Supporting Information

Structural and Spectroscopic Characterization of Rhenium Complexes Containing Neutral, Mono-, and Dianionic Ligands of 2,2'-Bipyridines and 2,2':6,2''-Terpyridines. An Experimental and DFT-Computational Study.

Mei Wang[†,‡], Thomas Weyhermüller[†], Eckhard Bill[†], Shengfa Ye[†,] and Karl Wieghardt[†,*]*

Page

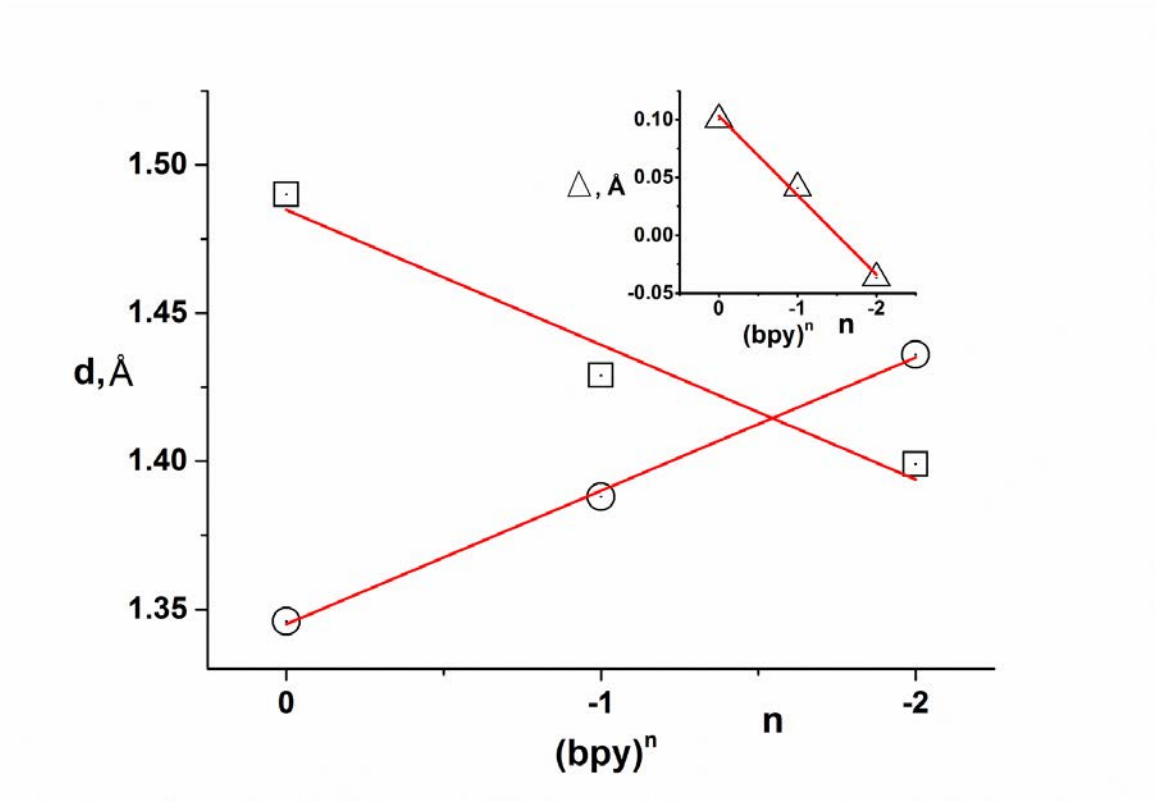


Figure S1. Average C_{py}-C_{py} (⊡) and C-N_{chel} (Θ) bond distances as a function of the charge n in uncoordinated bpy^0, its monoanionic π-radical $(bpy^{\bullet})^{1-}$, and the dianion $(bpy^{2-})^{2-}$. Data are taken from ref. 1 (R^2 values: 0.9255 and 0.9970). The inset shows the correlation of the difference Δ = [d(C_{py}-C_{py}) - d(C-N_{chel})] as a functions of the charge n of ((bpy), n = 0, 1-, 2-).

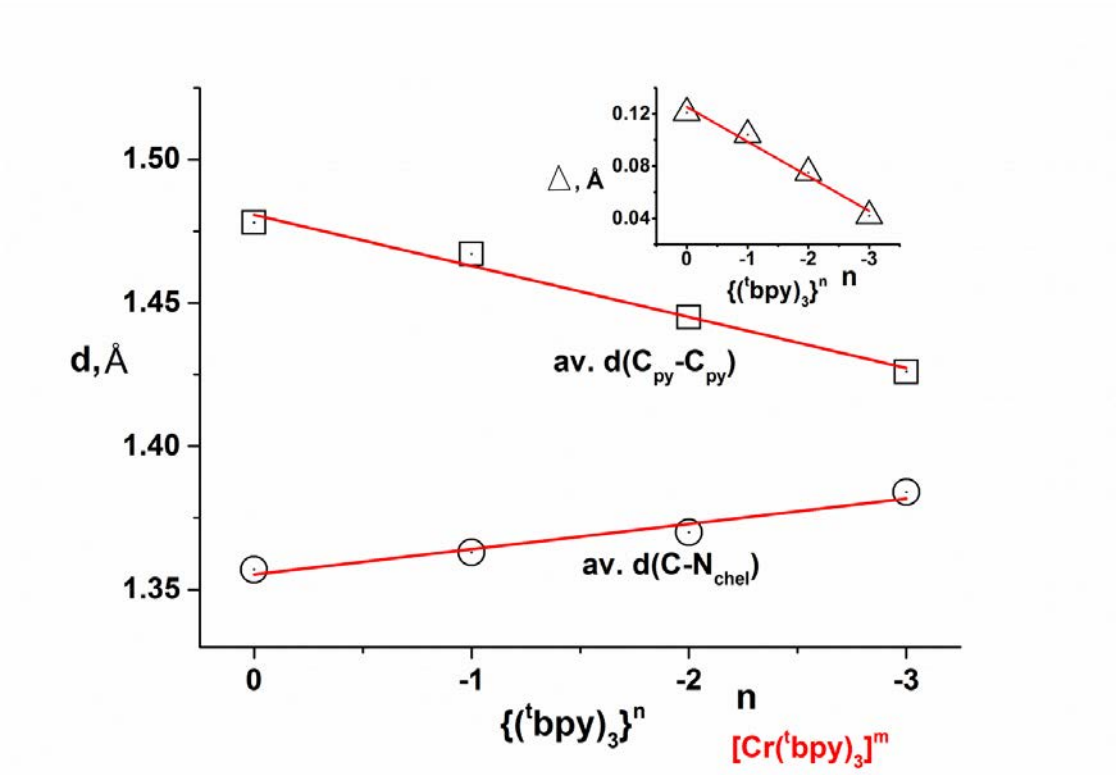


Figure S2. Averaged experimental bond distances (Å) d(C_{py}-C_{py}) (⊡) and d(C-N_{chel}) (Θ) in the members of the series $[Cr^{III}(^tbpy)_3]^m$ (m = 3+, 2+, 1+, 0) as a function of the charge n in $\{(^tbpy)_3\}^n$, The inset displays the correlation of the difference Δ = [d(C_{py}-C_{py}) - d(C-N_{chel})] of each species as a functions of the charge n in the $\{(bpy)_3\}^n$ unit. (R^2 values top to bottom: 0.974, 0.975, 0.934). (For all complexes m = n+3, since they all contain a central Cr(III) ion.) Data were taken from: Scarborough, C. C.; Sproules, S.; Weyhermüller, T.; DeBeer, S.; Wieghardt, K. *Inorg. Chem.* **2011**, *50*, 12446-12462.

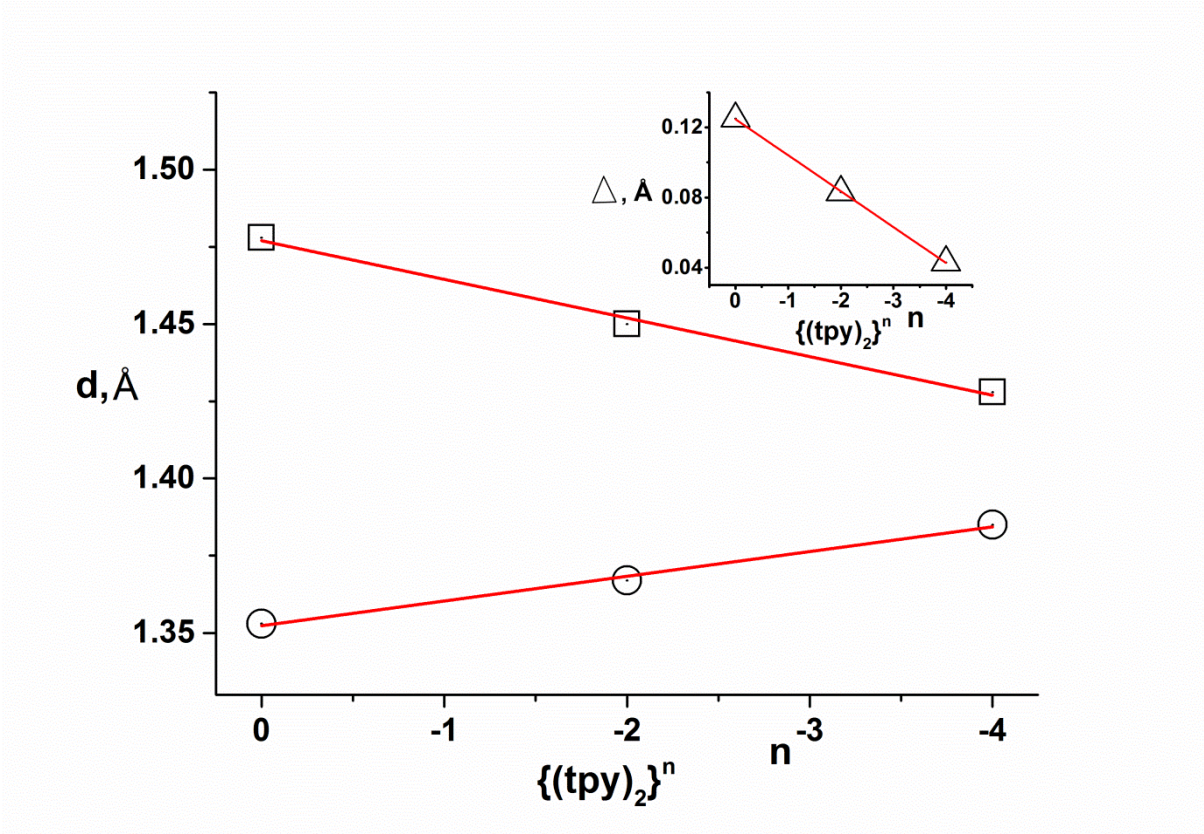


Figure S3. Average d(C_{py}-C_{py})(⊡) and average d(C-N_{chel}) (Θ) bond lengths in $[M(tpy)_2]^{n+}$ complexes as a function of the charge n of the two N, N',N''-coordinated ligands (R^2 = 0.9904 and 0.9896):

a) $(tpy^0)^0$: average of 6 octahedral structures (Co^{II}, Co^{I}, Cr^{III}, Ni^{II}, Mn^{II}, Fe^{II})
b) $(tpy^{\bullet})^{1-}$: average of 3 octahedral structures (Fe^{II}, Mn^{II}, Cr^{III})
c) $(tpy^{2-})^{2-}$: average of 3 octahedral structures (Ti^{IV}, V^{IV}, Mo^{IV})

The inset shows the empirical linear correlation of the difference Δ, Å of the av. C_{py}-C_{py} and C-N_{chel} distances and the charge n of the two $(tpy)^n$ ligands (R^2 = 0.9996). Data are from the following references:

$[M(tpy^{0})_2]^n$: a) Co(II), Co(I): England, J.; Bill, E.; Weyhermüller, T.; Neese, F.; Atanasov, M.; Wieghardt, K. *Inorg. Chem.* DOI: 10.1021/acs.inorgchem.5b02415. (b) Ni(II): Hamilton, J. M.; Anhorn, M. J.; Oscarson, K. A.; Reibenspies, J. H.; Hancock, R. D. *Inorg. Chem.* **2011**, *50*, 2764-2770. c) Cr(III): Wickramasinghe, W. A.; Bird, P. H.; Serpone, N. *Inorg. Chem.* **1982**, *21*, 2694-2698. d) Mn(II), Mn(III): Baffert, C.; Romero, I.; Pécaut, J.; Llobet, A.; Deronzier, A.; Collomb, M.-N. *Inorg. Chim. Acta* **2004**, *357*, 3430-3436. e) Romain, S.; Duboc, C.; Neese, F.; Riviére, E.; Hanton, L. R.; Blackman, A. G.; Philouze, C.; Leprêtre, J.-C.; Deronzier, A.; Collomb, M.-N. *Chem.-Eur. J.* **2009**, *15*, 980-988. f) Fe(II): Oshio, H.; Spiering, H.; Ksenofontov, V.; Renz, F.; Guetlich, P. *Inorg. Chem.* **2001**, *40*, 1143-1150.

$[M(tpy^{\bullet})_2]^m$: a) Cr(III): Scarborough, C. C.; Lancaster, K. M.; DeBeer, S.; Weyhermüller, T.; Sproules, S.; Wieghardt, K. *Inorg. Chem.* **2012**, *51*, 3718-3732. b) Mn(II): Wang, M.; England, J.; Weyhermüller, T.; Wieghardt, K. *Inorg. Chem.* **2014**, *53*, 2276-2287. c) Fe(II): England, J.; Scarborough, C. C.; Weyhermüller, T.; Sproules, S.; Wieghardt, K. *Eur. J. Inorg. Chem.* **2012**, 4605-4621.

$[Ni^{II}(tpy^{\bullet})(CH_3)]$: Jones, G. D.; Martin, J. L.; McFarland, C.; Allen, O. R.; Hall, R. E.; Haley, A. D.; Brandon, R. J.; Kanovalova, T.; Desrochers, P. J.; Pulay, P.; Vicic, D. A. *J. Am. Chem. Soc.* **2006**, *128*, 13175-13183.

$[Co^{II}(tpy^{\bullet})(BH_4)]$: Corey, E. J.; Cooper, N. J.; Canning, W. M.; Lipscomb, W. N.; Koetzle, T. F. *Inorg. Chem.* **1982**, *21*, 192-199.

$[M(tpy^{2-})_2]^q$: a) Ti(IV), V(IV), Mo(IV): Wang, M.; Weyhermüller, T.; England, J.; Wieghardt, K. *Inorg. Chem.* **2013**, *52*, 12763-12776.

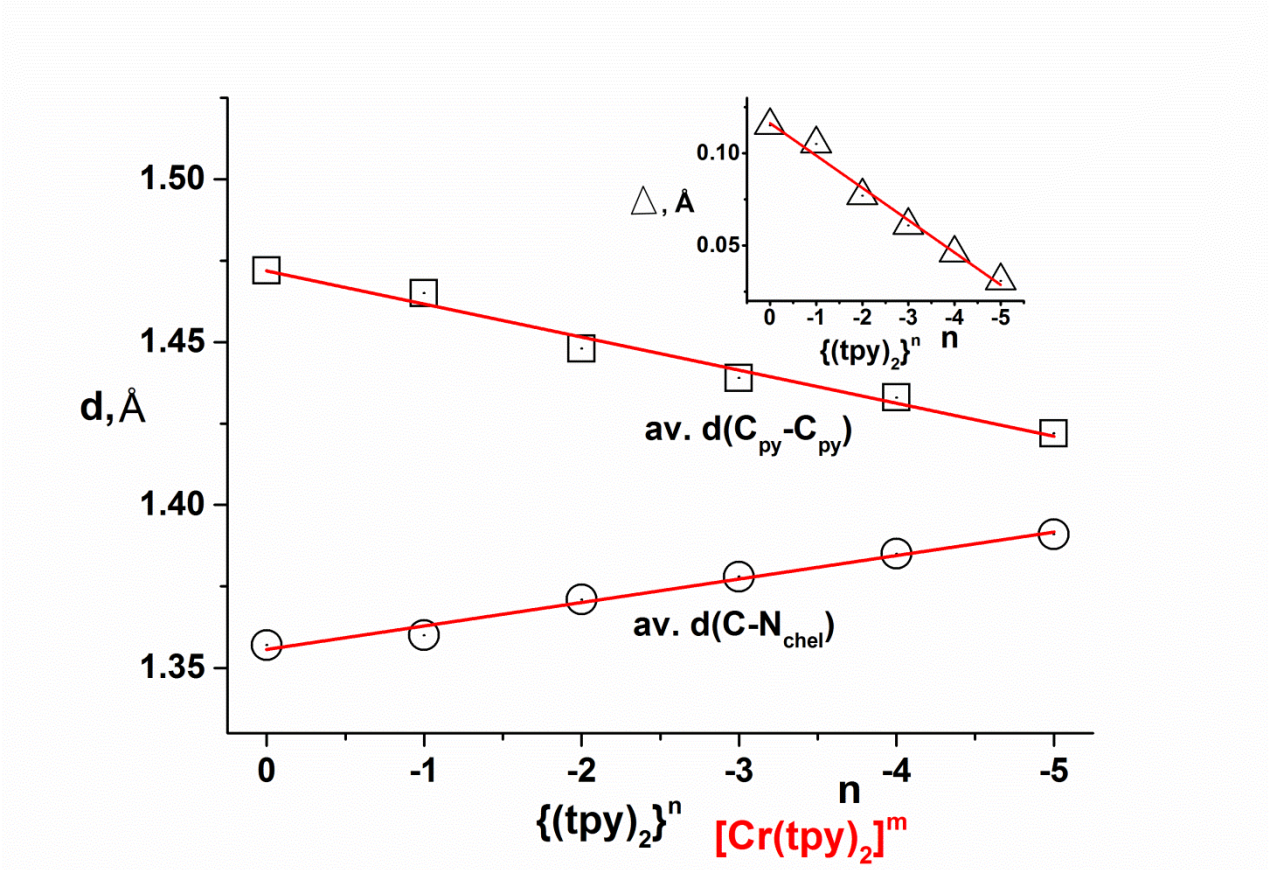


Figure S4. Averaged experimental C_{py}-C_{py} (⊡) and C-N_{chel} (Θ) bond lengths of the four members of the series $[Cr^{III}(tpy)_2]^m$ (m = 3+, 2+, 1+, 0) and of $[M(tpy)_2]^0$ (M = Mo, W) as a function of the charge n in $\{(tpy)_2\}^n$. The inset shows the correlation of the difference Δ = [d(C_{py}-C_{py}) - d(C-N_{chel})] in the same series of complexes (△) and the charge n of the respective $\{(tpy)_2\}^n$ unit (R^2 values top to bottom: 0.983, 0.977, 0.984). Note that m = n+3 for all chromium (III) complexes. For $[Mo(tpy)_2]^0$ n = 4- (two tpy^{2-} ligands) and $[W(tpy)_2]^0$ n = 5- (one $(tpy^{2-})^{2-}$ and one $(tpy^{3-})^{3-}$ ligand) . Data are taken from Scarborough, C. C.; Lancaster, K. M.; DeBeer, S.; Weyhermüller, T.; Sproules, S.; Wieghardt, K. *Inorg. Chem.* **2012**, *51*, 3718-3732.

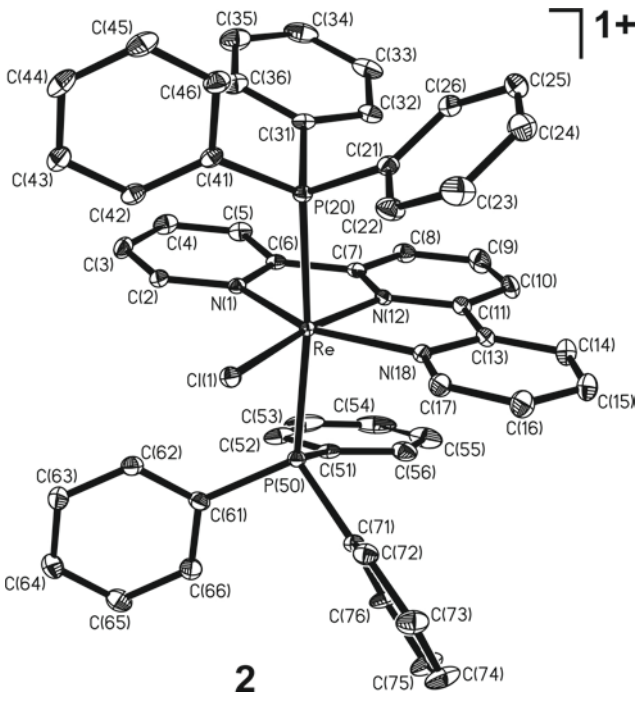


Figure S5. Structure of the monocation in crystals of **2** drawn at 40% probability.

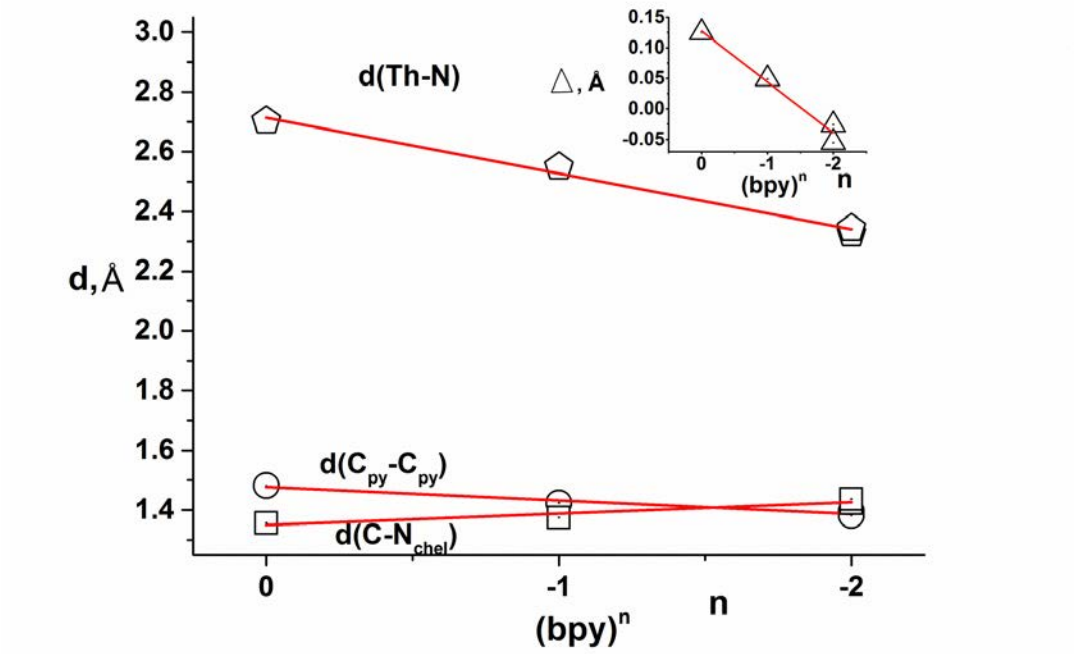


Figure S6. Empirical correlations of the average Th-N, C_{py}-C_{py} and C-N_{chel} bond distances in $[Th^{IV}(COT^{2-})_2(bpy^0)]^0$ (n = 0), $[Th^{IV}(COT^{2-})_2(bpy^{\bullet})]^{1-}$ (n = -1) and $[Th^{IV}(\eta^5\text{-}Cp^*)_2(bpy^{2-})]^0$ as a function of the charge n of the N, N'-coordinated $(bpy)^n$ ligand. (R^2 (top to bottom): 0.965, 0.987, 0.945, 0.880). The inset shows the difference $\Delta = [d(C_{py}\text{-}C_{py}) - d(C\text{-}N_{chel})]$ as a function of n. Data were taken from ref. 31 and 32.

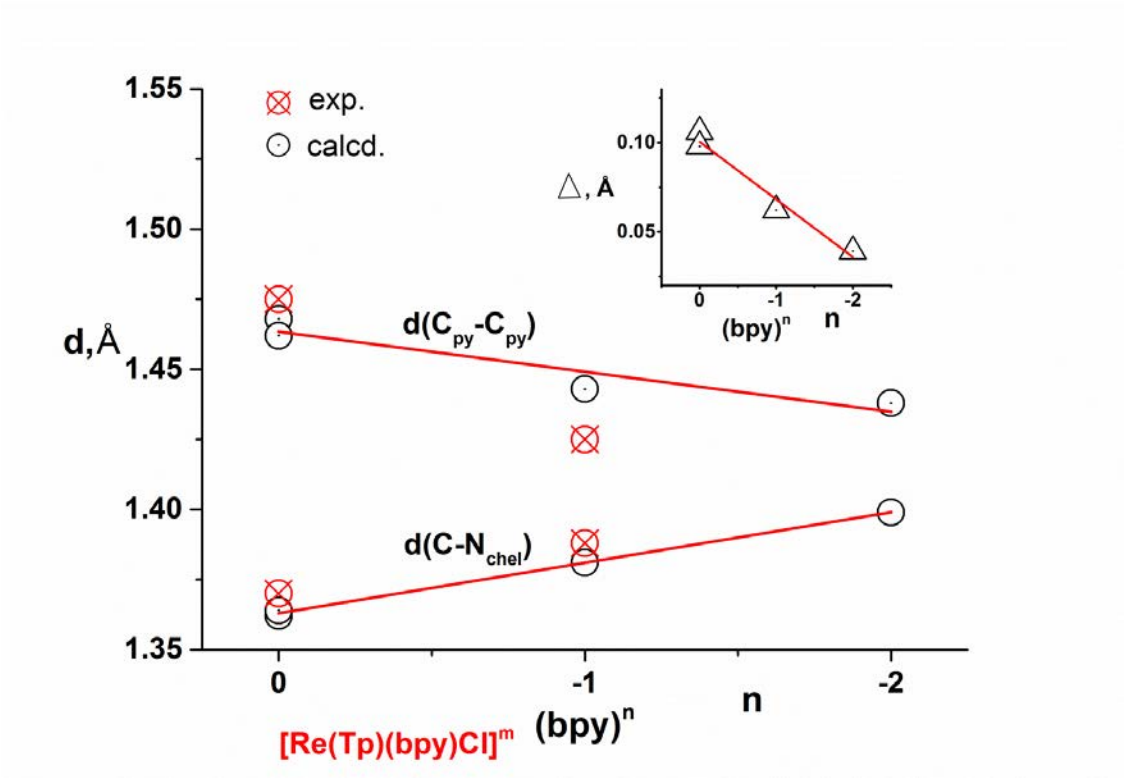


Figure S7. Calculated and experimental C_{py}-C_{py} and C-N_{chel} bond distances in the series $[Re(Tp)(bpy)Cl]^m$ (m = 2+, 1+, 0, 1-) as a function of the charge n of the ligand $(bpy)^n$ (n = 0,1-, 2-). The inset shows the correlation of the difference Δ = [d(C_{py}-C_{py}) - d(C-N_{chel})] and the charge n of the $(bpy)^n$. (Θ DFT calcd., ⊗ experimental value) (R^2 values from top to bottom: 0.957, 0.832, 0.997).

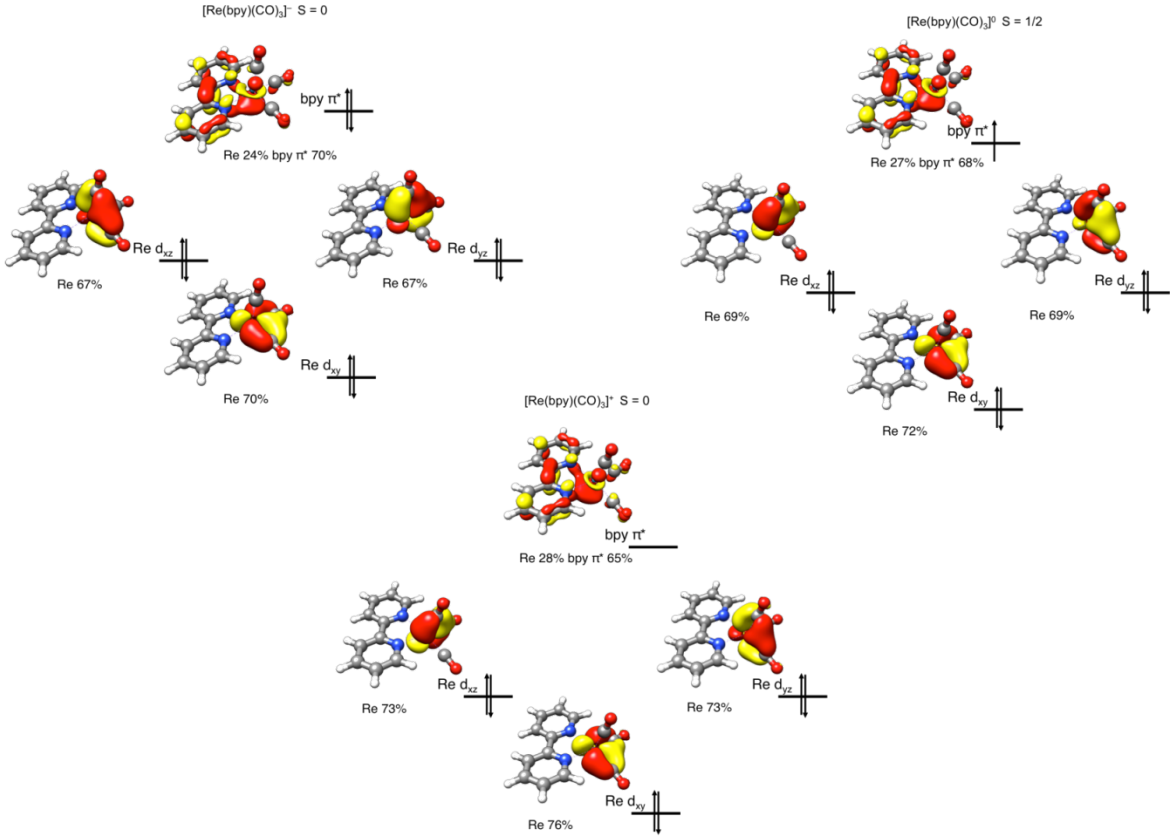


Figure S8. Schematic frontier molecular orbiral (FMO) diagrams of $[Re(bpy)(CO)_3]^{-,0,+}$.

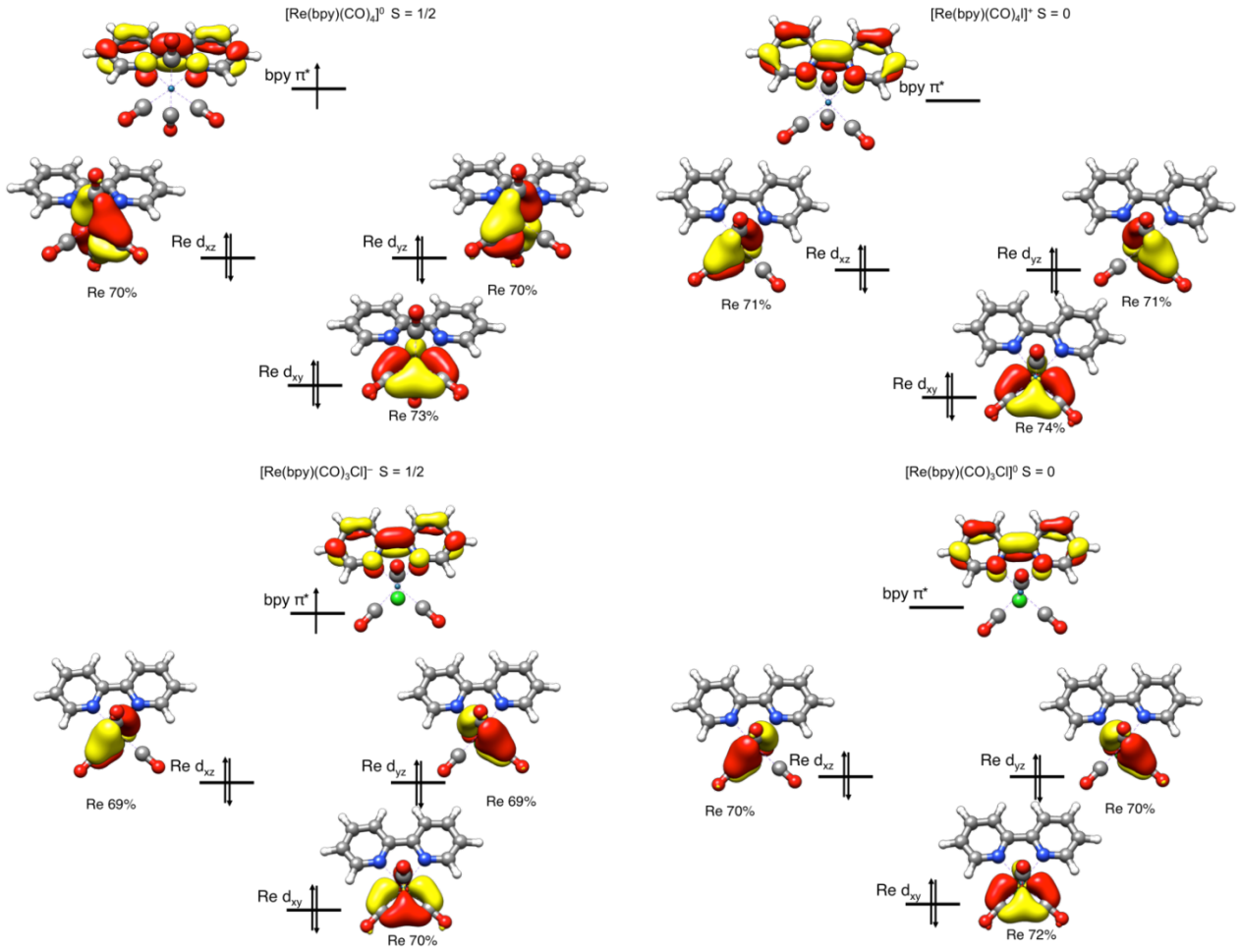


Figure S9. Schematic FMO diagrams of $[Re(bpy)(CO)_4]^{0,+}$ and $[Re(bpy)(CO)_3Cl]^{-,0}$.

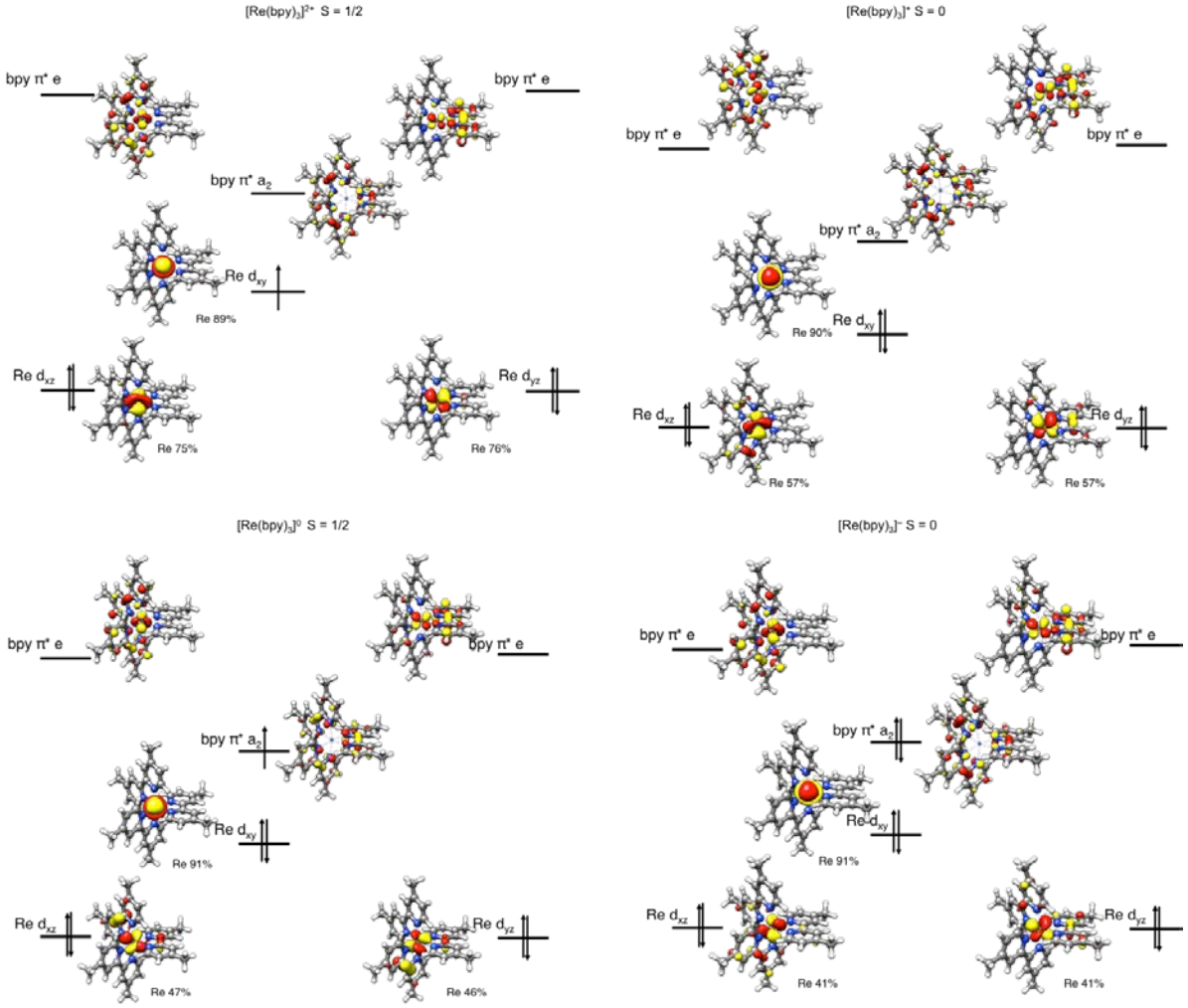


Figure S10. Schematic FMO diagrams of $[Re(bpy)_3]^{2+,+,0,-}$.

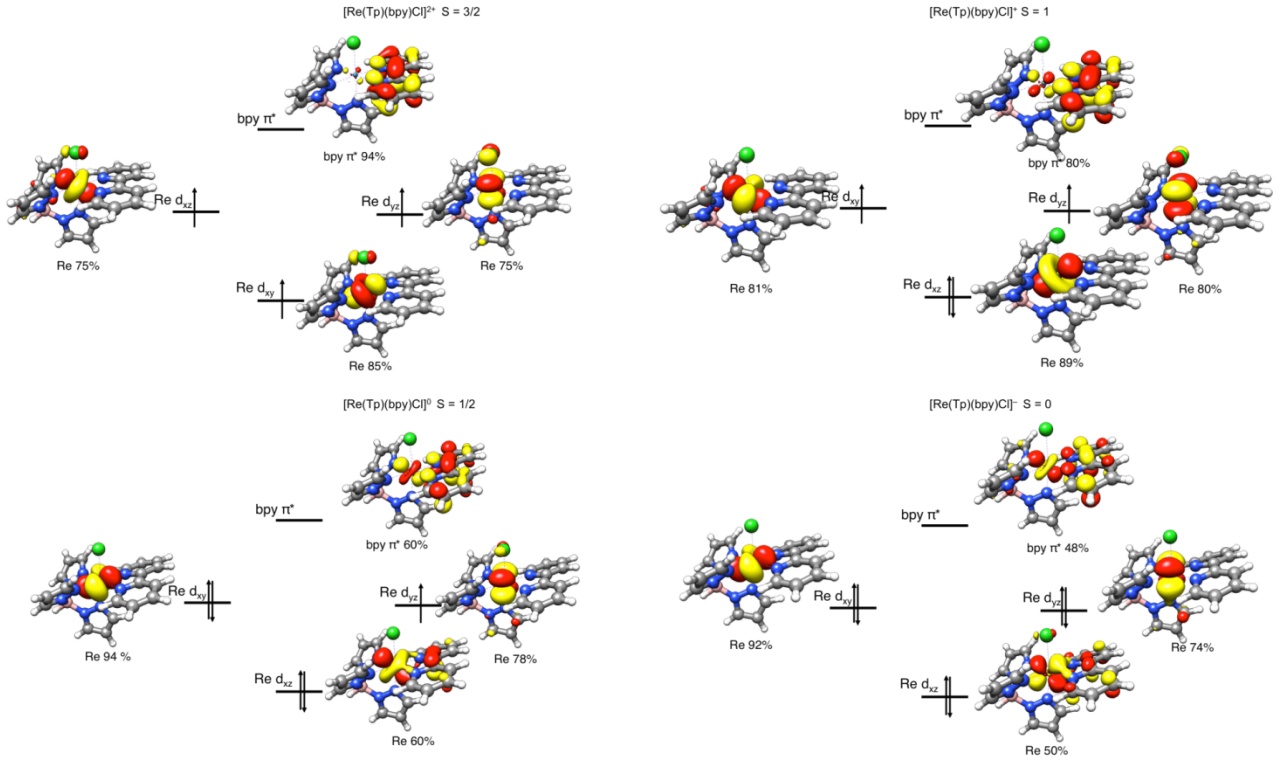


Figure S11. Schematic FMO diagrams of $[Re(Tp)(bpy)Cl]^{2+,+,0,-}$.

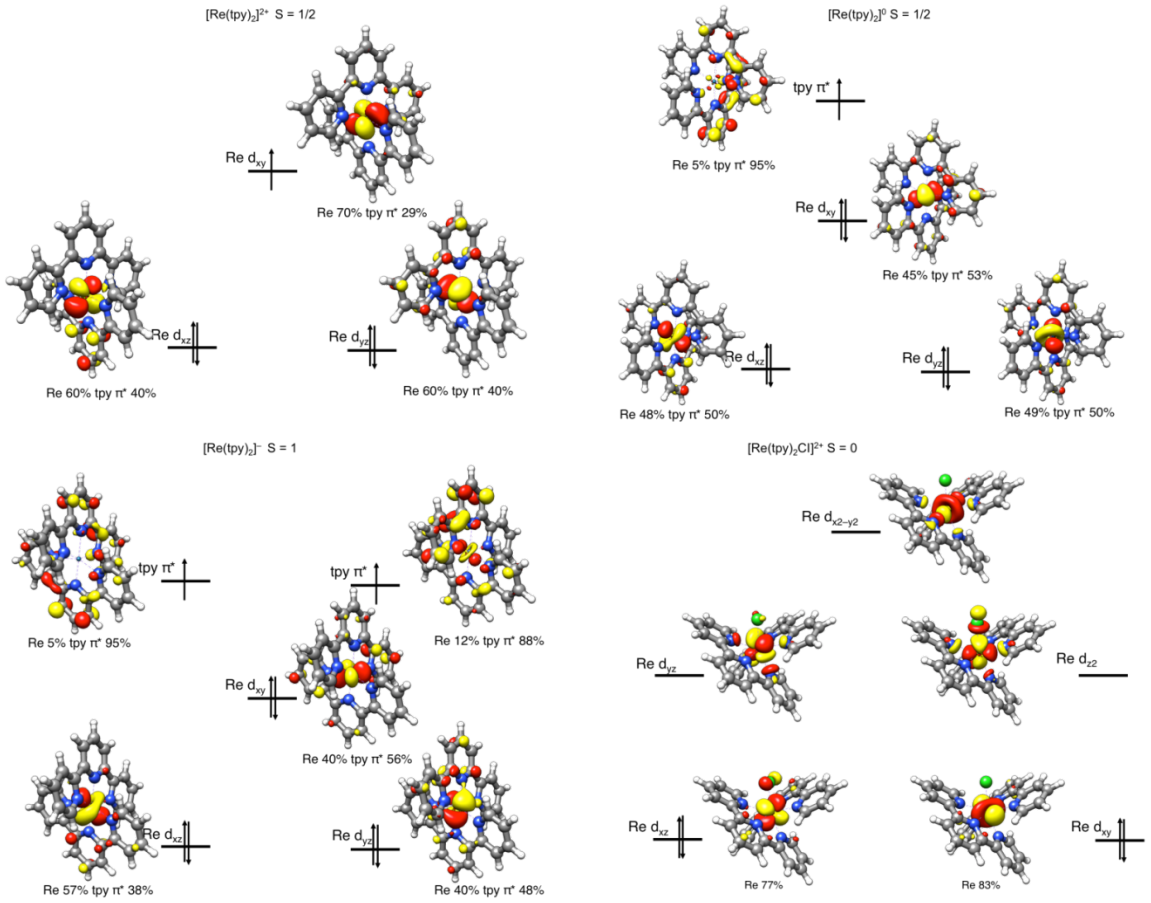


Figure S12. Schematic FMO diagrams of $[Re(tpy)_2]^n$ (n = 2+, 1+, 0, 1-) and $[Re(tpy)_2Cl]^{2+}$.

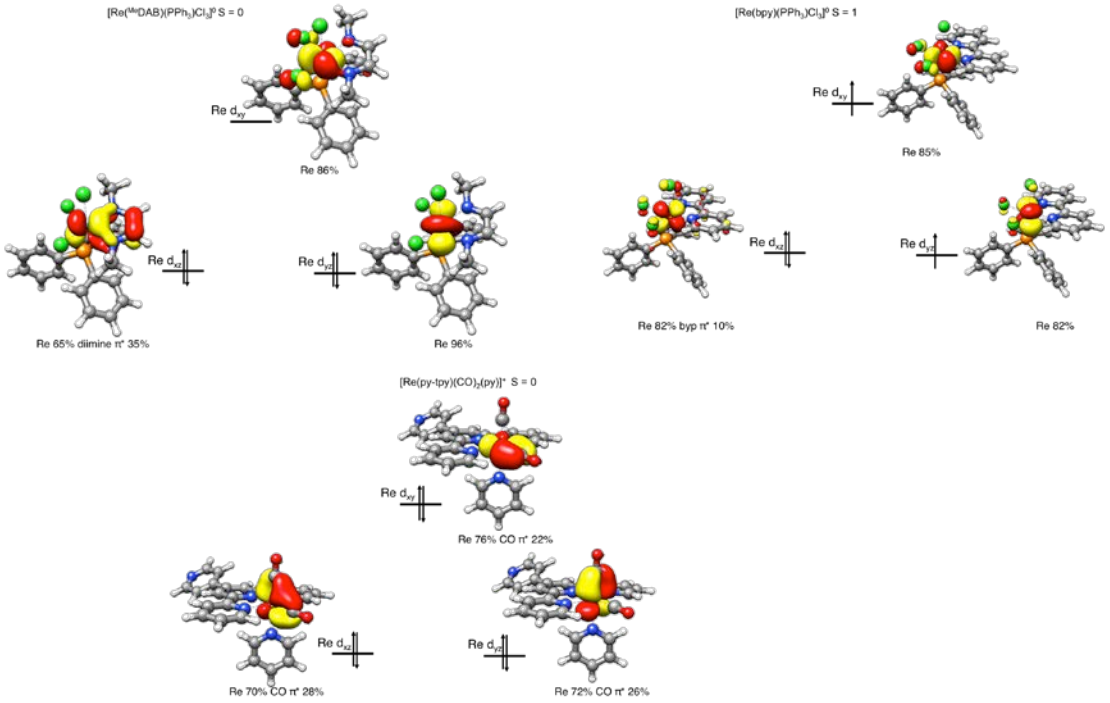


Figure S13. Schematic FMO diagrams of $[Re^{I}(py\text{-}tpy^{0})(CO)_2(py)]^{1+}$, $[Re(^{Me}DAB)(PPh_3)Cl_3]^{0}$, and $[Re(bpy^{0})Cl_3(PPh_3)]^{0}$.

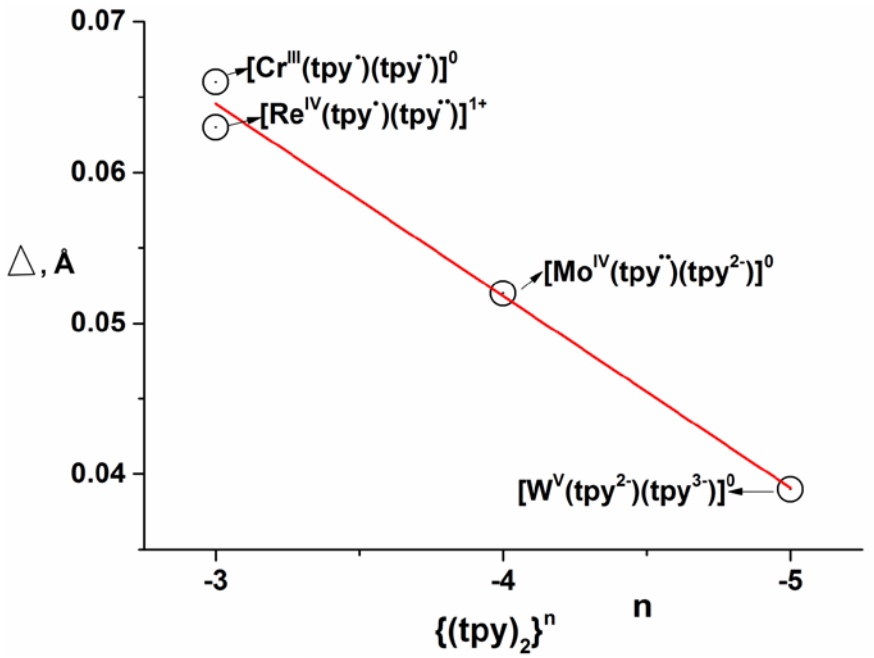


Figure S14. Empirical correlation of the difference Δ between the experimental average C_{py}- C_{py} and C-N_{chel} bond distances and the charge n of two coordinated terpyridine ligands $\{(tpy)_2\}^n$. Data for $[M(tpy)_2]^0$ (M=Cr, Mo, W) from ref. 10 (R^2 = 0.985), and for $[Re(tpy)_2]^{1+}$ in **5** and **6**.

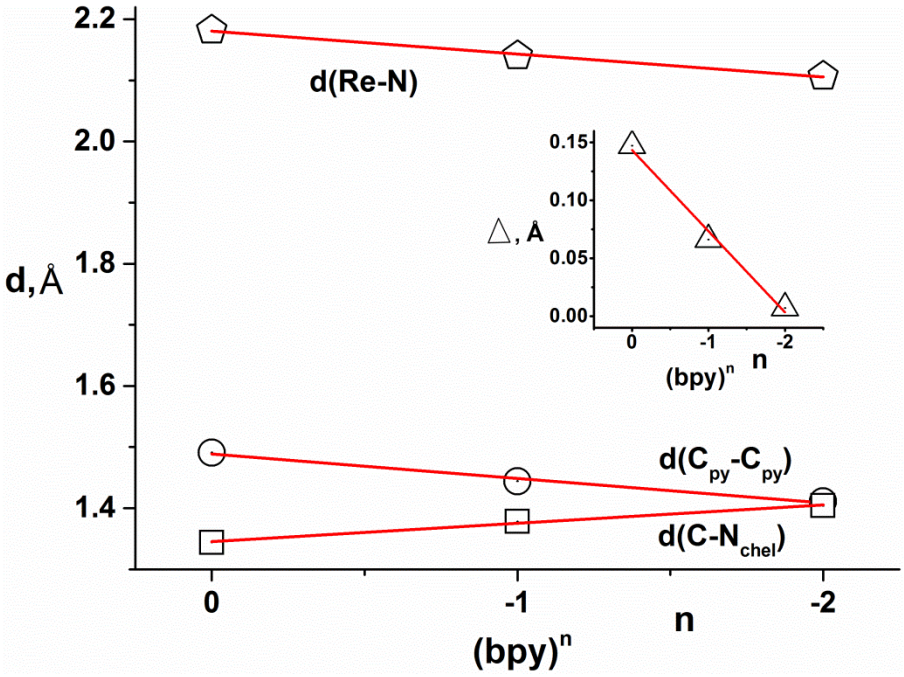


Figure S15. Linear correlations of the DFT-calculated average Re-N, C_{py}-C_{py}, and C-N_{chel} bond lengths and the Δ-values (inset) [d(C_{py}-C_{py}) - d(C-N_{chel})], Å for the series [Re(bpy)$(CO)_3$] (n = 1+, 0, 1-) as a function of the charge n of the $(bpy)^n$ ligand. (R^2 (top to bottom): 0.990, 0.984, 0.980, 0.988). Average *experimental* values for $[Re^{I}(bpy^{2-})(CO)_3]^{1-}$: Re-N: 2.081(5) Å, C_{py}-C_{py}: 1.402(6) Å, C-N_{chel}: 1.392(4) Å, Δ = 0.010 Å; data were taken from ref. 20e.

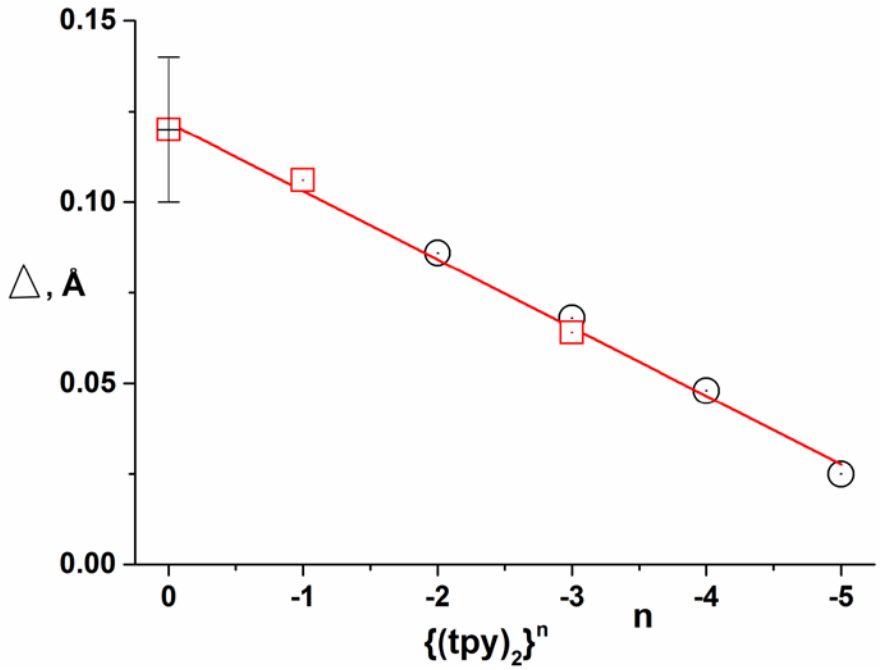


Figure S16. Linear correlation of calculated Δ-values *vs* the charge n of the $\{(tpy)_2\}^n$ unit in $[Re(tpy)_2]^m$ complexes (Θ) and experimental Δ-values for $[Cr^{III}(tpy^0)(tpy^{\bullet})]^{2+}$ (n=1), $[Re^{IV}\{(tpy)_2\}^{3-}]^{1+}$ (n=3), and an average Δ-value for a $\{(tpy^0)_2\}^0$ (n=0) unit (▪) (R^2 = 0.994).

Table S1. Fit Parameters for Magnetic Data.

Complex	***g***	%impurity (spin)	TIP (10^{-6} cm^3mol^{-1})	Θ, K
1	2.0	2.3 (*S* = 0.5)	60.1	0
2	1.993	1.2 (*S* = 1)	322.4	-0.28
3	1.986	1.2 (*S* = 1)	920.5	-3.5
4	2.0	0.6 (*S* = 2.5)	124.8	0
4a	1.989	0.9 (*S* = 1.5)	107.5	-0.2
6	2.0	1.1 (*S* = 1.5)	36.0	-1.33
8	2.0	0.2 (*S* = 1.5)	237.3	0

Table S2. UV-vis-NIR Spectra Recorded at 20°C in CH_3CN, thf or Methanol.

Complex	λ_{max}, nm (ε, 10^{-4} $M^{-1}cm^{-1}$)
$[Re^{II}(bpy)_3]^{2+}$ [a)]	495 (0.188), 375(0.25), 302(1.42)
$[Re^{II}(^{Me}bpy)_3]^{2+}$ **4a**	500 (0.7)
$[Re(^{Me}bpy)_3]^{1+}$ **4**	860 (sh), 740 (sh), 695 (1.1), ~600 (sh), ~580 (sh), 400 (1.8)
$[Re(^{Me}bpy)_3]^{0}$ **3**	2380, 1670, 1370 (0.2), ~1100 (sh), 860 (1.2), ~690 (sh),515 (1.9), 450 (2.4)
1	~1000 (sh), 900 (0.63), ~700 (sh), ~540 (sh), 470 (3.5)
2	~980 sh (0.5), 780 (0.8), 615 (1.3), ~410 (sh), 380 (2.1)
6	1000 (sh), 700 (0.85), 460 (2.2)
7	1180 (0.12), ~1000 (0.7), ~850 (sh), 600 (1.85), 420 (2.8)
7a	560 (0.76), 390 (1.1)
$[Re^{III}(Tp)(bpy^{2-})Cl]^{1-}$	1300 sh (0.25), 620 (sh), 470 (2.8), 390 (sh)
8	530 (0.5), 470 (sh)
$[Re^{I}(bpy^{2-})(CO)_3]^{1-}$	1320 (0.2), 1100 sh (0.3), 930 sh (0.75), 810 (1.4), 495 (1.95), 375 (2.1)
$[Re^{I}(bpy^{\bullet})(CO)_3]^{0}$ / $[Re^{I}(bpy^{\bullet})(CO)_3Cl]^{1-}$	800 (0.9), 605 (0.35), 480 (sh), 390 (2.4)

[a)] Stebler, M.; Gutierrez, A.; Ludi, A.; Buergi, H.- B. *Inorg. Chem.* **1987**, *26*, 1449-1451.

Table S3. Crystallographic Data for Complexes **1**, **2**, **3**, **4a**, **5**, **6**, **7**, **8**.

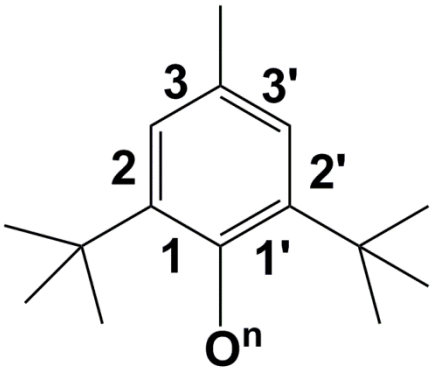
	1• Et_2O	**2**• 4MeOH	**3**	**4a**	**5**• THF
Chem. Formula	$C_{36}H_{49}Cl_3N_2OPRe$	$C_{55}H_{57}Cl_2N_3O_4P_2Re$	$C_{36}H_{36}N_6Re$	$C_{40}H_{44}F_6N_6O_8ReS$	$C_{45}H_{45}N_6ORe$[d]
Fw	849.29	1143.07	738.91	1101.13	872.07[d]
space group	*P*na2_1, No. 33	*P*bca, No. 61	*R*-3c, No. 167	*P*2_1/c, No. 14	*P*-1, No. 2
a, Å	12.9789(14)	17.640(2)	18.3091(10)	13.180(2)	9.3239(9)
b, Å	15.359(2)	22.476(2)	18.3091(10)	19.315(3)	15.0576(15)
c, Å	18.263(2)	25.573(3)	15.383(2)	17.588(2)	15.723(2)
α, deg	90	90	90	90	84.263(2)
β, deg	90	90	90	95.874(2)	80.615(2)
γ, deg	90	90	120	90	73.730(2)
V, Å^3	3640.6(7)	10139(2)	4465.9(8)	4453.9(11)	2087.2(4)
Z	4	8	6	4	2
T, K	100(2)	100(2)	100(2)	100(2)	100(2)
ρ calcd, g cm^{-3}	1.550	1.498	1.648	1.642	1.388[d]
refl. collected / $2\Theta_{max}$	100886 / 61.436	292290 / 62.072	39211 / 66.216	134879 / 63.170	62890 / 63.528
unique refl. / I>2σ(I)	11239 / 8739	16178 / 12368	1897 / 1443	14887 / 12608	14159 / 12914
No. of params / restr.	414 / 8	612 / 0	67 / 0	588 / 486	486 / 0
λ, Å / μ(Kα), cm^{-1}	0.71073 / 36.32	0.71073 / 26.14	0.71073 / 41.18	0.71073 / 29.04	0.71073 / 29.51[d]
R1 [a] / goodness of fit [b]	0.0365 / 1.020	0.0280 / 1.068	0.0287 / 1.090	0.0418 / 1.074	0.0242 / 1.047
wR2 [c] (I>2σ(I))	0.0734	0.0523	0.0691	0.1189	0.0581
residual density, eÅ^{-3}	+4.58 / -1.34	+0.94 / -1.17	+2.04 / -1.62	+2.30 / -1.54	+2.58 / -0.83

	6 • $2.5CH_2Cl_2$	**7**	**8**• Et_2O
Chem. Formula	$C_{32.5}H_{27}Cl_6N_6Re$	$C_{19.78}H_{20.35}BCl_{0.22}N8O_{0.78}$	$C_{32}H_{22}ClF_6N_6O_6ReS_2$
Fw	900.50	587.41	986.32[d]
space group	$P2_1/n$, No. 14	*P*nma, No. 62	*C*2/c, No. 15
a, Å	16.5197(9)	14.558(3)	14.1936(15)
b, Å	21.126(2)	14.386(2)	12.6799(13)
c, Å	20.0004(14)	9.793(2)	22.455(3)
α, deg	90	90	90
β, deg	101.754(5)	90	107.152(2)
γ, deg	90	90	90
V, Å^3	6833.7(9)	2051.0(7)	3861.6(8)
Z	8	4	4
T, K	100(2)	100	100(2)
ρ calcd, g cm^{-3}	1.751	1.902	1.697[d]
refl. collected / $2\Theta_{max}$	194722 / 66.296	62065 / 64.690	65891 / 68.108
unique refl. / I>2σ(I)	26005 / 20708	3781 / 3361	7877 / 7385
No. of params / restr.	841 / 10	157 / 0	245 / 0
λ, Å / μ(Kα), cm^{-1}	0.71073 / 40.59	0.71073 / 59.83	0.71073 / 34.02[d]
R1 [a] / goodness of fit [b]	0.0331 / 1.097	0.0212 / 1.108	0.0182 / 1.066
wR2 [c] (I>2σ(I))	0.0807	0.0520	0.0433
residual density, eÅ^{-3}	+1.95 / -1.72	+1.99 / -2.85	+1.17 / -0.65

a) Observation criterion: $I > 2\sigma(I)$. R1 = $\Sigma||F_o|-|F_c||/\Sigma|F_o|$, b) GooF = $[\Sigma[w(F_o^2-F_c^2)^2]/(n-p)]^{1/2}$

c) *w*R2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/\sigma^2(F_o^2)+(aP)^2+bP$, $P = (F_o^2+2F_c^2)/3$, d) calculated for the solvent-free complex

Table S4. DFT-B3LYP Calculated Bond Distances in the 2,6-di-tert-butyl-4-methyl-phenolate Monoanion and its Neutral Phenoxyl Radical.



Charge (n)	*S*	Method	Bond Lengths (Å)			
			C-O	1/1’	2-2’	3-3’
		Expt.	1.289	1.448, 1.452	1.392, 1.391	1.390, 1.401
1-	0	RKS(B3LYP)	1.296	1.455, 1.452	1.397, 1.400	1.403, 1.401
1-	0	RKS(BP)	1.304	1.462, 1.460	1.405, 1.407	1.411, 1.409
0	1/2	UKS(B3LYP)	1.258	1.477, 1.476	1.380, 1.384	1.416, 1.411
0	1/2	UKS(BP)	1.269	1.484, 1.482	1.388, 1.391	1.422, 1.418

Table S5. Summary of Experimental Structural Parameters of Complexes Containing (bpy^0), ($bpy^{\bullet}$)$^{1-}$, and (bpy^{2-})$^{2-}$ Ligands.

No	Complex	av. d(C_{py}-C_{py}), Å	av. d(C-N_{chel}), Å	Δ, Å[a)]	Ref.
0	$[Re^{I}(^{t}bpy^{0})(CO)_4]^{1+}$	1.473(5)	1.355(5)	0.118	[1]
1	$[Re_2{}^{0}(CO)_8(bpy^{0})]^{0}$	1.478	1.363	0.115	[2]
2	$[Re^{I}(^{CF3}bpy^{0})(CO)_3Cl]^{0}$	1.472(5)	1.353(6)	0.119	[3]
3	$[Re^{I}(^{Me}bpy^{0})(CO)_3Cl]^{0}$	1.476(6)	1.353(6)	0.119	[4]
4	$[Re^{I}(^{t}bpy^{0})(CO)_3(py)]^{1+}$	1.476(3)	1.358(4)	0.118	[5]
5	$[Re^{I}(^{t}bpy^{0})(CO)_3Cl]^{0}$	1.487(5)	1.361(5)	0.126	[5]
6	$[Re^{I}(^{OMe}bpy^{0})(CO)_3Cl]^{0}$	1.494(6)	1.356(6)	0.138	[4]
	$[Re^{I}(bpy^{0})(CO)_3X]^{n}$	> 200 structures		av. 0.118	CCDC
7	$[Re^{II}(^{Me}bpy^{0})(Br_2)(CO)_2]^{0}$	1.473	1.350	0.123	[6]
8	$[Re^{I}(^{Me}bpy^{0})(PEt_3)(PPh_3)(CO)_2]^{1+}$	1.484	1.356	0.128	[7]
9	$[Re^{I}(^{CF3}bpy^{\bullet})(CO)_3Cl]^{1-}$	1.433(6)	1.384(6)	0.049	[3]
10	$[Re_2(CO)_6(bpy)_2]^{1-}$	1.426(6)	1.382(6)	0.044	[8]
11	$[Re^{I}(bpy^{2-})(CO)_3]^{1-}$	1.402(6)	1.392(6)	0.010	[8]
12	$[Re^{I}(^{OMe}bpy^{2-})(CO)_3]^{1-}$	1.396(13)	1.382(14)	0.010	[3]
13	$[Re^{I}(^{Me}bpy^{2-})(CO)_3]^{1-}$	1.394(3)	1.408(3)	-0.008	[3]
14	$[Re^{I}(^{t}bpy^{2-})(CO)_3]^{1-}$	1.373(15)	1.412(15)	-0.039	[5]
15	$[Re^{III}(Tp)(bpy^{0})Cl]^{1+}$	1.475(9)	1.370(8)	0.105	[9]
16	$[Re^{III}(bpy^{0})_2Cl_2]^{1+}$	1.48(1)	1.357(9)	0.119	[10]
17	$[Re^{IV}(^{Me}bpy^{0})Cl_4]^{0}$	1.468	1.354	0.114	[11]
18	$[Re^{IV}(bpy^{0})Cl_4]^{0}$	1.475	1.355	0.120	[12]
19	$[Re^{V}(bpy^{0})_2(N\text{-}Ph)(OEt)]^{2+}$	1.469	1.363	0.106	[13]
20	$[Re^{V}(C_2O_4)(bpy^{0})O(OCH_3)]^{0}$	1.473	1.356	0.117	[14]
21	$[Re^{V}(O)_2(bpy^{0})\ (py)_2]^{1+}$	1.48(2)	1.37(2)	0.110	[15]
22	$[Re^{V}(bpy^{0})Cl_3(N\text{-}Ph)]^{0}$	1.475	1.358	0.117	[16]
23	$[Re^{V}(toly\text{-}S)_3O(bpy^{0})]^{0}$	1.455	1.336	0.119	[17]
24	$[Re^{V}(bpy^{0})(CH_3)_2O(CC\text{-}PMe_3)]^{1+}$	1.462	1.354	0.108	[18]
25	$[Re^{VII}(^{t}bpy^{0})(O)_3Br]^{0}$	1.472	1.359	0.113	[19]
26	$[Al^{III}(bpy^{2-})_2]^{1-}$	1.38	1.44	-0.080	[20]
27	$[Cp_2Zr^{IV}(bpy^{2-})]^{0}$	1.397(11)	1.389(20)	0.008	[21]
28	$[Zr^{IV}(bpy^{2-})_3]^{2-}$	1.361	1.437	-0.075	[22]
29	$[Ta^{V}(bpy^{2-})_3]^{1-}$	1.395(5)	1.415(5)	-0.020	[23]
30	$[Y^{III}(Tp^{Me2})(bpy^{2-})\ (thf)]^{0}$	1.350	1.428	-0.078	[24]
31	$[(C_5H_3\text{-}^{t}Bu_2)Th^{IV}(bpy^{2-})]^{0}$	1.397	1.422	-0.025	[25]
32	$[(C_5H_2\text{-}^{t}Bu_3)Th^{IV}(bpy^{2-})]^{0}$	1.382	1.437	-0.055	[26]
33	$[Th^{IV}(COT^{2-})_2(bpy^{0})]^{0}$	1.482(3)	1.357(3)	0.125	[27]
34	$[Th^{IV}(COT^{2-})_2(bpy^{\bullet})]^{1-}$	1.424(4)	1.391(4)	0.033	[27]

[a)] Δ = [d(C_{py}-C_{py}) - d(C-N_{chel})], Å

References:

(1) (a) Grice, K. A.; Gu, N. X.; Sampson, M. D.; Kubiak, C. P. *Dalton Trans.* **2013**, *42*, 8498-8503. (b) Morimoto, T.; Nishiura, C.; Tanaka, M.; Rohacova, J.; Nakagawa, Y.; Funada, Y.; Koike, K.; Yamamoto, Y.; Shishido, S.; Kojima, T. *J. Am. Chem. Soc.* **2013**, 1*35*, 13266-13269.

(2) Blake, A. J.; George, M. W.; Little, E. L.; Turner, J. J. *Acta Crystallogr., Section E: Struct. Rep. Online* **2001**, *57*, m378-m379.

(3) Benson, E. E.; Grice, K. A.; Smieja, J. M.; Kubiak, C. P. *Polyhedron* **2013**, *58*, 229-234.

(4) Smieja, J. M.; Kubiak, C. P. *Inorg. Chem.* **2010**, *49*, 9283-9289.

(5) Smieja J. M; Benson E. E; Kumar B.; Grice K. A; Seu C. S; Miller A. J. M.; Mayer J. M.; Kubiak C. P *Proc. Nat. Acad. Sci. USA* **2012**, *109*, 15646-15650.

(6) Zobi F.; Degonda A.; Schaub M. C.; Bogdanova A. Y. *Inorg. Chem.* **2010**, *49*, 7313-7322.

(7) Morimoto, T.; Ito, M.; Koike, K.; Kojima, T.; Ozeki, T.; Ishitani, O. *Chem.- Eur. J.* **2012**, *18*, 3292-3304.

(8) Benson, E. E.; Kubiak, C. P. *Chem. Commun.* **2012**, *48*, 7374-7376.

(9) Gunnoe T. B.; Meiere S. H.; Sabat M.; Harman W. D. *Inorg. Chem.* **2000**, *39*, 6127-6130.

(10) Helberg, L. E.; Orth, S. D.; Sabat, M.; Harman, W. D. *Inorg. Chem.* **1996**, *35*, 5584-5594.

(11) Martinez-Lillo, J.; Mastropietro, T. F.; Lappano, R.; Madeo, A.; Alberto, M. E.; Russo, N.; Maggiolini, M.; De Munno, G. *Chem. Commun.* **2011**, *47*, 5283-5285.

(12) Herrmann, W. A.; Thiel, W. R.; Herdtweck, E. *Chem. Ber.* **1990**, *123*, 271-276.

(13) Bakir, M.; Paulson, S.; Goodson, P.; Sullivan, B. P. *Inorg. Chem.* **1992**, *31*, 1127-1129.

(14) Chiozzone, R.; Gonzalez, R.; Kremer, C.; De Munno, G.; Faus, J. *Inorg. Chem. Acta* **2001**, *325*, 203-207.

(15) Blackbourn, R. L.; Jones, L. M.; Ram, M. S.; Sabat, M.; Hupp, J. T. *Inorg. Chem.* **1990**, *29*, 1791-1792.

(16) (a) Bakir, M.; Sullivan, B. P. *J. Chem. Soc., Dalton Trans.* **1995**, *10*, 1733-1738. (b) Ng, C.-O.; Tso-Lun Lo, L.; Ng, S.-M.; Ko, C.-C.; Zhu, N. *Inorg. Chem.* **2008**, *47*, 7447-7449.

(17) Papachristou, M.; Pirmettis, I. C.; Tsoukalas, C.; Papagiannopoulou, D.;

Raptopoulou, C.; Terzis, A.; Stassinopoulou, C. I.; Chiotellis, E.; Pelecanou, M.; Papadopoulos, M. *Inorg. Chem.* **2003**, *42*, 5778-5784.

(18) Jung, J.-H.; Hoffman, D. M.; Lee, T. R. *J. Organomet. Chem.* **2000**, *599*, 112-122.

(19) Kuehn, F. E.; Haider, J. J.; Herdtweck, E.; Herrmann, W. A.; Lopes, A. D.; Pillinger, M.; Romao, C. C. *Inorg. Chim. Acta* **1998**, *279*, 44-50.

(20) Nikiforov, G. B.; Roesky, H. W.; Noltemeyer, M.; Schmidt, H.-G. *Polyhedron* **2004**, *23*, 561-566.

(21) Nitschke, J. R.; Tilley, T. D. *Angew. Chem. Int. Ed.* **2001**, *40*, 2142-2145.

(22) Rosa, P.; Mézailles, N.; Ricard, L.; Mathey, F.; Le Floch, P. *Angew. Chem. Int. Ed.* **2000**, *39*, 1823-1826.

(23) Bowman, A. C.; England, J.; Sproules, S.; Weyhermüller, T.; Wieghardt, K. *Inorg. Chem.* **2013**, *52*, 2242-2256.

(24) Roitershtein, D.; Domingos, A.; Pereira, L. C. J.; Ascenso, J. R.; Marques, N. *Inorg. Chem.* **2003**, *42*, 7666-7673.

(25) Ren, W.; Song, H.; Zi, G.; Walter, M. D. *Dalton Trans.* **2012**, *41*, 5965-5973.

(26) Ren, W.; Zi, G.; Walter, M. D. *Organometallics* **2012**, *31*, 672-679.

(27) Berthet, J.-C.; Thuéry, P.; Ephritikhine, M. *C. R. Chimie* **2014**, *17*, 526-533.

Table S6. Computed key geometric parameters and energy gaps between different spin states.

		Re-N (Å)	Re-CO (Å)	Re-Cl (Å)	C–N_{chel} (Å)	C_{py}–C_{py} (Å)	C–O (Å)
$[Re(bpy)(CO)_3]^-$	S = 0	2.107, 2.113	1.884, 1.918, 1.922		1.404, 1.400	1.411	1.175, 1.175
$[Re(bpy)(CO)_3]^0$	S = 1/2	2.140, 2.140	1.879, 1.925, 1.926		1.378, 1.378	1.444	1.167, 1.164, 1.164
$[Re(bpy)(CO)_3]^+$	S = 0	2.181, 2.183	1.864, 1.943, 1.943		1.344, 1.344	1.491	1.156, 1.149, 1.149
$[Re(bpy)(CO)_4]^-$			CO dissociation				
$[Re(bpy)(CO)_4]^0$	S = 1/2	2.172, 2.171	2.014, 2.013, 1.942, 1.942		1.392, 1.392	1.424	1.143, 1.143, 1.157,1.157
$[Re(bpy)(CO)_4]^+$	S = 0	2.190, 2.190	2.016, 2.016, 1.943, 1.944		1.357, 1.357	1.474	1.140, 1.140, 1.152, 1.152
$[Re(bpy)(CO)_3Cl]^0$	S = 0	2.192, 2.193	1.907, 1.924, 1.923	2.514	1.355, 1.355	1.476	1.164, 1.159, 1.159
$[Re(bpy)(CO)_3Cl]^-$	S = 1/2	2.171, 2.172	1.894, 1.923, 1.923, 2.561		1.391, 1.390	1.425	1.169, 1.165, 1.165

$[Re(Tp)(bpy)Cl]^{2+}$	S = 3/2	
$[Re(Tp)(bpy)Cl]^{2+}$	S = 1/2	7.5 kcal/mol
$[Re(Tp)(bpy)Cl]^+$	S = 1	
$[Re(Tp)(bpy)Cl]^+$	S = 0	11.2 kcal/mol
$[Re(Tp)(bpy)Cl]^0$	S = 1/2	
$[Re(Tp)(bpy)Cl]^0$	S = 3/2	17.9 kcal/mol
$[Re(Tp)(bpy)Cl]^-$	S = 0	
$[Re(Tp)(bpy)Cl]^-$	S = 1	7.0 kcal/mol

		C–N_{chel} (Å)	C_{py}–C_{py} (Å)	Re-N_{bpy} (Å)	Re-N_{Tp} (Å)	Re-Cl (Å)
$[Re(Tp)(bpy)Cl]^{2+}$	S = 3/2	1.362, 1.363	1.468	2.119, 2.121	2.077, 2.077, 2.084	2.318
$[Re(Tp)(bpy)Cl]^{2+}$	S = 1/2	1.364, 1.363	1.468	2.116, 2.116	2.080, 2.075, 2.042	2.304
$[Re(Tp)(bpy)Cl]^{+}$	S = 1	1.364, 1.364	1.462	2.107, 2.105	2.101, 2.102, 2.085	2.408
$[Re(Tp)(bpy)Cl]^{+}$	S = 0	1.371, 1.369	1.454	2.077, 2.078	2.132, 2.124, 2.029	2.354
$[Re(Tp)(bpy)Cl]^{0}$	S = 1/2	1.381, 1.381	1.443	2.055, 2.053	2.131, 2.131, 2.079	2.440
$[Re(Tp)(bpy)Cl]^{0}$	S = 3/2	1.398, 1.397	1.417	2.101, 2.098	2.121, 2.120, 2.082	2.431
$[Re(Tp)(bpy)Cl]^{-}$	S = 0	1.399, 1.399	1.438	2.018, 2.019	2.130, 2.130, 2.054	2.511
$[Re(Tp)(bpy)Cl]^{-}$	S = 1	1.410, 1.409	1.407	2.077, 2.073	2.128, 2.128, 2.069	2.479

			C–N_{chel} (Å)	C_{py}–C_{py} (Å)	Re-N_{bpy} (Å)
$[Re(bpy)_3]^{2+}$	S = 1/2		1.366, 1.367, 1.367, 1.367, 1.366, 1.367	1.460, 1.461, 1.461	2.091, 2.090, 2.092, 2.092, 2.092, 2.091
$[Re(bpy)_3]^{+}$	S = 0		1.374, 1.374, 1.374, 1.374, 1.375, 1.374	1.456, 1.455, 1.455	2.076, 2.077, 2.077, 2.075, 2.075, 2.076
$[Re(bpy)_3]^{+}$	S = 1	12.5 kcal/mol	1.383, 1.384, 1.382, 1.382, 1.373, 1.373	1.435, 1.437, 1.448	2.083, 2.080, 2.079, 2.081, 2.083, 2.084
$[Re(bpy)_3]^{0}$	S = 1/2		1.389, 1.389, 1.390, 1.389, 1.389, 1.389	1.434, 1.433, 1.433	2.067, 2.072, 2.067, 2.073, 2.076, 2.076
$[Re(bpy)_3]^{0}$	S = 3/2	14.5 kcal/mol	1.388, 1.389, 1.400, 1.399, 1.388, 1.390	1.432, 1.414, 1.431	2.073, 2.076, 2.100, 2.101, 2.074, 2.079
$[Re(bpy)_3]^{-}$	S = 0		1.404, 1.403, 1.407, 1.404, 1.405, 1.407	1.416, 1.414, 1.413	2.059, 2.063, 2.059, 2.071, 2.070, 2.066
$[Re(bpy)_3]^{-}$	S = 1	5.6 kcal/mol	1.397, 1.397, 1.407, 1.403, 1.400, 1.403	1.431, 1.414, 1.423	2.064, 2.063, 2.084, 2.094, 2.074, 2.068
$[Re(bpy)_3]^{-}$	S = 2	13.6 kcal/mol	1.403, 1.404, 1.403, 1.405, 1.405, 1.404	1.413, 1.412, 1.412	2.096, 2.097, 2.092, 2.092, 2.092, 2.093

		$C–N_{chel}$ (Å)	$C_{py}–C_{py}$ (Å)	Re-N (Å)
$[Re(tpy)_2]^{2+}$	$S = 1/2$	1.375, 1.374, 1.371, 1.371 1.372, 1.379, 1.369, 1.366	1.456, 1.459 1.473, 1.454	2.085, 2.095, 2.081, 2.119, 2.016, 2.018
$[Re(tpy)_2]^{1+}$	$S = 0$	1.379, 1.380, 1.380, 1.380 1.383, 1.383, 1.383, 1.383	1.450, 1.450 1.450, 1.450	2.001, 1.998, 2.078, 2.078, 2.076, 2.076
$[Re(tpy)_2]^{0}$	$S = 1/2$	1.382, 1.402, 1.389, 1.399 1.378, 1.395, 1.379, 1.391	1.448, 1.429 1.440, 1.430	2.071, 2.066, 2.065, 2.075, 2.003, 2.008
$[Re(tpy)_2]^{1-}$	$S = 1$	1.429, 1.384, 1.418, 1.405 1.411, 1.371, 1.398 , 1.381	1.408, 1.451 1.417, 1.432	2.059, 2.049, 2.075, 2.055, 1.994, 2.037
$[Re(tpy)_2Cl]^{2+}$	$S = 0$	1.366, 1.363, 1.366, 1.363, 1.359, 1.358,1.359, 1.358	1.454, 1.458 1.454, 1.458	2.071, 2.069, 2.101, 2.168, 2.164, 2.101
$[[Re(tpy')(py)(CO)_2]^{+}$	$S = 0$	1.372, 1.371, 1.346, 1.345	1.478, 1.478	2.098, 2.139, 2.142, Re-N_{py} 2.255 Re-CO 1.900 (trans tpy), 1.893 (trans-py)
$[Re(^{Me}DAB)(PPh_3)Cl_3]$	$S = 0$	1.321, 1.326	1.399	2.028, 2.050, Re-Cl: 2.358, 2.361, 2.476 Re-P: 2.413
$[Re^{III}Cl_3(bpy^0)(PPh_3)]^0$	$S = 1$	1.360, 1.362	1.456	

Orca input file for geometry optimizations

```
! uks b3lyp rijcosx gridx6 def2-tzvp(-f) def2-tzvp/j tightscf zora cosmo(water) uno uco d3bj slowconv opt pal4

%basis newgto C "def2-SVP" end
       newgto H "def2-SVP" end
       end

%scf shift shift 0.5 erroff 0 end
          maxiter 250 end

*xyz 0 3
```

$[Re(bpy)(CO)_3]^-$

Re	13.477935	17.549708	3.792362
O	16.500404	17.926517	3.486653
O	13.374500	15.412421	1.559621
O	13.839338	15.321831	5.911500
N	12.616723	19.064412	2.597651
N	12.677074	18.930079	5.168371
C	15.336865	17.795103	3.606368
C	13.431605	16.215747	2.415110
C	13.714007	16.157090	5.095247
C	12.746230	18.812426	6.539181
H	13.236673	17.910806	6.904037
C	12.248174	19.738968	7.412543
H	12.342146	19.565747	8.486428
C	11.616324	20.916361	6.902238
H	11.208726	21.671136	7.577807
C	11.542603	21.072018	5.540716
H	11.074834	21.960675	5.113796
C	12.072104	20.089469	4.658149
C	12.040997	20.161876	3.249035
C	11.479306	21.229233	2.492954
H	11.032270	22.070375	3.024964
C	11.499242	21.211070	1.120554
H	11.068554	22.031091	0.542026
C	12.106127	20.094124	0.467234
H	12.158290	20.032211	-0.621434
C	12.634387	19.083391	1.223632
H	13.109332	18.222374	0.753989

$[Re(bpy)(CO)_3]^0$

Re	13.407065	17.505272	3.781104
O	16.412564	17.991739	3.708680
O	13.641158	15.450957	1.485483
O	13.764559	15.235338	5.844312
N	12.583102	19.067455	2.572151
N	12.666452	18.944504	5.181640
C	15.262738	17.794711	3.738621
C	13.569925	16.216693	2.358747
C	13.647173	16.084608	5.057787
C	12.751652	18.816625	6.534134
H	13.224162	17.905450	6.896961
C	12.279567	19.768020	7.411623
H	12.378298	19.603752	8.485479
C	11.677848	20.936712	6.896484
H	11.292753	21.709266	7.564297

C	11.588105	21.085311	5.524042
H	11.132143	21.978914	5.098502
C	12.087608	20.085073	4.668111
C	12.039129	20.151940	3.226489
C	11.480938	21.223260	2.502641
H	11.053525	22.070180	3.038778
C	11.476742	21.202871	1.119337
H	11.045465	22.030625	0.553331
C	12.045201	20.092198	0.458897
H	12.071452	20.029133	-0.629897
C	12.577956	19.067358	1.210312
H	13.027492	18.198299	0.732684

$[Re(bpy)(CO)_3]^+$

Re	13.266325	17.458021	3.777863
O	16.254218	17.897701	3.779165
O	13.610967	15.437948	1.463291
O	13.639535	15.163767	5.816335
N	12.671863	19.151643	2.539739
N	12.745624	19.016430	5.214785
C	15.115303	17.697480	3.776836
C	13.491561	16.179176	2.332927
C	13.513873	16.012189	5.051908
C	12.906381	18.900824	6.532405
H	13.456361	18.031821	6.890686
C	12.406926	19.860061	7.416245
H	12.574695	19.746805	8.488003
C	11.693342	20.924811	6.895663
H	11.268328	21.685804	7.553750
C	11.515127	21.027194	5.511547
H	10.957630	21.863273	5.092967
C	12.071496	20.054410	4.690737
C	12.014139	20.119307	3.201846
C	11.376338	21.143367	2.513244
H	10.832476	21.923101	3.043459
C	11.449916	21.164835	1.115995
H	10.958499	21.966421	0.560150
C	12.146917	20.171314	0.452262
H	12.235114	20.155454	-0.634761
C	12.734698	19.155082	1.208537
H	13.277118	18.338024	0.735147

$[Re(bpy)(CO)_4]^0$

Re	7.430228	7.217895	2.241378
O	6.426272	8.326656	-0.538208
O	4.575544	6.160066	2.820645

O	8.200592	4.525572	0.914666
O	8.422694	6.116098	5.026910
N	9.341309	8.204696	1.941507
N	7.157747	9.184216	3.121294
C	6.802528	7.938071	0.468478
C	5.644738	6.545959	2.603214
C	7.901242	5.527332	1.410813
C	8.072084	6.532014	4.021777
C	10.410266	7.654293	1.325838
H	10.280172	6.635364	0.961942
C	11.609276	8.313755	1.149822
H	12.435404	7.814084	0.643222
C	11.726585	9.641716	1.645057
C	10.649047	10.221311	2.273884
H	10.722938	11.238004	2.658855
C	9.428387	9.505272	2.430686
C	8.263632	10.027522	3.061016
C	8.167091	11.333043	3.621462
H	9.029876	11.997866	3.574174
C	7.001625	11.756854	4.217378
C	5.887111	10.874111	4.267488
H	4.943535	11.163766	4.730499
C	6.022426	9.619273	3.710053
H	5.191967	8.912911	3.727225
H	12.659868	10.197040	1.527399
H	6.935876	12.758380	4.647502

$[Re(bpy)(CO)_4]^+$

Re	7.428272	7.218167	2.237721
O	6.408302	8.306190	-0.543547
O	4.580809	6.153222	2.820070
O	8.196782	4.528626	0.912693
O	8.405046	6.101054	5.022984
N	9.349987	8.227064	1.944566
N	7.171397	9.204710	3.122598
C	6.790492	7.926081	0.461072
C	5.644009	6.537849	2.599568
C	7.893789	5.523593	1.408070
C	8.063622	6.521051	4.019600
C	10.403582	7.662175	1.333378
H	10.273995	6.644071	0.971776
C	11.609622	8.332201	1.161408
H	12.436064	7.829982	0.657678
C	11.727178	9.635700	1.643153
C	10.633562	10.221792	2.276935

H	10.704625	11.237550	2.660831
C	9.448157	9.495979	2.416692
C	8.242873	10.036354	3.070931
C	8.177948	11.321502	3.615010
H	9.041247	11.983198	3.567747
C	6.999339	11.752955	4.220527
C	5.907761	10.885590	4.267148
H	4.964099	11.173864	4.731011
C	6.035265	9.620169	3.705280
H	5.205584	8.915417	3.722072
H	12.658339	10.193385	1.527921
H	6.938311	12.753647	4.651078

$[Re(bpy)(CO)_3Cl]^-$

Re	7.528345	7.122753	2.355625
O	4.651295	6.084170	2.777078
O	8.268285	4.484564	0.932649
O	8.401170	5.980113	5.060196
N	9.414166	8.146035	2.015946
N	7.206508	9.122773	3.136612
C	5.741406	6.463616	2.619448
C	7.980131	5.472633	1.478190
C	8.067333	6.415986	4.027993
C	10.494406	7.600107	1.425426
H	10.387538	6.562252	1.108444
C	11.680158	8.279138	1.215070
H	12.517012	7.778015	0.727355
C	11.765870	9.629095	1.652213
C	10.672693	10.208124	2.255391
H	10.721234	11.242789	2.595566
C	9.469602	9.468854	2.440701
C	8.287760	9.991917	3.039741
C	8.154692	11.322485	3.529285
H	9.002282	12.004945	3.457693
C	6.970365	11.750565	4.084768
C	5.876444	10.845862	4.163620
H	4.916872	11.138056	4.591436
C	6.055681	9.563378	3.679304
H	5.243346	8.836758	3.720817
H	12.685928	10.201715	1.511842
H	6.875020	12.772634	4.458759
Cl	6.865790	8.178007	0.117741

$[Re(bpy)(CO)_3Cl]^0$

Re	7.521526	7.122437	2.337385
O	4.641196	6.093433	2.722650

O	8.268433	4.490858	0.916993
O	8.357790	5.948541	5.048355
N	9.432774	8.155403	2.046609
N	7.227807	9.131022	3.166882
C	5.729465	6.465057	2.577296
C	7.972711	5.473323	1.456795
C	8.039850	6.389056	4.019138
C	10.502386	7.589755	1.468494
H	10.403305	6.544901	1.178943
C	11.683903	8.287357	1.239814
H	12.525043	7.781790	0.764097
C	11.757100	9.625211	1.628732
C	10.646011	10.212964	2.229208
H	10.681571	11.255973	2.539182
C	9.487480	9.454994	2.426533
C	8.263872	9.996359	3.048828
C	8.152239	11.315902	3.497988
H	8.989037	12.005314	3.396838
C	6.958866	11.746904	4.073336
C	5.900963	10.844344	4.186822
H	4.946354	11.131991	4.628915
C	6.079040	9.545959	3.720095
H	5.278528	8.810668	3.787254
H	12.666565	10.206892	1.466661
H	6.859086	12.774730	4.426865
Cl	6.928430	8.266200	0.178206

$[Re(bpy)_3]^{2+}$

Re	0.047247	0.007444	3.819465
N	-0.096064	1.830336	4.835481
C	0.665527	2.171505	5.901747
H	1.432947	1.455648	6.192845
C	0.484735	3.350244	6.600292
H	1.125148	3.559383	7.458939
C	-0.511111	4.263841	6.201144
C	-1.275109	3.916151	5.086618
H	-2.054228	4.591993	4.733945
C	-1.060673	2.705204	4.420089
C	-0.737497	5.541800	6.954331
H	-1.476473	6.181837	6.452839
H	0.204468	6.103107	7.061707
H	-1.099424	5.325368	7.973319
N	-1.472773	1.016665	2.798312
C	-2.137678	0.513899	1.731565
H	-1.836282	-0.478324	1.401007

C	-3.142978	1.207779	1.085674
H	-3.636190	0.747037	0.228254
C	-3.524869	2.485870	1.539553
C	-2.841722	2.993000	2.645233
H	-3.102768	3.975715	3.036657
C	-1.824118	2.254482	3.259262
C	-4.620641	3.253098	0.859745
H	-4.796801	4.222962	1.344422
H	-5.560306	2.676899	0.873525
H	-4.368405	3.430768	-0.198347
N	-1.474738	-0.988410	4.853887
C	-2.136176	-0.474139	5.917224
H	-1.841720	0.525733	6.229908
C	-3.127878	-1.167481	6.584552
H	-3.617475	-0.697546	7.439115
C	-3.498647	-2.457723	6.157328
C	-2.820468	-2.976164	5.053555
H	-3.073348	-3.968974	4.682945
C	-1.817002	-2.237186	4.417238
C	-4.576912	-3.226668	6.862911
H	-4.740738	-4.210193	6.402064
H	-5.526000	-2.666239	6.842767
H	-4.314461	-3.375431	7.923032
N	-0.104454	-1.823880	2.820066
C	0.654745	-2.178849	1.756806
H	1.411660	-1.460132	1.445428
C	0.486822	-3.376317	1.087419
H	1.125948	-3.596800	0.230667
C	-0.492498	-4.294962	1.514947
C	-1.256737	-3.930578	2.623772
H	-2.023335	-4.609322	2.997658
C	-1.055947	-2.701260	3.259999
C	-0.699995	-5.597424	0.799434
H	-1.438727	-6.227807	1.313372
H	0.248002	-6.153603	0.721275
H	-1.051823	-5.416828	-0.229907
N	1.682428	-0.790134	4.849937
C	1.579231	-1.616921	5.917193
H	0.568935	-1.882556	6.223713
C	2.682226	-2.100291	6.594072
H	2.529082	-2.755149	7.453728
C	3.980677	-1.751617	6.171781
C	4.078980	-0.915027	5.059642
H	5.061290	-0.622382	4.689856

C	2.930552	-0.443246	4.414638
C	5.192018	-2.264109	6.893702
H	6.121128	-1.909390	6.427297
H	5.199815	-3.366461	6.904073
H	5.180699	-1.933626	7.945185
N	1.695819	0.791635	2.802552
C	1.607488	1.619724	1.734921
H	0.601282	1.888605	1.417610
C	2.719863	2.101549	1.072459
H	2.578852	2.758476	0.212326
C	4.012350	1.749242	1.510030
C	4.095205	0.909451	2.620818
H	5.072213	0.613566	3.001955
C	2.938095	0.439472	3.251124
C	5.233884	2.261524	0.805464
H	6.156025	1.901678	1.281695
H	5.245125	3.363914	0.801153
H	5.234677	1.936545	-0.247756

$[Re(bpy)_3]^+$

Re	0.027388	0.010079	3.844730
N	-0.148849	1.796474	4.886279
C	0.589244	2.133662	5.978140
H	1.318419	1.392168	6.301519
C	0.438237	3.329174	6.650730
H	1.065979	3.527536	7.522002
C	-0.514279	4.278107	6.216174
C	-1.263974	3.936005	5.093607
H	-2.009916	4.633774	4.710670
C	-1.076234	2.708628	4.441870
C	-0.705940	5.578363	6.944661
H	-1.387028	6.248970	6.401200
H	0.256330	6.096426	7.087383
H	-1.126608	5.404036	7.949785
N	-1.444650	1.035556	2.800646
C	-2.093111	0.555568	1.705693
H	-1.774314	-0.426238	1.360971
C	-3.094008	1.250168	1.057530
H	-3.569216	0.798720	0.184269
C	-3.493886	2.523607	1.520106
C	-2.829545	3.014891	2.641260
H	-3.100266	3.991826	3.042616
C	-1.818749	2.272212	3.268799
C	-4.583337	3.294360	0.829610
H	-4.764146	4.262726	1.317128

H	-5.527425	2.724006	0.829833
H	-4.323850	3.481425	-0.225712
N	-1.446178	-1.015792	4.887164
C	-2.104500	-0.530694	5.973768
H	-1.794476	0.455993	6.312085
C	-3.104190	-1.226623	6.622441
H	-3.587512	-0.770699	7.488934
C	-3.492661	-2.506586	6.168803
C	-2.818618	-3.002775	5.055467
H	-3.080759	-3.984688	4.660676
C	-1.809541	-2.258561	4.427370
C	-4.580643	-3.279049	6.859617
H	-4.753336	-4.251810	6.377906
H	-5.528137	-2.714434	6.851140
H	-4.324819	-3.457389	7.917382
N	-0.139728	-1.782724	2.810131
C	0.603633	-2.122144	1.722852
H	1.325228	-1.376049	1.393134
C	0.467046	-3.325845	1.061600
H	1.098459	-3.525754	0.193337
C	-0.475925	-4.280462	1.503715
C	-1.232271	-3.935000	2.620983
H	-1.971381	-4.637127	3.009112
C	-1.059050	-2.699342	3.260730
C	-0.650872	-5.590653	0.789062
H	-1.329948	-6.260939	1.335406
H	0.317033	-6.101671	0.659583
H	-1.065534	-5.431677	-0.221059
N	1.657739	-0.740495	4.889577
C	1.571443	-1.540733	5.986081
H	0.562413	-1.769503	6.324425
C	2.676710	-2.040603	6.643292
H	2.527145	-2.674647	7.519814
C	3.978208	-1.732301	6.187956
C	4.066144	-0.917618	5.061965
H	5.046287	-0.652474	4.664288
C	2.914178	-0.432443	4.426326
C	5.193925	-2.262910	6.893302
H	6.120565	-1.931505	6.403653
H	5.186392	-3.365728	6.915790
H	5.217106	-1.922817	7.942078
N	1.659275	0.752769	2.799414
C	1.575280	1.558344	1.706365
H	0.566802	1.805695	1.379607

C	2.681907	2.040076	1.038285
H	2.533955	2.678998	0.165023
C	3.982796	1.707358	1.478277
C	4.068568	0.889990	2.602391
H	5.048118	0.607119	2.989132
C	2.915203	0.423914	3.249893
C	5.199731	2.216344	0.759237
H	6.125807	1.865957	1.236562
H	5.213216	3.319160	0.739144
H	5.203504	1.878319	-0.290459

$[Re(bpy)_3]^0$

Re	-0.033007	-0.003554	3.845228
N	-0.210662	1.762496	4.915608
C	0.482189	2.062933	6.049947
H	1.172019	1.291561	6.391492
C	0.342244	3.247558	6.736261
H	0.935736	3.413325	7.638005
C	-0.567301	4.240210	6.270903
C	-1.270853	3.945740	5.115413
H	-1.977577	4.674778	4.714237
C	-1.094930	2.719368	4.434562
C	-0.740953	5.533553	7.018122
H	-1.436791	6.210004	6.499983
H	0.223999	6.055494	7.137795
H	-1.130164	5.354473	8.035545
N	-1.449829	1.061083	2.780529
C	-2.077415	0.616253	1.654654
H	-1.798756	-0.386171	1.332956
C	-2.997488	1.359558	0.952510
H	-3.457150	0.930470	0.059532
C	-3.339903	2.671925	1.388827
C	-2.713795	3.128480	2.535938
H	-2.943462	4.126017	2.914093
C	-1.780195	2.331438	3.236749
C	-4.336231	3.500421	0.626333
H	-4.477538	4.488587	1.087994
H	-5.318310	2.998219	0.581346
H	-4.011604	3.651941	-0.417555
N	-1.449673	-1.066699	4.910845
C	-2.074876	-0.621616	6.038073
H	-1.793402	0.379773	6.360501
C	-2.996334	-1.363315	6.739991
H	-3.454091	-0.934102	7.633887
C	-3.343075	-2.673946	6.302158

C	-2.719230	-3.130747	5.153809
H	-2.952215	-4.126994	4.774306
C	-1.784080	-2.335379	4.453402
C	-4.341277	-3.500502	7.064262
H	-4.487271	-4.486874	6.600256
H	-5.321255	-2.994563	7.112398
H	-4.015300	-3.656134	8.107116
N	-0.213772	-1.768232	2.774775
C	0.478173	-2.069109	1.639829
H	1.169995	-1.299075	1.299275
C	0.334530	-3.252234	0.951917
H	0.927354	-3.418384	0.049784
C	-0.578090	-4.242813	1.415557
C	-1.280424	-3.948045	2.571777
H	-1.989540	-4.675343	2.971905
C	-1.100538	-2.723401	3.254444
C	-0.756656	-5.533879	0.665629
H	-1.451296	-6.210721	1.184864
H	0.207010	-6.056810	0.540356
H	-1.150039	-5.351556	-0.349632
N	1.597135	-0.724813	4.908506
C	1.521237	-1.494677	6.029902
H	0.512220	-1.743242	6.356178
C	2.622825	-1.938497	6.725106
H	2.477183	-2.551555	7.617257
C	3.932852	-1.593942	6.283645
C	4.019631	-0.822842	5.137382
H	5.000245	-0.534620	4.754886
C	2.863915	-0.394513	4.444796
C	5.145986	-2.054391	7.042702
H	6.075107	-1.706080	6.568133
H	5.181692	-3.155861	7.106893
H	5.130203	-1.678816	8.080322
N	1.596503	0.720009	2.782210
C	1.519704	1.487033	1.659084
H	0.510294	1.728797	1.328873
C	2.620934	1.937043	0.967171
H	2.474594	2.547603	0.073445
C	3.931467	1.602335	1.414417
C	4.019069	0.833455	2.562183
H	5.000179	0.552781	2.949010
C	2.863591	0.398119	3.250783
C	5.144462	2.069702	0.659321
H	6.074154	1.733207	1.141257

H	5.169881	3.170973	0.588206
H	5.138037	1.687329	-0.375903

$[Re(bpy)_3]^-$

Re	0.087658	0.031494	3.866786
N	-0.176392	1.769418	4.939564
C	0.491208	2.102119	6.084079
H	1.267708	1.397053	6.383343
C	0.227341	3.223232	6.831351
H	0.813292	3.414486	7.733442
C	-0.811388	4.128842	6.426145
C	-1.478388	3.823142	5.260316
H	-2.275961	4.481734	4.907061
C	-1.168098	2.663643	4.495230
C	-1.137456	5.336722	7.260779
H	-1.912914	5.958314	6.787557
H	-0.244437	5.966256	7.423491
H	-1.499210	5.047639	8.264110
N	-1.344916	1.052806	2.774261
C	-1.911509	0.614823	1.614610
H	-1.549570	-0.349980	1.260877
C	-2.874381	1.306151	0.917935
H	-3.283675	0.877738	0.000384
C	-3.329720	2.577099	1.401229
C	-2.771074	3.033708	2.575877
H	-3.082828	3.998923	2.980971
C	-1.789197	2.282766	3.283370
C	-4.371190	3.352102	0.641328
H	-4.603428	4.308773	1.132526
H	-5.310247	2.777196	0.550930
H	-4.039246	3.568686	-0.389430
N	-1.342412	-1.012436	4.939090
C	-1.937537	-0.582223	6.087581
H	-1.601651	0.391479	6.442945
C	-2.896699	-1.290045	6.772116
H	-3.329034	-0.866160	7.681175
C	-3.319645	-2.572586	6.286642
C	-2.733389	-3.021571	5.123517
H	-3.020258	-3.993741	4.716405
C	-1.754793	-2.254672	4.427878
C	-4.357171	-3.365249	7.033382
H	-4.567382	-4.325464	6.538918
H	-5.307159	-2.806751	7.112889
H	-4.034606	-3.577610	8.068128
N	-0.132654	-1.717979	2.790149

C	0.551207	-2.038593	1.653472
H	1.314866	-1.318258	1.358848
C	0.317312	-3.166094	0.904188
H	0.914078	-3.346172	0.006959
C	-0.706705	-4.091334	1.302757
C	-1.390526	-3.797137	2.461382
H	-2.178664	-4.470597	2.807608
C	-1.111506	-2.628664	3.227195
C	-1.001997	-5.306524	0.466701
H	-1.769026	-5.943353	0.933406
H	-0.095297	-5.918289	0.311945
H	-1.360572	-5.025248	-0.540065
N	1.706135	-0.633612	4.958858
C	1.634204	-1.320400	6.135699
H	0.622603	-1.522782	6.487376
C	2.730757	-1.741504	6.848245
H	2.584260	-2.292306	7.780048
C	4.050533	-1.451540	6.368831
C	4.141857	-0.766632	5.175467
H	5.125086	-0.520246	4.768570
C	2.986280	-0.361687	4.452679
C	5.258882	-1.881614	7.153828
H	6.192488	-1.580683	6.655058
H	5.279997	-2.977545	7.290725
H	5.256510	-1.441483	8.166507
N	1.700778	0.685821	2.766973
C	1.625630	1.399232	1.604702
H	0.615286	1.669110	1.297619
C	2.716550	1.759274	0.852438
H	2.567474	2.333905	-0.064641
C	4.034142	1.373745	1.268844
C	4.130189	0.671559	2.451316
H	5.111039	0.354349	2.812267
C	2.982466	0.336081	3.220885
C	5.232458	1.728588	0.432699
H	6.164673	1.359767	0.886215
H	5.322897	2.821728	0.301761
H	5.156065	1.299262	-0.582053

$[Re(Tp)(bpy)Cl]^{2+}$

Re	0.571219	3.243040	4.056440
Cl	-0.128209	5.231814	5.019178
N	1.698170	2.754864	5.785868
N	2.475470	4.074721	3.640107
N	1.220229	1.464658	3.185913

N	0.371687	0.738180	2.406519
N	-1.199450	2.254266	4.505576
N	-1.726963	1.390971	3.586119
N	-0.372589	3.665066	2.255351
N	-0.989926	2.653341	1.575089
C	1.233782	1.995988	6.793637
C	1.987749	1.756157	7.935520
C	3.259982	2.320117	8.032551
C	3.747755	3.089258	6.974891
C	2.949491	3.289909	5.851722
C	3.383430	4.024963	4.654015
C	4.642279	4.601507	4.505818
C	4.974097	5.221171	3.299816
C	4.041222	5.237828	2.262488
C	2.799128	4.652035	2.470042
C	2.408527	0.825281	3.206381
C	2.322696	-0.327332	2.430083
C	1.011433	-0.341575	1.942430
C	-2.037607	2.288874	5.564303
C	-3.106588	1.428212	5.332451
C	-2.870647	0.887170	4.063571
C	-0.572644	4.807566	1.562673
C	-1.310846	4.526769	0.416909
C	-1.559619	3.150311	0.471567
B	-1.067858	1.236925	2.193896
H	0.238656	1.573164	6.675256
H	1.573466	1.135563	8.730334
H	3.876375	2.156227	8.917977
H	4.745295	3.521943	7.024289
H	5.364165	4.563805	5.320368
H	5.956753	5.677887	3.173108
H	4.261096	5.697613	1.298999
H	2.042961	4.639369	1.687503
H	3.248035	1.222621	3.769266
H	3.105360	-1.057147	2.242490
H	0.497997	-1.050692	1.298244
H	-1.827112	2.931304	6.415247
H	-3.947073	1.225287	5.990161
H	-3.451459	0.184491	3.471356
H	-0.183697	5.752237	1.932883
H	-1.633925	5.226021	-0.349013
H	-2.113581	2.500460	-0.201390
H	-1.689058	0.497199	1.501652

[Re(Tp)(bpy)Cl]+

Re	0.603449	3.220337	4.048760
Cl	-0.161854	5.286310	5.020130
N	1.717391	2.775864	5.781654
N	2.486362	4.081450	3.667646
N	1.220708	1.435892	3.165538
N	0.361832	0.717532	2.392726
N	-1.197043	2.234063	4.499903
N	-1.736450	1.382668	3.580620
N	-0.367461	3.646443	2.234736
N	-1.002310	2.642142	1.565690
C	1.236950	2.061294	6.819103
C	1.979291	1.828783	7.968527
C	3.279506	2.335620	8.050662
C	3.787006	3.057214	6.974036
C	2.986708	3.270881	5.848355
C	3.419032	4.004481	4.659483
C	4.683738	4.579374	4.506669
C	4.995204	5.251824	3.328314
C	4.031851	5.320384	2.317305
C	2.798920	4.716904	2.520567
C	2.397028	0.781619	3.173659
C	2.296641	-0.374138	2.395134
C	0.983353	-0.372560	1.918893
C	-2.032595	2.262575	5.554683
C	-3.116478	1.411377	5.322542
C	-2.886260	0.878065	4.052600
C	-0.563885	4.778622	1.533818
C	-1.323229	4.502872	0.393642
C	-1.581999	3.131874	0.459664
B	-1.074252	1.232435	2.192943
H	0.232144	1.660707	6.708348
H	1.540972	1.247226	8.780409
H	3.893120	2.163198	8.936545
H	4.800401	3.454239	7.006265
H	5.419638	4.501280	5.306237
H	5.977423	5.708768	3.198295
H	4.229821	5.826220	1.371766
H	2.033523	4.726868	1.747391
H	3.243338	1.172671	3.731514
H	3.069818	-1.112474	2.200191
H	0.455502	-1.074273	1.278329
H	-1.814063	2.899084	6.407989
H	-3.957079	1.210777	5.981252
H	-3.468846	0.180600	3.456098

H	-0.162940	5.721236	1.896372
H	-1.648442	5.201244	-0.372548
H	-2.144424	2.479350	-0.203477
H	-1.701405	0.490484	1.500681

[Re(Tp)(bpy)Cl]0

Re	0.690477	3.164932	4.025463
Cl	-0.057294	5.265214	5.016034
N	1.756786	2.729735	5.727067
N	2.522816	4.015320	3.657794
N	1.185898	1.366689	3.108321
N	0.270254	0.696588	2.354859
N	-1.163851	2.230659	4.510277
N	-1.777002	1.433210	3.593023
N	-0.320996	3.641086	2.211032
N	-1.041702	2.680691	1.569517
C	1.365728	1.865613	6.703236
C	2.063282	1.698529	7.882922
C	3.239039	2.445444	8.102099
C	3.677192	3.296092	7.100367
C	2.943333	3.413859	5.905945
C	3.372506	4.145329	4.738703
C	4.579388	4.859386	4.631100
C	4.956132	5.405390	3.415004
C	4.114223	5.210504	2.300682
C	2.930184	4.518819	2.461532
C	2.324897	0.653200	3.083349
C	2.146261	-0.495302	2.301929
C	0.824099	-0.423981	1.860104
C	-1.933294	2.225871	5.609362
C	-3.058817	1.409816	5.405426
C	-2.912926	0.921971	4.109299
C	-0.447315	4.768734	1.495774
C	-1.259068	4.537708	0.372450
C	-1.609885	3.192943	0.458940
B	-1.152884	1.277686	2.193895
H	0.444503	1.319926	6.507048
H	1.689412	0.999596	8.633288
H	3.800286	2.346303	9.033072
H	4.597670	3.867189	7.224054
H	5.218876	4.969859	5.507591
H	5.889784	5.962839	3.321074
H	4.374711	5.605476	1.317445
H	2.244922	4.362175	1.629605
H	3.198044	1.006912	3.624835

H	2.875040	-1.271798	2.084250
H	0.244597	-1.094988	1.231222
H	-1.641244	2.810132	6.477747
H	-3.863490	1.198827	6.105327
H	-3.533845	0.249859	3.522587
H	0.039802	5.679836	1.832346
H	-1.549150	5.249558	-0.396110
H	-2.218062	2.567495	-0.189559
H	-1.819665	0.558470	1.508333

[Re(Tp)(bpy)Cl]–

Re	0.698580	3.163038	4.029879
Cl	-0.109577	5.325675	5.017789
N	1.734778	2.729503	5.706472
N	2.493047	4.009189	3.654101
N	1.166821	1.379904	3.123799
N	0.250990	0.708766	2.366575
N	-1.156268	2.245656	4.533563
N	-1.782253	1.458700	3.610207
N	-0.294181	3.657534	2.211355
N	-1.036032	2.703457	1.578072
C	1.400058	1.801786	6.657475
C	2.091423	1.638147	7.838995
C	3.233390	2.433943	8.099118
C	3.644419	3.318295	7.112209
C	2.923885	3.438343	5.910016
C	3.347367	4.173750	4.749050
C	4.536209	4.917401	4.635751
C	4.928978	5.444087	3.413691
C	4.112243	5.181449	2.287359
C	2.943785	4.466136	2.444830
C	2.302114	0.652932	3.102448
C	2.114640	-0.503179	2.316482
C	0.802440	-0.429625	1.868750
C	-1.919436	2.223862	5.638354
C	-3.042193	1.399476	5.438170
C	-2.909745	0.930353	4.133652
C	-0.398014	4.776563	1.476446
C	-1.203367	4.543804	0.346366
C	-1.584028	3.208333	0.451751
B	-1.154833	1.301764	2.209429
H	0.506992	1.218351	6.436552
H	1.743335	0.897480	8.563001
H	3.787150	2.338735	9.035208
H	4.544849	3.919936	7.252255

H	5.155219	5.066183	5.523056
H	5.848931	6.024668	3.321138
H	4.386313	5.542659	1.293569
H	2.284605	4.260414	1.601953
H	3.174822	1.001895	3.646741
H	2.841604	-1.284137	2.104396
H	0.216955	-1.095555	1.240349
H	-1.616797	2.797774	6.509843
H	-3.838994	1.174493	6.143388
H	-3.537494	0.267515	3.543108
H	0.105709	5.681332	1.805114
H	-1.474880	5.248955	-0.435762
H	-2.205081	2.587274	-0.189231
H	-1.838824	0.592388	1.522827

$[Re(tpy)_2]^{2+}$ S = 1/2

Re	10.346092	11.751988	11.052438
N	9.888103	12.236019	9.076870
C	9.447207	13.447744	8.666528
H	9.274676	14.187932	9.447114
C	9.228507	13.739980	7.330864
H	8.878127	14.733607	7.049301
C	9.455596	12.744337	6.370184
H	9.286522	12.944970	5.310753
C	9.894542	11.492474	6.785351
H	10.075825	10.699604	6.059700
C	10.108291	11.247605	8.146044
C	10.552780	9.979486	8.705834
C	10.816374	8.800009	8.007761
H	10.705569	8.770769	6.923415
C	11.212299	7.658784	8.708330
H	11.422973	6.730842	8.175559
C	11.324555	7.711419	10.101512
H	11.616091	6.824439	10.664195
C	11.053131	8.904141	10.768530
N	10.685713	10.025170	10.069350
C	11.094927	9.129215	12.209149
C	11.452317	8.167379	13.158583
H	11.733004	7.165640	12.834231
C	11.448520	8.497409	14.510107
H	11.728995	7.753446	15.257619
C	11.075632	9.791916	14.895090
H	11.053042	10.091361	15.943724
C	10.720796	10.706949	13.916819
H	10.413865	11.720993	14.169859

N	10.738307	10.396972	12.601540
N	8.322143	11.704438	11.532582
C	7.464417	10.706176	11.214959
H	7.884869	9.877636	10.646133
C	6.131671	10.725311	11.589890
H	5.485555	9.893076	11.307525
C	5.641047	11.815943	12.324080
H	4.595998	11.855084	12.635164
C	6.510287	12.848954	12.650326
H	6.159716	13.711155	13.217880
C	7.850376	12.784313	12.248880
C	8.846062	13.804949	12.535407
C	8.653958	15.005125	13.232161
H	7.671152	15.256343	13.630035
C	9.730483	15.868260	13.408951
H	9.597697	16.807417	13.947100
C	10.992953	15.528151	12.893946
H	11.840234	16.199955	13.030376
C	11.148220	14.329663	12.212508
N	10.079975	13.491160	12.041530
C	12.394452	13.811256	11.622849
C	13.618768	14.475572	11.676562
H	13.690825	15.444635	12.168509
C	14.746638	13.889929	11.100445
H	15.709412	14.402686	11.138971
C	14.626772	12.645039	10.478365
H	15.482440	12.151175	10.017213
C	13.381508	12.029919	10.449336
H	13.236997	11.060954	9.973236
N	12.291105	12.591137	11.003526

$[Re(tpy)_2]^+$ S = 0

Re	10.349089	11.733964	11.083392
N	9.975510	12.259332	9.108005
C	9.612938	13.498922	8.687920
H	9.523880	14.257523	9.465080
C	9.366897	13.794347	7.359726
H	9.075739	14.808656	7.082135
C	9.494673	12.779903	6.394992
H	9.305409	12.984800	5.339714
C	9.865412	11.509161	6.811673
H	9.975102	10.699433	6.089404
C	10.102568	11.255313	8.170644
C	10.486638	9.970708	8.723415
C	10.693220	8.781193	8.026479

H	10.564113	8.757920	6.943474
C	11.064431	7.623219	8.717763
H	11.230957	6.688841	8.179891
C	11.222260	7.676993	10.106193
H	11.512787	6.784689	10.661942
C	11.008079	8.875981	10.784456
N	10.642674	10.018142	10.096331
C	11.122497	9.108495	12.211205
C	11.475073	8.136967	13.159580
H	11.686028	7.119572	12.828962
C	11.553208	8.471839	14.504106
H	11.827014	7.721163	15.247425
C	11.272610	9.795961	14.885345
H	11.320676	10.109072	15.929623
C	10.928063	10.720471	13.916673
H	10.701625	11.755227	14.171102
N	10.849403	10.404914	12.597780
N	8.324479	11.681539	11.543838
C	7.476364	10.672602	11.215709
H	7.919036	9.838077	10.672553
C	6.133229	10.690195	11.543624
H	5.500805	9.850748	11.250184
C	5.611457	11.790835	12.246872
H	4.556103	11.830360	12.522062
C	6.467455	12.829552	12.585025
H	6.095985	13.699396	13.127941
C	7.822968	12.769582	12.228628
C	8.806694	13.794467	12.518565
C	8.595357	15.002483	13.181300
H	7.599283	15.249557	13.549706
C	9.659081	15.890811	13.368064
H	9.501523	16.838698	13.883865
C	10.926556	15.551350	12.883693
H	11.767898	16.232620	13.016357
C	11.117728	14.337511	12.225858
N	10.063002	13.461115	12.046521
C	12.354439	13.831712	11.661574
C	13.586938	14.501094	11.688628
H	13.651712	15.480133	12.163196
C	14.708154	13.918901	11.114439
H	15.670137	14.434311	11.129796
C	14.578232	12.654509	10.513695
H	15.430259	12.155242	10.049924
C	13.343781	12.032017	10.509556

H	13.201727	11.053055	10.053604
N	12.239154	12.592821	11.065593

$[Re(tpy)_2]^0$ S = 1/2

Re	10.292652	11.707215	11.111497
N	9.850751	12.254779	9.168788
C	9.237281	13.402862	8.781942
H	8.954982	14.080387	9.588793
C	9.001676	13.724676	7.460916
H	8.523708	14.673827	7.213688
C	9.406029	12.814020	6.449856
H	9.239598	13.044550	5.395331
C	10.003861	11.626462	6.822781
H	10.310465	10.899721	6.068676
C	10.218149	11.326043	8.189154
C	10.748010	10.098606	8.695609
C	11.236567	8.997310	7.958429
H	11.260242	9.044553	6.868679
C	11.698551	7.863559	8.629189
H	12.083866	7.013875	8.060778
C	11.683263	7.816540	10.029297
H	12.059465	6.943999	10.563807
C	11.194346	8.925290	10.747655
N	10.741161	10.046651	10.085589
C	11.100665	9.068674	12.177216
C	11.370643	8.053257	13.115620
H	11.721169	7.083806	12.759193
C	11.179200	8.279663	14.467969
H	11.387177	7.494591	15.197564
C	10.702453	9.543674	14.881696
H	10.530741	9.769376	15.935807
C	10.460524	10.515645	13.931451
H	10.105963	11.508293	14.209822
N	10.664793	10.317903	12.601544
N	8.297625	11.733905	11.681265
C	7.426161	10.706051	11.495773
H	7.832114	9.833218	10.985245
C	6.111070	10.753626	11.917841
H	5.459625	9.897038	11.735900
C	5.638175	11.909352	12.569175
H	4.604694	11.974788	12.913701
C	6.517133	12.963868	12.768492
H	6.187826	13.871852	13.275294
C	7.846657	12.870374	12.325583
C	8.856847	13.894653	12.494113

C	8.685128	15.163852	13.053817
H	7.707155	15.469356	13.426480
C	9.782421	16.038125	13.117379
H	9.665025	17.033656	13.549141
C	11.020320	15.632986	12.620282
H	11.875194	16.310059	12.657890
C	11.176432	14.352477	12.061931
N	10.081493	13.490398	12.009477
C	12.364595	13.773342	11.517937
C	13.632476	14.399641	11.473184
H	13.730081	15.416376	11.856619
C	14.729065	13.738745	10.959551
H	15.706640	14.224148	10.924514
C	14.558949	12.411050	10.481494
H	15.394244	11.844181	10.067249
C	13.309843	11.832515	10.536857
H	13.143849	10.818740	10.175260
N	12.209324	12.469830	11.025022

$[Re(tpy)_2]^-$ S = 1

Re	10.302992	11.699698	11.129346
N	9.770272	12.268809	9.219403
C	9.110650	13.412388	8.877295
H	8.846490	14.066312	9.708763
C	8.800834	13.750853	7.578164
H	8.285249	14.691988	7.377463
C	9.164194	12.867955	6.523597
H	8.929228	13.110451	5.484936
C	9.807743	11.689347	6.846640
H	10.087727	10.978946	6.066200
C	10.104519	11.368978	8.192036
C	10.704388	10.156014	8.645594
C	11.214924	9.096323	7.855846
H	11.177859	9.162438	6.767365
C	11.790956	7.987402	8.489026
H	12.204628	7.173390	7.887258
C	11.847536	7.913786	9.883835
H	12.298776	7.052306	10.378921
C	11.308336	8.970228	10.662746
N	10.767682	10.087922	10.024939
C	11.209066	9.045944	12.077102
C	11.563962	8.018138	12.994344
H	12.040018	7.113256	12.611688
C	11.295198	8.153350	14.339309
H	11.570505	7.361853	15.040649

C	10.644587	9.333687	14.799814
H	10.399214	9.478125	15.853391
C	10.345472	10.324037	13.881904
H	9.872161	11.258404	14.187764
N	10.648981	10.238627	12.565659
N	8.328161	11.713549	11.781647
C	7.505461	10.642710	11.848370
H	7.951352	9.697660	11.534186
C	6.180570	10.719274	12.240829
H	5.561339	9.820755	12.241121
C	5.655700	11.989770	12.612603
H	4.610199	12.091142	12.913603
C	6.487073	13.088726	12.600753
H	6.113460	14.068927	12.902866
C	7.851067	12.962899	12.212799
C	8.829086	13.989937	12.264702
C	8.645284	15.347287	12.638385
H	7.646095	15.711368	12.882291
C	9.749155	16.202792	12.693151
H	9.610620	17.247279	12.985232
C	11.030010	15.736153	12.371512
H	11.891973	16.403815	12.401254
C	11.196051	14.384597	11.977997
N	10.104785	13.537922	11.920444
C	12.406885	13.735193	11.595360
C	13.697203	14.315098	11.624073
H	13.795800	15.356198	11.937097
C	14.813695	13.581828	11.274182
H	15.808515	14.032337	11.298044
C	14.637394	12.222807	10.891924
H	15.485992	11.597198	10.608726
C	13.367252	11.688822	10.872157
H	13.197483	10.652163	10.582205
N	12.246301	12.398854	11.186287

$[Re(tpy)_2Cl]^+$ S = 0

Re	-4.968933	0.317603	16.085435
Cl	-4.965248	-2.138134	16.084818
N	-3.670794	1.938109	16.406563
C	-3.841656	2.807047	17.425827
H	-4.781147	2.737054	17.970401
C	-2.865652	3.723603	17.779568
H	-3.048443	4.402641	18.613227
C	-1.659612	3.747567	17.064687
H	-0.867626	4.449290	17.331939

C	-1.485364	2.864085	16.006887
H	-0.562744	2.860926	15.426415
C	-2.510849	1.968088	15.684846
C	-2.504264	1.046206	14.560714
C	-1.528913	0.943401	13.567229
H	-0.599753	1.507371	13.646787
C	-1.779339	0.134224	12.458433
H	-1.028737	0.028357	11.673534
C	-3.028614	-0.477176	12.323231
H	-3.279862	-1.028145	11.417256
C	-3.967339	-0.337673	13.345193
N	-3.652166	0.321823	14.489819
C	-5.373671	-0.717606	13.287985
C	-5.970280	-1.426432	12.242379
H	-5.362428	-1.789979	11.414372
C	-7.340295	-1.665571	12.277807
H	-7.822602	-2.222704	11.472325
C	-8.086072	-1.184936	13.359747
H	-9.162000	-1.348385	13.430753
C	-7.432203	-0.494878	14.370414
H	-7.978006	-0.134594	15.240202
N	-6.109834	-0.262171	14.340811
N	-6.266825	1.940021	15.772563
C	-6.094977	2.815764	14.759502
H	-5.157223	2.745897	14.211964
C	-7.067174	3.740509	14.416432
H	-6.882956	4.425924	13.588359
C	-8.270838	3.765286	15.135157
H	-9.059477	4.474167	14.877054
C	-8.446683	2.873582	16.185794
H	-9.367061	2.871063	16.769848
C	-7.424737	1.970091	16.497477
C	-7.431947	1.043573	17.618022
C	-8.405031	0.942847	18.614118
H	-9.332915	1.509302	18.537645
C	-8.153179	0.133753	19.722652
H	-8.901607	0.030024	20.509981
C	-6.904230	-0.478662	19.854805
H	-6.650764	-1.027799	20.761287
C	-5.968181	-0.340720	18.829992
N	-6.285368	0.317205	17.685107
C	-4.560847	-0.716388	18.887973
C	-3.962323	-1.415018	19.939479
H	-4.569617	-1.775413	20.769278

C	-2.590784	-1.645717	19.909003
H	-2.106635	-2.193247	20.719987
C	-1.846334	-1.168136	18.824947
H	-0.769168	-1.324942	18.757543
C	-2.502511	-0.488861	17.808244
H	-1.956865	-0.130941	16.937409
N	-3.826111	-0.262901	17.833659

$[Re(py\text{-}tpy)(CO)_2(py)]^+$ S = 0

Re	4.428456	7.327199	8.370076
O	3.554924	8.887279	10.858945
C	3.598474	8.674227	7.318426
C	5.331678	3.636321	10.405165
H	4.784091	2.723454	10.630825
C	4.715703	4.666457	9.696524
N	5.403613	5.785931	9.407346
C	6.698272	5.946211	9.740277
C	7.362582	4.948241	10.450834
H	8.401775	5.084409	10.744168
C	6.672802	3.775582	10.802770
C	1.668587	5.878440	8.076731
H	1.390584	6.809678	7.586755
N	2.922556	5.814921	8.555735
C	3.326036	4.670185	9.193609
C	2.464099	3.584180	9.342531
H	2.806367	2.683024	9.849529
C	1.165989	3.655843	8.836225
H	0.484858	2.810062	8.944869
C	0.763563	4.826387	8.194148
H	-0.239543	4.936415	7.780712
C	4.092583	6.027898	5.526516
H	3.114478	6.478288	5.687075
N	5.004592	6.199470	6.504284
C	6.224845	5.658648	6.333851
H	6.951994	5.812316	7.128029
C	6.577140	4.933117	5.199741
H	7.582626	4.517636	5.121120
C	5.630520	4.755257	4.189927
H	5.874444	4.190872	3.287454
C	4.363797	5.317707	4.361897
H	3.584860	5.211272	3.605015
C	7.288529	7.208346	9.247684
N	6.447874	8.016988	8.525070
C	6.940024	9.151508	7.998288
H	6.238200	9.757544	7.428209

C	8.264681	9.546072	8.168000
H	8.605498	10.479434	7.718569
C	9.123296	8.738096	8.912586
H	10.166312	9.018021	9.068459
C	8.623775	7.553239	9.453331
H	9.273929	6.896269	10.030712
C	6.636953	1.898013	12.474547
H	5.572262	2.052342	12.657526
C	7.317469	0.902116	13.175237
H	6.778056	0.271956	13.889910
N	8.626638	0.660364	13.031577
C	9.305428	1.427429	12.168804
H	10.373485	1.213545	12.058433
C	8.720863	2.452340	11.424803
H	9.333148	3.023611	10.725025
C	7.347541	2.702897	11.570271
C	3.893049	8.281037	9.915363
O	3.094631	9.505516	6.657101

$[Re(^{Me}DAB)(PPh_3)Cl_3]$ S = 0

Re	13.575358	2.365130	0.085051
Cl	14.969282	4.411551	0.117650
Cl	14.877126	1.763039	-1.790693
Cl	14.687781	1.522715	1.985916
N	12.015038	2.987804	-1.050298
C	11.050717	3.704233	-0.490116
H	10.196874	4.059567	-1.066281
C	11.252806	3.954676	0.871438
H	10.589527	4.560827	1.489175
N	12.363501	3.426859	1.352628
P	12.563383	0.174664	0.079357
C	11.460031	-0.177983	-1.333832
C	10.089053	0.117688	-1.338440
H	9.591984	0.474318	-0.438345
C	9.332947	-0.054614	-2.502353
H	8.266002	0.180314	-2.488886
C	9.934321	-0.526577	-3.672298
H	9.341013	-0.660232	-4.580172
C	11.299133	-0.835317	-3.672776
H	11.777831	-1.211341	-4.580141
C	12.057225	-0.661297	-2.514210
H	13.122583	-0.894215	-2.530704
C	11.581513	-0.059240	1.604821
C	10.512360	0.814436	1.877655
H	10.239530	1.590472	1.165243

C	9.794929	0.712319	3.070487
H	8.961905	1.393669	3.258733
C	10.148493	-0.251042	4.021745
H	9.590894	-0.328060	4.958294
C	11.224697	-1.106540	3.771428
H	11.516583	-1.852995	4.514440
C	11.938481	-1.012497	2.572746
H	12.781624	-1.680291	2.401203
C	13.657943	-1.288420	0.031032
C	15.055764	-1.203460	0.058083
H	15.546139	-0.234333	0.110931
C	15.834115	-2.365506	0.013725
H	16.923876	-2.283604	0.033568
C	15.224783	-3.620302	-0.056035
H	15.834690	-4.526480	-0.088977
C	13.827863	-3.713783	-0.088156
H	13.342383	-4.691116	-0.146903
C	13.051025	-2.557029	-0.049584
H	11.962598	-2.641843	-0.082812
C	11.923566	2.786378	-2.503797
H	12.599299	3.499265	-2.997791
H	12.233882	1.776117	-2.771965
H	10.894083	2.959767	-2.843441
C	12.724050	3.774794	2.727001
H	11.996252	4.483063	3.145601
H	12.752056	2.861186	3.337431
H	13.725209	4.224054	2.735408

$[Re(bpy)(PPh_3)Cl_3]$ S = 1

Re	-1.852476	3.216401	6.992789
Cl	0.564060	3.636065	6.713489
Cl	-1.605055	3.312758	9.379614
Cl	-1.408930	0.853335	6.896588
P	-4.235062	2.900637	7.316054
C	-4.870492	1.783763	8.616189
C	-6.246154	1.806262	8.911689
H	-6.907392	2.508353	8.399330
C	-6.775990	0.937284	9.865000
H	-7.844563	0.968018	10.092694
C	-5.938806	0.030017	10.527700
H	-6.354312	-0.650910	11.275264
C	-4.573657	-0.001456	10.231744
H	-3.917031	-0.707814	10.746025
C	-4.037823	0.873307	9.279561
H	-2.973946	0.847506	9.051611

C	-4.955493	4.517967	7.741196
C	-5.215469	5.472477	6.742231
H	-5.092008	5.216548	5.689335
C	-5.626121	6.760242	7.087233
H	-5.827573	7.491294	6.301241
C	-5.770775	7.115483	8.432842
H	-6.090110	8.124943	8.701869
C	-5.494187	6.178150	9.431548
H	-5.593464	6.452104	10.484767
C	-5.084379	4.886509	9.089767
H	-4.859152	4.165096	9.876334
C	-5.144883	2.287899	5.853494
C	-6.381760	2.811657	5.441944
H	-6.836611	3.647261	5.973528
C	-7.050204	2.260133	4.345390
H	-8.008353	2.681105	4.032522
C	-6.500540	1.174470	3.656617
H	-7.023236	0.749636	2.796301
C	-5.284603	0.628961	4.080021
H	-4.854251	-0.228900	3.558038
C	-4.612703	1.178929	5.173457
H	-3.678347	0.730869	5.512000
N	-2.040643	3.458262	4.921748
C	-1.953558	2.452158	4.023417
H	-1.755432	1.465922	4.433673
C	-2.345098	3.950269	2.186393
H	-2.479282	4.142397	1.120411
C	-2.102320	2.656660	2.661354
H	-2.028750	1.804128	1.985133
C	-2.400885	4.994069	3.102170
H	-2.572399	6.014774	2.763537
C	-2.233191	4.732402	4.466681
C	-2.244176	5.755014	5.502138
C	-2.384269	7.124673	5.250545
H	-2.489798	7.479282	4.226265
C	-2.391620	8.022533	6.309427
H	-2.506284	9.092456	6.126846
C	-2.254862	7.523552	7.609970
H	-2.259640	8.183952	8.477615
C	-2.112503	6.159705	7.802471
H	-2.003847	5.728998	8.794075
N	-2.108855	5.281548	6.774978