5.404891    0.538636   –0.336038
    30          1           0        2.623021    0.794674   –4.819727
    31          1           0       –0.004135    0.709180   –5.443610
    32          1           0       –4.468996    0.118955   –2.683341
    33          1           0       –5.087748   –0.258453   –0.081892
    34          1           0        2.605155   –0.049275    3.655748
    35          1           0       –3.683317   –0.452885    2.172372
    36          1           0       –2.245558    0.469082   –4.018657
    37          1           0        3.994035    0.692020   –2.541524
    38          6           0        0.498899   –0.624331    5.322952
    39          1           0        1.210450   –1.458297    5.324594
    40          1           0        1.007664    0.275362    5.687685
    41          1           0       –0.331033   –0.860877    5.991287
    42          8           0        0.506773   –1.755856   –0.381459
    43          6           0        0.339417   –2.818534   –2.419881
    44          6           0       –1.376034   –3.022407   –0.808494
    45          6           0       –0.351805   –3.647855   –3.286704
    46          1           0        1.296482   –2.360631   –2.627269
    47          6           0       –2.093077   –3.852574   –1.653030
    48          1           0       –1.694157   –2.715961    0.178407
    49          6           0       –1.586833   –4.178728   –2.912156
    50          1           0        0.087444   –3.867823   –4.253562
    51          1           0       –3.048297   –4.236146   –1.311979
    52          1           0       –2.138536   –4.829152   –3.581782
    53          7           0       –0.170914   –2.514156   –1.193060
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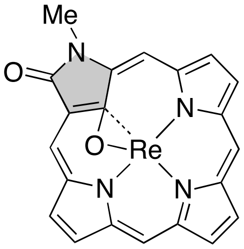
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
                           1                       2                       3
                           A                       A                       A
Frequencies --         19.4709                 38.6807                 50.5208
Red. masses --          5.5856                  5.6950                  5.5928
Frc consts  --          0.0012                  0.0050                  0.0084
IR Inten    --          0.4963                  1.2823                  0.3376
```

Re(oxo-NCPO)



```
E(RB3LYP) =    -1256.62903106        A.U.

Stoichiometry                       C21H13N4O2Re
Framework group                     C1[X(C21H13N4O2Re)]
Deg. of freedom                     117
Full point group                             C1
Largest Abelian subgroup                     C1        NOp    1
Largest concise Abelian subgroup             C1        NOp    1
                           Standard orientation:
---------------------------------------------------------------------
Center       Atomic        Atomic                Coordinates (Angstroms)
Number         Number        Type                 X              Y              Z
---------------------------------------------------------------------
1           75           0       –0.398505   –0.127717    0.638043
2            8           0        0.058198    0.028986    2.426222
3            8           0        4.724976    0.014089    2.711597
4            6           0        3.578512    0.315712    2.429629
5            6           0        2.430641   –0.512219    2.005942
6            6           0        1.319416    0.375840    1.805008
7            6           0        1.786779    1.728150    1.987017
8            6           0        1.070784    2.882544    1.703528
9            6           0       –0.137119    2.927359    0.983878
10           6           0       –0.855660    4.144954    0.725370
11           6           0       –1.953458    3.826628   –0.025020
12           6           0       –1.943788    2.405311   –0.229301
13           6           0       –2.883301    1.682212   –0.953474
14           6           0       –2.881514    0.300293   –1.172672
15           6           0       –3.807917   –0.417148   –1.999730
16           6           0       –3.433331   –1.734764   –1.983293
17           6           0       –2.268711   –1.838865   –1.150769
18           6           0       –1.523195   –2.995169   –0.937075
19           6           0       –0.330905   –3.100406   –0.214916
20           6           0        0.437733   –4.290064   –0.039970
21           6           0        1.544618   –3.959961    0.708104
22           6           0        1.477583   –2.564529    0.987055
23           6           0        2.475393   –1.849010    1.692801
24           6           0        3.992898    2.788372    2.606637
25           7           0        3.101963    1.664332    2.391347
26           7           0       –0.825689    1.864067    0.391181
27           7           0       –1.967432   –0.586987   –0.632245
28           7           0        0.303573   –2.046534    0.424280
29           1           0        1.488620    3.844909    1.981750
30           1           0       –0.553519    5.121554    1.079359
31           1           0       –2.709287    4.499052   –0.410105
32           1           0       –3.691050    2.247342   –1.408191
33           1           0       –4.626606    0.033307   –2.545511
34           1           0       –3.883667   –2.559170   –2.520649
35           1           0       –1.895913   –3.907057   –1.393598
36           1           0        0.175154   –5.261224   –0.439097
37           1           0        2.337881   –4.616006    1.041042
38           1           0        3.375350   –2.402618    1.947339
39           1           0        4.982198    2.377325    2.812450
40           1           0        3.665641    3.389914    3.460893
41           1           0        4.036521    3.424258    1.716163
---------------------------------------------------------------------

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
                          1                        2                        3
                          A                        A                        A
Frequencies --          41.9499                  63.6618                  77.6137
Red. masses --          5.5647                   7.3736                   5.2440
Frc consts  --          0.0058                   0.0176                   0.0186
IR Inten    --          0.0119                   2.9101                   1.1533
```