Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

Synthesis and Characterization of Oxorhenium(V) Diamido Pyridine Complexes that Catalyze Oxygen Atom Transfer Reactions

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X-ray Crystallographic Procedures and Data

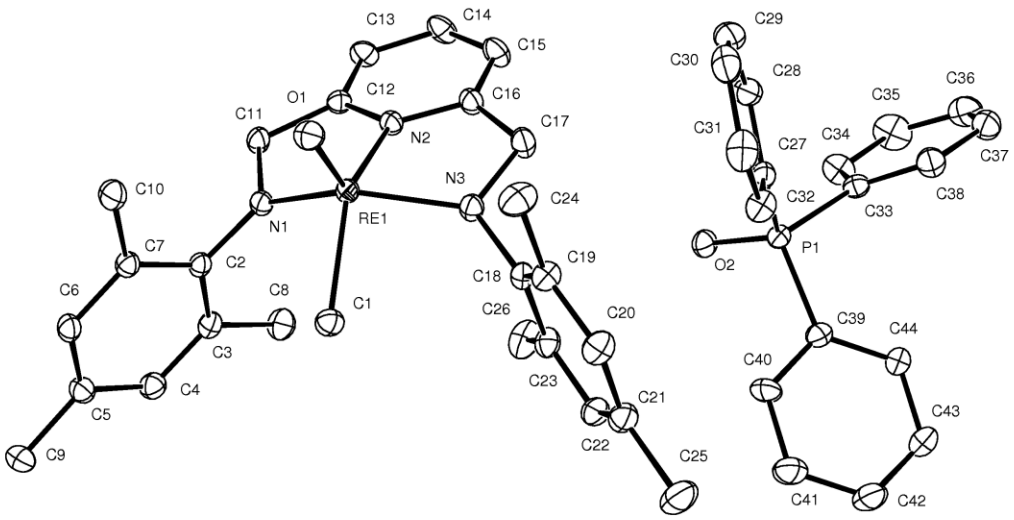

Figure S1. ORTEP drawing of **Re(O)Me(DAP)**.**OPPh$_3$**, **1** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

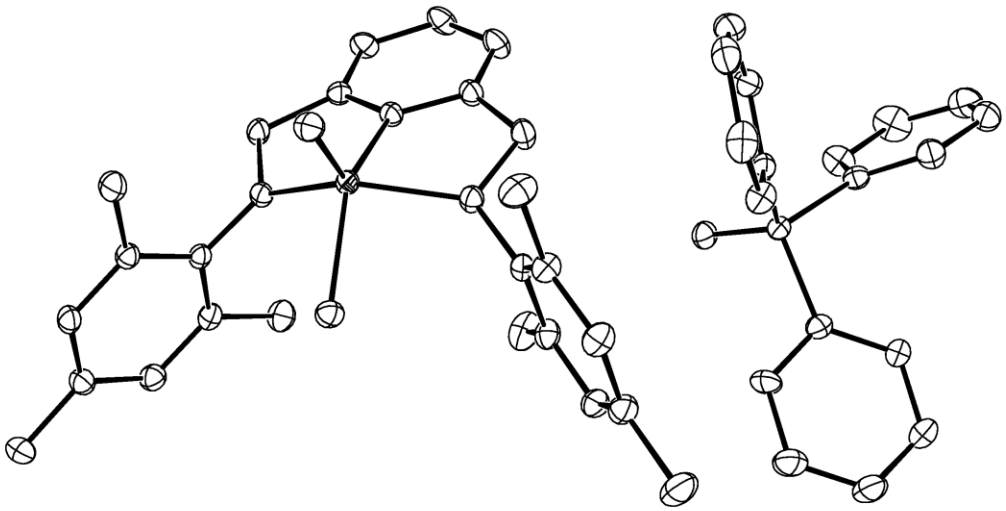

Figure S2. ORTEP drawing of **Re(O)Me(DAP)•OPPh$_3$, 1**. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

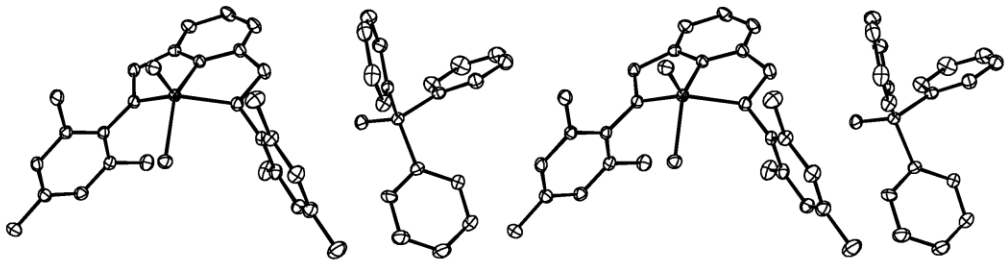

Figure S3. Stereoscopic ORTEP drawing of **Re(O)Me(DAP).OPPh$_3$, 1**. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

***Table S1*. Summary of Crystal Data for Re(O)Me(DAP).OPPh$_3$, 1**

Formula	$C_{44}H_{47}N_3O_2PRe$
Formula Weight (*g/mol*)	867.02
Crystal Dimensions (*mm*)	0.31 × 0.26 × 0.07
Crystal Color and Habit	red prism
Crystal System	triclinic
Space Group	P -1
Temperature, K	110
a, Å	8.5052(2)
b, Å	14.6432(4)
c, Å	16.3909(4)
α,°	111.4709(14)
β,°	94.3130(14)
γ,°	90.4943(13)
V, Å^3	1892.89(8)
Number of reflections to determine final unit cell	9799
Min and Max 2θ for cell determination, °	5.08, 73.36
Z	2
F(000)	876
ρ (*g/cm*)	1.521
λ, Å, (MoKα)	0.71073
μ, (cm^{-1})	3.293
Diffractometer Type	Bruker-Nonius Kappa Axis X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	78.8
Measured fraction of data	0.985
Number of reflections measured	77022
Unique reflections measured	20705
R_{merge}	0.0329
Number of reflections included in refinement	20705
Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc w=1/[sigma^2(Fo^2)+(0.0333P)^2+0.0000P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	467
R_1	0.0315
wR_2	0.0641
R_1 (all data)	0.0425
wR_2 (all data)	0.0679
GOF	1.037
Maximum shift/error	0.015
Min & Max peak heights on final ΔF Map (e^-/Å)	-1.231, 1.498

Where:

$R_1 = \Sigma(|F_o| - |F_c|) / \Sigma F_o$

$wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(w F_o^4)]^{½}$

$GOF = [\Sigma(w(F_o^2 - F_c^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

***Table S2*. Atomic Coordinates for Re(O)Me(DAP).OPPh$_3$, 1**

Atom	x	y	z	$U_{iso/equiv}$
Re1	0.404534(7)	0.330420(4)	1.101130(4)	0.01469(2)
O1	0.60268(14)	0.32778(10)	1.11940(8)	0.0216(2)
C1	0.3127(2)	0.22106(13)	1.14343(12)	0.0204(3)
N1	0.31336(16)	0.43088(10)	1.20146(9)	0.0164(2)
N2	0.31824(16)	0.43098(10)	1.04943(9)	0.0166(2)
N3	0.32980(17)	0.24889(10)	0.97889(9)	0.0176(2)
C2	0.26483(18)	0.42268(11)	1.28013(10)	0.0157(3)
C3	0.10443(19)	0.41416(12)	1.29205(11)	0.0186(3)
C4	0.0619(2)	0.39983(13)	1.36714(11)	0.0209(3)
C5	0.1744(2)	0.39620(13)	1.43216(11)	0.0201(3)
C6	0.3322(2)	0.40897(12)	1.42063(11)	0.0196(3)
C7	0.38025(18)	0.42174(12)	1.34611(11)	0.0171(3)
C8	-0.0213(2)	0.41765(15)	1.22346(13)	0.0259(4)
C9	0.1289(2)	0.37659(15)	1.51153(12)	0.0268(4)
C10	0.5528(2)	0.43286(15)	1.33506(12)	0.0241(3)
C11	0.2977(2)	0.52991(12)	1.19906(11)	0.0191(3)
C12	0.28695(19)	0.52166(12)	1.10490(11)	0.0178(3)
C13	0.2434(2)	0.59352(13)	1.07213(12)	0.0215(3)
C14	0.2300(2)	0.56850(14)	0.98142(12)	0.0238(3)
C15	0.2569(2)	0.47395(14)	0.92539(12)	0.0235(3)
C16	0.2991(2)	0.40458(12)	0.96102(11)	0.0187(3)
C17	0.3202(2)	0.29687(13)	0.91398(11)	0.0217(3)
C18	0.28468(18)	0.14672(12)	0.94109(10)	0.0165(3)
C19	0.40018(19)	0.07669(12)	0.91514(11)	0.0194(3)
C20	0.3538(2)	-0.02249(13)	0.87900(12)	0.0229(3)
C21	0.1961(2)	-0.05434(13)	0.86966(12)	0.0222(3)
C22	0.0839(2)	0.01680(13)	0.89671(11)	0.0211(3)
C23	0.12479(19)	0.11690(13)	0.93105(11)	0.0194(3)
C24	0.5722(2)	0.10792(15)	0.92558(14)	0.0274(4)
C25	0.1501(3)	-0.16220(14)	0.83226(14)	0.0311(4)
C26	-0.0003(2)	0.19203(15)	0.95714(14)	0.0294(4)
P1	-0.11537(5)	0.17263(3)	0.66366(3)	0.01579(7)
O2	-0.17582(15)	0.24820(9)	0.74240(8)	0.0221(2)
C27	0.09741(18)	0.17145(12)	0.67220(10)	0.0175(3)
C28	0.1771(2)	0.25418(14)	0.66968(12)	0.0235(3)
C29	0.3411(2)	0.26218(17)	0.68102(13)	0.0289(4)
C30	0.4266(2)	0.18801(17)	0.69529(12)	0.0296(4)
C31	0.3487(2)	0.10626(16)	0.69819(13)	0.0288(4)
C32	0.1839(2)	0.09784(14)	0.68699(12)	0.0231(3)
C33	-0.16602(18)	0.19714(12)	0.56481(11)	0.0177(3)
C34	-0.2642(2)	0.27475(14)	0.57184(13)	0.0262(4)
C35	-0.3063(3)	0.29827(17)	0.49835(15)	0.0359(5)
C36	-0.2531(2)	0.24319(16)	0.41760(14)	0.0316(4)
C37	-0.1527(3)	0.16690(15)	0.41059(13)	0.0281(4)

C38	-0.1083(2)	0.14467(13)	0.48440(12)	0.0241(3)
C39	-0.19433(19)	0.05093(12)	0.64541(11)	0.0184(3)
C40	-0.1821(2)	0.01917(14)	0.71532(13)	0.0249(3)
C41	-0.2446(3)	-0.07024(15)	0.70914(14)	0.0308(4)
C42	-0.3258(3)	-0.12989(15)	0.63160(14)	0.0305(4)
C43	-0.3444(2)	-0.09889(15)	0.56071(13)	0.0302(4)
C44	-0.2784(2)	-0.00901(13)	0.56709(12)	0.0233(3)
H1A	0.3338	0.1558	1.1013	0.031
H1B	0.1986	0.2276	1.1469	0.031
H1C	0.3635	0.2294	1.2015	0.031
H4	-0.0467	0.3923	1.3742	0.025
H6	0.4102	0.4090	1.4653	0.024
H8A	-0.1191	0.3857	1.2296	0.039
H8B	0.0137	0.3833	1.1647	0.039
H8C	-0.0403	0.4862	1.2315	0.039
H9A	0.1330	0.3061	1.4998	0.040
H9B	0.0217	0.3982	1.5240	0.040
H9C	0.2026	0.4127	1.5624	0.040
H10A	0.6146	0.4445	1.3911	0.036
H10B	0.5695	0.4886	1.3167	0.036
H10C	0.5865	0.3727	1.2902	0.036
H11A	0.3903	0.5724	1.2320	0.023
H11B	0.2017	0.5596	1.2268	0.023
H13	0.2232	0.6580	1.1106	0.026
H14	0.2020	0.6169	0.9576	0.029
H15	0.2465	0.4570	0.8634	0.028
H17A	0.2299	0.2680	0.8697	0.026
H17B	0.4179	0.2867	0.8831	0.026
H20	0.4321	-0.0699	0.8601	0.027
H22	-0.0240	-0.0035	0.8916	0.025
H24A	0.6362	0.0496	0.9073	0.041
H24B	0.6027	0.1481	0.9873	0.041
H24C	0.5896	0.1463	0.8889	0.041
H25A	0.0867	-0.1782	0.8731	0.047
H25B	0.2454	-0.2006	0.8238	0.047
H25C	0.0883	-0.1780	0.7756	0.047
H26A	-0.0164	0.2219	0.9127	0.044
H26B	0.0335	0.2430	1.0142	0.044
H26C	-0.0993	0.1600	0.9615	0.044
H28	0.1191	0.3051	0.6602	0.028
H29	0.3948	0.3184	0.6790	0.035
H30	0.5385	0.1936	0.7030	0.035
H31	0.4073	0.0556	0.7078	0.035
H32	0.1308	0.0417	0.6895	0.028
H34	-0.3025	0.3117	0.6269	0.031
H35	-0.3715	0.3521	0.5036	0.043
H36	-0.2854	0.2576	0.3670	0.038
H37	-0.1144	0.1300	0.3555	0.034

H38	-0.0380	0.0933	0.4798	0.029
H40	-0.1286	0.0606	0.7695	0.030
H41	-0.2319	-0.0907	0.7579	0.037
H42	-0.3691	-0.1920	0.6265	0.037
H43	-0.4023	-0.1394	0.5077	0.036
H44	-0.2905	0.0116	0.5184	0.028

***Table S3*. Anisotropic Displacement Parameters for Re(O)Me(DAP).OPPh$_3$, 1**

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
Re1	0.01570(3)	0.01395(3)	0.01489(3)	0.00041(2)	-0.00095(2)	0.00631(2)
O1	0.0180(5)	0.0249(6)	0.0241(6)	0.0006(4)	-0.0001(4)	0.0118(5)
C1	0.0222(7)	0.0175(7)	0.0221(8)	0.0003(6)	0.0010(6)	0.0084(6)
N1	0.0206(6)	0.0141(6)	0.0153(6)	0.0004(5)	-0.0015(5)	0.0068(5)
N2	0.0198(6)	0.0156(6)	0.0150(6)	0.0004(5)	0.0006(4)	0.0065(5)
N3	0.0219(6)	0.0149(6)	0.0154(6)	0.0011(5)	-0.0008(5)	0.0055(5)
C2	0.0188(6)	0.0128(6)	0.0150(6)	0.0002(5)	-0.0017(5)	0.0049(5)
C3	0.0189(7)	0.0167(7)	0.0183(7)	0.0006(5)	-0.0022(5)	0.0050(6)
C4	0.0188(7)	0.0216(8)	0.0213(8)	-0.0006(6)	0.0019(6)	0.0068(6)
C5	0.0250(8)	0.0180(7)	0.0178(7)	0.0005(6)	0.0021(6)	0.0070(6)
C6	0.0229(7)	0.0195(7)	0.0164(7)	0.0001(6)	-0.0029(5)	0.0074(6)
C7	0.0177(6)	0.0164(7)	0.0172(7)	0.0005(5)	-0.0012(5)	0.0066(6)
C8	0.0191(7)	0.0315(10)	0.0270(9)	0.0009(6)	-0.0047(6)	0.0119(8)
C9	0.0333(9)	0.0275(9)	0.0218(8)	-0.0048(7)	0.0046(7)	0.0114(7)
C10	0.0190(7)	0.0331(10)	0.0215(8)	-0.0027(6)	-0.0032(6)	0.0125(7)
C11	0.0263(8)	0.0141(7)	0.0159(7)	-0.0004(6)	-0.0015(6)	0.0051(6)
C12	0.0211(7)	0.0147(7)	0.0181(7)	-0.0012(5)	0.0003(5)	0.0070(6)
C13	0.0265(8)	0.0166(7)	0.0247(8)	0.0034(6)	0.0034(6)	0.0113(6)
C14	0.0309(9)	0.0235(8)	0.0235(8)	0.0062(7)	0.0058(7)	0.0154(7)
C15	0.0316(9)	0.0247(8)	0.0187(8)	0.0044(7)	0.0036(6)	0.0129(7)
C16	0.0221(7)	0.0196(7)	0.0156(7)	0.0009(6)	0.0009(5)	0.0080(6)
C17	0.0301(8)	0.0195(8)	0.0152(7)	0.0025(6)	0.0011(6)	0.0063(6)
C18	0.0180(6)	0.0167(7)	0.0135(6)	0.0004(5)	-0.0002(5)	0.0042(5)
C19	0.0172(6)	0.0183(7)	0.0211(7)	0.0014(5)	0.0015(5)	0.0053(6)
C20	0.0227(7)	0.0177(7)	0.0263(8)	0.0042(6)	-0.0001(6)	0.0062(6)
C21	0.0263(8)	0.0188(8)	0.0219(8)	-0.0016(6)	-0.0032(6)	0.0088(6)
C22	0.0178(7)	0.0241(8)	0.0209(8)	-0.0037(6)	-0.0025(6)	0.0084(6)
C23	0.0162(6)	0.0223(8)	0.0177(7)	0.0018(5)	-0.0008(5)	0.0055(6)
C24	0.0181(7)	0.0254(9)	0.0353(10)	0.0013(6)	0.0054(7)	0.0065(8)
C25	0.0365(10)	0.0196(8)	0.0357(11)	-0.0061(7)	-0.0079(8)	0.0105(8)
C26	0.0189(7)	0.0306(10)	0.0309(10)	0.0054(7)	-0.0014(7)	0.0026(8)
P1	0.01495(16)	0.01500(18)	0.01645(18)	0.00043(13)	0.00121(13)	0.00465(14)
O2	0.0233(6)	0.0198(6)	0.0201(6)	0.0019(4)	0.0056(4)	0.0026(5)
C27	0.0162(6)	0.0202(7)	0.0145(7)	0.0000(5)	0.0005(5)	0.0044(6)
C28	0.0207(7)	0.0291(9)	0.0220(8)	-0.0031(6)	-0.0012(6)	0.0116(7)
C29	0.0225(8)	0.0392(11)	0.0250(9)	-0.0088(7)	-0.0006(7)	0.0126(8)
C30	0.0157(7)	0.0470(12)	0.0205(8)	0.0002(7)	0.0005(6)	0.0062(8)
C31	0.0217(8)	0.0343(10)	0.0251(9)	0.0094(7)	0.0002(6)	0.0051(8)
C32	0.0201(7)	0.0214(8)	0.0251(8)	0.0031(6)	0.0004(6)	0.0057(7)
C33	0.0156(6)	0.0171(7)	0.0212(7)	0.0000(5)	-0.0001(5)	0.0082(6)
C34	0.0239(8)	0.0280(9)	0.0306(9)	0.0088(7)	0.0047(7)	0.0145(8)
C35	0.0306(10)	0.0409(12)	0.0439(12)	0.0125(9)	0.0000(9)	0.0250(10)
C36	0.0327(10)	0.0358(11)	0.0321(10)	-0.0037(8)	-0.0077(8)	0.0216(9)
C37	0.0397(10)	0.0237(9)	0.0222(9)	-0.0014(8)	0.0008(7)	0.0104(7)

C38	0.0314(9)	0.0189(8)	0.0232(8)	0.0043(6)	0.0031(7)	0.0090(7)
C39	0.0164(6)	0.0168(7)	0.0210(7)	-0.0003(5)	0.0017(5)	0.0058(6)
C40	0.0338(9)	0.0194(8)	0.0259(9)	-0.0019(7)	0.0055(7)	0.0129(7)
C41	0.0383(11)	0.0260(9)	0.0320(10)	-0.0066(8)	-0.0018(8)	0.0165(8)
C42	0.0354(10)	0.0193(8)	0.0353(11)	-0.0055(7)	0.0042(8)	0.0081(8)
C43	0.0357(10)	0.0234(9)	0.0254(9)	-0.0101(7)	0.0006(7)	0.0025(7)
C44	0.0275(8)	0.0212(8)	0.0183(8)	-0.0040(6)	0.0003(6)	0.0043(6)

***Table S4*. Bond Lengths for Re(O)Me(DAP).OPPh$_3$, 1**

Re1-O1	1.6926(12)	C20-H20	0.9500
Re1-N3	1.9718(14)	C21-C22	1.391(3)
Re1-N1	1.9774(14)	C21-C25	1.506(3)
Re1-N2	2.0648(13)	C22-C23	1.394(2)
Re1-C1	2.1278(17)	C22-H22	0.9500
C1-H1A	0.9800	C23-C26	1.506(2)
C1-H1B	0.9800	C24-H24A	0.9800
C1-H1C	0.9800	C24-H24B	0.9800
N1-C2	1.428(2)	C24-H24C	0.9800
N1-C11	1.472(2)	C25-H25A	0.9800
N2-C12	1.349(2)	C25-H25B	0.9800
N2-C16	1.352(2)	C25-H25C	0.9800
N3-C18	1.430(2)	C26-H26A	0.9800
N3-C17	1.472(2)	C26-H26B	0.9800
C2-C3	1.404(2)	C26-H26C	0.9800
C2-C7	1.409(2)	P1-O2	1.4895(13)
C3-C4	1.394(2)	P1-C27	1.8053(16)
C3-C8	1.508(2)	P1-C33	1.8063(17)
C4-C5	1.394(2)	P1-C39	1.8097(17)
C4-H4	0.9500	C27-C32	1.393(2)
C5-C6	1.390(2)	C27-C28	1.398(3)
C5-C9	1.507(2)	C28-C29	1.391(3)
C6-C7	1.391(2)	C28-H28	0.9500
C6-H6	0.9500	C29-C30	1.392(3)
C7-C10	1.507(2)	C29-H29	0.9500
C8-H8A	0.9800	C30-C31	1.381(3)
C8-H8B	0.9800	C30-H30	0.9500
C8-H8C	0.9800	C31-C32	1.398(3)
C9-H9A	0.9800	C31-H31	0.9500
C9-H9B	0.9800	C32-H32	0.9500
C9-H9C	0.9800	C33-C38	1.390(2)
C10-H10A	0.9800	C33-C34	1.392(2)
C10-H10B	0.9800	C34-C35	1.392(3)
C10-H10C	0.9800	C34-H34	0.9500
C11-C12	1.499(2)	C35-C36	1.386(3)
C11-H11A	0.9900	C35-H35	0.9500
C11-H11B	0.9900	C36-C37	1.389(3)
C12-C13	1.387(2)	C36-H36	0.9500
C13-C14	1.390(3)	C37-C38	1.391(3)
C13-H13	0.9500	C37-H37	0.9500
C14-C15	1.385(3)	C38-H38	0.9500
C14-H14	0.9500	C39-C40	1.383(2)
C15-C16	1.382(2)	C39-C44	1.399(2)
C15-H15	0.9500	C40-C41	1.375(3)
C16-C17	1.500(2)	C40-H40	0.9500

C17-H17A	0.9900	C41-C42	1.379(3)
C17-H17B	0.9900	C41-H41	0.9500
C18-C19	1.399(2)	C42-C43	1.393(3)
C18-C23	1.404(2)	C42-H42	0.9500
C19-C20	1.393(2)	C43-C44	1.391(3)
C19-C24	1.508(2)	C43-H43	0.9500
C20-C21	1.395(3)	C44-H44	0.9500

***Table S5*. Bond Angles for Re(O)Me(DAP)·OPPh$_3$, 1**

O1-Re1-N3	111.76(6)	C20-C19-C24	120.37(15)
O1-Re1-N1	111.41(6)	C18-C19-C24	120.61(15)
N3-Re1-N1	135.88(6)	C19-C20-C21	122.06(16)
O1-Re1-N2	117.59(6)	C19-C20-H20	119.0
N3-Re1-N2	76.29(5)	C21-C20-H20	119.0
N1-Re1-N2	76.23(5)	C22-C21-C20	117.71(16)
O1-Re1-C1	104.61(6)	C22-C21-C25	121.49(17)
N3-Re1-C1	89.37(6)	C20-C21-C25	120.80(17)
N1-Re1-C1	88.41(6)	C21-C22-C23	122.07(15)
N2-Re1-C1	137.79(6)	C21-C22-H22	119.0
Re1-C1-H1A	109.5	C23-C22-H22	119.0
Re1-C1-H1B	109.5	C22-C23-C18	118.94(15)
H1A-C1-H1B	109.5	C22-C23-C26	120.66(15)
Re1-C1-H1C	109.5	C18-C23-C26	120.40(16)
H1A-C1-H1C	109.5	C19-C24-H24A	109.5
H1B-C1-H1C	109.5	C19-C24-H24B	109.5
C2-N1-C11	113.53(13)	H24A-C24-H24B	109.5
C2-N1-Re1	128.88(10)	C19-C24-H24C	109.5
C11-N1-Re1	117.54(10)	H24A-C24-H24C	109.5
C12-N2-C16	122.17(14)	H24B-C24-H24C	109.5
C12-N2-Re1	118.92(11)	C21-C25-H25A	109.5
C16-N2-Re1	118.88(11)	C21-C25-H25B	109.5
C18-N3-C17	112.83(13)	H25A-C25-H25B	109.5
C18-N3-Re1	129.78(11)	C21-C25-H25C	109.5
C17-N3-Re1	117.38(11)	H25A-C25-H25C	109.5
C3-C2-C7	119.65(15)	H25B-C25-H25C	109.5
C3-C2-N1	121.06(13)	C23-C26-H26A	109.5
C7-C2-N1	119.29(14)	C23-C26-H26B	109.5
C4-C3-C2	119.37(14)	H26A-C26-H26B	109.5
C4-C3-C8	119.99(15)	C23-C26-H26C	109.5
C2-C3-C8	120.62(15)	H26A-C26-H26C	109.5
C5-C4-C3	121.84(16)	H26B-C26-H26C	109.5
C5-C4-H4	119.1	O2-P1-C27	111.95(7)
C3-C4-H4	119.1	O2-P1-C33	111.84(8)
C6-C5-C4	117.72(16)	C27-P1-C33	104.60(8)
C6-C5-C9	120.40(15)	O2-P1-C39	111.72(8)
C4-C5-C9	121.87(16)	C27-P1-C39	108.96(8)
C5-C6-C7	122.42(15)	C33-P1-C39	107.43(8)
C5-C6-H6	118.8	C32-C27-C28	119.27(16)
C7-C6-H6	118.8	C32-C27-P1	124.30(14)
C6-C7-C2	118.92(15)	C28-C27-P1	116.27(13)
C6-C7-C10	120.81(14)	C29-C28-C27	120.20(18)
C2-C7-C10	120.27(15)	C29-C28-H28	119.9
C3-C8-H8A	109.5	C27-C28-H28	119.9
C3-C8-H8B	109.5	C28-C29-C30	120.12(19)
H8A-C8-H8B	109.5	C28-C29-H29	119.9

C3-C8-H8C	109.5	C30-C29-H29	119.9
H8A-C8-H8C	109.5	C31-C30-C29	120.04(17)
H8B-C8-H8C	109.5	C31-C30-H30	120.0
C5-C9-H9A	109.5	C29-C30-H30	120.0
C5-C9-H9B	109.5	C30-C31-C32	120.14(18)
H9A-C9-H9B	109.5	C30-C31-H31	119.9
C5-C9-H9C	109.5	C32-C31-H31	119.9
H9A-C9-H9C	109.5	C27-C32-C31	120.24(18)
H9B-C9-H9C	109.5	C27-C32-H32	119.9
C7-C10-H10A	109.5	C31-C32-H32	119.9
C7-C10-H10B	109.5	C38-C33-C34	119.48(16)
H10A-C10-H10B	109.5	C38-C33-P1	123.30(13)
C7-C10-H10C	109.5	C34-C33-P1	117.19(14)
H10A-C10-H10C	109.5	C33-C34-C35	120.09(19)
H10B-C10-H10C	109.5	C33-C34-H34	120.0
N1-C11-C12	108.51(13)	C35-C34-H34	120.0
N1-C11-H11A	110.0	C36-C35-C34	120.09(19)
C12-C11-H11A	110.0	C36-C35-H35	120.0
N1-C11-H11B	110.0	C34-C35-H35	120.0
C12-C11-H11B	110.0	C35-C36-C37	120.03(18)
H11A-C11-H11B	108.4	C35-C36-H36	120.0
N2-C12-C13	120.15(15)	C37-C36-H36	120.0
N2-C12-C11	112.47(14)	C36-C37-C38	119.81(19)
C13-C12-C11	127.31(15)	C36-C37-H37	120.1
C12-C13-C14	118.16(16)	C38-C37-H37	120.1
C12-C13-H13	120.9	C33-C38-C37	120.44(17)
C14-C13-H13	120.9	C33-C38-H38	119.8
C15-C14-C13	120.83(16)	C37-C38-H38	119.8
C15-C14-H14	119.6	C40-C39-C44	118.33(16)
C13-C14-H14	119.6	C40-C39-P1	117.91(13)
C16-C15-C14	118.97(16)	C44-C39-P1	123.53(13)
C16-C15-H15	120.5	C41-C40-C39	122.27(19)
C14-C15-H15	120.5	C41-C40-H40	118.9
N2-C16-C15	119.57(16)	C39-C40-H40	118.9
N2-C16-C17	112.02(14)	C40-C41-C42	119.39(19)
C15-C16-C17	128.33(15)	C40-C41-H41	120.3
N3-C17-C16	108.78(13)	C42-C41-H41	120.3
N3-C17-H17A	109.9	C41-C42-C43	119.82(18)
C16-C17-H17A	109.9	C41-C42-H42	120.1
N3-C17-H17B	109.9	C43-C42-H42	120.1
C16-C17-H17B	109.9	C44-C43-C42	120.37(18)
H17A-C17-H17B	108.3	C44-C43-H43	119.8
C19-C18-C23	120.18(15)	C42-C43-H43	119.8
C19-C18-N3	119.91(14)	C43-C44-C39	119.78(17)
C23-C18-N3	119.91(14)	C43-C44-H44	120.1
C20-C19-C18	119.01(15)	C39-C44-H44	120.1

***Table S6*. Torsion Angles for Re(O)Me(DAP).$OPPh_3$, 1**

O1-Re1-N1-C2	-85.81(14)	N2-C16-C17-N3	9.3(2)
N3-Re1-N1-C2	106.71(13)	C15-C16-C17-N3	-167.33(18)
N2-Re1-N1-C2	159.60(14)	C17-N3-C18-C19	95.94(18)
C1-Re1-N1-C2	19.27(13)	Re1-N3-C18-C19	-82.69(19)
O1-Re1-N1-C11	91.24(12)	C17-N3-C18-C23	-84.80(19)
N3-Re1-N1-C11	-76.23(14)	Re1-N3-C18-C23	96.57(17)
N2-Re1-N1-C11	-23.35(11)	C23-C18-C19-C20	0.3(3)
C1-Re1-N1-C11	-163.68(12)	N3-C18-C19-C20	179.57(15)
O1-Re1-N2-C12	-89.27(13)	C23-C18-C19-C24	179.97(16)
N3-Re1-N2-C12	163.09(13)	N3-C18-C19-C24	-0.8(2)
N1-Re1-N2-C12	17.94(12)	C18-C19-C20-C21	-1.5(3)
C1-Re1-N2-C12	89.71(15)	C24-C19-C20-C21	178.88(17)
O1-Re1-N2-C16	88.93(13)	C19-C20-C21-C22	0.9(3)
N3-Re1-N2-C16	-18.70(12)	C19-C20-C21-C25	-178.58(18)
N1-Re1-N2-C16	-163.85(14)	C20-C21-C22-C23	0.9(3)
C1-Re1-N2-C16	-92.08(15)	C25-C21-C22-C23	-179.69(17)
O1-Re1-N3-C18	87.89(14)	C21-C22-C23-C18	-2.0(3)
N1-Re1-N3-C18	-104.66(14)	C21-C22-C23-C26	178.12(17)
N2-Re1-N3-C18	-157.53(15)	C19-C18-C23-C22	1.3(2)
C1-Re1-N3-C18	-17.61(14)	N3-C18-C23-C22	-177.91(15)
O1-Re1-N3-C17	-90.68(13)	C19-C18-C23-C26	-178.73(16)
N1-Re1-N3-C17	76.76(15)	N3-C18-C23-C26	2.0(2)
N2-Re1-N3-C17	23.89(12)	O2-P1-C27-C32	107.73(15)
C1-Re1-N3-C17	163.82(13)	C33-P1-C27-C32	-130.98(15)
C11-N1-C2-C3	78.35(19)	C39-P1-C27-C32	-16.36(17)
Re1-N1-C2-C3	-104.50(16)	O2-P1-C27-C28	-67.63(15)
C11-N1-C2-C7	-102.58(17)	C33-P1-C27-C28	53.66(15)
Re1-N1-C2-C7	74.57(18)	C39-P1-C27-C28	168.29(13)
C7-C2-C3-C4	-3.3(2)	C32-C27-C28-C29	0.6(3)
N1-C2-C3-C4	175.81(15)	P1-C27-C28-C29	176.21(14)
C7-C2-C3-C8	178.39(16)	C27-C28-C29-C30	-0.3(3)
N1-C2-C3-C8	-2.5(2)	C28-C29-C30-C31	0.0(3)
C2-C3-C4-C5	1.7(3)	C29-C30-C31-C32	-0.1(3)
C8-C3-C4-C5	-179.96(17)	C28-C27-C32-C31	-0.7(3)
C3-C4-C5-C6	1.0(3)	P1-C27-C32-C31	-175.94(14)
C3-C4-C5-C9	-177.45(17)	C30-C31-C32-C27	0.5(3)
C4-C5-C6-C7	-2.2(3)	O2-P1-C33-C38	172.17(14)
C9-C5-C6-C7	176.32(16)	C27-P1-C33-C38	50.80(17)
C5-C6-C7-C2	0.6(3)	C39-P1-C33-C38	-64.90(16)
C5-C6-C7-C10	-178.48(17)	O2-P1-C33-C34	-5.82(16)
C3-C2-C7-C6	2.2(2)	C27-P1-C33-C34	-127.19(14)
N1-C2-C7-C6	-176.93(15)	C39-P1-C33-C34	117.11(14)
C3-C2-C7-C10	-178.77(16)	C38-C33-C34-C35	1.2(3)
N1-C2-C7-C10	2.1(2)	P1-C33-C34-C35	179.25(16)
C2-N1-C11-C12	-157.27(13)	C33-C34-C35-C36	1.3(3)

Re1-N1-C11-C12	25.23(17)	C34-C35-C36-C37	-2.6(3)
C16-N2-C12-C13	-4.3(3)	C35-C36-C37-C38	1.3(3)
Re1-N2-C12-C13	173.82(13)	C34-C33-C38-C37	-2.4(3)
C16-N2-C12-C11	172.91(15)	P1-C33-C38-C37	179.62(15)
Re1-N2-C12-C11	-8.94(19)	C36-C37-C38-C33	1.2(3)
N1-C11-C12-N2	-9.5(2)	O2-P1-C39-C40	-51.45(16)
N1-C11-C12-C13	167.50(17)	C27-P1-C39-C40	72.77(16)
N2-C12-C13-C14	1.4(3)	C33-P1-C39-C40	-174.46(14)
C11-C12-C13-C14	-175.43(17)	O2-P1-C39-C44	122.93(15)
C12-C13-C14-C15	1.1(3)	C27-P1-C39-C44	-112.86(15)
C13-C14-C15-C16	-0.7(3)	C33-P1-C39-C44	-0.08(17)
C12-N2-C16-C15	4.7(3)	C44-C39-C40-C41	2.4(3)
Re1-N2-C16-C15	-173.42(13)	P1-C39-C40-C41	177.05(16)
C12-N2-C16-C17	-172.22(15)	C39-C40-C41-C42	-1.6(3)
Re1-N2-C16-C17	9.64(19)	C40-C41-C42-C43	-0.3(3)
C14-C15-C16-N2	-2.2(3)	C41-C42-C43-C44	1.4(3)
C14-C15-C16-C17	174.22(18)	C42-C43-C44-C39	-0.6(3)
C18-N3-C17-C16	155.55(14)	C40-C39-C44-C43	-1.2(3)
Re1-N3-C17-C16	-25.64(18)	P1-C39-C44-C43	-175.60(15)

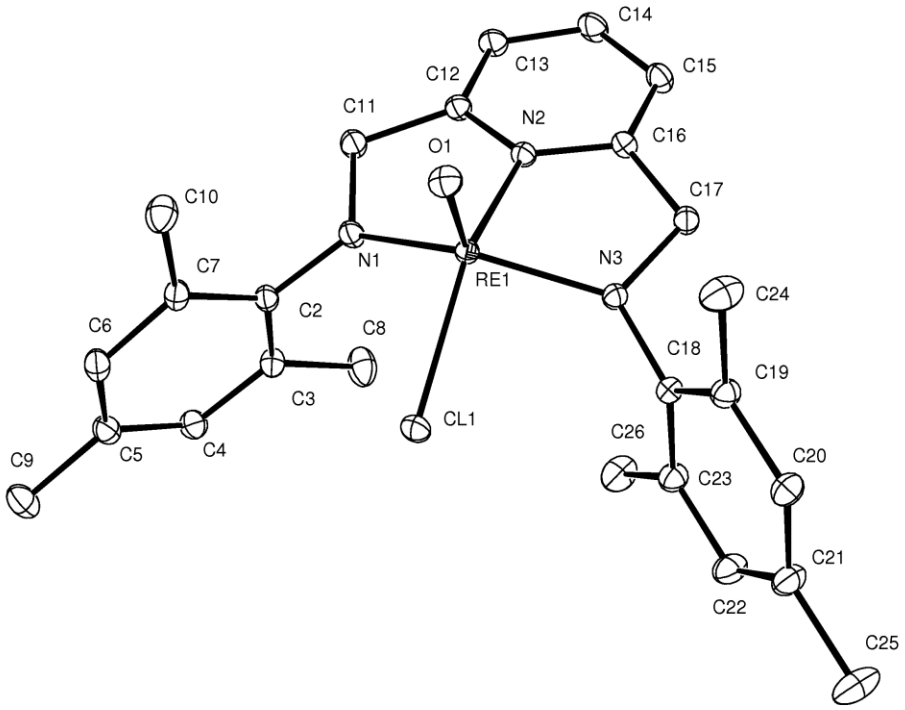

Figure S4. ORTEP drawing of **Re(O)Cl(DAP), 2** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

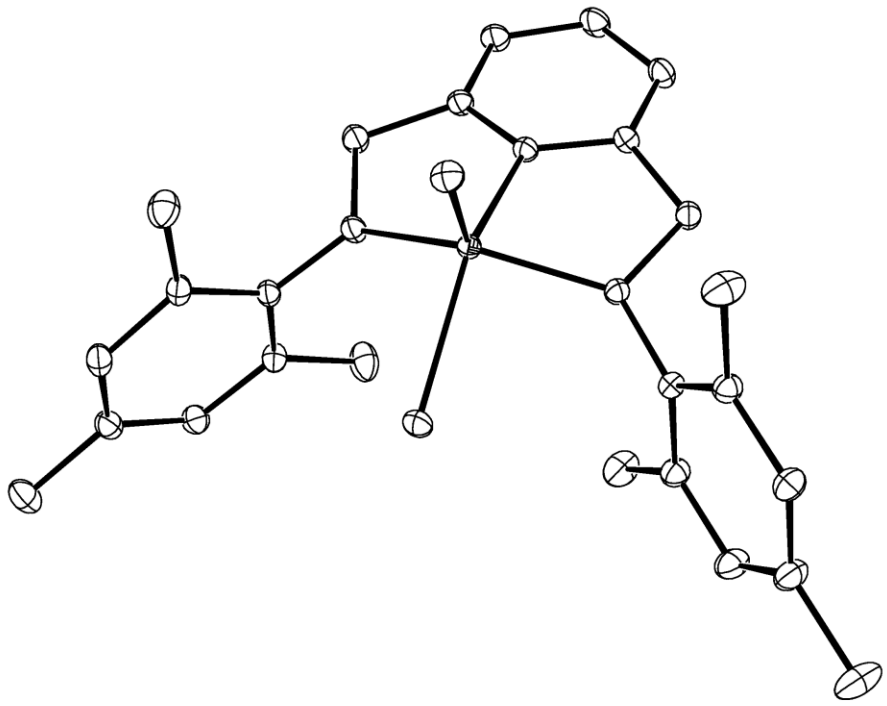

Figure S5. ORTEP drawing of **Re(O)Cl(DAP), 2**. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

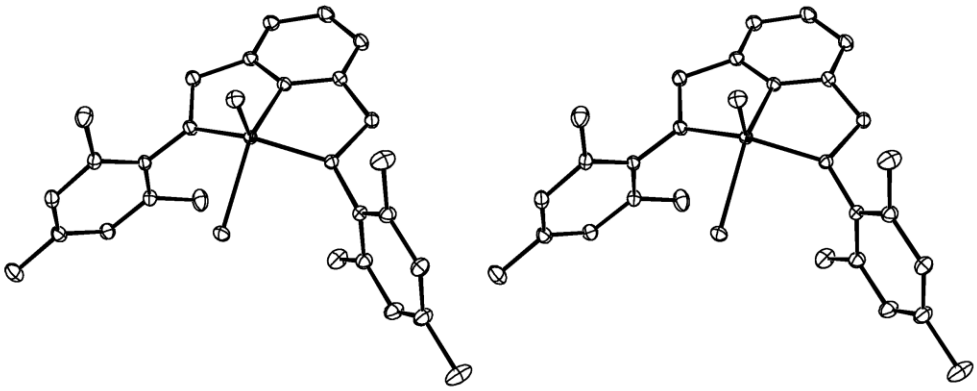

Figure S6. Stereoscopic ORTEP drawing of **Re(O)Cl(DAP), 2**. Ellipsoids are at the 50% probability level and hydrogen atoms were omitted for clarity.

***Table S7*. Summary of Crystal Data for Re(O)Cl(DAP), 2**

Formula	$C_{25.50}H_{30}Cl_2N_3ORe$
Formula Weight (*g/mol*)	651.62
Crystal Dimensions (*mm*)	0.37 × 0.16 × 0.10
Crystal Color and Habit	green prism
Crystal System	triclinic
Space Group	P -1
Temperature, K	110
a, Å	9.6153(5)
b, Å	11.9246(6)
c, Å	12.6634(6)
α,°	63.761(2)
β,°	73.053(2)
γ,°	81.327(2)
V, Å^3	1245.39(11)
Number of reflections to determine final unit cell	9996
Min and Max 2θ for cell determination, °	6.46, 82.94
Z	2
F(000)	642
ρ (*g/cm*)	1.738
λ, Å, (MoKα)	0.71073
μ, (*cm*$^{-1}$)	5.116
Diffractometer Type	Bruker-Nonius Kappa Axis X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	85.6
Measured fraction of data	0.990
Number of reflections measured	76499
Unique reflections measured	16306
R_{merge}	0.0316
Number of reflections included in refinement	16306
Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc $w=1/[sigma^2(Fo^2)+(0.0302P)^2+0.0000P]$ where $P=(Fo^2+2Fc^2)/3$
Number of parameters in least-squares	305
R_1	0.0255
wR_2	0.0555
R_1 (all data)	0.0311
wR_2 (all data)	0.0569
GOF	1.087
Maximum shift/error	0.006
Min & Max peak heights on final ΔF Map (*e*$^-$/Å)	-0.774, 2.558

Where:

$R_1 = \Sigma(|F_o| - |F_c|) / \Sigma F_o$

$wR_2 = [\ \Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(w F_o^4)\ ]^{½}$

$GOF = [\ \Sigma(w(F_o^2 - F_c^2)^2) / (\text{No. of reflns. - No. of params. })\ ]^{½}$

***Table S8*. Atomic Coordinates for Re(O)Cl(DAP), 2**

Atom	x	y	z	$U_{iso/equiv}$
Re1	0.889966(5)	0.629989(5)	0.621741(4)	0.00991(1)
Cl1	0.65311(3)	0.70595(3)	0.67505(3)	0.01520(5)
O1	0.87387(12)	0.49047(10)	0.62246(10)	0.01591(18)
N1	0.92263(12)	0.60743(12)	0.77678(10)	0.01315(19)
N2	1.10527(12)	0.66670(11)	0.57567(10)	0.01149(17)
N3	0.91788(12)	0.76431(11)	0.45584(10)	0.01184(18)
C2	0.82038(14)	0.61216(13)	0.88249(11)	0.0124(2)
C3	0.80340(16)	0.72227(14)	0.90014(12)	0.0145(2)
C4	0.69936(16)	0.72677(15)	1.00161(13)	0.0162(2)
C5	0.60952(15)	0.62689(15)	1.08336(12)	0.0155(2)
C6	0.62953(16)	0.51825(15)	1.06437(12)	0.0155(2)
C7	0.73667(15)	0.50790(14)	0.96692(12)	0.0139(2)
C8	0.8898(2)	0.83578(16)	0.80850(15)	0.0231(3)
C9	0.49360(18)	0.63586(18)	1.18974(14)	0.0213(3)
C10	0.76210(19)	0.38595(15)	0.95539(14)	0.0200(3)
C11	1.07302(15)	0.57973(15)	0.78957(12)	0.0154(2)
C12	1.17505(14)	0.62830(13)	0.66480(12)	0.0130(2)
C13	1.32329(15)	0.64440(15)	0.63505(13)	0.0159(2)
C14	1.39649(16)	0.70388(16)	0.51194(14)	0.0180(2)
C15	1.32016(15)	0.74892(15)	0.42255(13)	0.0158(2)
C16	1.17180(14)	0.73114(13)	0.45724(12)	0.0124(2)
C17	1.06797(15)	0.78474(14)	0.37818(12)	0.0133(2)
C18	0.81391(14)	0.83893(13)	0.39018(11)	0.0120(2)
C19	0.76657(15)	0.79748(14)	0.31825(12)	0.0139(2)
C20	0.67026(16)	0.87276(14)	0.25022(13)	0.0162(2)
C21	0.61580(17)	0.98699(15)	0.25323(14)	0.0181(2)
C22	0.66289(17)	1.02561(15)	0.32599(14)	0.0182(2)
C23	0.76190(16)	0.95401(14)	0.39358(13)	0.0148(2)
C24	0.81724(19)	0.67283(16)	0.31545(16)	0.0211(3)
C25	0.5105(2)	1.06644(18)	0.17955(18)	0.0281(4)
C26	0.80958(15)	1.00045(8)	0.47037(8)	0.0215(3)
C1Y	1.03012(11)	0.95389(8)	0.96843(7)	0.0373(9)
Cl1Y	1.15888(10)	0.91927(9)	1.05647(8)	0.0410(3)
Cl2Y	0.92713(10)	1.08697(11)	0.96096(8)	0.0617(4)
H4	0.6897	0.8001	1.0152	0.019
H6	0.5687	0.4494	1.1192	0.019
H8A	0.8581	0.9052	0.8323	0.035
H8B	0.8742	0.8592	0.7282	0.035
H8C	0.9933	0.8170	0.8052	0.035
H9A	0.5396	0.6340	1.2501	0.032
H9B	0.4286	0.5651	1.2269	0.032
H9C	0.4374	0.7143	1.1611	0.032
H10A	0.6815	0.3303	1.0111	0.030
H10B	0.8535	0.3467	0.9760	0.030

H10C	0.7679	0.4012	0.8716	0.030
H11A	1.0885	0.4884	0.8328	0.018
H11B	1.0913	0.6204	0.8374	0.018
H13	1.3742	0.6158	0.6967	0.019
H14	1.4987	0.7135	0.4894	0.022
H15	1.3690	0.7912	0.3391	0.019
H17A	1.0838	0.8754	0.3285	0.016
H17B	1.0843	0.7438	0.3224	0.016
H20	0.6406	0.8456	0.2002	0.019
H22	0.6266	1.1028	0.3297	0.022
H24A	0.7766	0.6615	0.2583	0.032
H24B	0.7844	0.6059	0.3970	0.032
H24C	0.9237	0.6699	0.2892	0.032
H25A	0.4391	1.0128	0.1841	0.042
H25B	0.5637	1.1115	0.0945	0.042
H25C	0.4602	1.1267	0.2121	0.042
H26A	0.8151	1.0918	0.4296	0.032
H26B	0.9055	0.9639	0.4815	0.032
H26C	0.7392	0.9758	0.5499	0.032
H1Y1	1.0826	0.9644	0.8849	0.045
H1Y2	0.9648	0.8824	1.0046	0.045

***Table S9*. Anisotropic Displacement Parameters for Re(O)Cl(DAP), 2**

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
Re1	0.00896(2)	0.01063(2)	0.00983(2)	-0.00064(1)	-0.00252(2)	-0.00382(2)
Cl1	0.00981(11)	0.01916(14)	0.01492(12)	0.00060(10)	-0.00229(10)	-0.00648(11)
O1	0.0158(4)	0.0136(4)	0.0185(4)	-0.0014(3)	-0.0045(4)	-0.0065(4)
N1	0.0105(4)	0.0179(5)	0.0110(4)	-0.0001(4)	-0.0028(4)	-0.0062(4)
N2	0.0106(4)	0.0122(4)	0.0114(4)	-0.0002(3)	-0.0025(4)	-0.0049(4)
N3	0.0104(4)	0.0130(5)	0.0107(4)	-0.0002(3)	-0.0029(4)	-0.0036(4)
C2	0.0112(5)	0.0149(5)	0.0098(4)	-0.0007(4)	-0.0023(4)	-0.0043(4)
C3	0.0164(5)	0.0140(5)	0.0117(5)	-0.0016(4)	-0.0028(4)	-0.0044(4)
C4	0.0172(6)	0.0177(6)	0.0141(5)	0.0008(5)	-0.0037(5)	-0.0075(5)
C5	0.0130(5)	0.0211(6)	0.0127(5)	0.0003(5)	-0.0036(4)	-0.0074(5)
C6	0.0144(5)	0.0186(6)	0.0113(5)	-0.0034(5)	-0.0025(4)	-0.0039(4)
C7	0.0139(5)	0.0153(6)	0.0109(4)	-0.0025(4)	-0.0033(4)	-0.0034(4)
C8	0.0299(8)	0.0178(7)	0.0185(6)	-0.0081(6)	0.0005(6)	-0.0067(5)
C9	0.0168(6)	0.0299(8)	0.0177(6)	-0.0010(6)	-0.0009(5)	-0.0126(6)
C10	0.0263(7)	0.0155(6)	0.0172(6)	-0.0027(5)	-0.0042(6)	-0.0061(5)
C11	0.0123(5)	0.0202(6)	0.0125(5)	0.0001(4)	-0.0037(4)	-0.0056(5)
C12	0.0113(5)	0.0151(5)	0.0132(5)	0.0004(4)	-0.0038(4)	-0.0061(4)
C13	0.0112(5)	0.0204(6)	0.0163(5)	0.0010(4)	-0.0048(4)	-0.0075(5)
C14	0.0105(5)	0.0244(7)	0.0182(6)	-0.0006(5)	-0.0020(5)	-0.0093(5)
C15	0.0119(5)	0.0209(6)	0.0137(5)	-0.0016(5)	-0.0011(4)	-0.0074(5)
C16	0.0121(5)	0.0136(5)	0.0118(4)	-0.0007(4)	-0.0021(4)	-0.0062(4)
C17	0.0125(5)	0.0150(5)	0.0109(4)	-0.0009(4)	-0.0026(4)	-0.0041(4)
C18	0.0122(5)	0.0120(5)	0.0112(4)	0.0006(4)	-0.0037(4)	-0.0042(4)
C19	0.0143(5)	0.0144(5)	0.0140(5)	0.0007(4)	-0.0050(4)	-0.0064(4)
C20	0.0171(6)	0.0169(6)	0.0159(5)	0.0002(5)	-0.0076(5)	-0.0061(5)
C21	0.0176(6)	0.0179(6)	0.0179(6)	0.0029(5)	-0.0088(5)	-0.0050(5)
C22	0.0206(6)	0.0144(6)	0.0201(6)	0.0039(5)	-0.0084(5)	-0.0072(5)
C23	0.0169(5)	0.0136(5)	0.0151(5)	0.0010(4)	-0.0053(5)	-0.0067(4)
C24	0.0268(7)	0.0177(6)	0.0271(7)	0.0051(6)	-0.0145(6)	-0.0137(6)
C25	0.0310(9)	0.0234(8)	0.0327(8)	0.0088(7)	-0.0219(8)	-0.0088(7)
C26	0.0294(8)	0.0176(7)	0.0229(6)	0.0015(6)	-0.0119(6)	-0.0106(6)
C1Y	0.045(2)	0.036(2)	0.0294(18)	-0.0088(19)	-0.0017(18)	-0.0153(17)
Cl1Y	0.0667(8)	0.0342(5)	0.0218(4)	-0.0014(6)	-0.0126(5)	-0.0107(4)
Cl2Y	0.0605(9)	0.0593(9)	0.0367(6)	0.0176(8)	0.0029(7)	-0.0103(6)

***Table S10*. Bond Lengths for Re(O)Cl(DAP), 2**

Re1-O1	1.6898(11)	C12-C13	1.3842(19)
Re1-N3	1.9690(11)	C13-C14	1.401(2)
Re1-N1	1.9730(11)	C13-H13	0.9500
Re1-N2	2.0399(11)	C14-C15	1.392(2)
Re1-Cl1	2.3420(3)	C14-H14	0.9500
N1-C2	1.4299(17)	C15-C16	1.3843(19)
N1-C11	1.4736(18)	C15-H15	0.9500
N2-C16	1.3486(17)	C16-C17	1.4940(19)
N2-C12	1.3512(17)	C17-H17A	0.9900
N3-C18	1.4299(17)	C17-H17B	0.9900
N3-C17	1.4751(17)	C18-C23	1.403(2)
C2-C7	1.4005(19)	C18-C19	1.4102(18)
C2-C3	1.405(2)	C19-C20	1.391(2)
C3-C4	1.396(2)	C19-C24	1.505(2)
C3-C8	1.502(2)	C20-C21	1.396(2)
C4-C5	1.391(2)	C20-H20	0.9500
C4-H4	0.9500	C21-C22	1.396(2)
C5-C6	1.395(2)	C21-C25	1.508(2)
C5-C9	1.511(2)	C22-C23	1.397(2)
C6-C7	1.398(2)	C22-H22	0.9500
C6-H6	0.9500	C23-C26	1.5083(16)
C7-C10	1.502(2)	C24-H24A	0.9800
C8-H8A	0.9800	C24-H24B	0.9800
C8-H8B	0.9800	C24-H24C	0.9800
C8-H8C	0.9800	C25-H25A	0.9800
C9-H9A	0.9800	C25-H25B	0.9800
C9-H9B	0.9800	C25-H25C	0.9800
C9-H9C	0.9800	C26-H26A	0.9800
C10-H10A	0.9800	C26-H26B	0.9800
C10-H10B	0.9800	C26-H26C	0.9800
C10-H10C	0.9800	C1Y-Cl2Y	1.7192
C11-C12	1.5010(19)	C1Y-Cl1Y	1.7861
C11-H11A	0.9900	C1Y-H1Y1	0.9900
C11-H11B	0.9900	C1Y-H1Y2	0.9900

***Table S11*. Bond Angles for Re(O)Cl(DAP), 2**

O1-Re1-N3	110.83(5)	N2-C12-C11	112.52(11)
O1-Re1-N1	110.89(5)	C13-C12-C11	127.44(12)
N3-Re1-N1	136.22(5)	C12-C13-C14	118.47(13)
O1-Re1-N2	108.98(5)	C12-C13-H13	120.8
N3-Re1-N2	77.53(5)	C14-C13-H13	120.8
N1-Re1-N2	77.01(5)	C15-C14-C13	120.31(13)
O1-Re1-Cl1	106.56(4)	C15-C14-H14	119.8
N3-Re1-Cl1	90.10(4)	C13-C14-H14	119.8
N1-Re1-Cl1	90.42(4)	C16-C15-C14	118.90(13)
N2-Re1-Cl1	144.47(3)	C16-C15-H15	120.6
C2-N1-C11	113.37(11)	C14-C15-H15	120.6
C2-N1-Re1	129.55(9)	N2-C16-C15	119.69(12)
C11-N1-Re1	117.07(8)	N2-C16-C17	112.95(11)
C16-N2-C12	122.45(12)	C15-C16-C17	127.17(12)
C16-N2-Re1	118.57(9)	N3-C17-C16	109.04(10)
C12-N2-Re1	118.97(9)	N3-C17-H17A	109.9
C18-N3-C17	112.03(10)	C16-C17-H17A	109.9
C18-N3-Re1	130.55(9)	N3-C17-H17B	109.9
C17-N3-Re1	117.00(9)	C16-C17-H17B	109.9
C7-C2-C3	120.41(12)	H17A-C17-H17B	108.3
C7-C2-N1	119.97(13)	C23-C18-C19	119.75(12)
C3-C2-N1	119.61(12)	C23-C18-N3	120.97(12)
C4-C3-C2	118.84(13)	C19-C18-N3	119.25(12)
C4-C3-C8	120.22(14)	C20-C19-C18	119.19(13)
C2-C3-C8	120.86(13)	C20-C19-C24	119.84(13)
C5-C4-C3	121.87(14)	C18-C19-C24	120.97(13)
C5-C4-H4	119.1	C19-C20-C21	122.05(13)
C3-C4-H4	119.1	C19-C20-H20	119.0
C4-C5-C6	118.10(13)	C21-C20-H20	119.0
C4-C5-C9	120.92(14)	C22-C21-C20	117.80(14)
C6-C5-C9	120.98(14)	C22-C21-C25	121.09(15)
C5-C6-C7	121.83(13)	C20-C21-C25	121.10(14)
C5-C6-H6	119.1	C21-C22-C23	121.87(14)
C7-C6-H6	119.1	C21-C22-H22	119.1
C6-C7-C2	118.79(13)	C23-C22-H22	119.1
C6-C7-C10	120.03(13)	C22-C23-C18	119.31(13)
C2-C7-C10	121.18(13)	C22-C23-C26	119.67(12)
C3-C8-H8A	109.5	C18-C23-C26	121.01(12)
C3-C8-H8B	109.5	C19-C24-H24A	109.5
H8A-C8-H8B	109.5	C19-C24-H24B	109.5
C3-C8-H8C	109.5	H24A-C24-H24B	109.5
H8A-C8-H8C	109.5	C19-C24-H24C	109.5
H8B-C8-H8C	109.5	H24A-C24-H24C	109.5
C5-C9-H9A	109.5	H24B-C24-H24C	109.5
C5-C9-H9B	109.5	C21-C25-H25A	109.5
H9A-C9-H9B	109.5	C21-C25-H25B	109.5

C5-C9-H9C	109.5	H25A-C25-H25B	109.5
H9A-C9-H9C	109.5	C21-C25-H25C	109.5
H9B-C9-H9C	109.5	H25A-C25-H25C	109.5
C7-C10-H10A	109.5	H25B-C25-H25C	109.5
C7-C10-H10B	109.5	C23-C26-H26A	109.5
H10A-C10-H10B	109.5	C23-C26-H26B	109.5
C7-C10-H10C	109.5	H26A-C26-H26B	109.5
H10A-C10-H10C	109.5	C23-C26-H26C	109.5
H10B-C10-H10C	109.5	H26A-C26-H26C	109.5
N1-C11-C12	108.49(11)	H26B-C26-H26C	109.5
N1-C11-H11A	110.0	Cl2Y-C1Y-Cl1Y	112.7
C12-C11-H11A	110.0	Cl2Y-C1Y-H1Y1	109.1
N1-C11-H11B	110.0	Cl1Y-C1Y-H1Y1	109.1
C12-C11-H11B	110.0	Cl2Y-C1Y-H1Y2	109.1
H11A-C11-H11B	108.4	Cl1Y-C1Y-H1Y2	109.1
N2-C12-C13	119.87(12)	H1Y1-C1Y-H1Y2	107.8

***Table S12*. Torsion Angles for Re(O)Cl(DAP), 2**

O1-Re1-N1-C2	-96.04(13)	N1-C2-C7-C10	6.1(2)
N3-Re1-N1-C2	102.47(13)	C2-N1-C11-C12	-156.66(12)
N2-Re1-N1-C2	158.35(13)	Re1-N1-C11-C12	24.14(15)
Cl1-Re1-N1-C2	11.89(12)	C16-N2-C12-C13	-6.1(2)
O1-Re1-N1-C11	83.01(11)	Re1-N2-C12-C13	175.45(11)
N3-Re1-N1-C11	-78.49(13)	C16-N2-C12-C11	169.48(13)
N2-Re1-N1-C11	-22.61(10)	Re1-N2-C12-C11	-8.93(16)
Cl1-Re1-N1-C11	-169.06(10)	N1-C11-C12-N2	-9.03(17)
O1-Re1-N2-C16	91.20(11)	N1-C11-C12-C13	166.19(15)
N3-Re1-N2-C16	-16.80(10)	N2-C12-C13-C14	1.7(2)
N1-Re1-N2-C16	-160.89(11)	C11-C12-C13-C14	-173.15(15)
Cl1-Re1-N2-C16	-88.95(11)	C12-C13-C14-C15	2.0(2)
O1-Re1-N2-C12	-90.33(11)	C13-C14-C15-C16	-1.6(2)
N3-Re1-N2-C12	161.67(11)	C12-N2-C16-C15	6.6(2)
N1-Re1-N2-C12	17.58(10)	Re1-N2-C16-C15	-175.02(11)
Cl1-Re1-N2-C12	89.52(12)	C12-N2-C16-C17	-168.89(13)
O1-Re1-N3-C18	86.48(12)	Re1-N2-C16-C17	9.53(15)
N1-Re1-N3-C18	-112.02(12)	C14-C15-C16-N2	-2.6(2)
N2-Re1-N3-C18	-167.72(13)	C14-C15-C16-C17	172.15(14)
Cl1-Re1-N3-C18	-21.31(12)	C18-N3-C17-C16	165.51(11)
O1-Re1-N3-C17	-85.32(10)	Re1-N3-C17-C16	-21.20(14)
N1-Re1-N3-C17	76.19(12)	N2-C16-C17-N3	6.90(16)
N2-Re1-N3-C17	20.48(9)	C15-C16-C17-N3	-168.13(14)
Cl1-Re1-N3-C17	166.89(9)	C17-N3-C18-C23	-96.31(15)
C11-N1-C2-C7	-98.22(15)	Re1-N3-C18-C23	91.58(15)
Re1-N1-C2-C7	80.86(16)	C17-N3-C18-C19	81.82(15)
C11-N1-C2-C3	82.53(16)	Re1-N3-C18-C19	-90.30(15)
Re1-N1-C2-C3	-98.39(15)	C23-C18-C19-C20	0.9(2)
C7-C2-C3-C4	-1.5(2)	N3-C18-C19-C20	-177.21(12)
N1-C2-C3-C4	177.72(13)	C23-C18-C19-C24	-178.30(14)
C7-C2-C3-C8	-178.37(14)	N3-C18-C19-C24	3.5(2)
N1-C2-C3-C8	0.9(2)	C18-C19-C20-C21	-1.7(2)
C2-C3-C4-C5	-1.9(2)	C24-C19-C20-C21	177.57(15)
C8-C3-C4-C5	174.94(15)	C19-C20-C21-C22	1.0(2)
C3-C4-C5-C6	2.5(2)	C19-C20-C21-C25	-179.45(15)
C3-C4-C5-C9	-177.51(14)	C20-C21-C22-C23	0.4(2)
C4-C5-C6-C7	0.3(2)	C25-C21-C22-C23	-179.13(16)
C9-C5-C6-C7	-179.63(14)	C21-C22-C23-C18	-1.1(2)
C5-C6-C7-C2	-3.7(2)	C21-C22-C23-C26	179.76(14)
C5-C6-C7-C10	175.27(14)	C19-C18-C23-C22	0.4(2)
C3-C2-C7-C6	4.2(2)	N3-C18-C23-C22	178.53(13)
N1-C2-C7-C6	-175.01(12)	C19-C18-C23-C26	179.53(12)
C3-C2-C7-C10	-174.70(13)	N3-C18-C23-C26	-2.4(2)

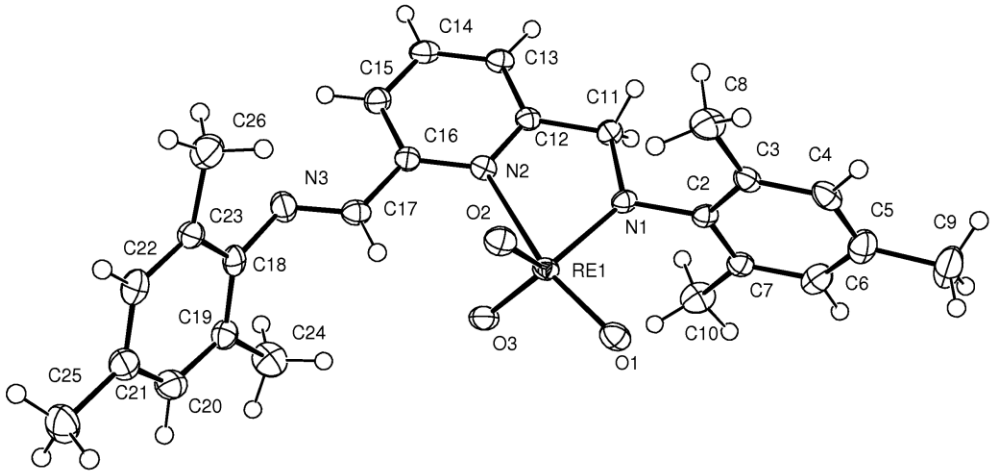

Figure S7. ORTEP drawing of **$Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

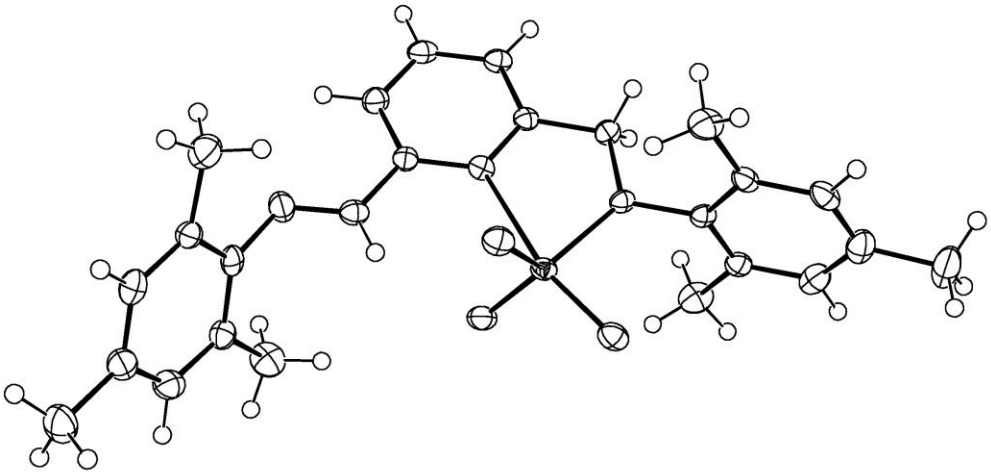

Figure S8. ORTEP drawing of **$Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity

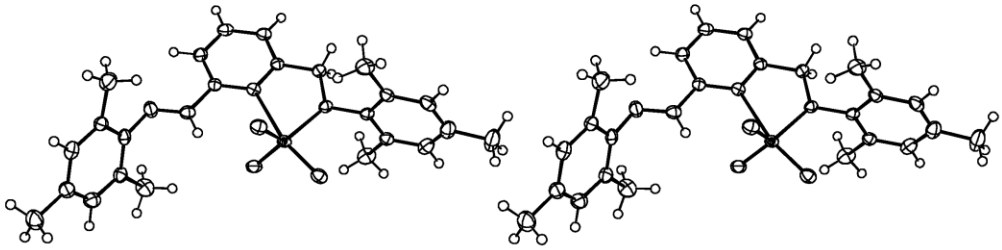

Figure S9. Stereoscopic ORTEP drawing of **$Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity

***Table S13*. Summary of Crystal Data for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

Formula	$C_{25}H_{28}N_3O_3Re$
Formula Weight (*g/mol*)	604.70
Crystal Dimensions (*mm*)	0.28 × 0.15 × 0.01
Crystal Color and Habit	pale yellow plate
Crystal System	monoclinic
Space Group	P 2_1/c
Temperature, K	110
a, Å	15.9434(13)
b, Å	13.1771(10)
c, Å	11.4807(9)
α,°	90.00
β,°	92.956(4)
γ,°	90.00
V, $Å^3$	2408.7(3)
Number of reflections to determine final unit cell	9904
Min and Max 2θ for cell determination, °	4.7, 48.84
Z	4
F(000)	1192
ρ (*g/cm*)	1.667
λ, Å, (MoKα)	0.71073
μ, (cm^{-1})	5.075
Diffractometer Type	Bruker-Nonius Kappa Axis X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	65.12
Measured fraction of data	0.994
Number of reflections measured	74284
Unique reflections measured	8715
R_{merge}	0.0896
Number of reflections included in refinement	8715
Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc w=1/[sigma^2(Fo^2)+(0.0414P)^2+0.0000P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	295
R_1	0.0414
wR_2	0.0805
R_1 (all data)	0.0840
wR_2 (all data)	0.0924
GOF	1.007
Maximum shift/error	0.002
Min & Max peak heights on final ΔF Map (e^-/Å)	-2.412, 4.222

Where:

$R_1 = \Sigma(|F_o| - |F_c|) / \Sigma F_o$

$wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(w F_o^4)]^{½}$

$GOF = [\Sigma(w(F_o^2 - F_c^2)^2) / (\text{No. of reflns. - No. of params.})]^{½}$

***Table S14*. Atomic Coordinates for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

Atom	x	y	z	$U_{iso/equiv}$
Re1	1.001309(10)	0.266369(12)	0.077842(13)	0.01878(6)
O1	1.08522(18)	0.3233(2)	0.0155(2)	0.0267(7)
O2	0.93907(19)	0.2184(2)	-0.0355(2)	0.0273(7)
O3	0.95118(18)	0.3642(2)	0.1457(2)	0.0263(7)
N1	1.0768(2)	0.1713(2)	0.1606(3)	0.0185(7)
N2	0.9189(2)	0.1717(2)	0.1962(3)	0.0184(7)
N3	0.7097(2)	0.2654(3)	0.1283(3)	0.0286(8)
C2	1.1649(2)	0.1638(3)	0.1370(3)	0.0187(8)
C3	1.1908(3)	0.0908(3)	0.0572(3)	0.0221(9)
C4	1.2754(3)	0.0867(3)	0.0351(3)	0.0267(10)
C5	1.3341(3)	0.1519(4)	0.0845(4)	0.0321(10)
C6	1.3061(3)	0.2228(3)	0.1644(4)	0.0299(10)
C7	1.2226(3)	0.2299(3)	0.1925(3)	0.0219(8)
C8	1.1288(3)	0.0206(3)	-0.0048(4)	0.0318(10)
C9	1.4251(3)	0.1496(4)	0.0515(4)	0.0437(13)
C10	1.1954(3)	0.3060(4)	0.2811(4)	0.0326(10)
C11	1.0524(2)	0.0980(3)	0.2495(3)	0.0206(8)
C12	0.9605(2)	0.1053(3)	0.2659(3)	0.0190(8)
C13	0.9208(3)	0.0472(3)	0.3486(3)	0.0217(8)
C14	0.8351(3)	0.0577(3)	0.3569(4)	0.0249(9)
C15	0.7915(3)	0.1256(3)	0.2839(3)	0.0246(9)
C16	0.8346(2)	0.1819(3)	0.2039(3)	0.0193(8)
C17	0.7884(3)	0.2520(3)	0.1220(4)	0.0232(9)
C18	0.6682(2)	0.3322(3)	0.0461(3)	0.0221(9)
C19	0.6729(3)	0.4371(3)	0.0609(4)	0.0244(9)
C20	0.6268(3)	0.4973(3)	-0.0179(4)	0.0299(10)
C21	0.5767(3)	0.4579(3)	-0.1092(4)	0.0291(10)
C22	0.5737(3)	0.3526(3)	-0.1216(4)	0.0279(10)
C23	0.6192(3)	0.2892(3)	-0.0450(4)	0.0236(9)
C24	0.7269(3)	0.4840(4)	0.1587(4)	0.0367(11)
C25	0.5280(3)	0.5263(4)	-0.1936(4)	0.0400(12)
C26	0.6202(3)	0.1755(4)	-0.0637(4)	0.0366(11)
H4	1.2936	0.0361	-0.0169	0.032
H6	1.3458	0.2680	0.2008	0.036
H8A	1.1152	-0.0353	0.0473	0.048
H8B	1.1533	-0.0069	-0.0747	0.048
H8C	1.0775	0.0582	-0.0275	0.048
H9A	1.4429	0.0791	0.0416	0.066
H9B	1.4606	0.1816	0.1134	0.066
H9C	1.4307	0.1867	-0.0217	0.066
H10A	1.1758	0.2701	0.3493	0.049
H10B	1.1497	0.3477	0.2465	0.049
H10C	1.2430	0.3496	0.3050	0.049
H11A	1.0839	0.1124	0.3243	0.025
H11B	1.0666	0.0284	0.2248	0.025

H13	0.9520	0.0015	0.3980	0.026
H14	0.8063	0.0189	0.4121	0.030
H15	0.7325	0.1335	0.2885	0.029
H17	0.8179	0.2870	0.0644	0.028
H20	0.6296	0.5689	-0.0088	0.036
H22	0.5399	0.3237	-0.1836	0.033
H24A	0.7191	0.5577	0.1581	0.055
H24B	0.7860	0.4681	0.1479	0.055
H24C	0.7106	0.4564	0.2335	0.055
H25A	0.5107	0.5876	-0.1529	0.060
H25B	0.4781	0.4905	-0.2256	0.060
H25C	0.5636	0.5453	-0.2572	0.060
H26A	0.5805	0.1577	-0.1285	0.055

***Table S15*. Anisotropic Displacement Parameters for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
Re1	0.02321(9)	0.01653(8)	0.01688(8)	0.00089(7)	0.00366(6)	0.00174(6)
O1	0.0326(17)	0.0256(17)	0.0224(14)	0.0044(13)	0.0043(12)	0.0040(12)
O2	0.0322(17)	0.0276(17)	0.0223(15)	0.0000(13)	0.0026(12)	0.0033(12)
O3	0.0309(17)	0.0197(15)	0.0288(16)	-0.0001(12)	0.0065(13)	0.0033(12)
N1	0.0213(18)	0.0185(17)	0.0163(15)	-0.0018(13)	0.0050(13)	0.0005(13)
N2	0.0234(18)	0.0193(17)	0.0129(15)	0.0014(14)	0.0034(13)	-0.0002(12)
N3	0.0226(19)	0.033(2)	0.030(2)	0.0048(16)	0.0031(15)	0.0076(16)
C2	0.022(2)	0.019(2)	0.0151(17)	-0.0012(16)	0.0039(15)	0.0025(15)
C3	0.027(2)	0.019(2)	0.0205(19)	0.0048(17)	0.0062(16)	0.0030(16)
C4	0.035(3)	0.024(2)	0.022(2)	0.0096(19)	0.0101(18)	0.0039(17)
C5	0.025(2)	0.043(3)	0.028(2)	0.001(2)	0.0033(19)	0.012(2)
C6	0.027(2)	0.036(3)	0.026(2)	-0.0068(19)	-0.0036(18)	0.0065(19)
C7	0.025(2)	0.021(2)	0.0192(19)	0.0004(17)	0.0013(16)	0.0038(16)
C8	0.040(3)	0.025(2)	0.031(2)	-0.002(2)	0.008(2)	-0.0093(19)
C9	0.024(3)	0.064(4)	0.044(3)	0.001(2)	0.007(2)	0.011(3)
C10	0.041(3)	0.031(2)	0.026(2)	-0.007(2)	0.0018(19)	-0.010(2)
C11	0.023(2)	0.023(2)	0.0169(18)	0.0001(16)	0.0042(15)	0.0028(15)
C12	0.022(2)	0.017(2)	0.0184(18)	-0.0001(15)	0.0031(15)	-0.0026(15)
C13	0.028(2)	0.019(2)	0.0178(19)	-0.0004(17)	0.0049(16)	0.0011(15)
C14	0.033(3)	0.018(2)	0.025(2)	-0.0024(17)	0.0098(18)	-0.0016(16)
C15	0.024(2)	0.023(2)	0.027(2)	-0.0006(17)	0.0079(17)	-0.0016(17)
C16	0.021(2)	0.018(2)	0.0191(18)	-0.0004(15)	0.0008(15)	-0.0041(15)
C17	0.028(2)	0.020(2)	0.022(2)	-0.0009(16)	0.0039(17)	-0.0014(15)
C18	0.016(2)	0.032(2)	0.0184(19)	0.0029(17)	0.0049(15)	0.0026(17)
C19	0.021(2)	0.027(2)	0.025(2)	-0.0002(17)	0.0024(17)	-0.0033(17)
C20	0.032(3)	0.024(2)	0.035(3)	0.0015(19)	0.009(2)	-0.0028(19)
C21	0.026(2)	0.034(3)	0.028(2)	0.0024(19)	0.0067(18)	0.0080(19)
C22	0.021(2)	0.038(3)	0.024(2)	-0.0022(19)	0.0000(17)	-0.0016(18)
C23	0.021(2)	0.023(2)	0.028(2)	0.0005(16)	0.0076(17)	0.0021(17)
C24	0.042(3)	0.035(3)	0.033(3)	0.002(2)	-0.001(2)	-0.007(2)
C25	0.034(3)	0.050(3)	0.036(3)	0.006(2)	0.001(2)	0.014(2)
C26	0.030(3)	0.033(3)	0.046(3)	-0.004(2)	0.002(2)	-0.005(2)

***Table S16*. Bond Lengths for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

Re1-O2	1.716(3)	C11-H11A	0.9900
Re1-O1	1.722(3)	C11-H11B	0.9900
Re1-O3	1.724(3)	C12-C13	1.397(5)
Re1-N1	1.950(3)	C13-C14	1.382(6)
Re1-N2	2.305(3)	C13-H13	0.9500
N1-C2	1.449(5)	C14-C15	1.389(6)
N1-C11	1.472(5)	C14-H14	0.9500
N2-C12	1.338(5)	C15-C16	1.390(5)
N2-C16	1.359(5)	C15-H15	0.9500
N3-C17	1.273(6)	C16-C17	1.485(6)
N3-C18	1.428(5)	C17-H17	0.9500
C2-C7	1.396(6)	C18-C23	1.393(6)
C2-C3	1.405(5)	C18-C19	1.395(6)
C3-C4	1.386(6)	C19-C20	1.386(6)
C3-C8	1.507(6)	C19-C24	1.511(6)
C4-C5	1.372(6)	C20-C21	1.385(6)
C4-H4	0.9500	C20-H20	0.9500
C5-C6	1.398(6)	C21-C22	1.395(6)
C5-C9	1.519(6)	C21-C25	1.509(6)
C6-C7	1.390(6)	C22-C23	1.390(6)
C6-H6	0.9500	C22-H22	0.9500
C7-C10	1.507(6)	C23-C26	1.514(6)
C8-H8A	0.9800	C24-H24A	0.9800
C8-H8B	0.9800	C24-H24B	0.9800
C8-H8C	0.9800	C24-H24C	0.9800
C9-H9A	0.9800	C25-H25A	0.9800
C9-H9B	0.9800	C25-H25B	0.9800
C9-H9C	0.9800	C25-H25C	0.9800
C10-H10A	0.9800	C26-H26A	0.9800
C10-H10B	0.9800	C26-H26B	0.9800
C10-H10C	0.9800	C26-H26C	0.9800
C11-C12	1.490(5)		

***Table S17*. Bond Angles for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

O2-Re1-O1	106.05(13)	C12-C11-H11B	109.7
O2-Re1-O3	110.78(14)	H11A-C11-H11B	108.2
O1-Re1-O3	104.50(13)	N2-C12-C13	122.4(4)
O2-Re1-N1	116.79(13)	N2-C12-C11	115.3(3)
O1-Re1-N1	90.54(13)	C13-C12-C11	122.3(4)
O3-Re1-N1	123.32(13)	C14-C13-C12	118.5(4)
O2-Re1-N2	85.58(12)	C14-C13-H13	120.7
O1-Re1-N2	163.68(12)	C12-C13-H13	120.7
O3-Re1-N2	81.20(12)	C13-C14-C15	119.3(4)
N1-Re1-N2	73.79(12)	C13-C14-H14	120.4
C2-N1-C11	112.2(3)	C15-C14-H14	120.4
C2-N1-Re1	122.2(2)	C14-C15-C16	119.6(4)
C11-N1-Re1	125.5(3)	C14-C15-H15	120.2
C12-N2-C16	119.2(3)	C16-C15-H15	120.2
C12-N2-Re1	115.2(2)	N2-C16-C15	120.9(4)
C16-N2-Re1	125.5(2)	N2-C16-C17	118.7(3)
C17-N3-C18	118.2(4)	C15-C16-C17	120.3(4)
C7-C2-C3	121.1(4)	N3-C17-C16	120.5(4)
C7-C2-N1	119.6(3)	N3-C17-H17	119.7
C3-C2-N1	119.3(3)	C16-C17-H17	119.7
C4-C3-C2	117.9(4)	C23-C18-C19	121.3(4)
C4-C3-C8	120.7(4)	C23-C18-N3	118.0(4)
C2-C3-C8	121.4(4)	C19-C18-N3	120.7(4)
C5-C4-C3	123.3(4)	C20-C19-C18	117.7(4)
C5-C4-H4	118.4	C20-C19-C24	120.9(4)
C3-C4-H4	118.4	C18-C19-C24	121.4(4)
C4-C5-C6	117.2(4)	C21-C20-C19	123.0(4)
C4-C5-C9	121.6(4)	C21-C20-H20	118.5
C6-C5-C9	121.2(4)	C19-C20-H20	118.5
C7-C6-C5	122.6(4)	C20-C21-C22	117.7(4)
C7-C6-H6	118.7	C20-C21-C25	121.3(4)
C5-C6-H6	118.7	C22-C21-C25	121.0(4)
C6-C7-C2	117.9(4)	C23-C22-C21	121.3(4)
C6-C7-C10	120.9(4)	C23-C22-H22	119.4
C2-C7-C10	121.1(4)	C21-C22-H22	119.4
C3-C8-H8A	109.5	C22-C23-C18	119.0(4)
C3-C8-H8B	109.5	C22-C23-C26	121.0(4)
H8A-C8-H8B	109.5	C18-C23-C26	119.9(4)
C3-C8-H8C	109.5	C19-C24-H24A	109.5
H8A-C8-H8C	109.5	C19-C24-H24B	109.5
H8B-C8-H8C	109.5	H24A-C24-H24B	109.5
C5-C9-H9A	109.5	C19-C24-H24C	109.5
C5-C9-H9B	109.5	H24A-C24-H24C	109.5
H9A-C9-H9B	109.5	H24B-C24-H24C	109.5
C5-C9-H9C	109.5	C21-C25-H25A	109.5
H9A-C9-H9C	109.5	C21-C25-H25B	109.5

H9B-C9-H9C	109.5	H25A-C25-H25B	109.5
C7-C10-H10A	109.5	C21-C25-H25C	109.5
C7-C10-H10B	109.5	H25A-C25-H25C	109.5
H10A-C10-H10B	109.5	H25B-C25-H25C	109.5
C7-C10-H10C	109.5	C23-C26-H26A	109.5
H10A-C10-H10C	109.5	C23-C26-H26B	109.5
H10B-C10-H10C	109.5	H26A-C26-H26B	109.5
N1-C11-C12	110.0(3)	C23-C26-H26C	109.5
N1-C11-H11A	109.7	H26A-C26-H26C	109.5
C12-C11-H11A	109.7	H26B-C26-H26C	109.5
N1-C11-H11B	109.7		

***Table S18*. Torsion Angles for $Re(O)_3(MesNCH_2)(MesNCH)NC_5H_3$, 8**

O2-Re1-N1-C2	99.3(3)	C16-N2-C12-C13	-1.5(5)
O1-Re1-N1-C2	-9.1(3)	Re1-N2-C12-C13	175.4(3)
O3-Re1-N1-C2	-116.9(3)	C16-N2-C12-C11	178.9(3)
N2-Re1-N1-C2	175.6(3)	Re1-N2-C12-C11	-4.2(4)
O2-Re1-N1-C11	-78.9(3)	N1-C11-C12-N2	2.3(5)
O1-Re1-N1-C11	172.8(3)	N1-C11-C12-C13	-177.4(3)
O3-Re1-N1-C11	65.0(3)	N2-C12-C13-C14	1.2(6)
N2-Re1-N1-C11	-2.6(3)	C11-C12-C13-C14	-179.2(4)
O2-Re1-N2-C12	123.3(3)	C12-C13-C14-C15	-0.4(6)
O1-Re1-N2-C12	-13.0(6)	C13-C14-C15-C16	-0.1(6)
O3-Re1-N2-C12	-124.9(3)	C12-N2-C16-C15	0.9(5)
N1-Re1-N2-C12	3.7(2)	Re1-N2-C16-C15	-175.6(3)
O2-Re1-N2-C16	-60.1(3)	C12-N2-C16-C17	-176.9(3)
O1-Re1-N2-C16	163.7(4)	Re1-N2-C16-C17	6.5(5)
O3-Re1-N2-C16	51.8(3)	C14-C15-C16-N2	-0.1(6)
N1-Re1-N2-C16	-179.6(3)	C14-C15-C16-C17	177.7(4)
C11-N1-C2-C7	-96.8(4)	C18-N3-C17-C16	-178.9(4)
Re1-N1-C2-C7	84.8(4)	N2-C16-C17-N3	-178.3(4)
C11-N1-C2-C3	84.0(4)	C15-C16-C17-N3	3.9(6)
Re1-N1-C2-C3	-94.4(4)	C17-N3-C18-C23	104.5(5)
C7-C2-C3-C4	-0.2(6)	C17-N3-C18-C19	-79.1(5)
N1-C2-C3-C4	179.0(3)	C23-C18-C19-C20	0.4(6)
C7-C2-C3-C8	-178.8(4)	N3-C18-C19-C20	-175.9(4)
N1-C2-C3-C8	0.4(5)	C23-C18-C19-C24	-179.2(4)
C2-C3-C4-C5	-2.0(6)	N3-C18-C19-C24	4.5(6)
C8-C3-C4-C5	176.7(4)	C18-C19-C20-C21	0.1(6)
C3-C4-C5-C6	2.6(6)	C24-C19-C20-C21	179.7(4)
C3-C4-C5-C9	-175.6(4)	C19-C20-C21-C22	-0.4(6)
C4-C5-C6-C7	-1.2(6)	C19-C20-C21-C25	-179.5(4)
C9-C5-C6-C7	177.1(4)	C20-C21-C22-C23	0.1(6)
C5-C6-C7-C2	-0.8(6)	C25-C21-C22-C23	179.2(4)
C5-C6-C7-C10	178.7(4)	C21-C22-C23-C18	0.4(6)
C3-C2-C7-C6	1.5(6)	C21-C22-C23-C26	-175.9(4)
N1-C2-C7-C6	-177.7(3)	C19-C18-C23-C22	-0.7(6)
C3-C2-C7-C10	-178.0(4)	N3-C18-C23-C22	175.8(4)
N1-C2-C7-C10	2.8(6)	C19-C18-C23-C26	175.7(4)
C2-N1-C11-C12	-177.1(3)	N3-C18-C23-C26	-7.9(6)
Re1-N1-C11-C12	1.2(4)		

O1-Re1-N1-C2	-96.04(13)	N1-C2-C7-C10	6.1(2)
N3-Re1-N1-C2	102.47(13)	C2-N1-C11-C12	-156.66(12)
N2-Re1-N1-C2	158.35(13)	Re1-N1-C11-C12	24.14(15)
Cl1-Re1-N1-C2	11.89(12)	C16-N2-C12-C13	-6.1(2)
O1-Re1-N1-C11	83.01(11)	Re1-N2-C12-C13	175.45(11)
N3-Re1-N1-C11	-78.49(13)	C16-N2-C12-C11	169.48(13)

N2-Re1-N1-C11	-22.61(10)	Re1-N2-C12-C11	-8.93(16)
Cl1-Re1-N1-C11	-169.06(10)	N1-C11-C12-N2	-9.03(17)
O1-Re1-N2-C16	91.20(11)	N1-C11-C12-C13	166.19(15)
N3-Re1-N2-C16	-16.80(10)	N2-C12-C13-C14	1.7(2)
N1-Re1-N2-C16	-160.89(11)	C11-C12-C13-C14	-173.15(15)
Cl1-Re1-N2-C16	-88.95(11)	C12-C13-C14-C15	2.0(2)
O1-Re1-N2-C12	-90.33(11)	C13-C14-C15-C16	-1.6(2)
N3-Re1-N2-C12	161.67(11)	C12-N2-C16-C15	6.6(2)
N1-Re1-N2-C12	17.58(10)	Re1-N2-C16-C15	-175.02(11)
Cl1-Re1-N2-C12	89.52(12)	C12-N2-C16-C17	-168.89(13)
O1-Re1-N3-C18	86.48(12)	Re1-N2-C16-C17	9.53(15)
N1-Re1-N3-C18	-112.02(12)	C14-C15-C16-N2	-2.6(2)
N2-Re1-N3-C18	-167.72(13)	C14-C15-C16-C17	172.15(14)
Cl1-Re1-N3-C18	-21.31(12)	C18-N3-C17-C16	165.51(11)
O1-Re1-N3-C17	-85.32(10)	Re1-N3-C17-C16	-21.20(14)
N1-Re1-N3-C17	76.19(12)	N2-C16-C17-N3	6.90(16)
N2-Re1-N3-C17	20.48(9)	C15-C16-C17-N3	-168.13(14)
Cl1-Re1-N3-C17	166.89(9)	C17-N3-C18-C23	-96.31(15)
C11-N1-C2-C7	-98.22(15)	Re1-N3-C18-C23	91.58(15)
Re1-N1-C2-C7	80.86(16)	C17-N3-C18-C19	81.82(15)
C11-N1-C2-C3	82.53(16)	Re1-N3-C18-C19	-90.30(15)
Re1-N1-C2-C3	-98.39(15)	C23-C18-C19-C20	0.9(2)
C7-C2-C3-C4	-1.5(2)	N3-C18-C19-C20	-177.21(12)
N1-C2-C3-C4	177.72(13)	C23-C18-C19-C24	-178.30(14)
C7-C2-C3-C8	-178.37(14)	N3-C18-C19-C24	3.5(2)
N1-C2-C3-C8	0.9(2)	C18-C19-C20-C21	-1.7(2)
C2-C3-C4-C5	-1.9(2)	C24-C19-C20-C21	177.57(15)
C8-C3-C4-C5	174.94(15)	C19-C20-C21-C22	1.0(2)
C3-C4-C5-C6	2.5(2)	C19-C20-C21-C25	-179.45(15)
C3-C4-C5-C9	-177.51(14)	C20-C21-C22-C23	0.4(2)
C4-C5-C6-C7	0.3(2)	C25-C21-C22-C23	-179.13(16)
C9-C5-C6-C7	-179.63(14)	C21-C22-C23-C18	-1.1(2)
C5-C6-C7-C2	-3.7(2)	C21-C22-C23-C26	179.76(14)
C5-C6-C7-C10	175.27(14)	C19-C18-C23-C22	0.4(2)
C3-C2-C7-C6	4.2(2)	N3-C18-C23-C22	178.53(13)
N1-C2-C7-C6	-175.01(12)	C19-C18-C23-C26	179.53(12)
C3-C2-C7-C10	-174.70(13)	N3-C18-C23-C26	-2.4(2)