Electronic Supplementary Information For:

Photophysics and Ultrafast Processes in Rhenium(I) Diimine Dicarbonyls

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Experimental Details for Synthesis

cis-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**). This molecule was prepared using a modified procedure originally described by Smithback and coworkers.[S1] *fac*-Re(3,4,7,8-Me_4Phen)(CO)$_3$(CF_3SO_3) (100 mg, 0.15 mmol) and 2.2 eq of 3,4,7,8-tetramethyl-1,10-phenanthroline (3,4,7,8-Me_4phen) were placed in a heavy walled reaction tube equipped with a stir bar. The tube was sealed with a rubber septum and purged with N_2 gas for 30 min. The combined solids were heated at 275°C for 15 min under stirring. The mixture was then cooled to RT and MeOH (5 mL) was added, resulting in a solid orange precipitate. The orange precipitate was filtered. Purification was achieved by column chromatography over acidic alumina, starting with a 95:5 ratio (v:v) of dichloromethane (CH_2Cl_2)/acetonitrile (CH_3CN) and gradually increasing the percent composition of CH_3CN in the eluent. The final product was recrystallized by first dissolving the isolated solid in methylene chloride and adding this solution dropwise to a stirring solution of diethyl ether, resulting in the generation of an orange precipitate. Yield: 61 mg (46%).

cis-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**). The synthesis conditions for **2** were exactly the same as for **1**, using 100 mg (0.16 mmol) of *fac*-Re(4,7-Me_2phen)(CO)$_3$(CF_3SO_3) and 2.2 eq of 4,7-dimethyl-1,10-phenanthroline (4,7-Me_2phen). The cooled reaction mixture was purified by dissolving in MeOH, and the product was precipitated by the addition of an aqueous solution of ammonium hexafluorophosphate. The mixture was maintained in a refrigerator at 3-5°C for one hour, filtered, and washed with deionized H_2O. Following the filtration step, purification was achieved by column chromatography over acidic alumina, starting with a 95:5 ratio (v:v) of CH_2Cl_2/CH_3CN and gradually increasing the percent composition of CH_3CN in the eluent. The final product was recrystallized by first dissolving the isolated solid in methylene chloride and adding this solution dropwise to a stirring solution of diethyl ether. Yield: 65 mg (51%).

cis-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**). The synthesis and purification for **3** was exactly the same as for **2** using 100 mg (0.16 mmol) of *fac*-Re(5,6-Me_2phen)(CO)$_3$(CF_3SO_3) and 2.2 eq of 5,6-dimethyl-1,10-phenanthroline (5,6-Me_2phen). Yield: 33 mg (24%).

cis-[Re(phen)$_2$(CO)$_2$](CF_3SO_3) (**4**).[S1] The synthesis and purification of **4** was exactly the same as for **1** using 400 mg (0.67 mmol) of *fac*-Re(phen)(CO)$_3$(CF_3SO_3) and 2.2 eq of 1,10-phenanthroline. Yield: 356 mg (71%).

cis-[Re(4,7-Ph_2phen)$_2$(CO)$_2$]PF_6 (**5**).[S1] The synthesis and purification of **5** was exactly the same as for **2** using 355 mg (0.49 mmol) of *fac*-[Re(4,7-Ph_2phen)(CO)$_3$(MeCN)]BF_4 and 2.2 eq of 4,7-diphenyl-1,10-phenanthroline (4,7-Ph_2phen). The final product was reprecipitated with hexanes instead of diethyl ether. Yield: 182 mg (36%).

cis-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**). The synthesis and purification of **6** was the same as for **2** using 100 mg (0.17 mmol) of *fac*-[Re(5,5′-Me_2bpy)(CO)$_3$(MeCN)](BF_4) and 2.2 eq of 5,5′-dimethyl-2,2′-bipyridine (5,5′-Me_2bpy). However, the reaction time was increased to 4 hours. Yield: 84 mg (65 %).

cis-[Re(4,4′-dtbbpy)$_2$(CO)$_2$]PF$_6$ (**7**). The synthesis and purification of **7** was the same as for **6** using 608 mg (0.91 mmol) of *fac*-[Re(4,4′-dtbbpy)(CO)$_3$(MeCN)](BF$_4$) and 2.2 eq of 4 4'-di-*tert*-butyl-2 2'-bipyridine (4,4′-dtbbpy). Reprecipitation was performed in hexanes instead of diethyl ether. Yield: 517 mg (61%).

cis-[Re(bpy)$_2$(CO)$_2$]PF$_6$ (**8**).[S1] The synthesis and purification of **8** was the same as for **6** using 285 mg (0.51 mmol) of *fac*-[Re(bpy)(CO)$_3$(MeCN)](BF$_4$) and 3 eq of 2,2′-bipyridine. Yield: 181 mg (51%).

cis-[Re(4,4′-Me$_2$bpy)$_2$(CO)$_2$]PF$_6$ (**9**). The synthesis and purification of **9** was the same as for **6** using 100 mg (0.17 mmol) of *fac*-[Re(4,4′-Me$_2$bpy)(CO)$_3$(MeCN)](BF$_4$) and 2.2 eq of 4,4′-dimethyl-2,2′-bipyridine (4,4′-Me$_2$bpy). Yield: 32 mg (25%).

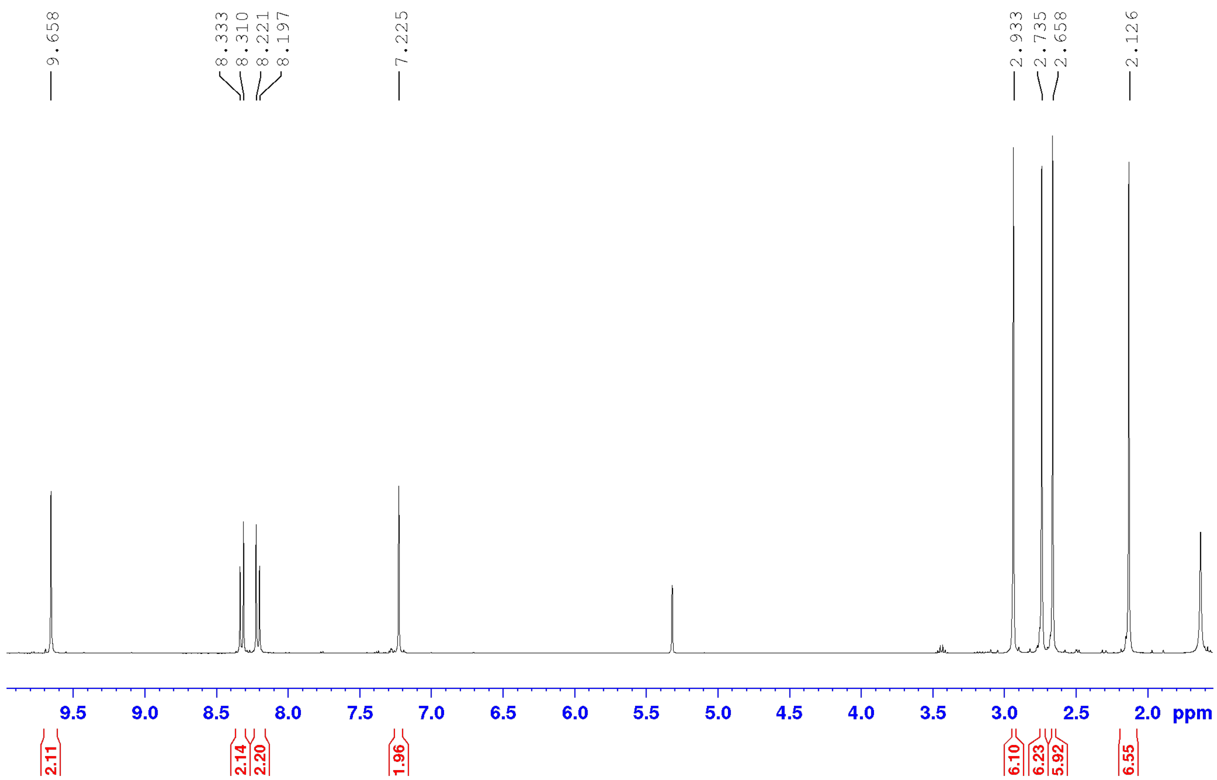

Figure S1. ^{1}H NMR spectrum of *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**) in CH_2Cl_2-*d_2* (400 MHz).

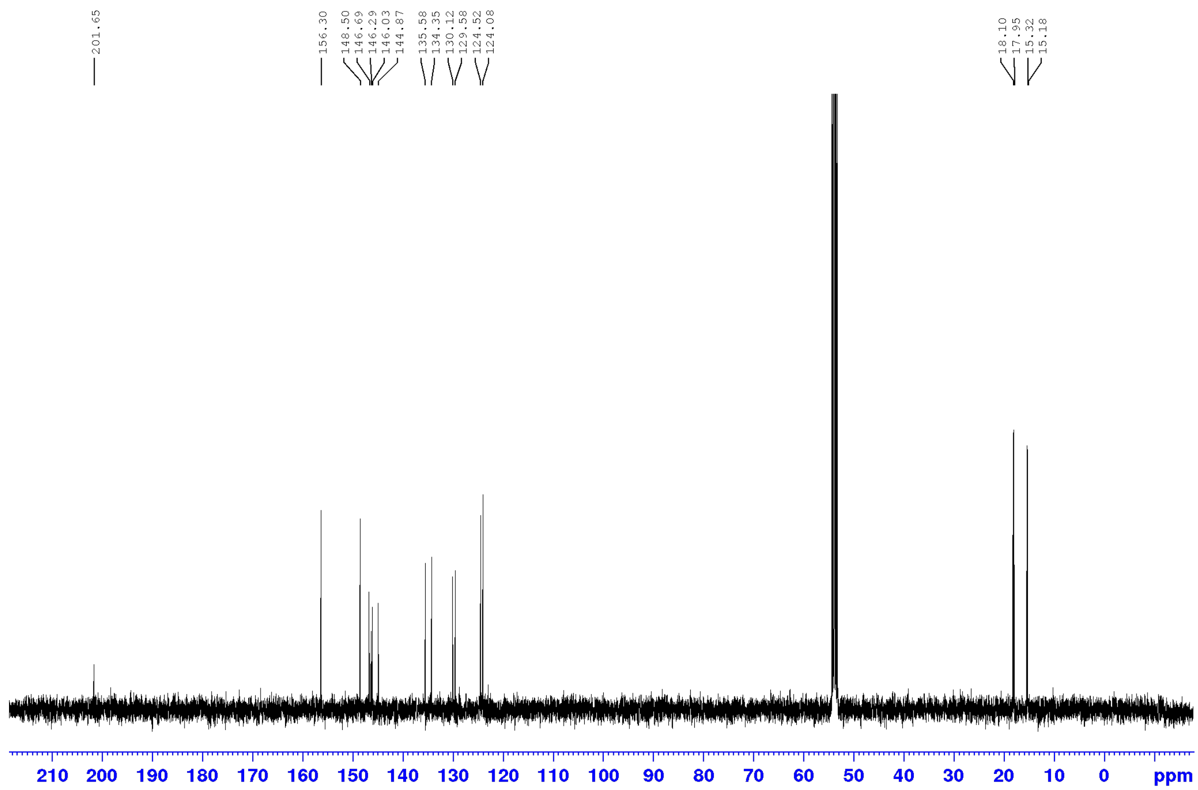

Figure S2. ^{13}C NMR spectrum of *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**) in CH_2Cl_2-d_2 (100 MHz).

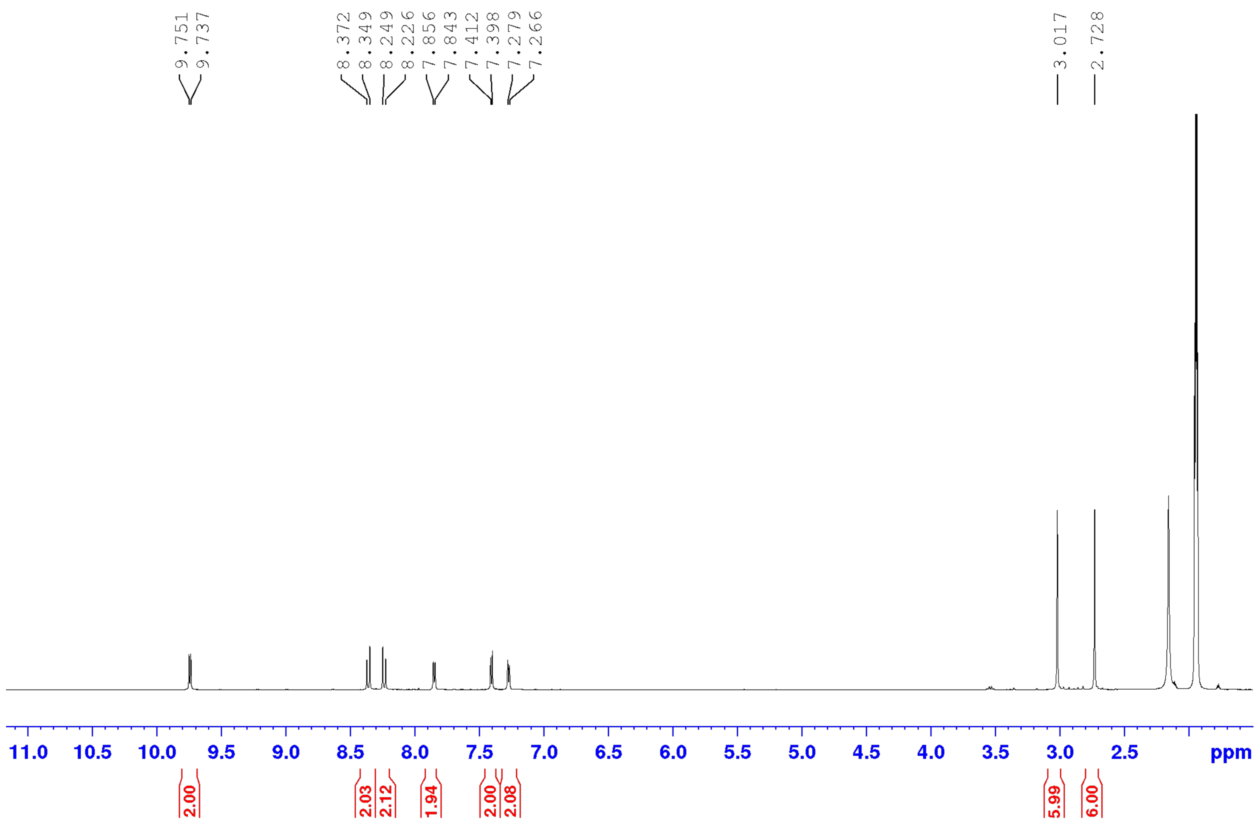

Figure S3. ^{1}H NMR spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**) in CH_3CN-d_3 (400 MHz).

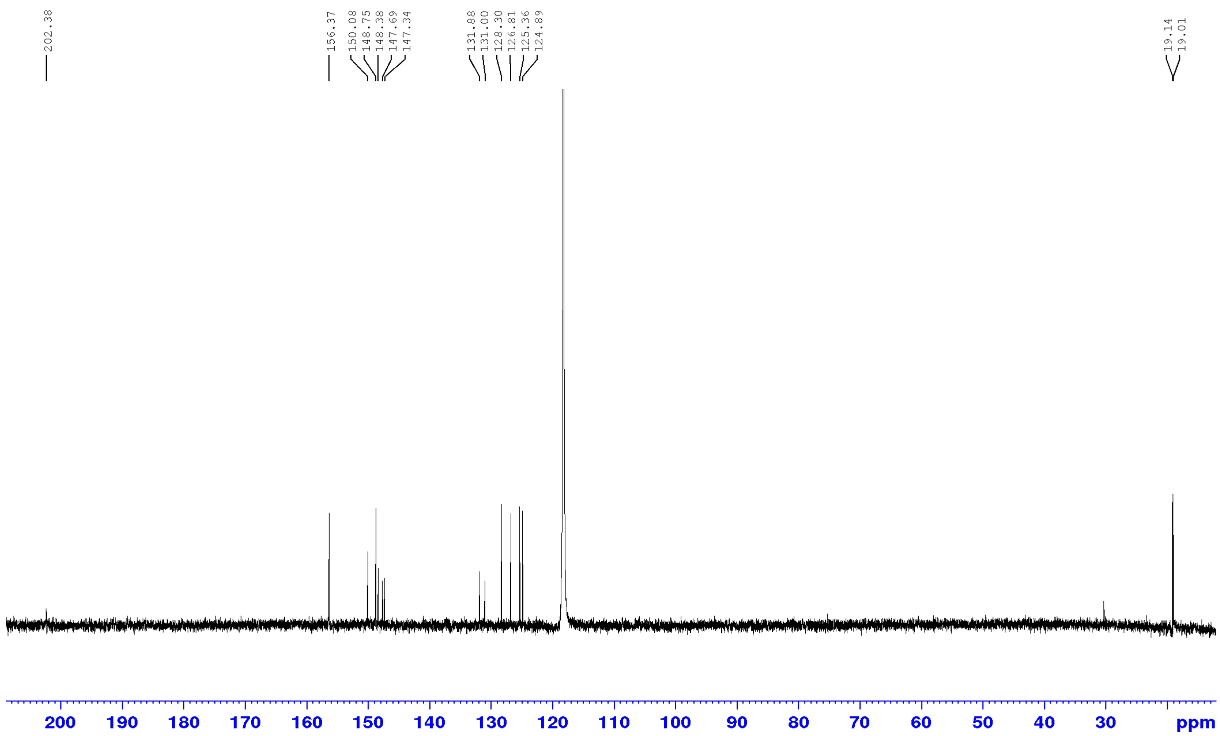

Figure S4. ^{13}C NMR spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**) in CH_3CN-d_3 (100 MHz).

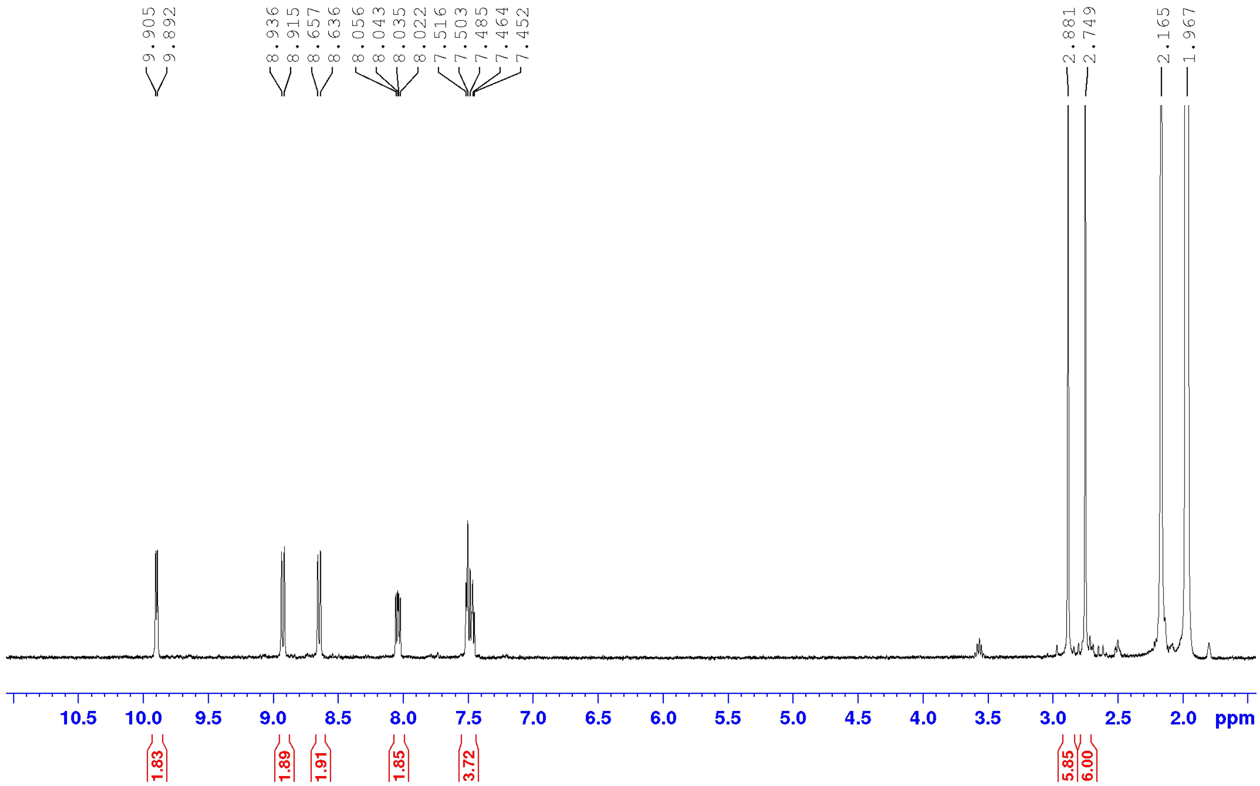

Figure S5. [1]H NMR spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**) in CH_3CN-d_3 (400 MHz).

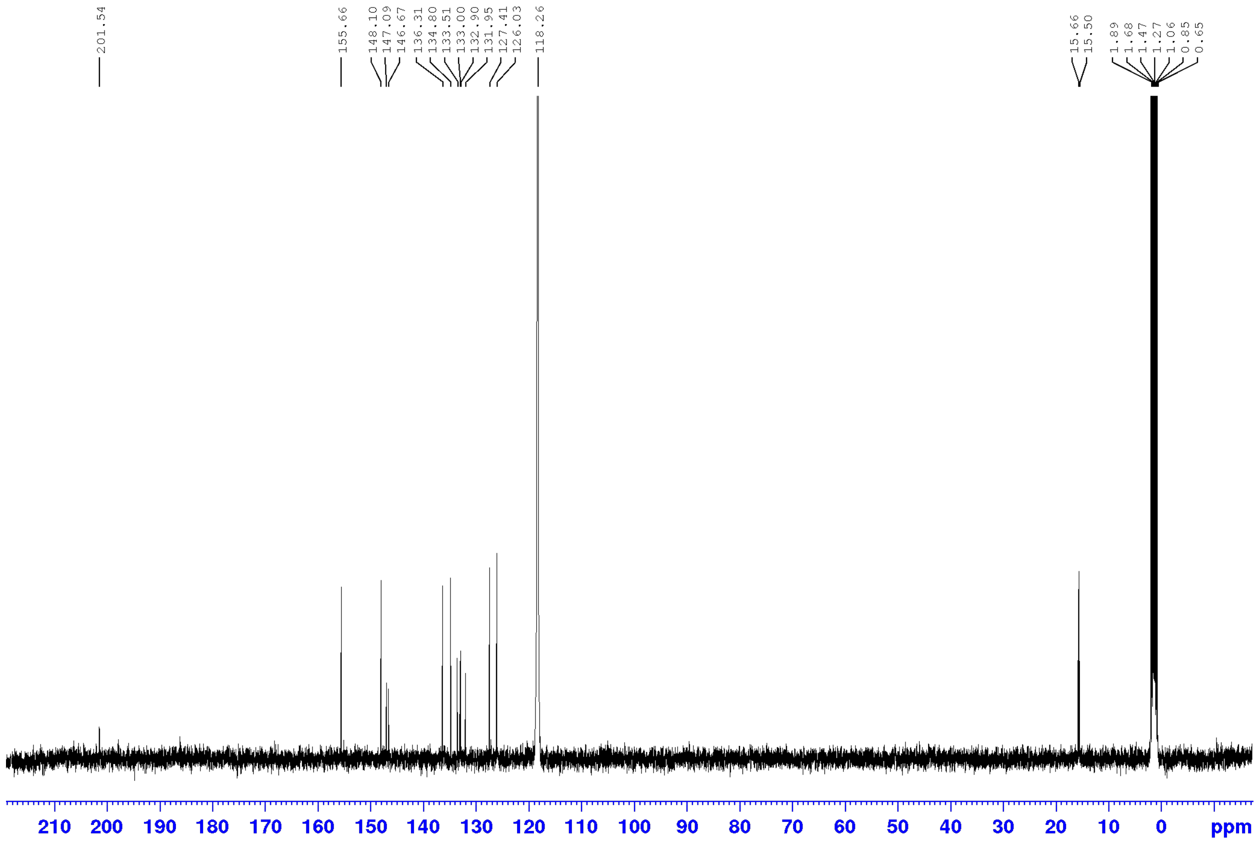

Figure S6. ^{13}C NMR spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**) in CH_3CN-d_3 (100 MHz).

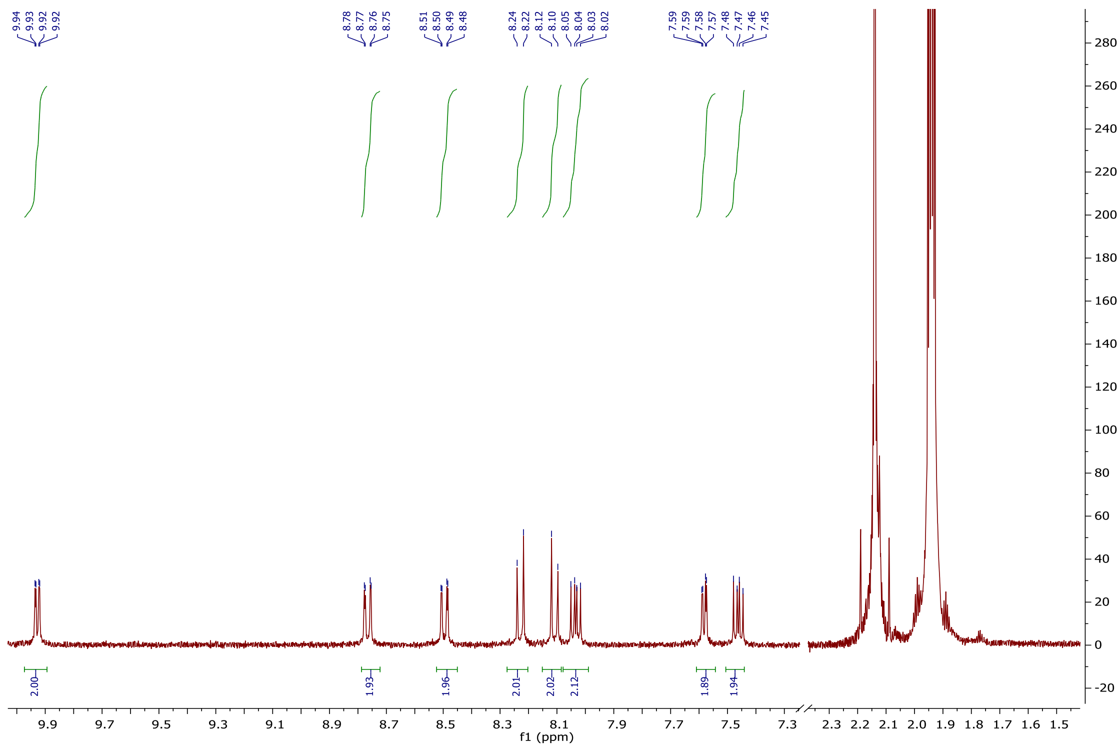

Figure S7. ^{1}H NMR spectrum of *cis*-[Re(phen)$_2$(CO)$_2$](CF$_3$SO$_3$) (**4**) in CH$_3$CN-d_3 (400 MHz).

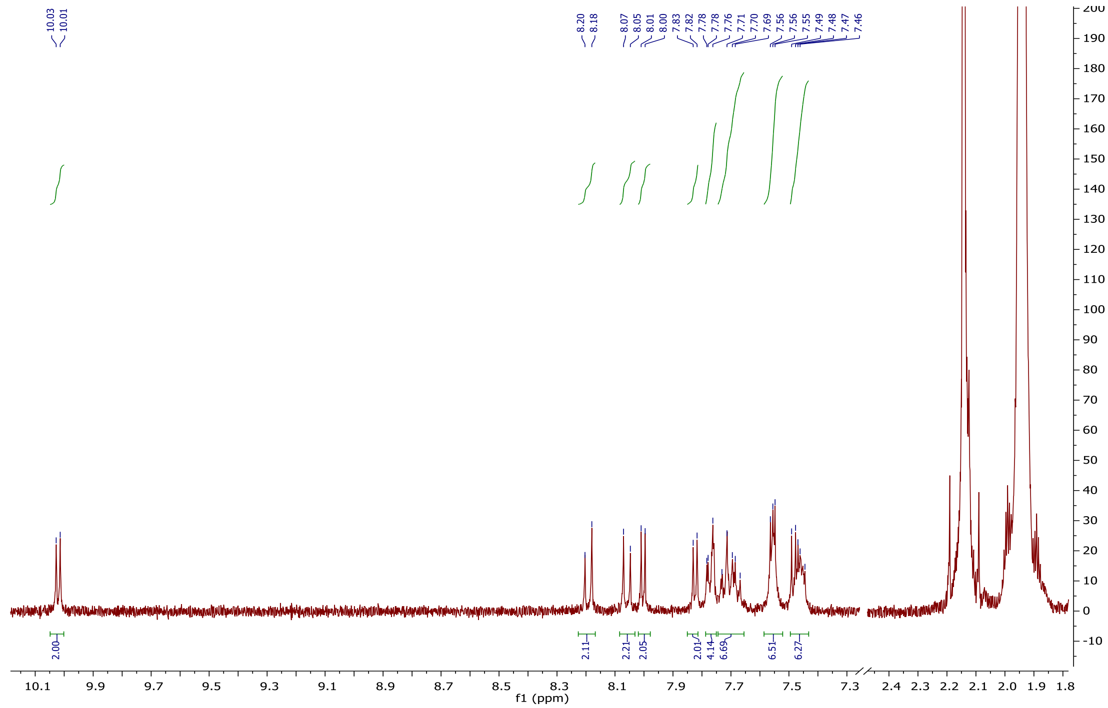

Figure S8. ^{1}H NMR spectrum of *cis*-[Re(4,7-Ph_2phen)$_2$(CO)$_2$]PF_6 (**5**) in CH_3CN-*d_3* (400 MHz).

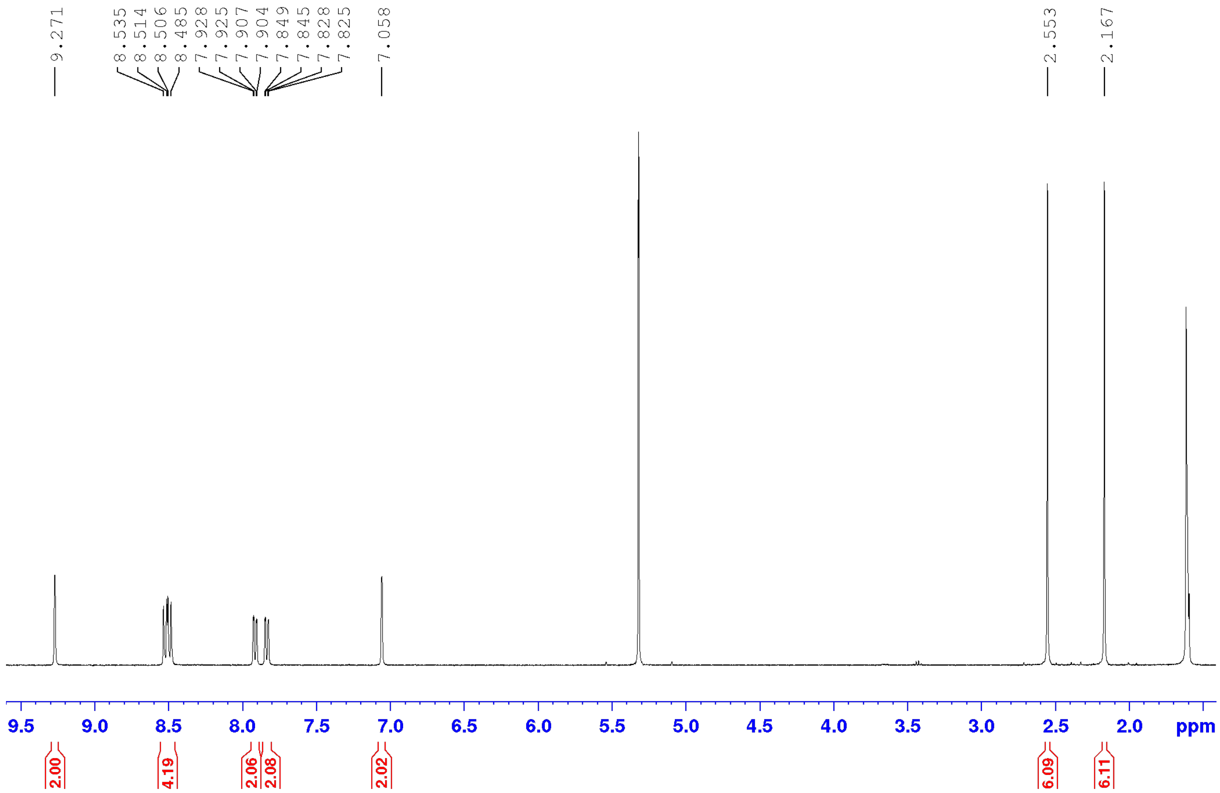

Figure S9. [1]H NMR spectrum of *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**) in CH_2Cl_2-d_2 (400 MHz).

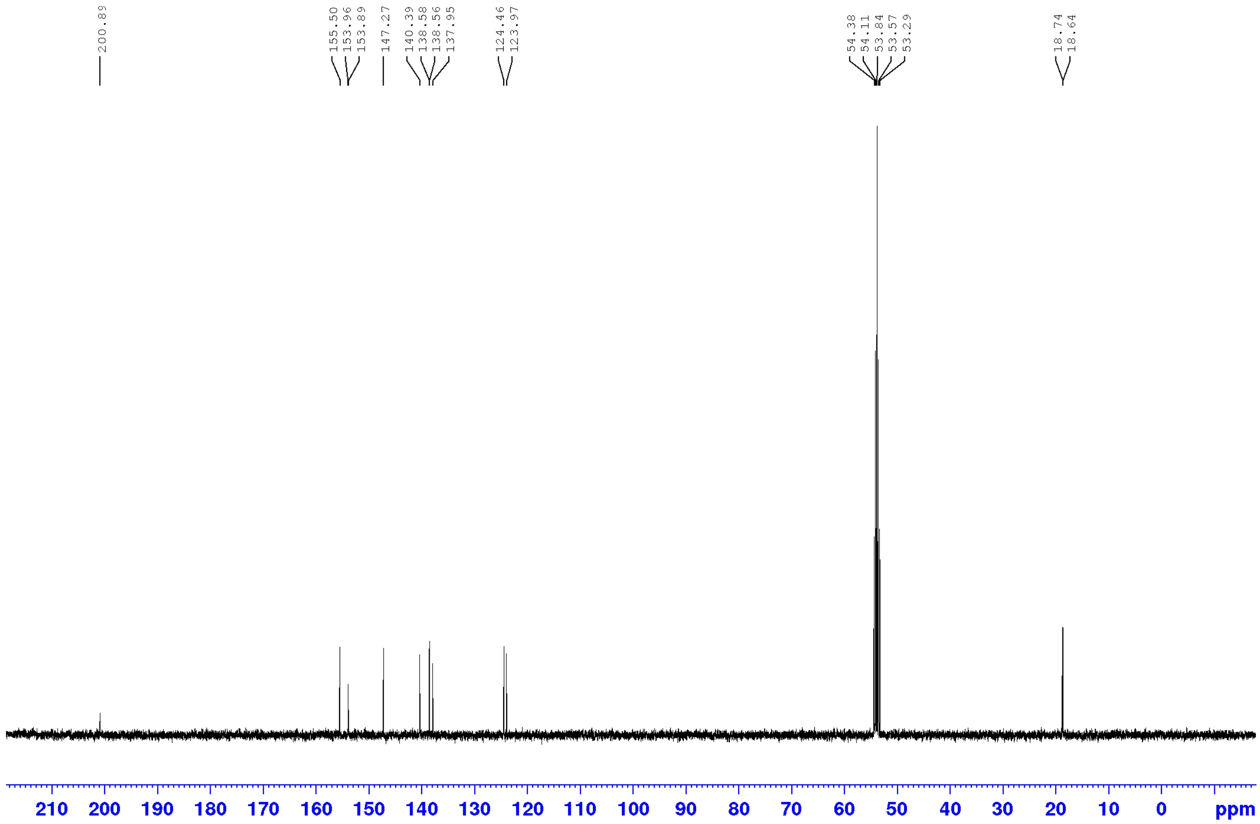

Figure S10. ^{13}C NMR spectrum of *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**) in CH_2Cl_2-d_2 (100 MHz).

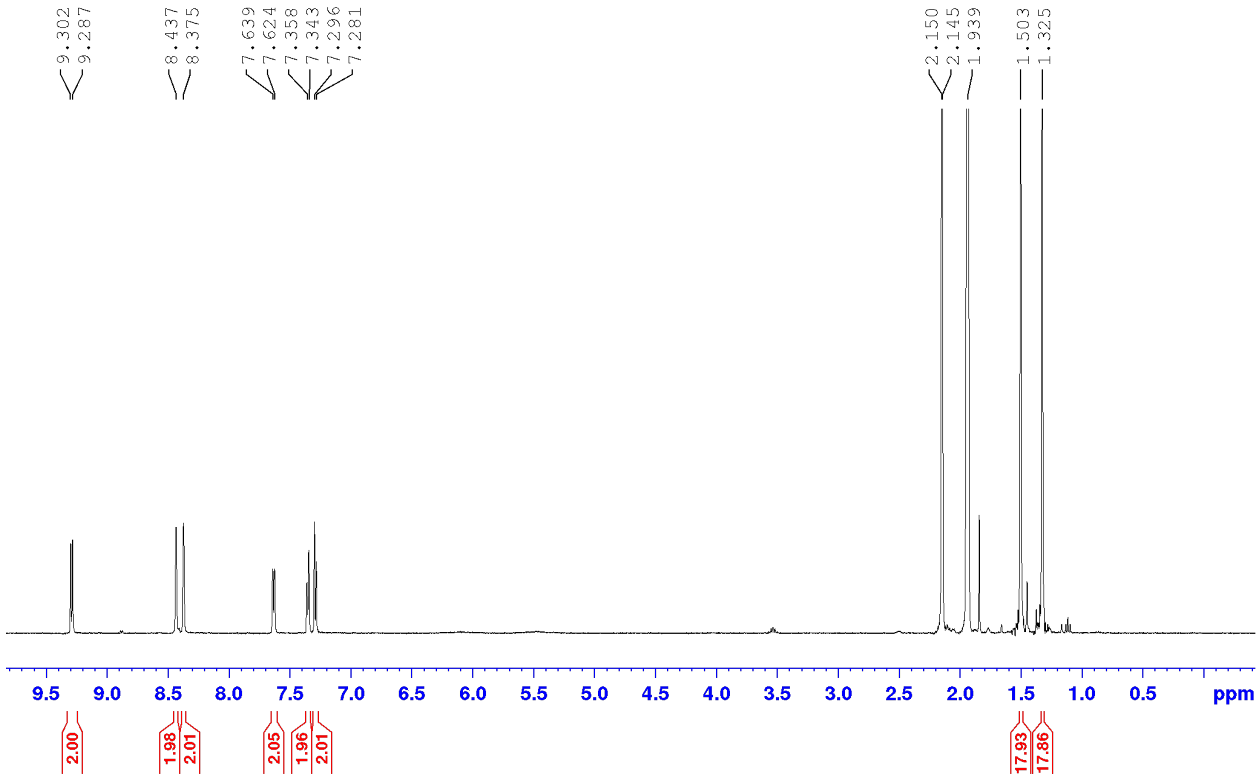

Figure S11. ^{1}H NMR spectrum of *cis*-[Re(4,4′-dtbbpy)$_2$(CO)$_2$]PF$_6$ (**7**) in CH$_3$CN-d_3 (400 MHz).

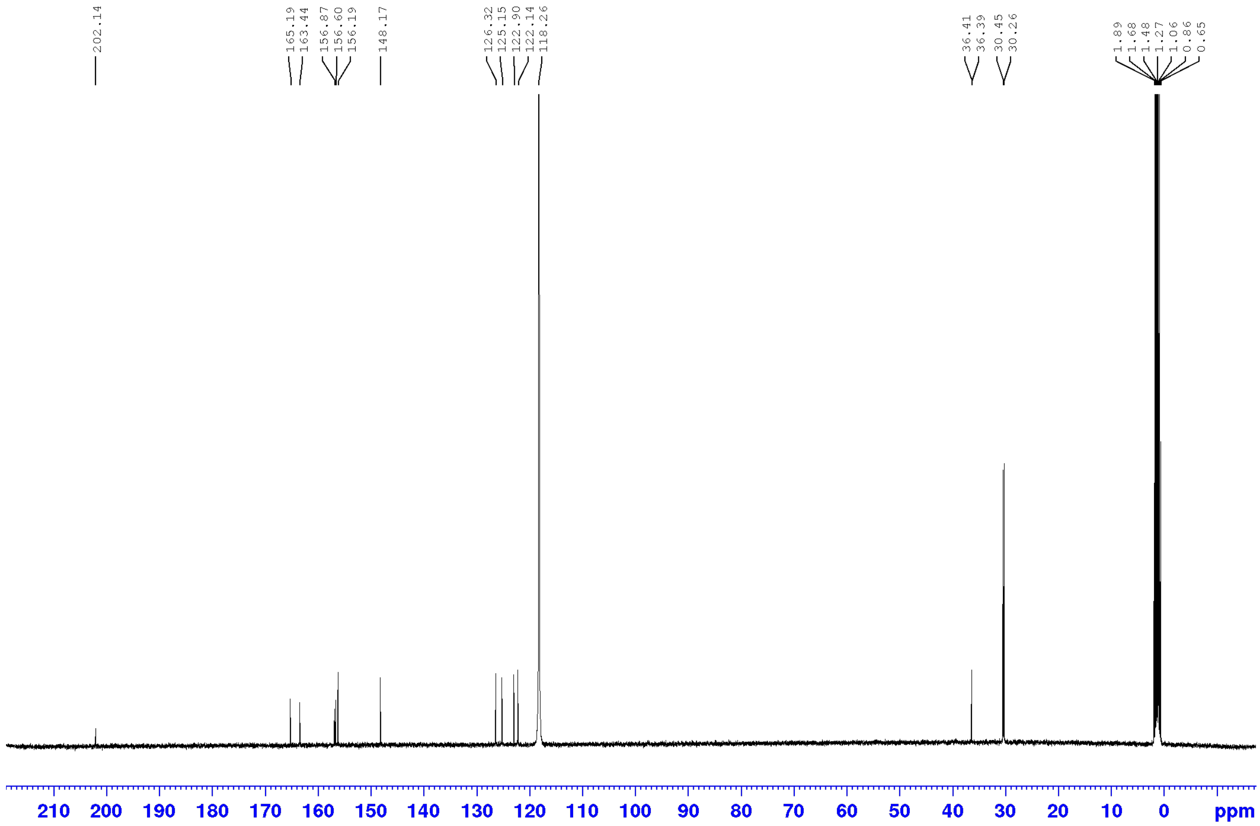

Figure S12. ^{13}C NMR spectrum of *cis*-$[Re(4,4'\text{-dtbbpy})_2(CO)_2]PF_6$ (**7**) in CH_3CN-d_3 (100 MHz).

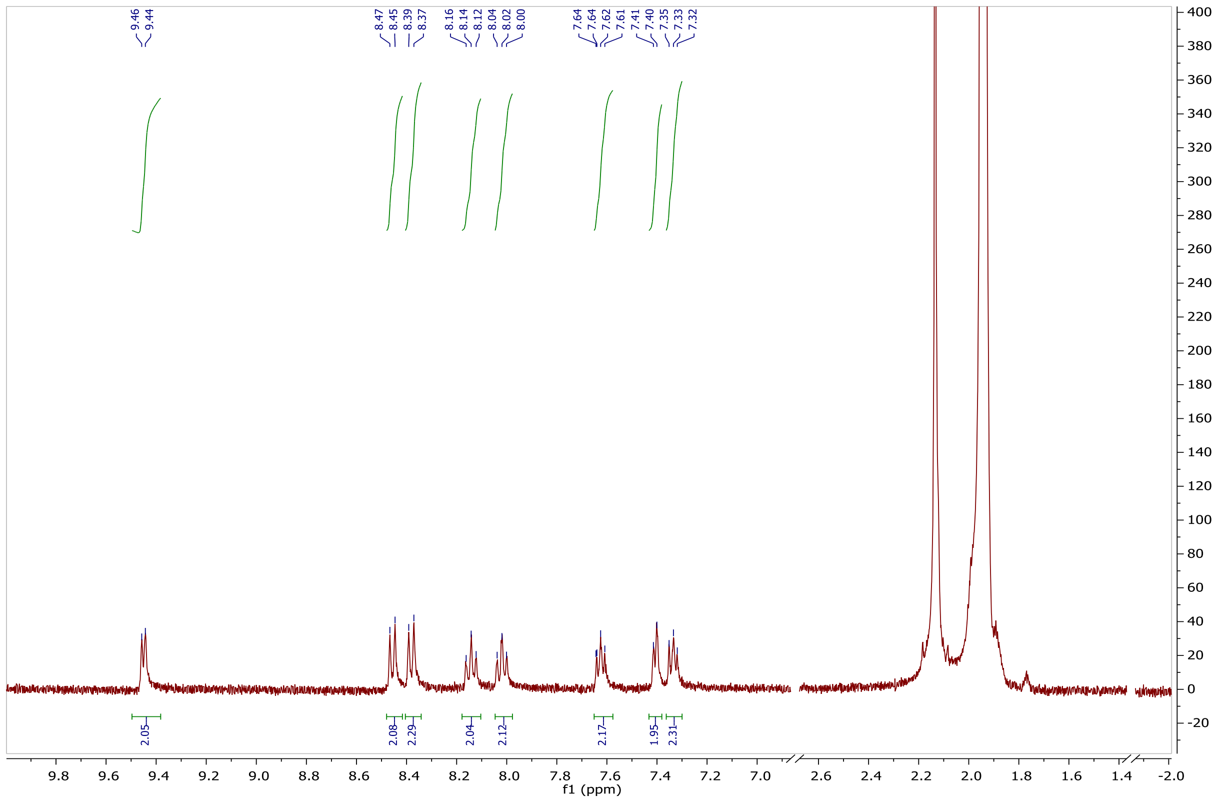

Figure S13. ^{1}H NMR spectrum of *cis*-$[Re(bpy)_2(CO)_2]PF_6$ (**8**) in CH_3CN-d_3 (400 MHz).

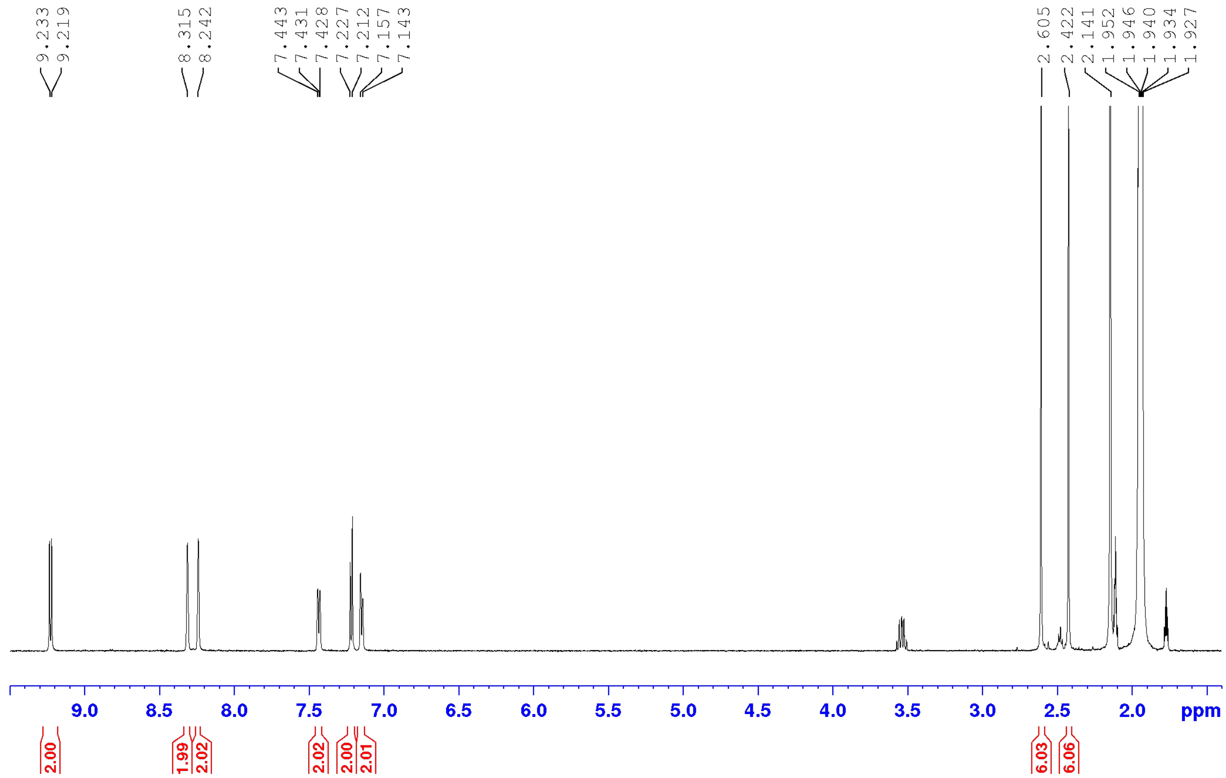

Figure S14. ^{1}H NMR spectrum of *cis*-[Re(4,4'-Me_2bpy)$_2$(CO)$_2$]PF_6 (**9**) in CH_3CN-d_3 (400 MHz).

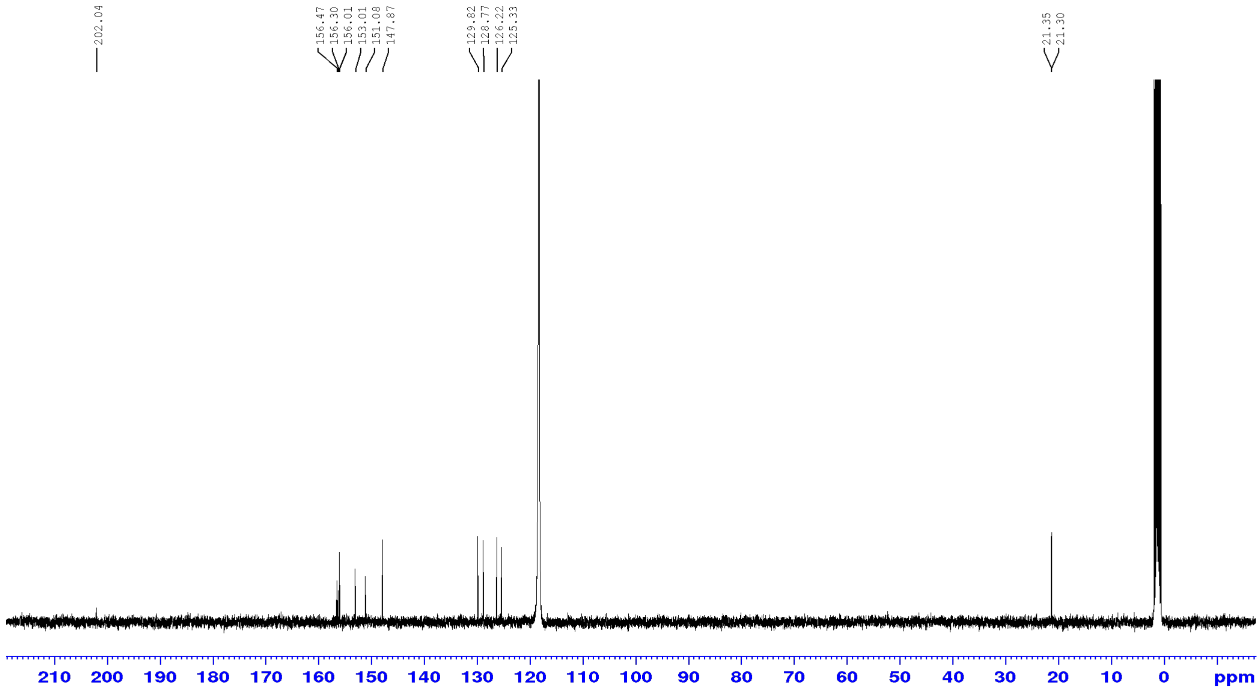

Figure S15. ^{13}C NMR spectrum of *cis*-[Re(4,4′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**9**) in CH_3CN-*d_3* (100 MHz).

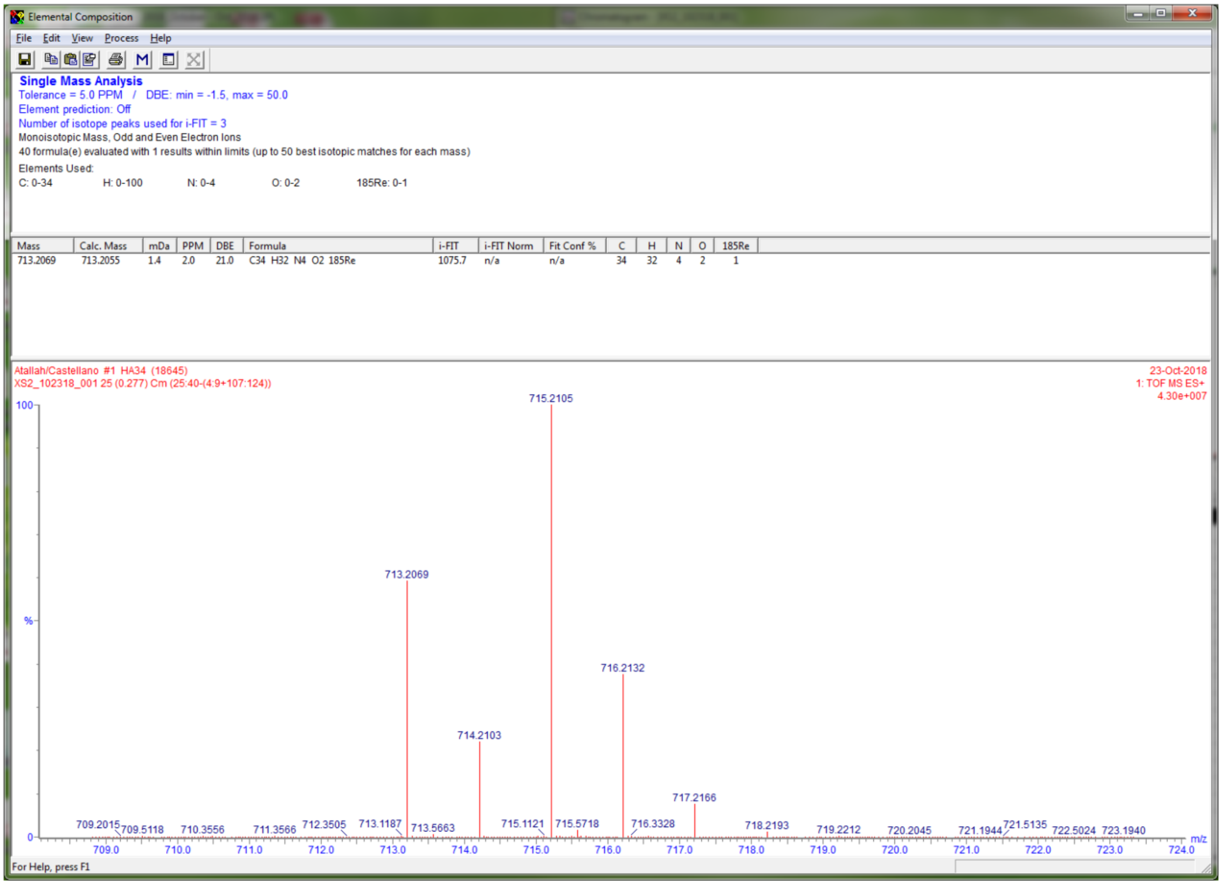

Figure S16. HRMS spectrum of *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**).

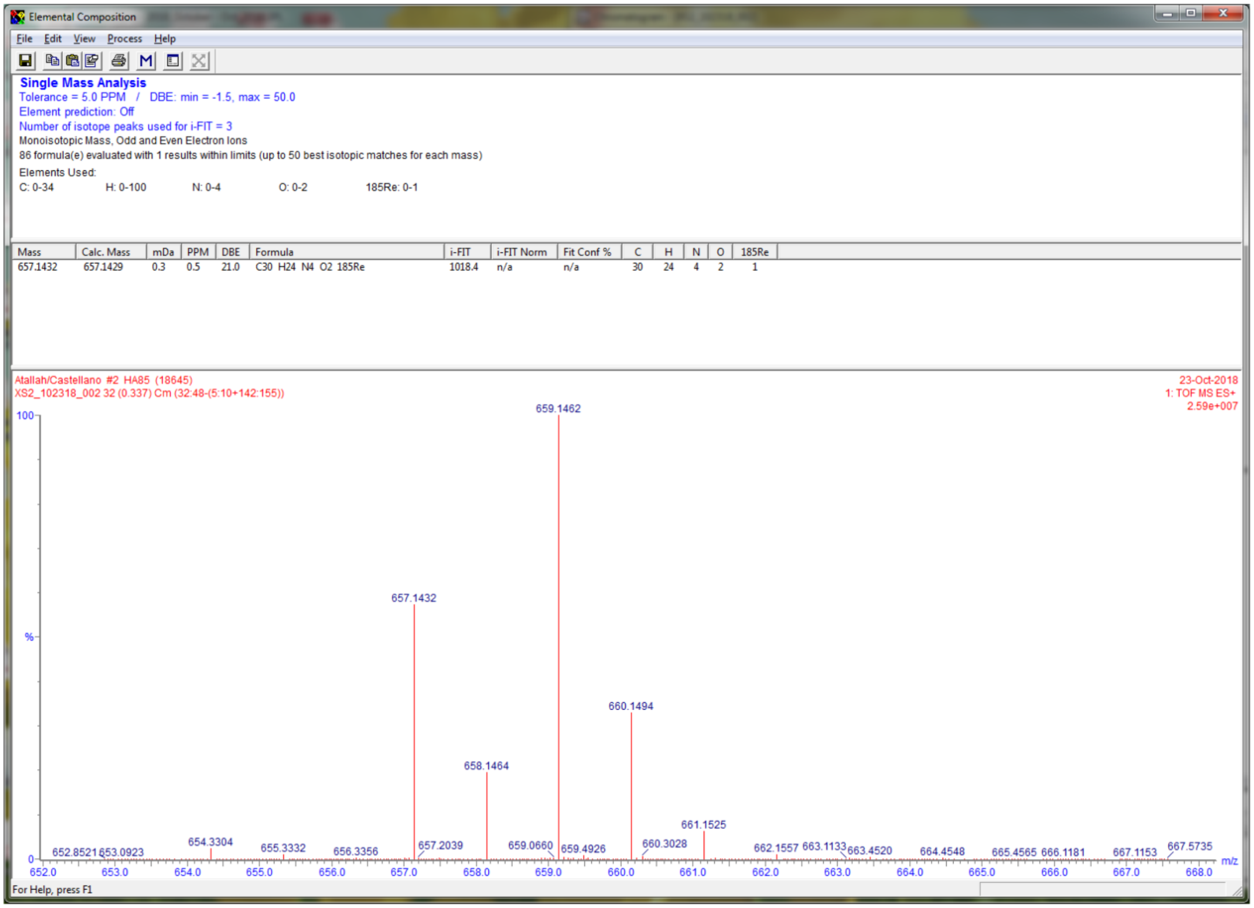

Figure S17. HRMS spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**).

Figure S18. HRMS spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**).

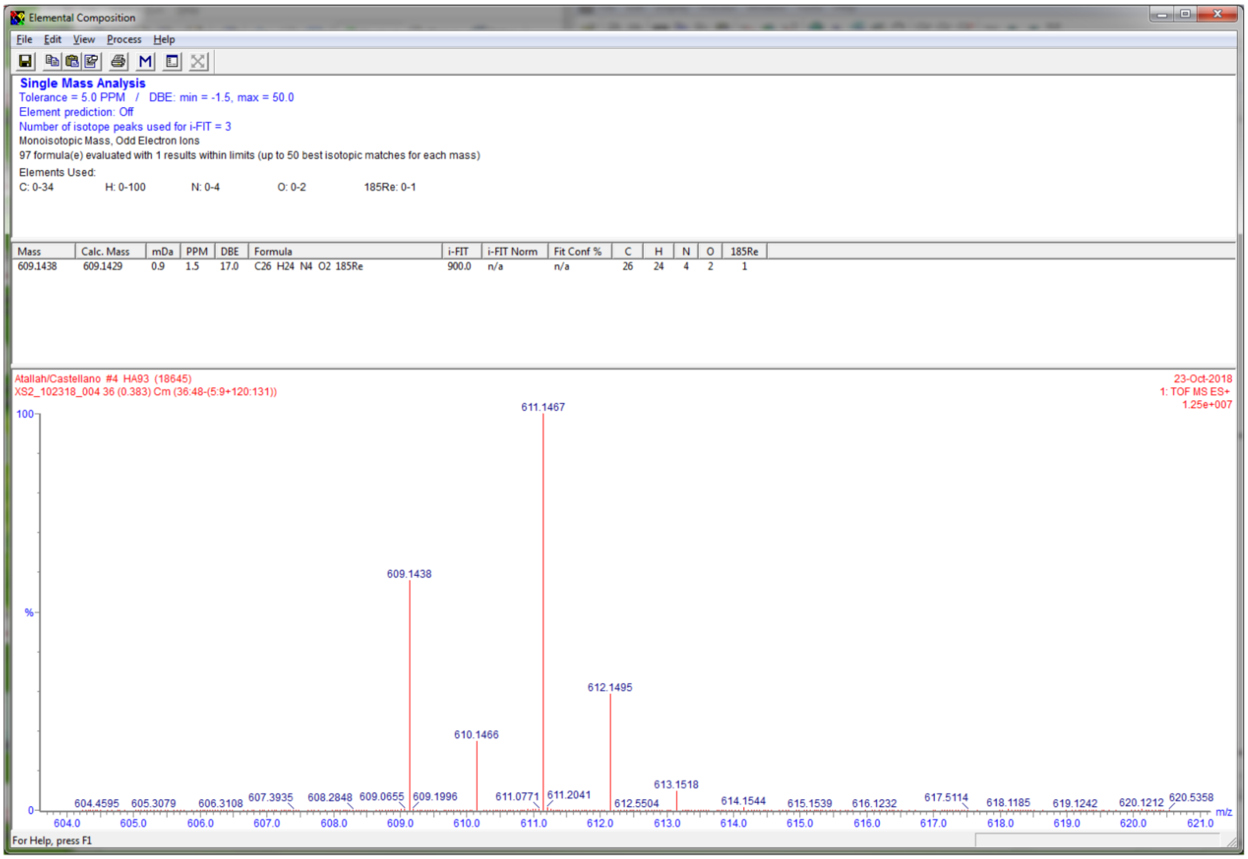

Figure S19. HRMS spectrum of *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**).

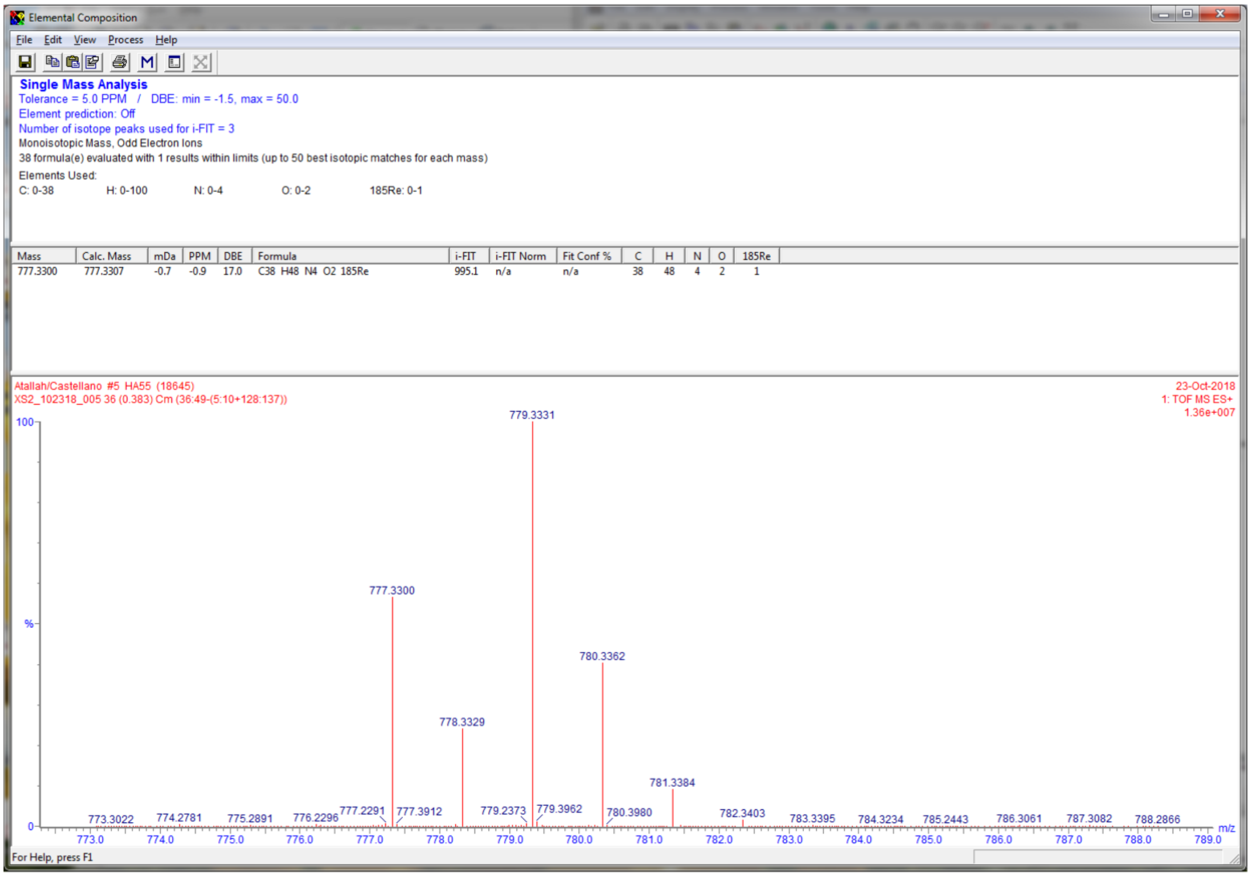

Figure S20. HRMS spectrum of *cis*-[Re(4,4'-dtbbpy)$_2$(CO)$_2$]PF_6 (**7**).

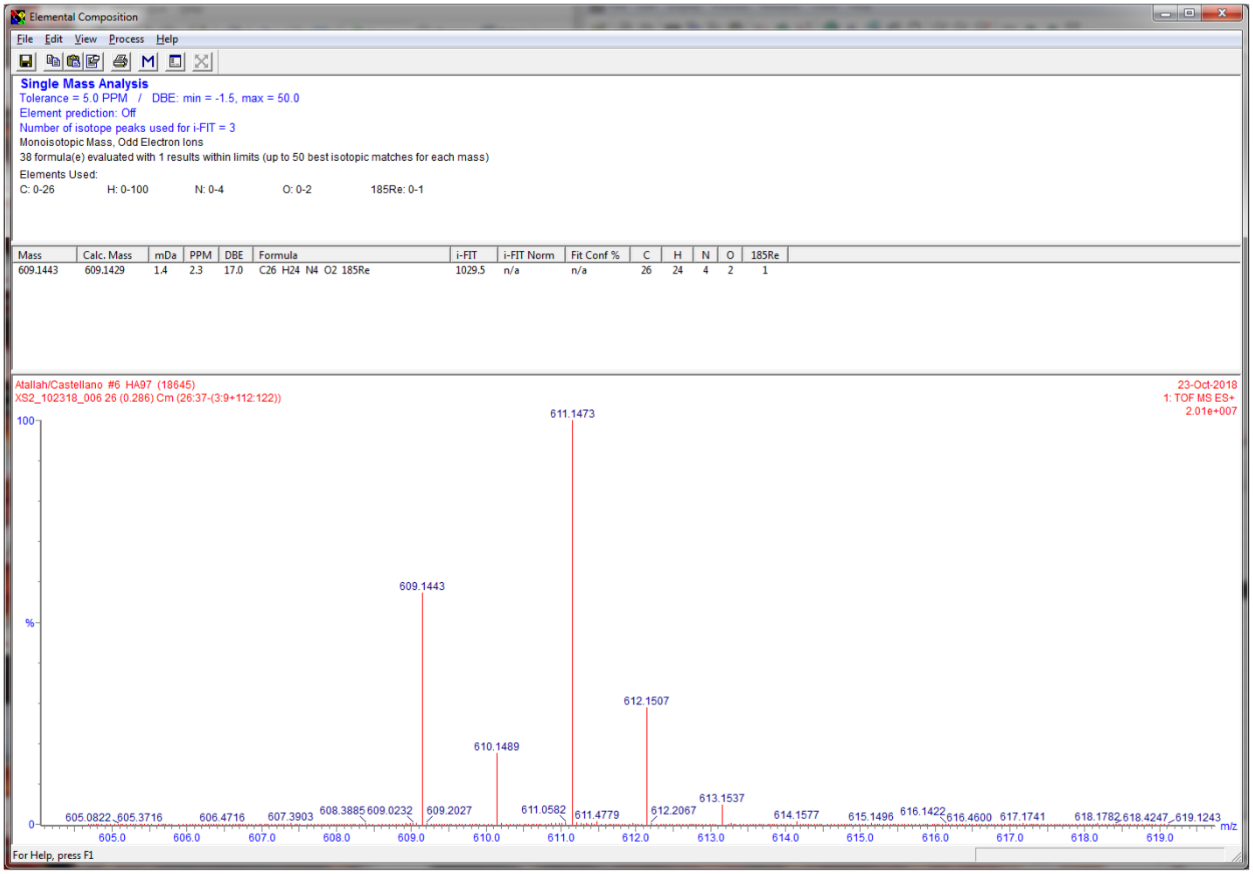

Figure S21. HRMS spectrum of *cis*-[Re(4,4′-Me$_2$bpy)$_2$(CO)$_2$]PF$_6$ (**9**).

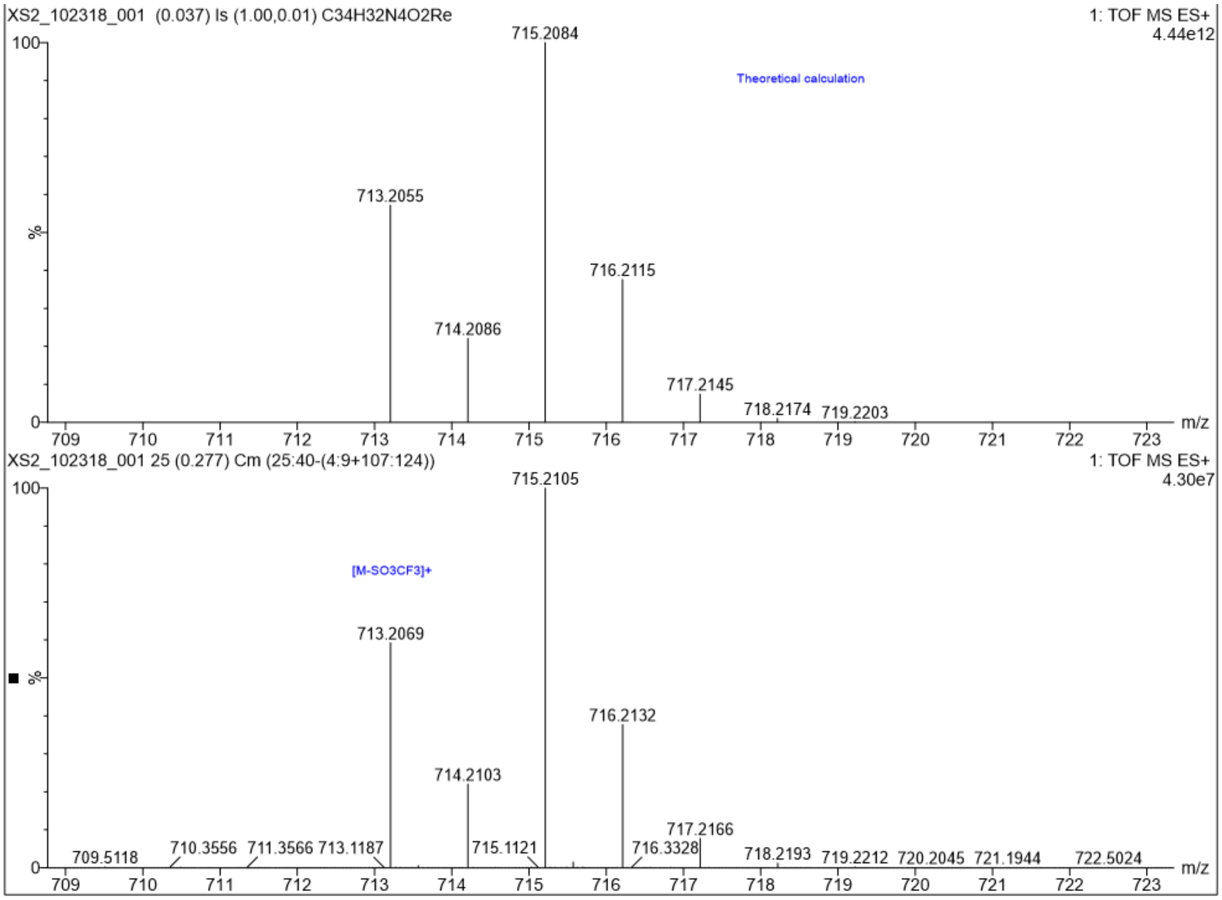

Figure S22. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**).

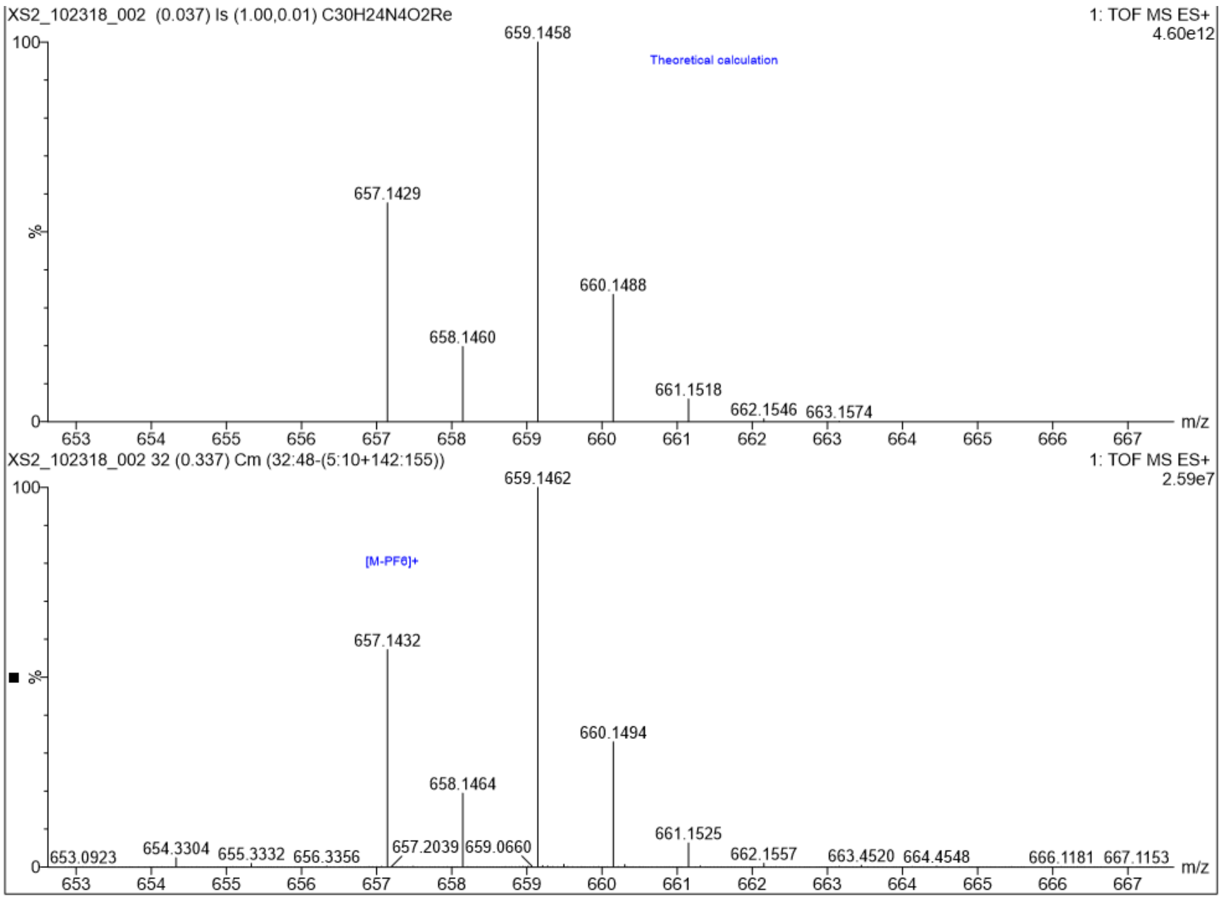

Figure S23. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**).

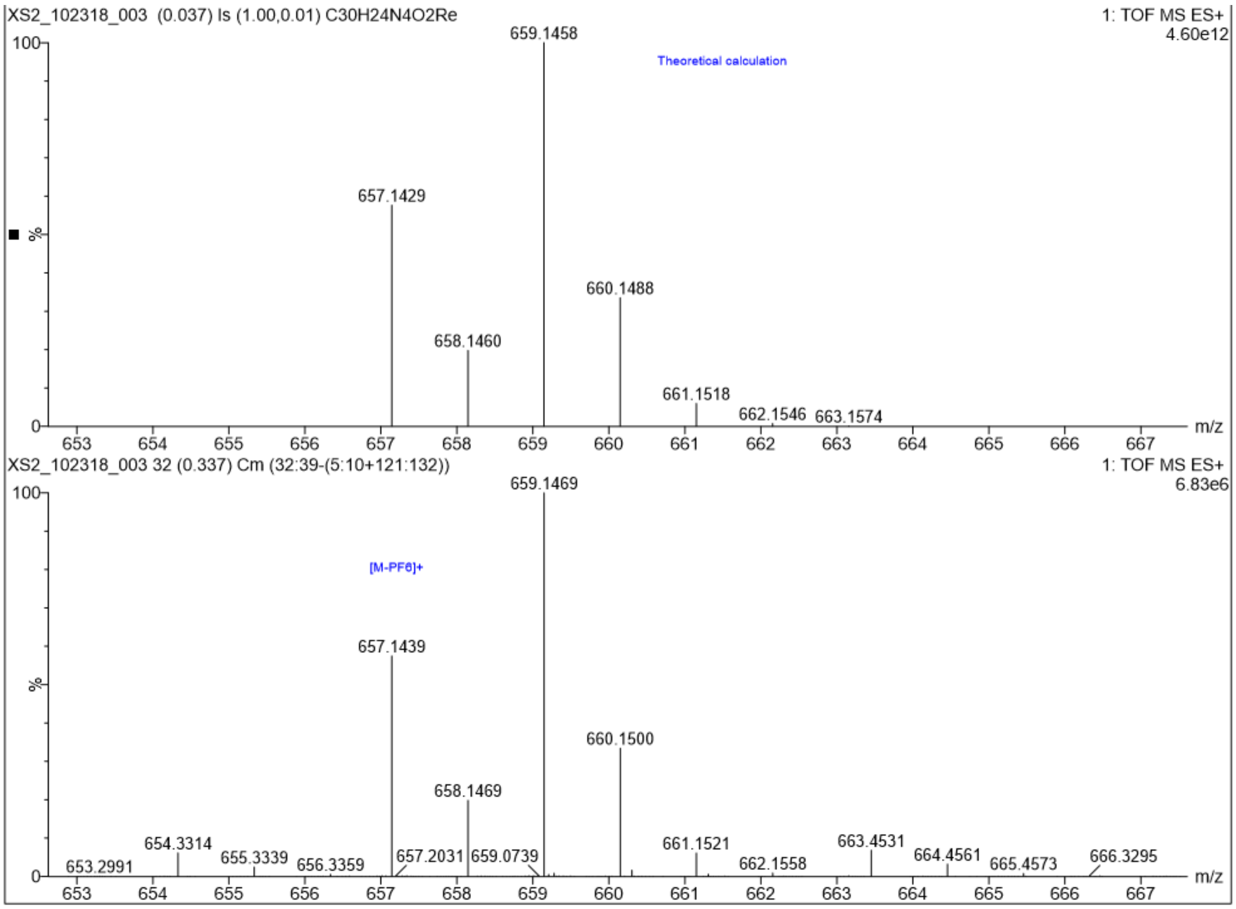

Figure S24. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**).

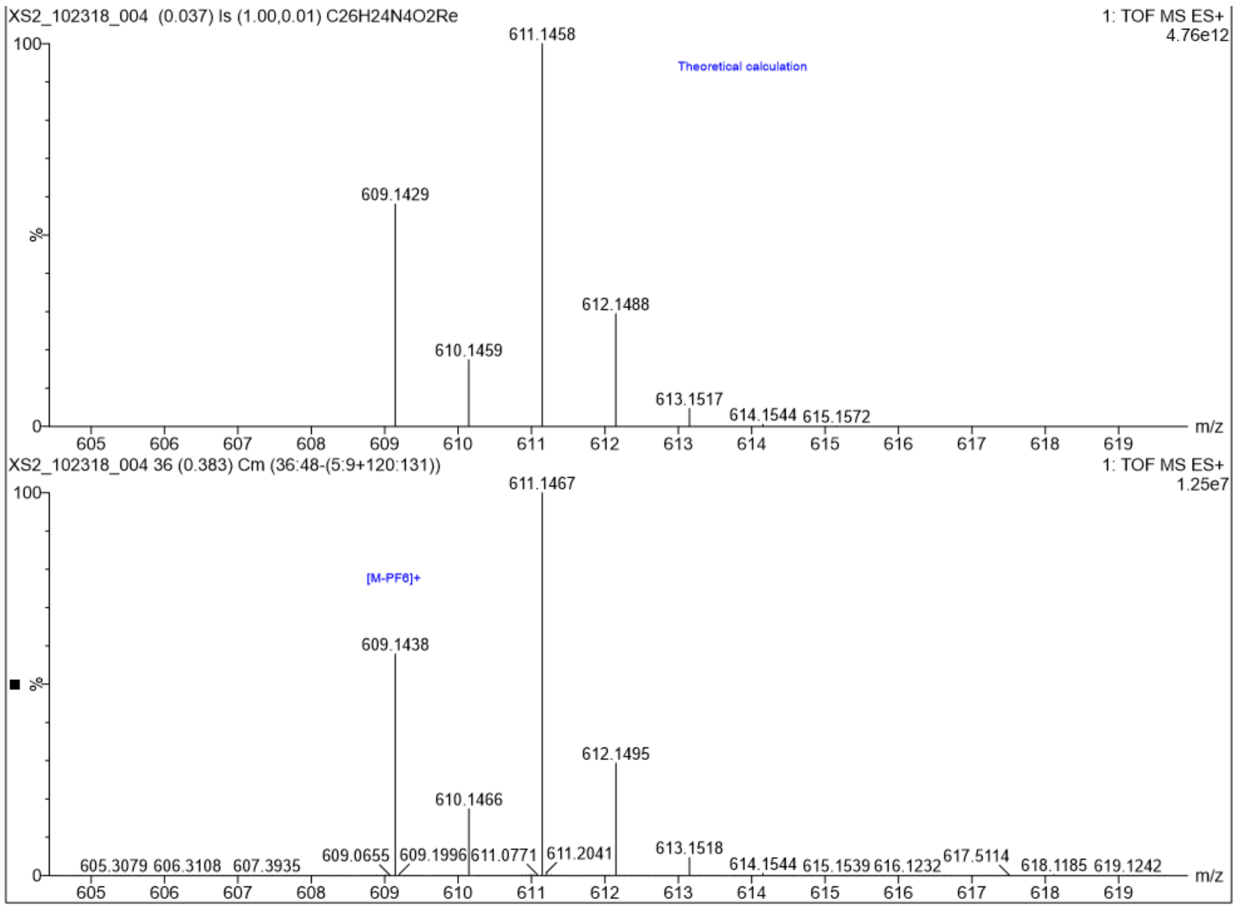

Figure S25. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(5,5'-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**).

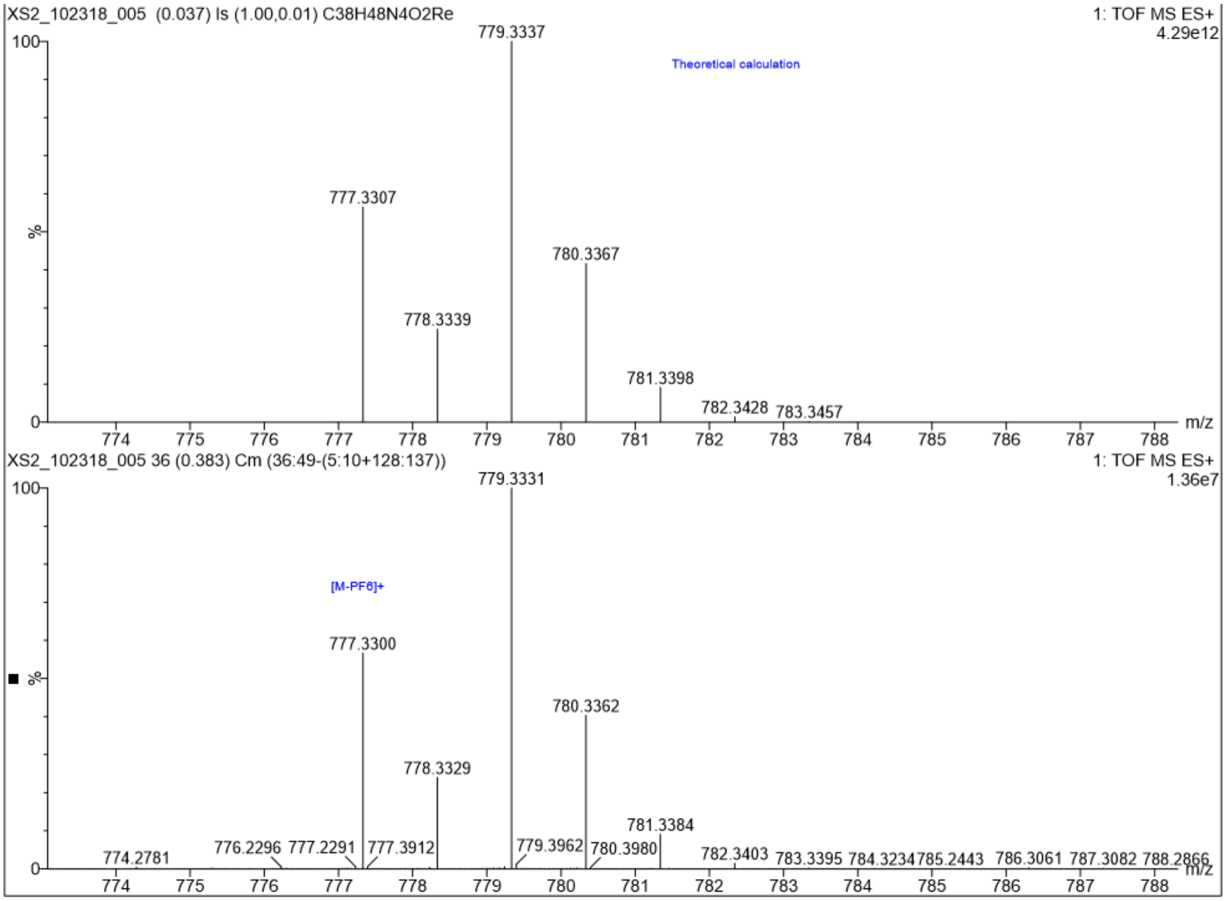

Figure S26. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(4,4′-dtbbpy)$_2$(CO)$_2$]PF$_6$ (**7**).

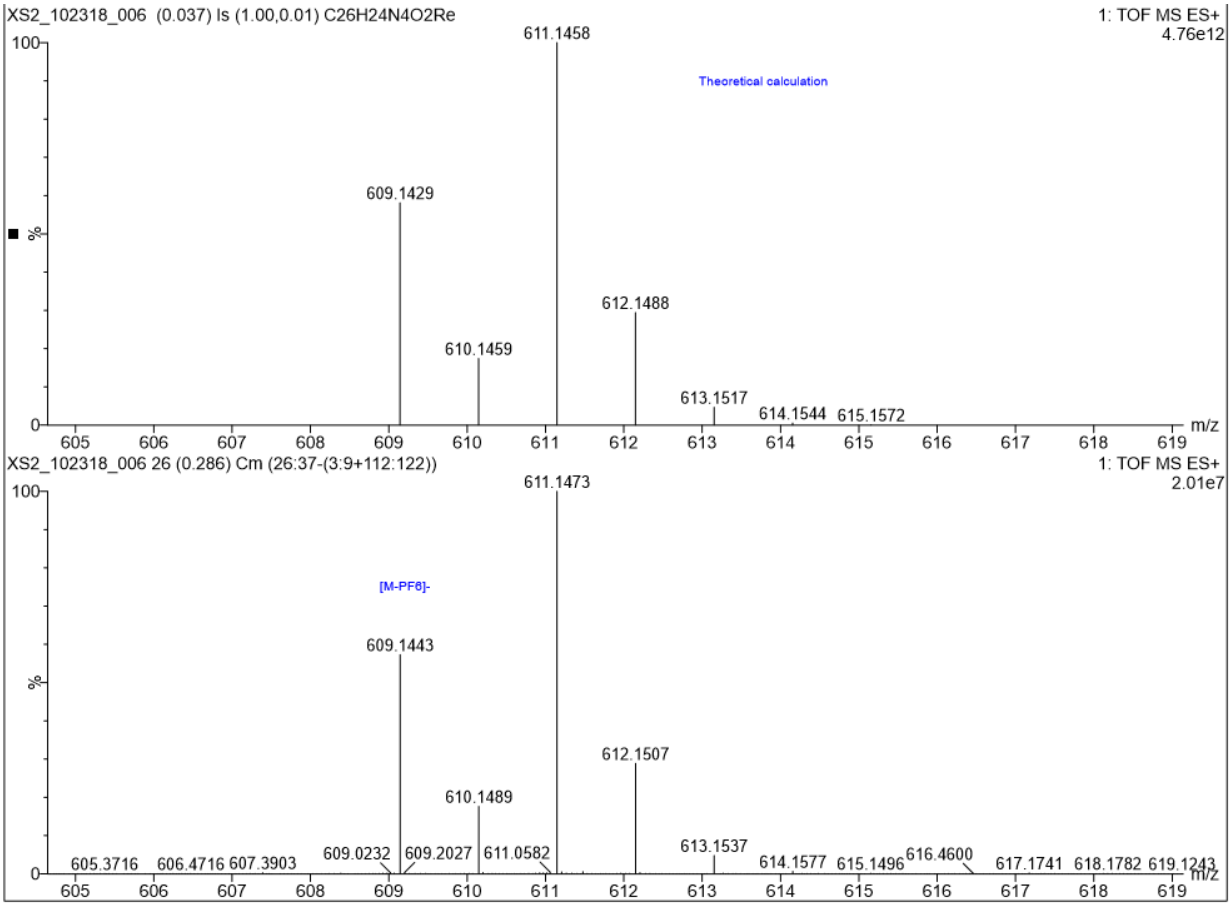

Figure S27. The simulated isotopic pattern of the ESI-MS spectrum in comparison with the experimental data for *cis*-[Re(4,4'-Me_2bpy)$_2$(CO)$_2$]PF_6 (**9**).

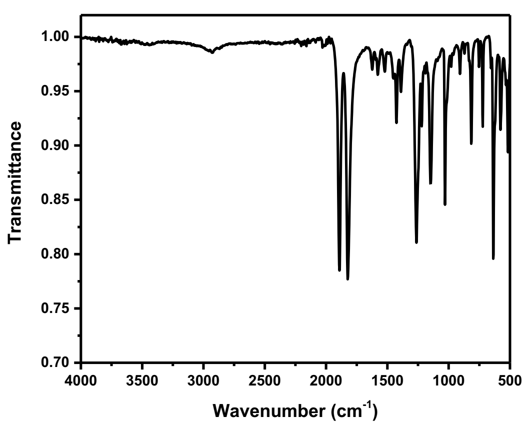

Figure S28. FTIR spectrum of *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**).

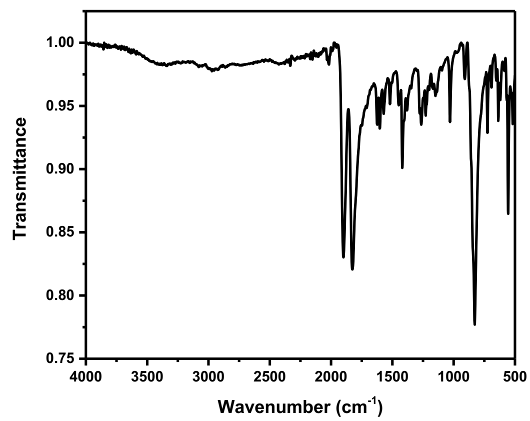

Figure S29. FTIR spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**).

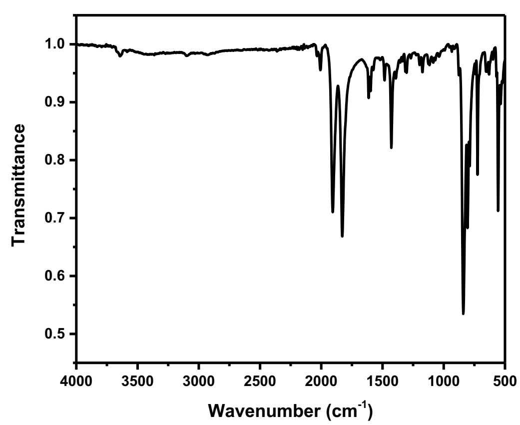

Figure S30. FTIR spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**).

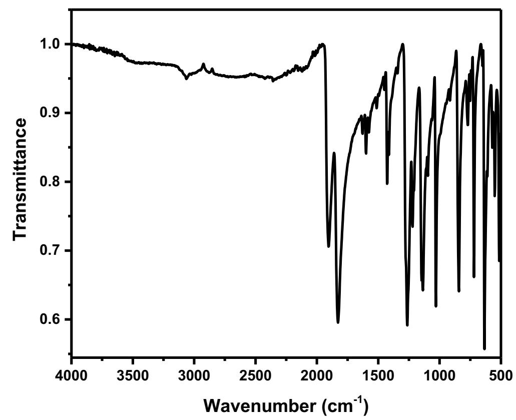

Figure S31. FTIR spectrum of *cis*-[Re(phen)$_2$(CO)$_2$](CF$_3$SO$_3$) (**4**).

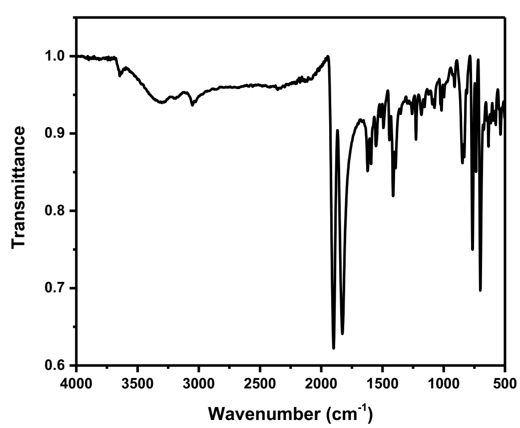

Figure S32. FTIR spectrum of *cis*-[Re(4,7-Ph$_2$phen)$_2$(CO)$_2$]PF$_6$ (**5**).

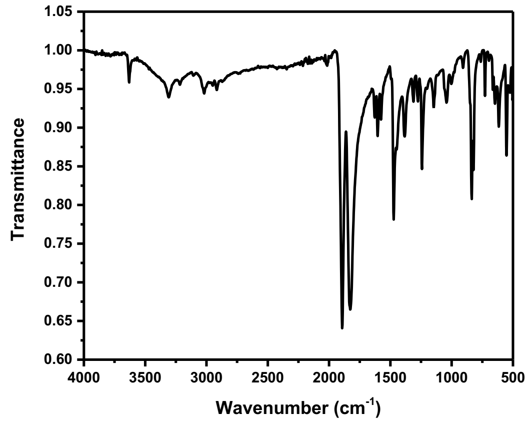

Figure S33. FTIR spectrum of *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**).

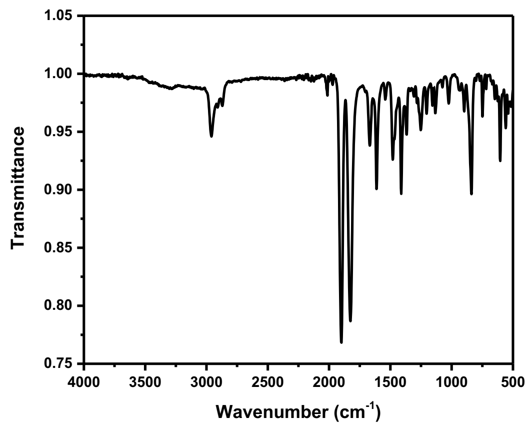

Figure S34. FTIR spectrum of *cis*-[Re(4,4′-dtbbpy)$_2$(CO)$_2$]PF_6 (**7**).

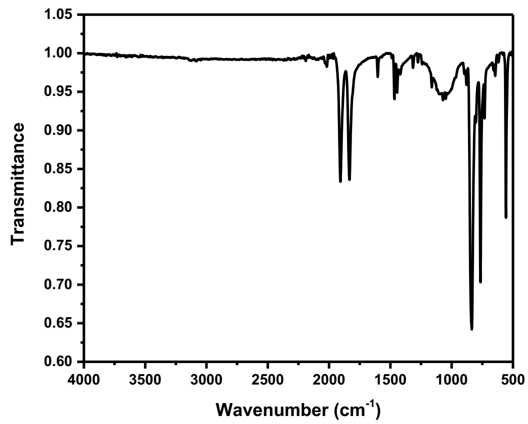

Figure S35. FTIR spectrum of *cis*-[Re(bpy)$_2$(CO)$_2$]PF_6 (**8**).

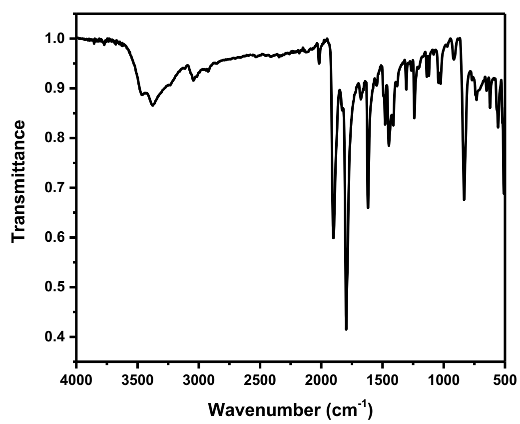

Figure S36. FTIR spectrum of *cis*-[Re(4,4′-Me$_2$bpy)$_2$(CO)$_2$]PF_6 (**9**).

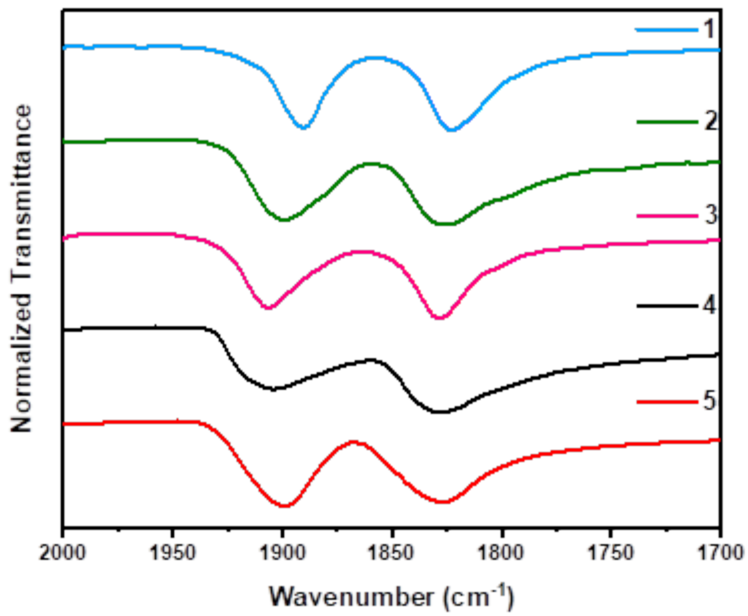

Figure S37. Comparison of the carbonyl stretching frequencies for **1**, **2**, **3**, **4**, and **5**.

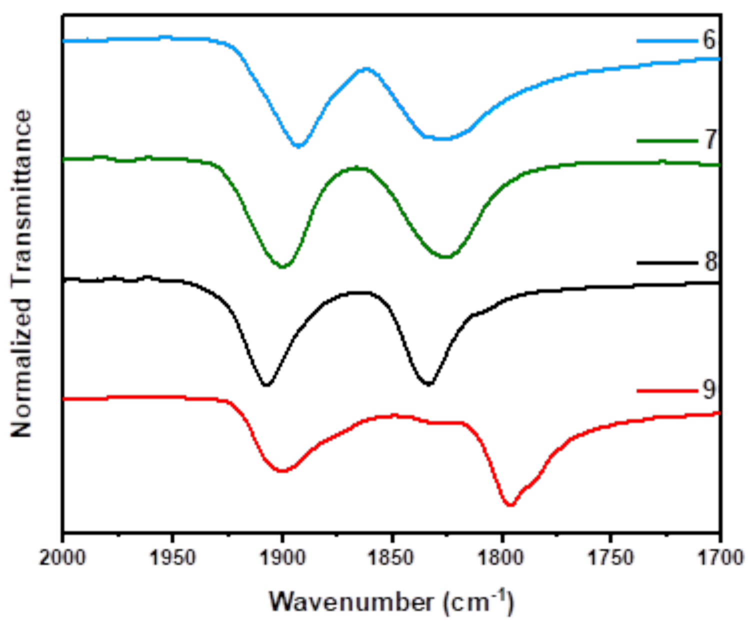

Figure S38. Comparison of the carbonyl stretching frequencies for **6**, **7**, **8**, and **9**.

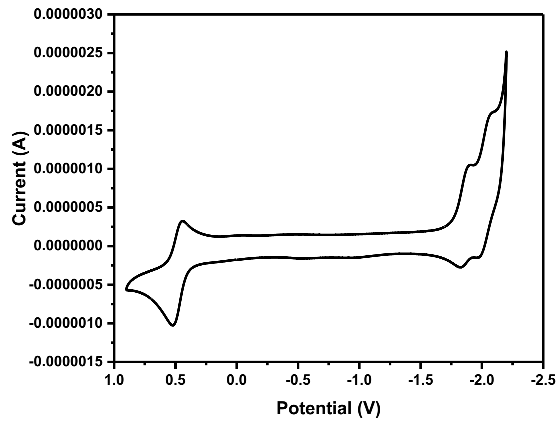

Figure S39. Cyclic voltammogram spectrum for *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

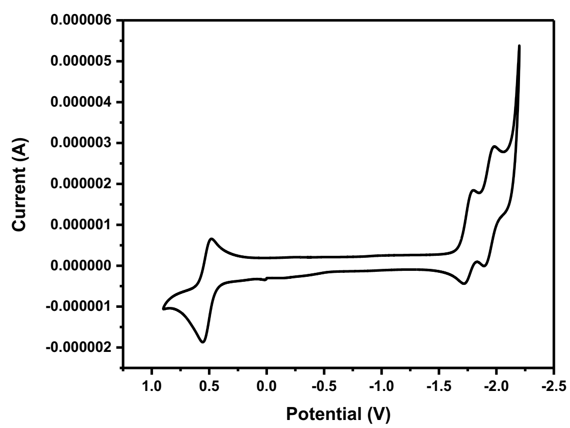

Figure S40. Cyclic voltammogram spectrum for *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

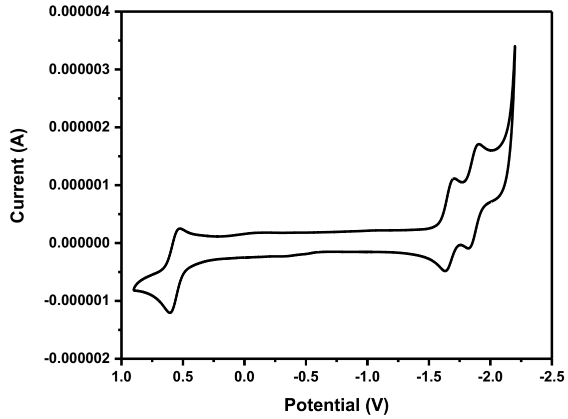

Figure S41. Cyclic voltammogram spectrum for *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

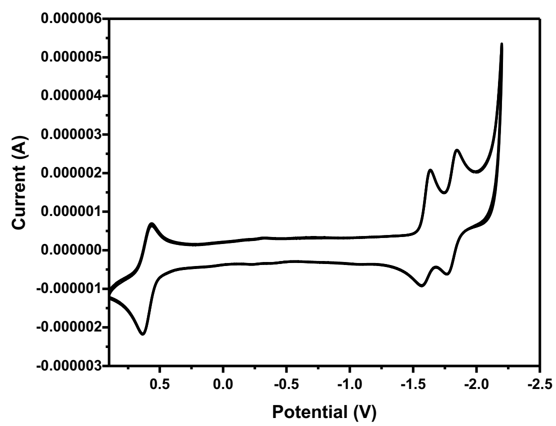

Figure S42. Cyclic voltammogram spectrum for *cis*-[Re(phen)$_2$(CO)$_2$](CF_3SO_3) (**4**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

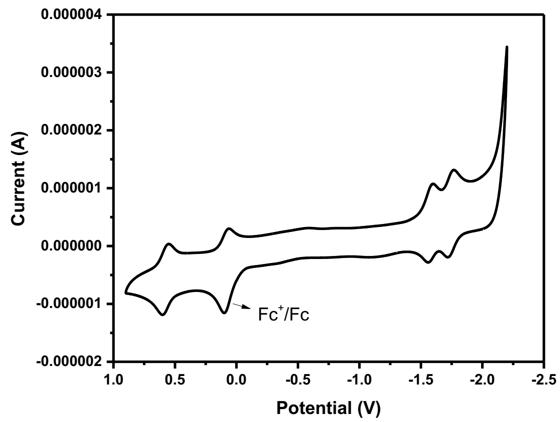

Figure S43. Cyclic voltammogram spectrum for *cis*-[Re(4,7-Ph_2phen)$_2$(CO)$_2$]PF_6 (**5**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

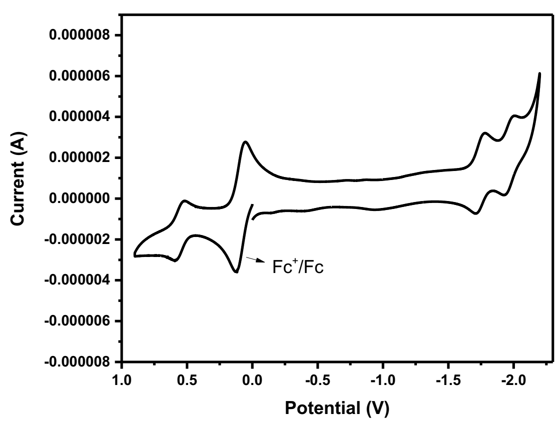

Figure S44. Cyclic voltammogram spectrum for *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

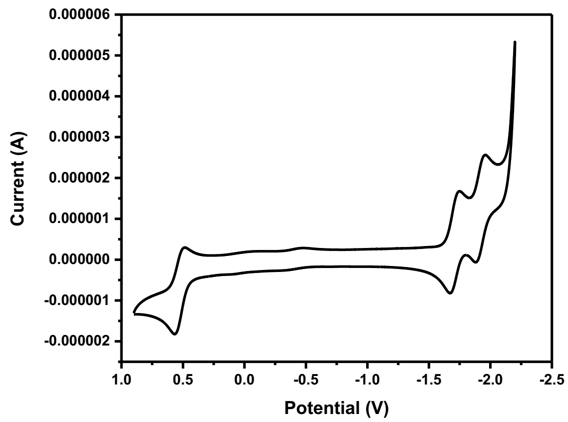

Figure S45. Cyclic voltammogram spectrum for *cis*-[Re(4,4'-dtbbpy)$_2$(CO)$_2$]PF$_6$ (**7**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M TBAPF$_6$ supporting electrolyte. Pt was used as the working electrode with Ag/AgNO$_3$ reference electrode.

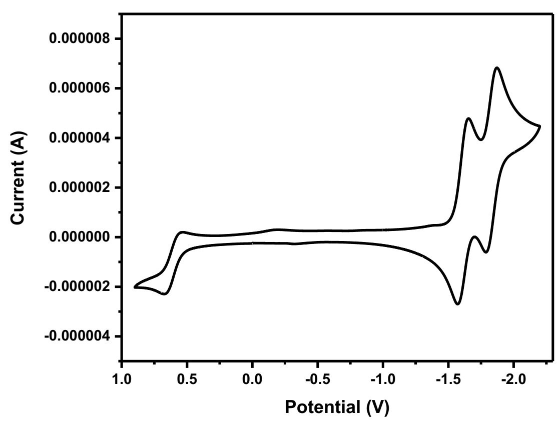

Figure S46. Cyclic voltammogram spectrum for *cis*-[Re(bpy)$_2$(CO)$_2$]PF$_6$ (**8**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M TBAPF$_6$ supporting electrolyte. Pt was used as the working electrode with Ag/AgNO$_3$ reference electrode.

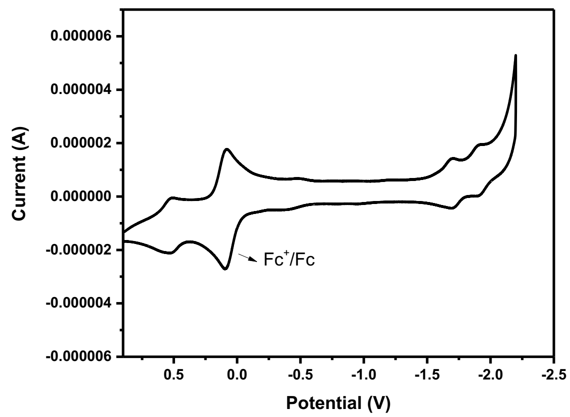

Figure S47. Cyclic voltammogram spectrum for *cis*-[Re(4,4′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**9**). Scans were taken at 20 mV/s in CH_3CN with a 0.1 M $TBAPF_6$ supporting electrolyte. Pt was used as the working electrode with Ag/$AgNO_3$ reference electrode.

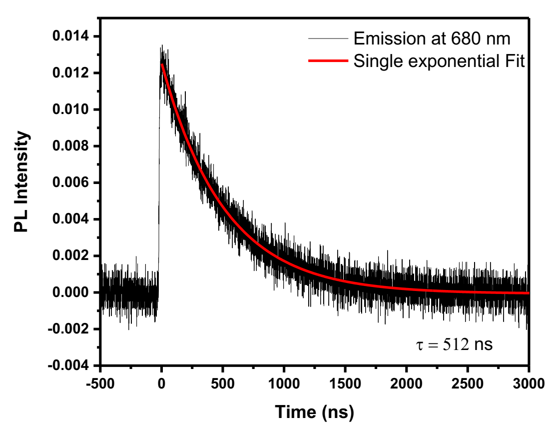

Figure S48. Room temperature PL emission intensity decay spectrum of *cis*-[Re(3,4,7,8-Me_4phen)$_2$(CO)$_2$](CF_3SO_3) (**1**) at 680 nm in deaerated CH_2Cl_2.

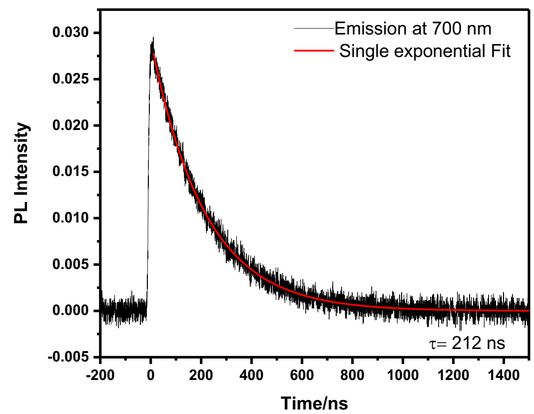

Figure S49. Room temperature PL emission intensity decay spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**) at 700 nm in deaerated CH_2Cl_2.

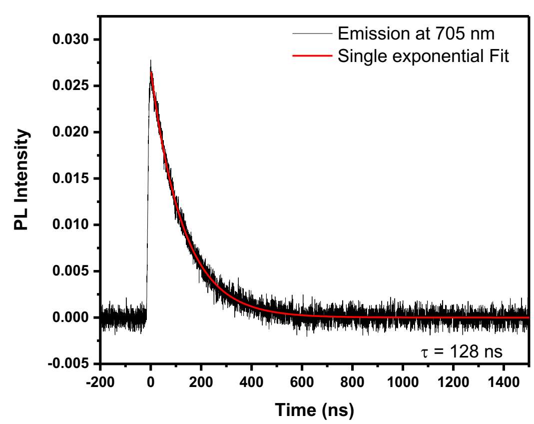

Figure S50. Room temperature PL emission intensity decay spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**) at 705 nm in deaerated CH_2Cl_2.

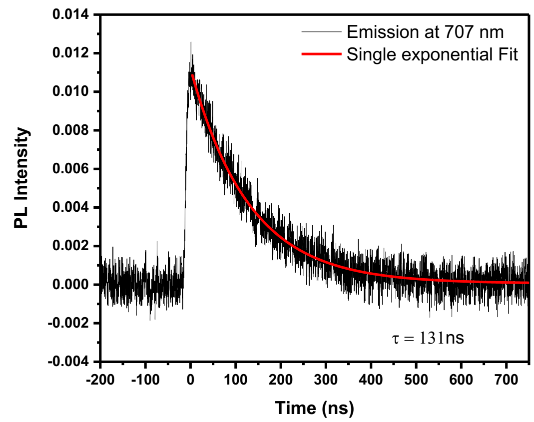

Figure S51. Room temperature PL emission intensity decay spectrum of *cis*-[Re(phen)$_2$(CO)$_2$](CF$_3$SO$_3$) (**4**) at 707 nm in deaerated CH_2Cl_2.

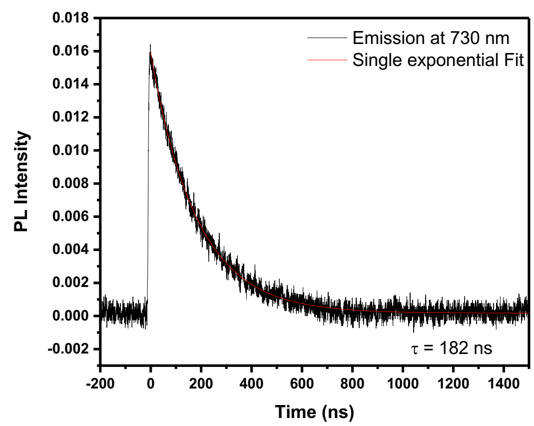

Figure S52. Room temperature PL emission intensity decay spectrum of *cis*-[Re(4,7-Ph$_2$phen)$_2$(CO)$_2$]PF$_6$ (**5**) at 730 nm in deaerated CH_2Cl_2.

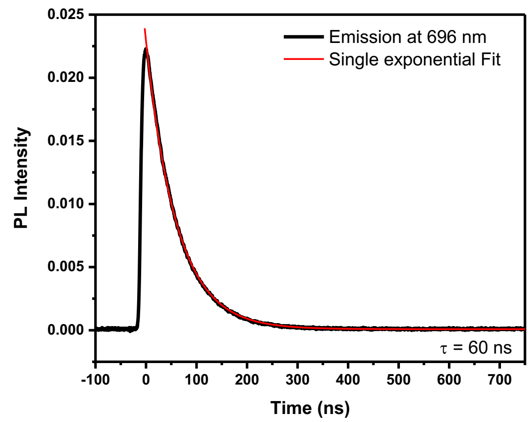

Figure S53. Room temperature PL emission intensity decay spectrum of *cis*-[Re(5,5'-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**) at 696 nm in deaerated CH_2Cl_2.

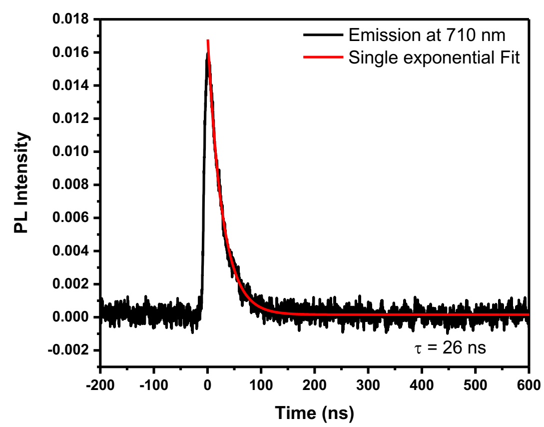

Figure S54. Room temperature PL emission intensity decay spectrum of *cis*-[Re(4,4'-dtbbpy)$_2$(CO)$_2$]PF_6 (**7**) at 710 nm in deaerated CH_2Cl_2**.**

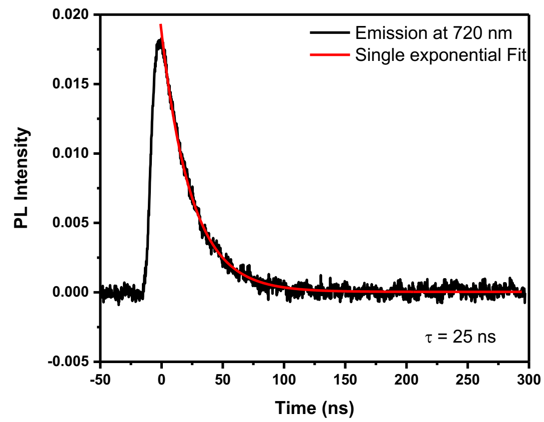

Figure S55. Room temperature PL emission intensity decay spectrum of *cis*-$[Re(bpy)_2(CO)_2]PF_6$ (**8**) at 720 nm in deaerated CH_2Cl_2.

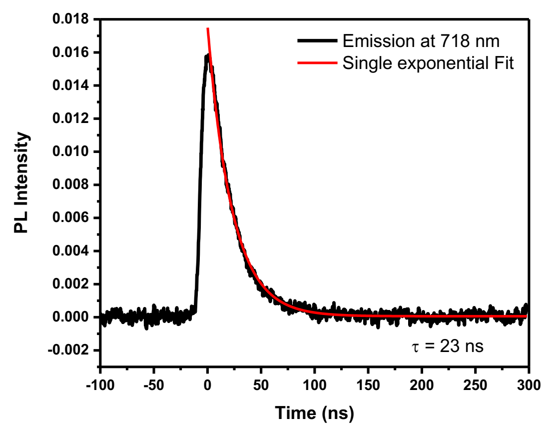

Figure S56. Room temperature PL emission intensity decay spectrum of *cis*-$[Re(4,4'\text{-}Me_2bpy)_2(CO)_2]PF_6$ (**9**) at 718 nm in deaerated CH_2Cl_2.

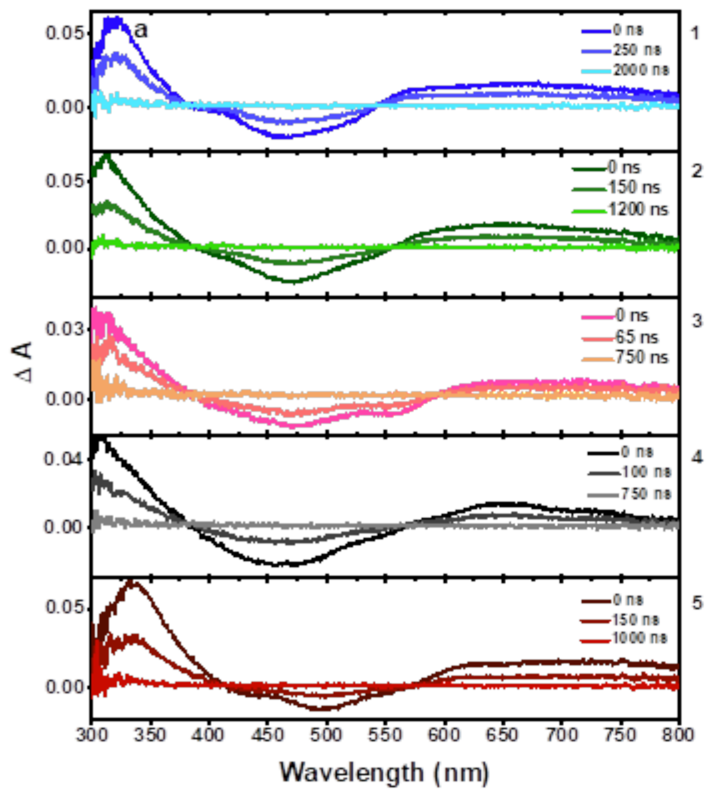

Figure S57. Excited-state absorption difference spectra in deaerated CH_2Cl_2 with 500 nm pulsed excitation (2 mJ/pulse) for complexes **1- 5**.

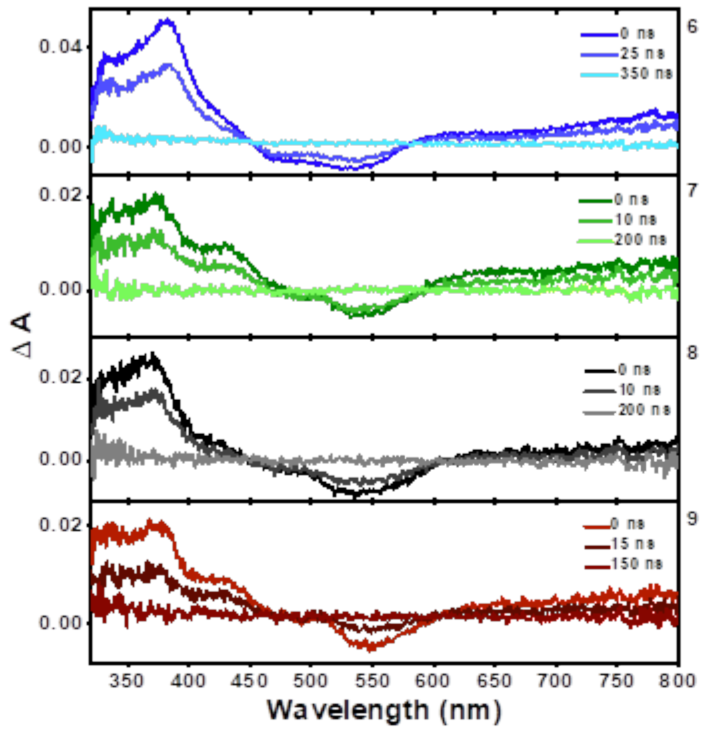

Figure S58. Excited-state absorption difference spectra in deaerated CH_2Cl_2 with 500 nm pulsed excitation (2 mJ/pulse) for complexes **6**- **9**.

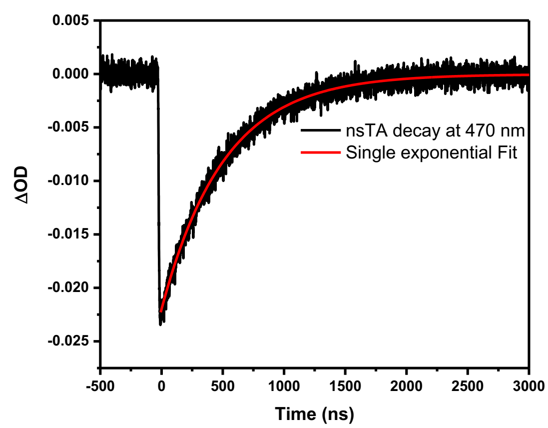

Figure S59. Room temperature nsTA decay spectrum of *cis*-[Re(3,4,7,8-Me_4phen$)_2$(CO$)_2$](CF_3SO_3) (**1**) at 470 nm in deaerated CH_2Cl_2.

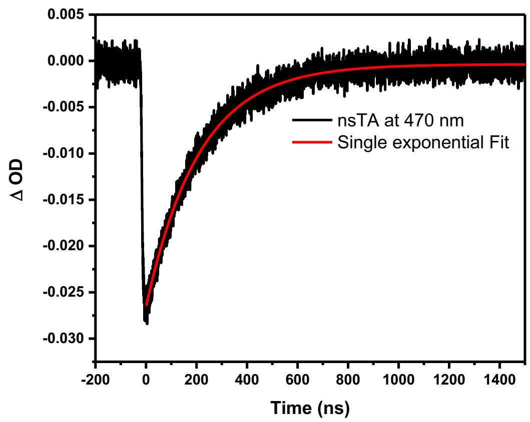

Figure S60. Room temperature nsTA decay spectrum of *cis*-[Re(4,7-Me_2phen)$_2$(CO)$_2$]PF_6 (**2**) at 470 nm in deaerated CH_2Cl_2.

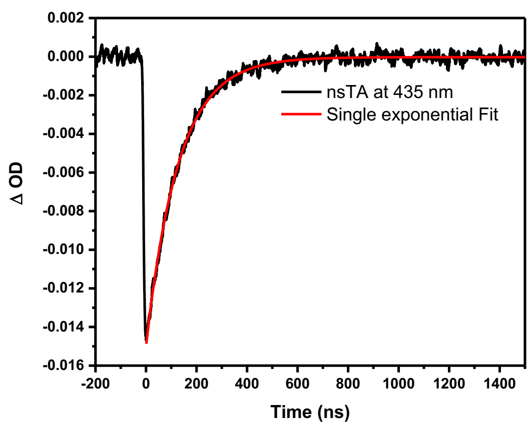

Figure S61. Room temperature nsTA decay spectrum of *cis*-[Re(5,6-Me_2phen)$_2$(CO)$_2$]PF_6 (**3**) at 435 nm in deaerated CH_2Cl_2.

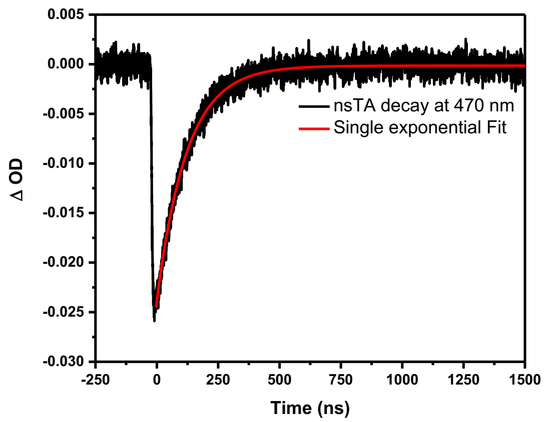

Figure S62. Room temperature nsTA decay spectrum of *cis*-[Re(CO)$_2$(phen)$_2$](CF$_3$SO$_3$) (**4**) at 470 nm in deaerated CH_2Cl_2.

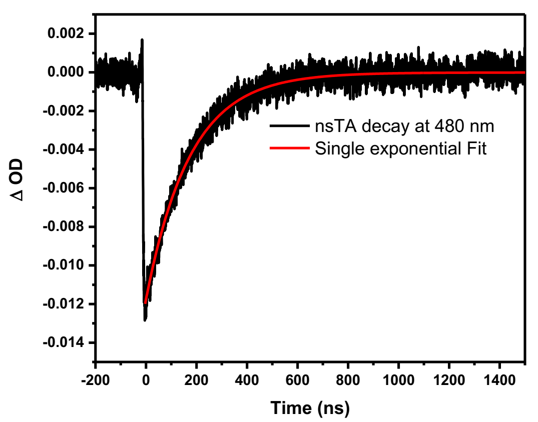

Figure S63. Room temperature nsTA decay spectrum of *cis*-[Re(4,7-Ph$_2$phen)$_2$(CO)$_2$]PF$_6$ (**5**) at 480 nm in deaerated CH_2Cl_2.

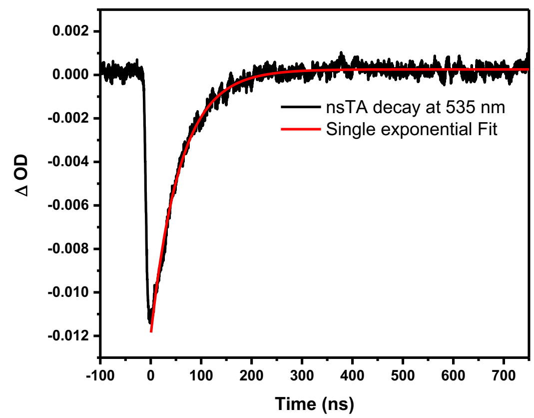

Figure S64. Room temperature nsTA decay spectrum of *cis*-[Re(5,5′-Me_2bpy)$_2$(CO)$_2$]PF_6 (**6**) at 535 nm in deaerated CH_2Cl_2.

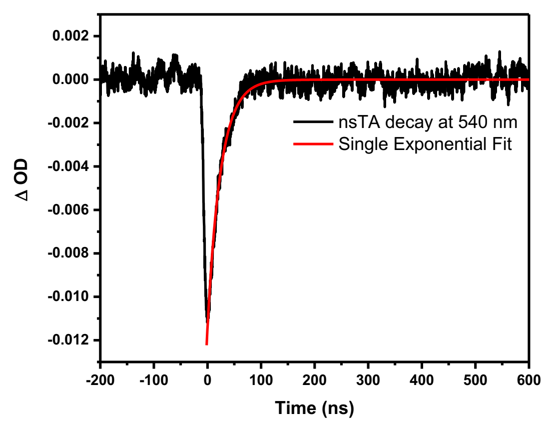

Figure S65. Room temperature nsTA decay spectrum of *cis*-[Re (4,4′-dtbbpy)$_2$(CO)$_2$]PF_6 (**7**) at 540 nm in deaerated CH_2Cl_2.

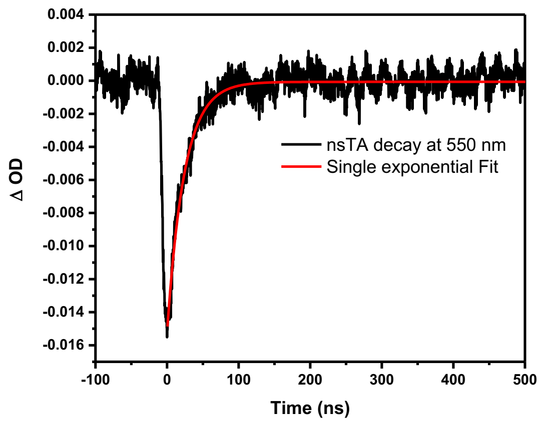

Figure S66. Room temperature nsTA decay spectrum of *cis*-$[Re(bpy)_2(CO)_2]PF_6$ (**8**) at 550 nm in deaerated CH_2Cl_2.

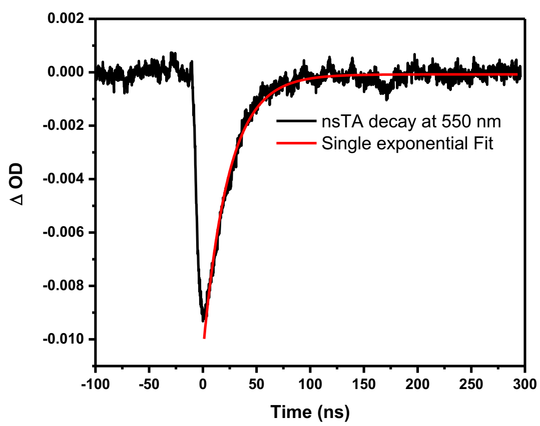

Figure S67. Room temperature nsTA decay spectrum of *cis*-$[Re(4,4'\text{-}Me_2bpy)_2(CO)_2]PF_6$ (**9**) at 550 nm in deaerated CH_2Cl_2.

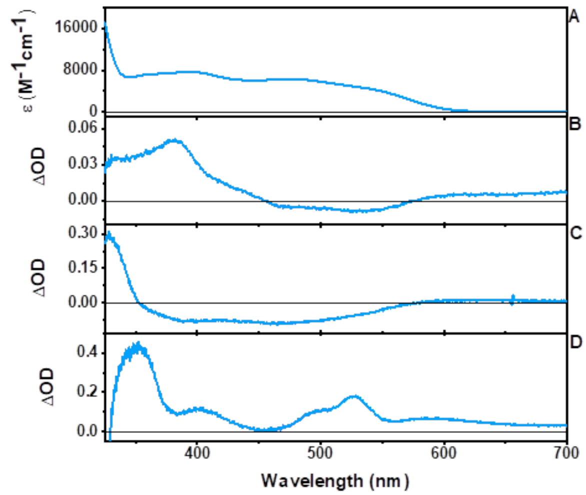

Figure S68. (A) Electronic absorption spectrum of **6** measured in CH_2Cl_2. (B) The nsTA difference spectrum of **6** measured in CH_2Cl_2. (C) Differential absorption spectrum of one-electron oxidized **6**. (D) Differential absorption spectrum of one-electron reduced **6**.

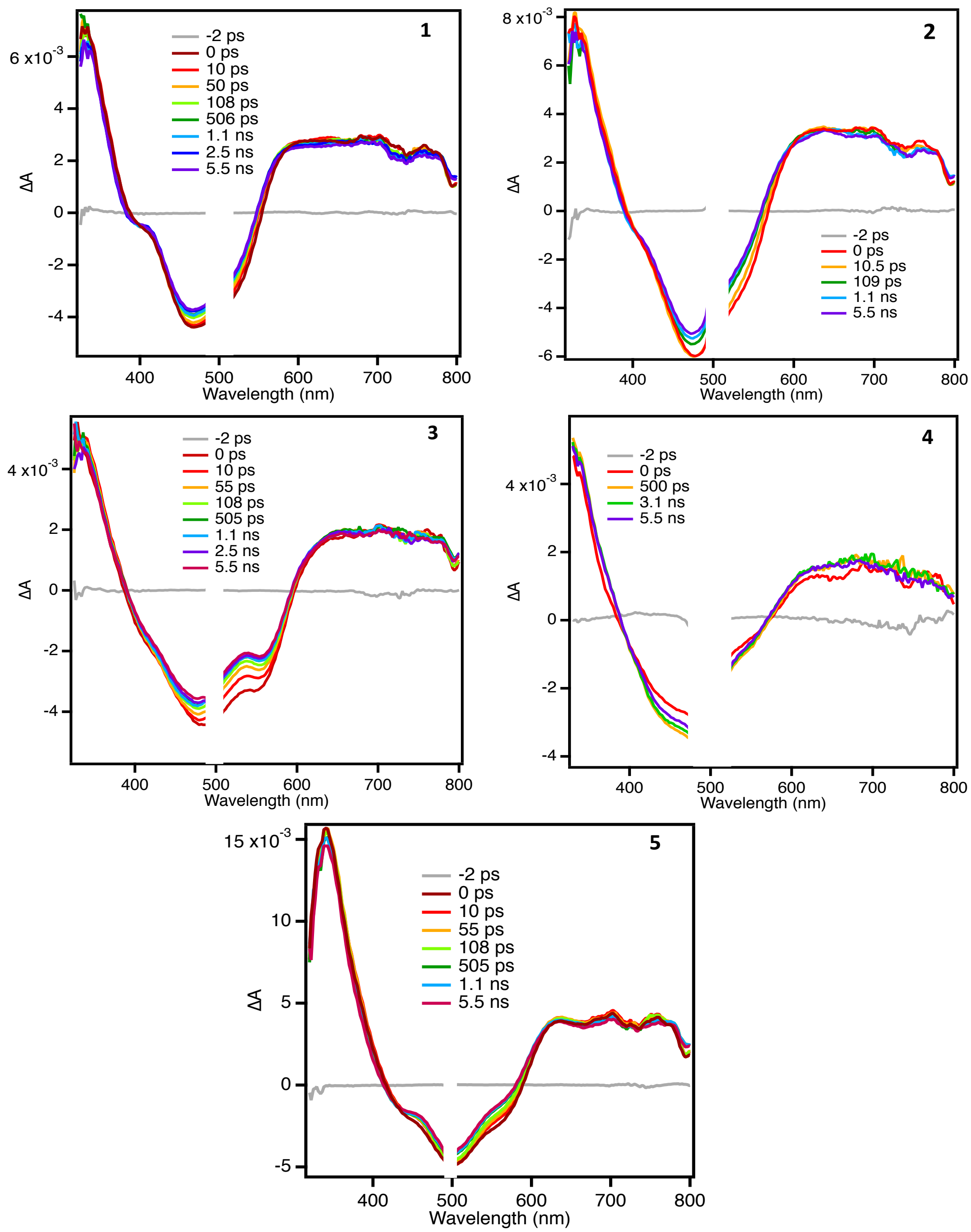

Figure S69. Ultrafast transient absorption difference spectra of phen-containing complexes **1**–**5** in dichloromethane (λ_{ex} = 500 nm, 100 fs fwhm, 0.5 μJ/pulse). The laser scatter at 500 nm removed for clarity.

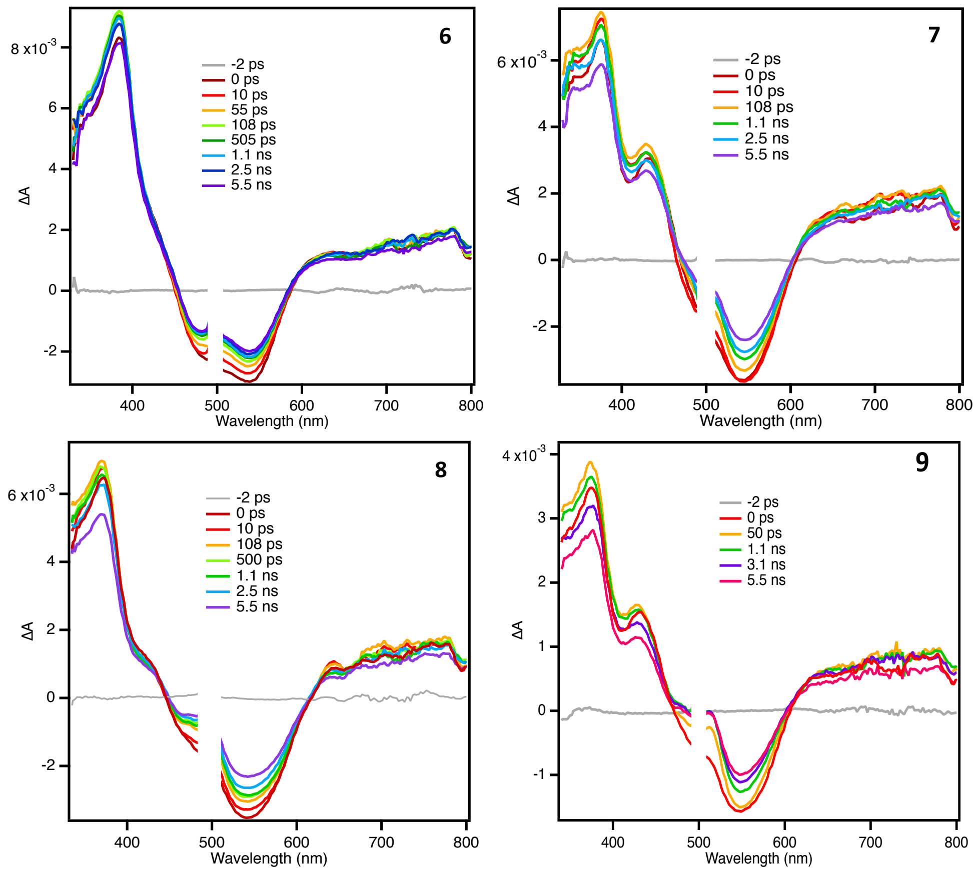

Figure S70. Ultrafast transient absorption difference spectra of bpy-containing complexes **6**–**9** in dichloromethane (λ_{ex} = 500 nm, 100 fs fwhm, 0.5 μJ/pulse). The laser scatter at 500 nm removed for clarity.

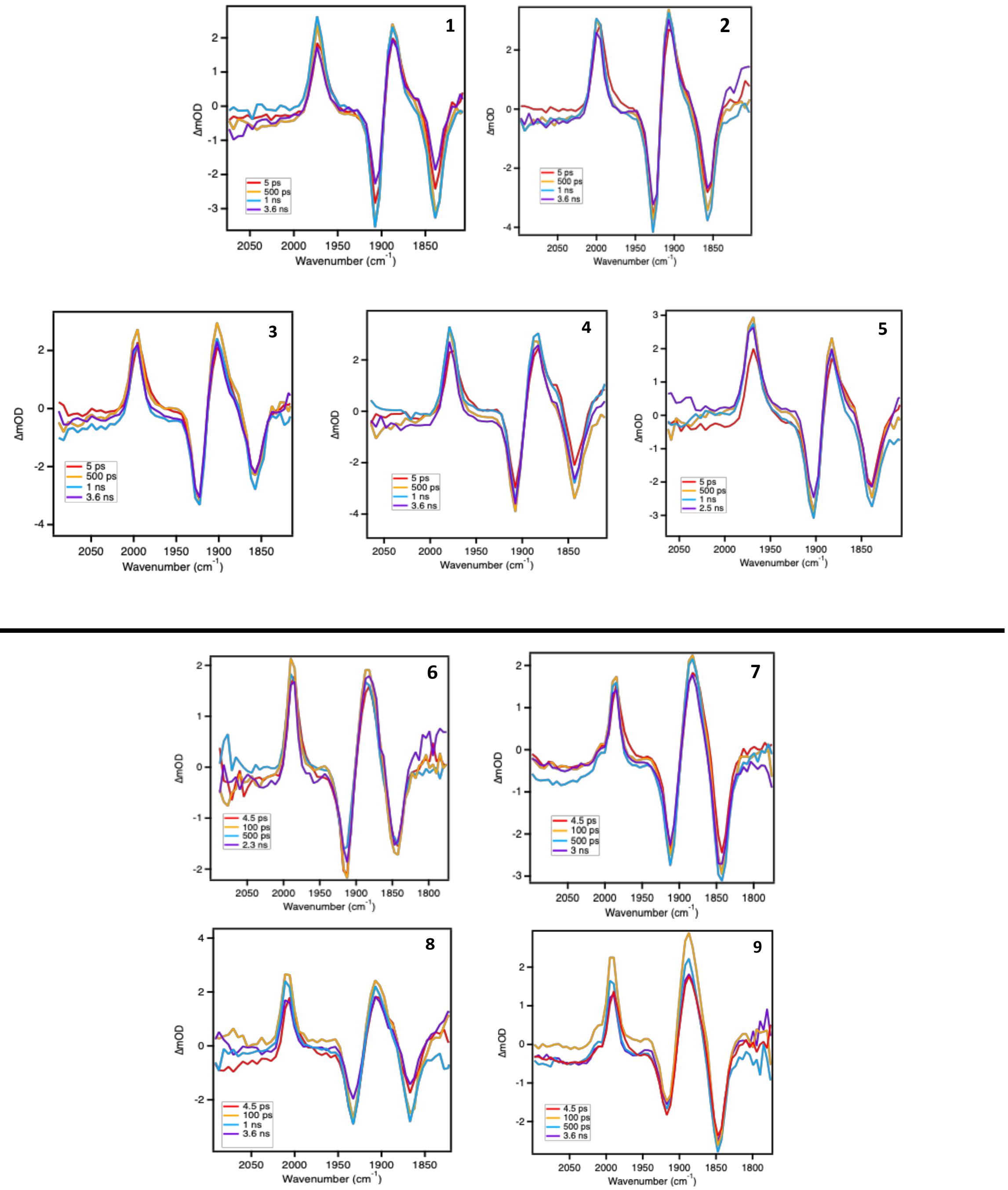

Figure S71. Ultrafast TR-IR difference spectra following 500 nm (0.7 μJ/pulse) excitation (of the *cis*-$[Re(N^\wedge N)_2(CO)_2]^+$ complexes **1**–**9** in dichloromethane, where N^N is phen-based (top) or bpy-based (bottom). (Spacer width = 750 μm)

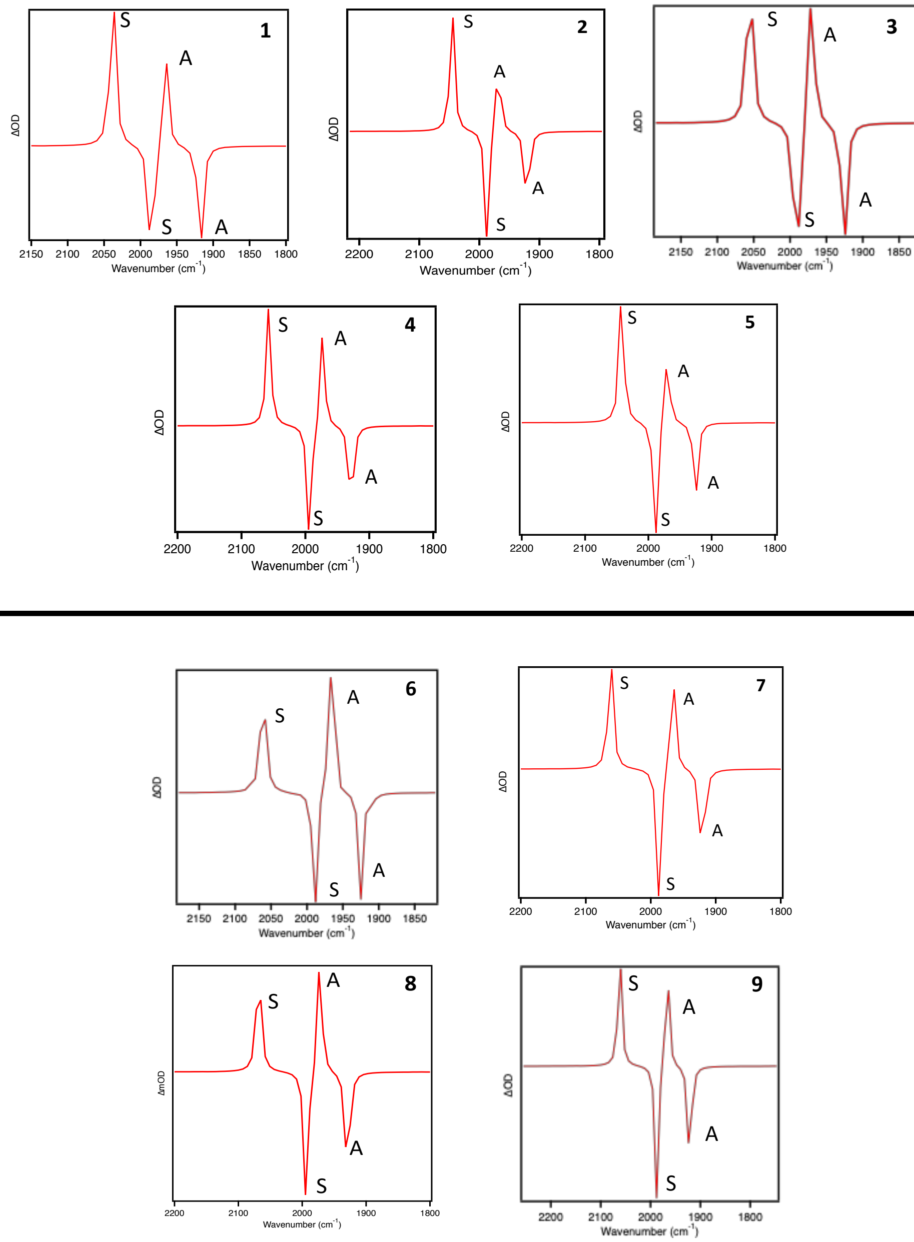

Figure S72. Simulated TR-IR spectra of complexes **1**–**9**. Symmetric (S) and antisymmetric (A) modes are labeled on the figure. Calculated at the B3LYP/D3/6-31G*/LANL2DZ (PCM solvent=dichloromethane) level of theory.

S73. Optimized S_0 and T_1 geometries of **1**–**9**

Optimized S_0 geometry of **1**

Re	0.00004000	1.36435900	-0.00000100
N	0.34133800	-0.30709500	1.40321800
N	2.11469200	1.02797700	-0.09311400
N	-0.34138300	-0.30699000	-1.40331000
N	-2.11463200	1.02810600	0.09312100
C	-0.56146300	-0.94121000	2.14752100
C	-0.27948200	-2.07364700	2.93398200
C	1.02656300	-2.57239300	2.94359800
C	2.00953000	-1.90073100	2.16093900
C	1.62182500	-0.77132800	1.40610600
C	2.57371900	-0.05763600	0.60589100
C	3.92245500	-0.47572000	0.55339400
C	4.84245700	0.25505100	-0.25032300
C	4.36068300	1.36604500	-0.94875900
C	3.00055400	1.70305700	-0.83409800
C	0.56136400	-0.94110100	-2.14767800
C	0.27929700	-2.07345900	-2.93422100
C	-1.02677600	-2.57213200	-2.94384100
C	-2.00967600	-1.90050300	-2.16106500
C	-1.62189000	-0.77116800	-1.40617400
C	-2.57372100	-0.05749100	-0.60587000
C	-3.92244900	-0.47558400	-0.55325200
C	-4.84236500	0.25514200	0.25061500
C	-4.36055700	1.36620600	0.94891300
C	-3.00044100	1.70322700	0.83412500
H	-1.56676500	-0.53537800	2.12065600
H	2.60637500	2.55743400	-1.37093800
H	1.56669200	-0.53532900	-2.12080300
H	-2.60622400	2.55762500	1.37090600
C	-0.06832200	2.70402600	-1.34233400
C	0.06850200	2.70395400	1.34239800
O	0.05480400	3.52185800	2.18478800
O	-0.05459600	3.52199500	-2.18466000
C	4.29147900	-1.63105900	1.32457800
H	5.31981500	-1.97207700	1.30194700
C	3.38495900	-2.30786800	2.08821300
H	3.71255400	-3.17136300	2.65513000
C	-3.38511000	-2.30761400	-2.08826500
H	-3.71277100	-3.17105300	-2.65522900
C	-4.29155500	-1.63086100	-1.32449000

H	-5.31989800	-1.97185600	-1.30182100
C	-1.40482700	-2.69845600	3.72328400
H	-2.34201200	-2.15917400	3.55933500
H	-1.56500700	-3.74298700	3.43344900
H	-1.19469900	-2.68454900	4.79860700
C	1.41398400	-3.78406500	3.75129400
H	1.81435900	-4.57197200	3.10240600
H	2.19761600	-3.53274700	4.47553300
H	0.57177500	-4.20171600	4.30261200
C	6.28391700	-0.17717800	-0.32621700
H	6.74647700	-0.16770800	0.66783200
H	6.36395700	-1.20110600	-0.71020500
H	6.87539700	0.46883200	-0.97468000
C	5.23683700	2.22465200	-1.82985000
H	6.06215000	2.66711200	-1.26103300
H	5.67638600	1.64091000	-2.64656500
H	4.66223100	3.04150000	-2.27482300
C	1.40459100	-2.69827100	-3.72359300
H	2.34182400	-2.15909600	-3.55955800
H	1.56467000	-3.74285400	-3.43389200
H	1.19448100	-2.68420100	-4.79891700
C	-1.41428200	-3.78371400	-3.75163300
H	-1.81454200	-4.57171300	-3.10278400
H	-2.19802100	-3.53233000	-4.47573100
H	-0.57213900	-4.20127400	-4.30312100
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H	-6.06220600	2.66701000	1.26123300
C	-6.28377600	-0.17719900	0.32677900
H	-6.74675200	-0.16698400	-0.66707600
H	-6.36362200	-1.20141400	0.71002100
H	-6.87500900	0.46829000	0.97598700

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Optimized S_0 geometry of **2**

Re	0.00000900	1.29994200	-0.00000800
N	0.63594000	-0.35849600	1.31137900
N	2.05211300	0.97738900	-0.52493100
N	-0.63599600	-0.35843000	-1.31143700
N	-2.05210000	0.97743600	0.52492400
C	-0.09271500	-0.99169700	2.22937100
C	0.39432800	-2.08425200	2.95871000
C	1.68020300	-2.56057500	2.74718600
C	2.47535200	-1.89234700	1.77049700
C	1.90926000	-0.79475200	1.08046500
C	2.67044100	-0.08102500	0.09573600
C	3.99757100	-0.47467000	-0.19860400
C	4.72472400	0.25762000	-1.18068100
C	4.07242900	1.32233300	-1.78484500
C	2.75708500	1.65314400	-1.44089800
C	0.09262900	-0.99162400	-2.22945900
C	-0.39444400	-2.08416300	-2.95880200
C	-1.68032200	-2.56047200	-2.74725900
C	-2.47543900	-1.89225100	-1.77053900

C	-1.90931500	-0.79467700	-1.08050200
C	-2.67046100	-0.08095600	-0.09574400
C	-3.99759200	-0.47458200	0.19861700
C	-4.72470900	0.25770600	1.18072300
C	-4.07238100	1.32239900	1.78488700
C	-2.75703900	1.65319300	1.44091400
H	-1.09703700	-0.61646700	2.38877000
H	-0.25332300	-2.55331100	3.69180200
H	4.57436600	1.91951100	-2.53874100
H	2.25004600	2.48421500	-1.91464500
H	1.09695300	-0.61640700	-2.38887300
H	0.25318400	-2.55321700	-3.69191700
H	-4.57429100	1.91957500	2.53880300
H	-2.24997200	2.48424600	1.91466200
C	-0.35851100	2.64170200	-1.29483400
C	0.35849300	2.64175900	1.29478600
O	0.53355700	3.46134500	2.11636700
O	-0.53300200	3.46184700	-2.11598000
C	4.54411400	-1.59633800	0.50979000
H	5.55873200	-1.90999600	0.29300500
C	3.81998500	-2.27223700	1.44911300
H	4.26843600	-3.11265400	1.96613700
C	-3.82007100	-2.27212500	-1.44913300
H	-4.26854700	-3.11252500	-1.96616200
C	-4.54416900	-1.59622900	-0.50978300
H	-5.55878800	-1.90987300	-0.29298200
C	-2.21485000	-3.73404200	-3.52182100
H	-2.50280300	-4.55116800	-2.84997400
H	-3.10808500	-3.45377000	-4.09241300
H	-1.46833400	-4.11495000	-4.22266000
C	-6.13817200	-0.10335300	1.54676500
H	-6.79882900	-0.04141900	0.67401300
H	-6.19769300	-1.13031400	1.92614900
H	-6.52709400	0.56764900	2.31635800
C	2.21469600	-3.73417100	3.52173300
H	2.50265400	-4.55128600	2.84987500
H	3.10792100	-3.45392500	4.09235300
H	1.46815800	-4.11508500	4.22254600
C	6.13818700	-0.10346000	-1.54669800
H	6.79882600	-0.04155400	-0.67393000
H	6.19769700	-1.13041800	-1.92609700
H	6.52714000	0.56754600	-2.31627200

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Optimized S_0 geometry of **3**

Re	0.00000200	1.37641800	0.00000500
N	0.76946300	-0.28107300	1.23735400
N	1.99005900	1.06308300	-0.72948500
N	-0.76946500	-0.28106500	-1.23735100
N	-1.99005500	1.06308000	0.72949600
C	0.13048000	-0.90653700	2.22706600
C	0.69133100	-2.00069800	2.89665100
C	1.94446400	-2.45538300	2.52651800
C	2.65459100	-1.81194600	1.48540100
C	2.00961000	-0.71522800	0.87050600
C	2.66398300	0.00037000	-0.18053900
C	3.95200100	-0.40258300	-0.60072400
C	4.54609700	0.35273500	-1.63790500
C	3.86462200	1.42675000	-2.18210600
C	2.59119000	1.75552100	-1.70768100
C	-0.13048600	-0.90652300	-2.22707000
C	-0.69134200	-2.00067600	-2.89666300
C	-1.94447500	-2.45536100	-2.52653300

C	-2.65459900	-1.81193000	-1.48540900
C	-2.00961300	-0.71521900	-0.87050700
C	-2.66398300	0.00037300	0.18054400
C	-3.95200100	-0.40257900	0.60072900
C	-4.54609400	0.35273300	1.63791500
C	-3.86461500	1.42674300	2.18212200
C	-2.59118200	1.75551300	1.70769800
H	-0.84884400	-0.52319900	2.48745100
H	0.13641600	-2.47933100	3.69557800
H	4.30169600	2.02188900	-2.97598600
H	2.03346700	2.58826500	-2.11623600
H	0.84883800	-0.52318500	-2.48745300
H	-0.13642900	-2.47930400	-3.69559500
H	-4.30168500	2.02187800	2.97600700
H	-2.03345600	2.58825300	2.11625700
H	2.37471200	-3.30415600	3.04359800
H	5.53137400	0.10240800	-2.01012400
H	-5.53137100	0.10240800	2.01013400
H	-2.37472700	-3.30412800	-3.04361800
C	-0.48816600	2.71995600	-1.25225300
C	0.48816500	2.71992800	1.25229400
O	0.74286200	3.53990700	2.05110500
O	-0.74283000	3.53984100	-2.05117200
C	4.60556400	-1.54115900	0.02613000
C	3.97563100	-2.22596900	1.04398900
C	-3.97564000	-2.22595200	-1.04399800
C	-4.60556800	-1.54114800	-0.02613300
C	4.58170200	-3.41117900	1.76061800
H	4.68435900	-3.20522600	2.83278300
H	3.94290300	-4.29657900	1.65931000
H	5.56796000	-3.67855000	1.38757000
C	5.97731800	-1.89878900	-0.49987000
H	6.67583900	-1.06454100	-0.36370300
H	6.41081200	-2.76749800	-0.00902200
H	5.93777600	-2.11780300	-1.57351800
C	-4.58171600	-3.41115500	-1.76063500
H	-4.68437600	-3.20519300	-2.83279800
H	-3.94291900	-4.29655700	-1.65933600
H	-5.56797300	-3.67852600	-1.38758600
C	-5.97732400	-1.89877800	0.49986500
H	-6.67584000	-1.06452300	0.36371100
H	-6.41082400	-2.76747700	0.00900600
H	-5.93778000	-2.11780600	1.57351100

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2 6 1.5 10 1.5
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Optimized S_0 geometry of **4**

Re	0.00001200	-1.07228300	-0.00002300
N	-0.67001600	0.58720800	1.30035800
N	-2.03811500	-0.75936700	-0.58674000
N	0.66998800	0.58724600	-1.30035800
N	2.03814200	-0.75936400	0.58668600
C	0.02872500	1.21977000	2.24432000
C	-0.48653600	2.31326100	2.95848300
C	-1.76446100	2.76327700	2.68150000
C	-2.53137300	2.11009700	1.69174300
C	-1.93587400	1.01434200	1.02346700
C	-2.66591300	0.30012300	0.02000500
C	-3.98478500	0.69670200	-0.30490100
C	-4.66832100	-0.04218200	-1.29405500
C	-4.02946500	-1.11091500	-1.89548500
C	-2.71955900	-1.44049400	-1.51951800
C	-0.02877200	1.21980400	-2.24431400
C	0.48646200	2.31331700	-2.95845700
C	1.76437500	2.76336200	-2.68146200
C	2.53129700	2.11019300	-1.69170600

C	1.93583000	1.01440600	-1.02345300
C	2.66589700	0.30017600	-0.02000900
C	3.98475100	0.69679800	0.30492000
C	4.66831100	-0.04209700	1.29404600
C	4.02949800	-1.11088600	1.89542400
C	2.71961200	-1.44051100	1.51943400
H	1.02672100	0.84332000	2.43563200
H	0.12661700	2.78919200	3.71520300
H	-4.52132500	-1.70481300	-2.65750800
H	-2.19797800	-2.27148700	-1.97695600
H	-1.02676400	0.84333500	-2.43561500
H	-0.12669500	2.78923900	-3.71518000
H	4.52138200	-1.70479200	2.65742500
H	2.19807400	-2.27155500	1.97682300
H	-2.18621000	3.60854800	3.21682800
H	-5.68239700	0.23129600	-1.56844400
H	5.68237100	0.23141700	1.56846000
H	2.18610300	3.60864800	-3.21678200
C	0.39499900	-2.41589000	-1.28462200
C	-0.39511900	-2.41615600	1.28428700
O	-0.59457500	-3.23606700	2.09803100
O	0.59495000	-3.23644200	-2.09760200
C	-4.56258000	1.81949000	0.37972900
H	-5.57375500	2.11589700	0.11840400
C	-3.86730100	2.49736400	1.33735700
H	-4.31454000	3.34193500	1.85233000
C	3.86720600	2.49749900	-1.33729300
H	4.31442200	3.34209800	-1.85224100
C	4.56250300	1.81963200	-0.37967200
H	5.57365900	2.11608800	-0.11833000

1 38 1.0 39 1.0 3 1.0 2 1.0 4 1.0 5 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 34 1.0
9 10 1.5 44 1.5
10 11 1.5
11 12 1.5
12 13 1.5 42 1.5
13 14 1.5 35 1.0

14 15 1.5 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 1.5 31 1.0
18 19 1.5 37 1.0
19 20 1.5 46 1.5
20 21 1.5
21 22 1.5
22 23 1.5 48 1.5
23 24 1.5 36 1.0
24 25 1.5 32 1.0
25 33 1.0
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38 41 3.0
39 40 3.0
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42 43 1.0 44 1.5
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44 45 1.0
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46 47 1.0 48 1.5
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48 49 1.0
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Optimized S_0 geometry of **5**

Re	0.00001500	2.14729600	0.00002700
N	0.50920000	0.47879800	1.34512000
N	2.08747500	1.82400000	-0.33460000
N	-0.50919600	0.47883900	-1.34510800
N	-2.08744600	1.82400600	0.33465600
C	-0.30614700	-0.15115200	2.19181700
C	0.07586900	-1.30128300	2.88804600
C	1.34440100	-1.84756400	2.71605000
C	2.25074100	-1.15305700	1.85767500
C	1.77941300	0.00373200	1.18968400
C	2.63991700	0.74318300	0.30890400
C	3.98981100	0.34927600	0.13532800
C	4.81562200	1.12677900	-0.73139900
C	4.21648000	2.19947400	-1.38508400
C	2.87473000	2.51771900	-1.16894400
C	0.30614200	-0.15109100	-2.19183000
C	-0.07589200	-1.30119500	-2.88809600
C	-1.34442600	-1.84746700	-2.71610700
C	-2.25075100	-1.15298800	-1.85769600
C	-1.77940900	0.00377700	-1.18967700
C	-2.63990100	0.74320900	-0.30886800
C	-3.98979400	0.34930000	-0.13528600
C	-4.81559400	1.12679000	0.73146400
C	-4.21644000	2.19946900	1.38516600
C	-2.87468900	2.51770900	1.16902400
H	-1.30171600	0.26276700	2.30091800
H	-0.64470900	-1.78762900	3.53585900
H	4.79806500	2.82534500	-2.05275000
H	2.41563200	3.36197700	-1.66740700
H	1.30171100	0.26282700	-2.30092500
H	0.64467200	-1.78752100	-3.53594100
H	-4.79801700	2.82533200	2.05284600
H	-2.41558000	3.36195100	1.66750400
C	-0.23375200	3.49282300	-1.32213000
C	0.23377100	3.49271900	1.32228900
O	0.32498500	4.31399000	2.15447800
O	-0.32485200	4.31379400	-2.15462700
C	4.43942800	-0.82679000	0.82446100
H	5.46131600	-1.15470100	0.68022300
C	3.61590400	-1.53889000	1.64616400
H	3.99937100	-2.41080600	2.16136400
C	-3.61590700	-1.53883800	-1.64616300
H	-3.99936900	-2.41075700	-2.16136300
C	-4.43941800	-0.82675800	-0.82443000

H	-5.46129800	-1.15468200	-0.68017100
C	6.25331500	0.84195800	-0.95502100
C	6.74858100	0.74221800	-2.26617800
C	7.14852600	0.72110900	0.12215800
C	8.10463700	0.50895600	-2.49427700
H	6.06323700	0.83017900	-3.10459300
C	8.50541900	0.49605700	-0.10954800
H	6.78400600	0.82911200	1.13947100
C	8.98617700	0.38473500	-1.41705200
H	8.47189200	0.42322100	-3.51287300
H	9.18738000	0.41419900	0.73181700
H	10.04254400	0.20584200	-1.59544200
C	1.70047800	-3.10540500	3.41576600
C	2.21370200	-4.20805000	2.71081300
C	1.47453600	-3.22458500	4.79724900
C	2.50092400	-5.39943700	3.37673800
H	2.36400500	-4.13787600	1.63742300
C	1.77184900	-4.41428800	5.46172500
H	1.08397200	-2.37525100	5.35054700
C	2.28552000	-5.50410100	4.75364800
H	2.88831800	-6.24689800	2.81875200
H	1.60406800	-4.48894500	6.53219100
H	2.51446000	-6.43099600	5.27150100
C	-6.25328800	0.84198100	0.95508400
C	-6.74853200	0.74211700	2.26624000
C	-7.14852400	0.72126400	-0.12209000
C	-8.10459000	0.50886400	2.49434100
H	-6.06317100	0.82997500	3.10465200
C	-8.50541900	0.49622100	0.10961900
H	-6.78402300	0.82936600	-1.13939900
C	-8.98615400	0.38477600	1.41712100
H	-8.47182600	0.42303300	3.51293600
H	-9.18739800	0.41446700	-0.73174100
H	-10.04252200	0.20588900	1.59551400
C	-1.70053800	-3.10527200	-3.41587700
C	-2.21379400	-4.20792400	-2.71096100
C	-1.47460600	-3.22440000	-4.79736400
C	-2.50105500	-5.39927700	-3.37693100
H	-2.36409600	-4.13778300	-1.63756900
C	-1.77196000	-4.41406900	-5.46188400
H	-1.08401000	-2.37505900	-5.35062700
C	-2.28566000	-5.50389400	-4.75384600
H	-2.88847500	-6.24674800	-2.81897700
H	-1.60418600	-4.48869000	-6.53235400

H -2.51463100 -6.43076200 -5.27173500

1 34 1.0 35 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 57 1.0
9 10 1.5 40 1.5
10 11 1.5
11 12 1.5
12 13 1.5 38 1.5
13 14 1.5 46 1.0
14 15 1.5 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 1.5 31 1.0
18 19 1.5 79 1.0
19 20 1.5 42 1.5
20 21 1.5
21 22 1.5
22 23 1.5 44 1.5
23 24 1.5 68 1.0
24 25 1.5 32 1.0
25 33 1.0
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34 37 2.0
35 36 2.0
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38 39 1.0 40 2.0
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40 41 1.0
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42 43 1.0 44 2.0

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44 45 1.0
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46 47 1.5 48 1.5
47 49 1.5 50 1.0
48 51 1.5 52 1.0
49 53 1.5 54 1.0
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51 53 1.5 55 1.0
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53 56 1.0
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57 58 1.5 59 1.5
58 60 1.5 61 1.0
59 62 1.5 63 1.0
60 64 1.5 65 1.0
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62 64 1.5 66 1.0
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64 67 1.0
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68 69 1.5 70 1.5
69 71 1.5 72 1.0
70 73 1.5 74 1.0
71 75 1.5 76 1.0
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73 75 1.5 77 1.0
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75 78 1.0
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79 80 1.5 81 1.5
80 82 1.5 83 1.0
81 84 1.5 85 1.0
82 86 1.5 87 1.0
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84 86 1.5 88 1.0
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86 89 1.0

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Optimized S_0 geometry of **6**

Re	0.00005100	-0.91537500	0.00017400
N	-0.00306300	0.73292900	1.45999800
N	-2.06976300	-0.59720500	0.44751500
N	0.00299100	0.73208000	-1.46058000
N	2.06981600	-0.59729900	-0.44738500
C	1.10003500	1.32074900	1.95649900
C	1.06705900	2.40542900	2.83104900
C	-1.34422200	2.28575400	2.68633600
C	-1.22821500	1.19439600	1.81743500
C	-2.37395800	0.46496800	1.25002800
C	-3.70702000	0.80685900	1.50278400
C	-4.43037200	-1.03882200	0.12876300
C	-3.08328500	-1.31978800	-0.08277500
C	-1.10016500	1.31960000	-1.95730500
C	-1.06730600	2.40414300	-2.83202200
C	1.34399200	2.28475400	-2.68728600
C	1.22809600	1.19362800	-1.81807700
C	2.37391000	0.46453300	-1.25039100
C	3.70694200	0.80642100	-1.50332000
C	4.43046500	-1.03861000	-0.12851300
C	3.08340800	-1.31957800	0.08319100
H	2.04450000	0.89730900	1.63546300
H	-2.31833000	2.66127600	2.97368100
H	-3.94211100	1.65451100	2.13429800
H	-2.78476400	-2.15438100	-0.70451300
H	-2.04457500	0.89598000	-1.63635600
H	2.31806100	2.66027100	-2.97476700
H	3.94195300	1.65381300	-2.13521300
H	2.78495900	-2.15390900	0.70531600
C	-0.25016000	-2.26116000	-1.31867000
C	0.25040300	-2.26015700	1.32001700
O	0.46329200	-3.08192000	2.12947700
O	-0.46297500	-3.08360100	-2.12746200

C	-4.73405100	0.06155100	0.94300500
H	-5.76850600	0.32784600	1.13830400
C	0.19882700	2.88819000	-3.18964000
H	0.28644500	3.73425600	-3.86507800
C	4.73404200	0.06144200	-0.94323100
H	5.76847300	0.32774500	-1.13864700
C	-0.19912200	2.88944300	3.18853500
H	-0.28684000	3.73570500	3.86371600
C	2.33484800	3.01976300	3.36134600
H	2.36524000	2.96217700	4.45545600
H	3.22137300	2.51342600	2.96921400
H	2.39722400	4.07978200	3.08974400
C	-5.50762000	-1.88303400	-0.49823100
H	-6.13459800	-1.27866100	-1.16408500
H	-5.08665300	-2.70740900	-1.08036800
H	-6.16390900	-2.30656300	0.27052000
C	5.50779400	-1.88253200	0.49873300
H	6.13542800	-1.27767800	1.16352700
H	5.08688800	-2.70612800	1.08201500
H	6.16342900	-2.30715000	-0.26998000
C	-2.33517000	3.01859400	-3.36200900
H	-2.36322300	2.96643800	-4.45643000
H	-3.22153100	2.50874200	-2.97407500
H	-2.40011700	4.07714700	-3.08522700

1 30 1.0 31 1.0 2 1.0 5 1.0 3 1.0 4 1.0
2 6 1.5 9 1.5
3 10 1.5 13 1.5
4 14 1.5 17 1.5
5 18 1.5 21 1.5
6 7 1.5 22 1.0
7 40 1.5 42 1.0
8 9 1.5 23 1.0 40 1.5
9 10 1.0
10 11 1.5
11 24 1.0 34 1.5
12 13 1.5 34 1.5 46 1.0
13 25 1.0
14 15 1.5 26 1.0
15 36 1.5 54 1.0
16 17 1.5 27 1.0 36 1.5
17 18 1.0
18 19 1.5
19 28 1.0 38 1.5

20 21 1.5 38 1.5 50 1.0
21 29 1.0
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30 33 3.0
31 32 3.0
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34 35 1.0
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36 37 1.0
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38 39 1.0
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40 41 1.0
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42 43 1.0 44 1.0 45 1.0
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46 47 1.0 48 1.0 49 1.0
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50 51 1.0 52 1.0 53 1.0
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54 55 1.0 56 1.0 57 1.0
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Optimized S_0 geometry of **7**

Re 0.00032900 -1.75868200 0.00010100

N	0.48512700	-0.09685300	-1.36038200
N	2.09665700	-1.43099300	0.27011100
N	-0.48518500	-0.09705100	1.36051100
N	-2.09608000	-1.43175500	-0.27009900
C	-0.37688500	0.50904200	-2.19202900
C	-0.04408700	1.63214700	-2.93916600
C	1.23982000	2.18277700	-2.83888800
C	2.13151500	1.52900900	-1.97693800
C	1.74654700	0.40022800	-1.25613300
C	2.64725900	-0.34470400	-0.35292600
C	3.97780100	0.01056900	-0.13993600
C	4.81005800	-0.72876700	0.70993400
C	4.22494000	-1.84596000	1.31959400
C	2.89409300	-2.15783600	1.08068700
C	0.37650300	0.50895000	2.19241700
C	0.04309200	1.63156300	2.94001000
C	-1.24112900	2.18151500	2.83998200
C	-2.13243500	1.52771000	1.97765700
C	-1.74682100	0.39947400	1.25633300
C	-2.64706400	-0.34552100	0.35270700
C	-3.97750100	0.00971300	0.13901800
C	-4.80932800	-0.72972000	-0.71118900
C	-4.22389300	-1.84698200	-1.32042500
C	-2.89312700	-2.15874600	-1.08092200
H	-1.36704600	0.07312800	-2.25145900
H	-0.79920000	2.06035800	-3.58533700
H	3.13880600	1.90839800	-1.86827700
H	4.37498100	0.88003200	-0.64725000
H	4.78343200	-2.48906000	1.98738400
H	2.43060700	-3.01505100	1.55163700
H	1.36688100	0.07350000	2.25168800
H	0.79796000	2.05992500	3.58636500
H	-3.13993600	1.90660900	1.86916400
H	-4.37488400	0.87929400	0.64596800
H	-4.78204900	-2.49018200	-1.98839500
H	-2.42937100	-3.01595700	-1.55161500
C	-0.19975200	-3.10252600	1.32766200
C	0.20100800	-3.10266800	-1.32723400
O	0.26678600	-3.92437300	-2.16255900
O	-0.26520500	-3.92412500	2.16311700
C	6.26585000	-0.30613600	0.92857700
C	1.69049600	3.42670100	-3.61157400
C	7.00336800	-1.25334700	1.89203600
H	7.03928900	-2.27819100	1.50589000

H	8.03551900	-0.91103400	2.01913100
H	6.53550300	-1.27078600	2.88286300
C	6.28972100	1.12169400	1.52487200
H	5.81858100	1.85207700	0.85882100
H	5.76812500	1.15214200	2.48811800
H	7.32620800	1.43800200	1.68662700
C	7.00255400	-0.31424700	-0.43226800
H	8.04539300	-0.00938300	-0.28999800
H	6.99560000	-1.31679000	-0.87417900
H	6.54751300	0.37703100	-1.14932600
C	2.13257400	4.51332600	-2.60220700
H	2.96769000	4.17954600	-1.97740300
H	2.45917900	5.40804800	-3.14366900
H	1.30444500	4.79556800	-1.94251600
C	2.88289700	3.04781900	-4.52223300
H	3.21608600	3.92988300	-5.08025700
H	3.73627700	2.67514500	-3.94614800
H	2.59479200	2.27454200	-5.24281400
C	0.56371000	4.00193500	-4.48850000
H	0.22960200	3.28323800	-5.24521600
H	-0.30250200	4.30488200	-3.88937900
H	0.92964200	4.88979500	-5.01410800
C	-1.69254900	3.42471700	3.61339800
C	-0.56607300	4.00017300	4.49057300
H	-0.23150700	3.28130800	5.24693000
H	0.29994100	4.30390900	3.89156200
H	-0.93249600	4.88756700	5.01662300
C	-2.13547900	4.51163500	2.60475200
H	-1.30760500	4.79487500	1.94516800
H	-2.97040300	4.17763600	1.97981200
H	-2.46268400	5.40578100	3.14680200
C	-2.88463000	3.04445200	4.52394000
H	-2.59593600	2.27097200	5.24406400
H	-3.21841900	3.92596000	5.08248600
H	-3.73776100	2.67149600	3.94767000
C	-6.26495900	-0.30701700	-0.93076900
C	-7.00241800	-0.31432400	0.42966500
H	-6.54773100	0.37727900	1.14663500
H	-8.04513700	-0.00941100	0.28662700
H	-6.99583700	-1.31664000	0.87210100
C	-6.28824700	1.12052900	-1.52776600
H	-5.81722700	1.85110700	-0.86184300
H	-5.76620800	1.15039800	-2.49078900
H	-7.32458900	1.43699500	-1.69014600

C	-7.00212500	-1.25457000	-1.89416900
H	-7.03836300	-2.27923800	-1.50758300
H	-8.03417100	-0.91218500	-2.02192800
H	-6.53378400	-1.27251300	-2.88476100

1 38 1.0 39 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 43 1.0
9 10 1.5 28 1.0
10 11 1.0
11 12 1.5
12 13 1.5 29 1.0
13 14 1.5 42 1.0
14 15 1.5 30 1.0
15 31 1.0
16 17 1.5 32 1.0
17 18 1.5 33 1.0
18 19 1.5 68 1.0
19 20 1.5 34 1.0
20 21 1.0
21 22 1.5
22 23 1.5 35 1.0
23 24 1.5 81 1.0
24 25 1.5 36 1.0
25 37 1.0
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38 41 2.0
39 40 2.0

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42 44 1.0 48 1.0 52 1.0
43 56 1.0 60 1.0 64 1.0
44 45 1.0 46 1.0 47 1.0
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48 49 1.0 50 1.0 51 1.0
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52 53 1.0 54 1.0 55 1.0
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56 57 1.0 58 1.0 59 1.0
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60 61 1.0 62 1.0 63 1.0
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64 65 1.0 66 1.0 67 1.0
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68 69 1.0 73 1.0 77 1.0
69 70 1.0 71 1.0 72 1.0
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73 74 1.0 75 1.0 76 1.0
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77 78 1.0 79 1.0 80 1.0
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81 82 1.0 86 1.0 90 1.0
82 83 1.0 84 1.0 85 1.0
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86 87 1.0 88 1.0 89 1.0
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90 91 1.0 92 1.0 93 1.0
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Optimized S_0 geometry of **8**

Re	0.00006800	0.84855500	-0.00004100
N	0.47211600	-0.80210200	1.37793700
N	2.10494100	0.53992300	-0.22926500
N	-0.47251700	-0.80135300	-1.37877400
N	-2.10492200	0.54077300	0.22910600
C	-0.41497100	-1.39822200	2.19500600
C	-0.08660100	-2.49462000	2.98269200
C	1.21367700	-2.99575700	2.91785400
C	2.13747900	-2.37657700	2.08138200
C	1.74677400	-1.27090800	1.31858100
C	2.65575100	-0.52612000	0.42743600
C	4.00341000	-0.85955900	0.25827300
C	4.80780900	-0.09870900	-0.58231100
C	4.24302200	0.99569300	-1.23836800
C	2.89991400	1.27961400	-1.03679400
C	0.41433200	-1.39744000	-2.19612300
C	0.08567500	-2.49378300	-2.98375400
C	-1.21466000	-2.99474900	-2.91863700
C	-2.13823500	-2.37555600	-2.08191300
C	-1.74721600	-1.27001500	-1.31905900
C	-2.65589200	-0.52526900	-0.42747700
C	-4.00335200	-0.85904900	-0.25745000
C	-4.80742300	-0.09842700	0.58368000
C	-4.24255100	0.99622300	1.23924800
C	-2.89962200	1.28045900	1.03686400
H	-1.41096100	-0.97284100	2.20672400
H	-0.83638600	-2.94015500	3.62637500
H	3.15098300	-2.75303700	2.02847600

H	4.42465200	-1.70854900	0.78147000
H	4.82695000	1.62548400	-1.89990300
H	2.42242600	2.11687000	-1.52827100
H	1.41034500	-0.97211200	-2.20798900
H	0.83524700	-2.93942900	-3.62760500
H	-3.15180400	-2.75186500	-2.02896200
H	-4.42459600	-1.70821000	-0.78034900
H	-4.82624500	1.62595300	1.90104400
H	-2.42207300	2.11799400	1.52781600
H	1.50833200	-3.85354000	3.51323400
H	5.85357700	-0.35269500	-0.71790600
H	-5.85298000	-0.35283000	0.72010800
H	-1.50951500	-3.85249900	-3.51397100
C	-0.18067700	2.19479800	-1.33138000
C	0.18166600	2.19405700	1.33200600
O	0.23466500	3.01501800	2.16692400
O	-0.23344200	3.01656300	-2.16552500

1 42 1.0 43 1.0 3 1.0 2 1.0 4 1.0 5 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 38 1.0
9 10 1.5 28 1.0
10 11 1.0
11 12 1.5
12 13 1.5 29 1.0
13 14 1.5 39 1.0
14 15 1.5 30 1.0
15 31 1.0
16 17 1.5 32 1.0
17 18 1.5 33 1.0
18 19 1.5 41 1.0
19 20 1.5 34 1.0
20 21 1.0
21 22 1.5
22 23 1.5 35 1.0
23 24 1.5 40 1.0
24 25 1.5 36 1.0
25 37 1.0
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Optimized S_0 geometry of **9**

Re	-0.00049300	-1.11991200	-0.00039600
N	0.49049700	0.53507200	-1.36800400
N	2.09991800	-0.80144400	0.25955100
N	-0.49013700	0.53276500	1.37031700
N	-2.10079700	-0.79975400	-0.25930000
C	-0.37983000	1.14008000	-2.19764500
C	-0.03686000	2.23593200	-2.97376600
C	2.16148800	2.11415700	-2.04607900
C	1.76122200	1.00805400	-1.29117600
C	2.65849300	0.26597200	-0.38402900
C	3.99962700	0.60793100	-0.18801700
C	4.22387900	-1.23477900	1.30506100
C	2.89063800	-1.53095600	1.08133000
C	0.38103700	1.13675900	2.19914700
C	0.04054300	2.23544200	2.97305000
C	-2.15784500	2.11662800	2.04508300
C	-1.76032900	1.00826600	1.29284900
C	-2.65866100	0.26697400	0.38597800
C	-4.00010700	0.60892000	0.19198300

C	-4.22572300	-1.23192200	-1.30325100
C	-2.89226800	-1.52828800	-1.08123800
H	-1.37822500	0.72065600	-2.22667600
H	-0.78074500	2.68461800	-3.62389800
H	3.17603500	2.48625500	-1.97149500
H	4.41847600	1.46225900	-0.70578500
H	4.79803600	-1.86179500	1.97936300
H	2.41416300	-2.37219800	1.56736300
H	1.37868800	0.71561000	2.22881100
H	0.78560000	2.68411300	3.62172800
H	-3.17131500	2.49162600	1.96944300
H	-4.41864800	1.46232600	0.71154900
H	-4.80054100	-1.85812900	-1.97774100
H	-2.41623300	-2.36893800	-1.56872000
C	-0.19728200	-2.46602000	1.32552800
C	0.19559200	-2.46271800	-1.32982300
O	0.25692100	-3.28352500	-2.16618100
O	-0.25899800	-3.28911700	2.15962100
C	1.26501900	2.75216700	-2.90608200
C	4.81475100	-0.13513000	0.66555600
C	-4.81605300	-0.13321600	-0.66161800
C	-1.25943500	2.75490200	2.90362000
C	-1.67554800	3.93383400	3.74110000
H	-0.87482200	4.67779300	3.79900100
H	-2.57393100	4.41381500	3.34331400
H	-1.89415500	3.60895400	4.76613900
C	-6.26346700	0.21335900	-0.88197000
H	-6.54168600	1.13647400	-0.36655600
H	-6.47419200	0.33467700	-1.95057300
H	-6.91019000	-0.59275200	-0.51542000
C	6.26184100	0.21153100	0.88788100
H	6.53967000	1.13672800	0.37598700
H	6.47209100	0.32896400	1.95699300
H	6.90922000	-0.59277200	0.51850100
C	1.67918100	3.93082300	-3.74491700
H	0.93256600	4.73012200	-3.69131600
H	2.64565100	4.33257000	-3.42917900
H	1.76230100	3.63488700	-4.79791300

1 34 1.0 35 1.0 4 1.0 5 1.0 2 1.0 3 1.0
2 6 1.5 9 1.5
3 10 1.5 13 1.5
4 14 1.5 17 1.5
5 18 1.5 21 1.5

6 7 1.5 22 1.0
7 23 1.0 38 1.5
8 9 1.5 24 1.0 38 1.5
9 10 1.0
10 11 1.5
11 25 1.0 39 1.5
12 13 1.5 26 1.0 39 1.5
13 27 1.0
14 15 1.5 28 1.0
15 29 1.0 41 1.5
16 17 1.5 30 1.0 41 1.5
17 18 1.0
18 19 1.5
19 31 1.0 40 1.5
20 21 1.5 32 1.0 40 1.5
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34 37 3.0
35 36 3.0
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38 54 1.0
39 50 1.0
40 46 1.0
41 42 1.0
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54 55 1.0 56 1.0 57 1.0
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Optimized T_1 geometry of **1**

Re	0.02569800	1.38684000	0.02429200
N	0.26965600	-0.29548200	1.41101100
N	2.05370600	1.07842200	-0.02110000
N	-0.27243500	-0.30815700	-1.34826900
N	-2.11384300	1.06050600	0.02224300
C	-0.65112000	-0.94111400	2.11355100
C	-0.41249000	-2.13449200	2.82891800
C	0.87582900	-2.67954900	2.80538700
C	1.89067800	-2.00467100	2.07010000
C	1.54982900	-0.80238200	1.37802300
C	2.49669900	-0.07956300	0.62554800
C	3.83506200	-0.52091300	0.54071200
C	4.78393100	0.24864300	-0.20601900
C	4.33447700	1.49039900	-0.77950800
C	3.02283800	1.86079300	-0.65648100
C	0.66931100	-0.95340000	-2.03195900
C	0.43170900	-2.12577400	-2.77411100
C	-0.86427800	-2.64947800	-2.80340200
C	-1.88637700	-1.96248500	-2.08500300
C	-1.54307000	-0.79521400	-1.37042000
C	-2.53107800	-0.06454500	-0.63505500
C	-3.87420700	-0.49661300	-0.61011000
C	-4.82912500	0.26617100	0.12269200
C	-4.38915500	1.42563400	0.77074000
C	-3.03068300	1.77500700	0.68427600
H	-1.64282300	-0.50050100	2.11604200
H	2.65305900	2.78845400	-1.07457500
H	1.66335200	-0.52413000	-1.98507900

H	-2.66777000	2.66892600	1.17784700
C	-0.04624300	2.75317700	-1.32302100
C	0.06633800	2.83688700	1.31281300
O	0.05344300	3.71598600	2.07050700
O	-0.07257400	3.58137300	-2.14054200
C	4.16366700	-1.73074200	1.23291500
H	5.18282900	-2.09773600	1.18530300
C	3.23784000	-2.44291100	1.96500000
H	3.54995900	-3.35011800	2.47004300
C	-3.25665900	-2.38919900	-2.03686500
H	-3.55106500	-3.28399600	-2.57242600
C	-4.19975800	-1.69342200	-1.33596200
H	-5.22246500	-2.05077300	-1.33120300
C	-1.56344400	-2.76389300	3.57898100
H	-2.47746600	-2.17539200	3.45473000
H	-1.77293700	-3.77913200	3.22223200
H	-1.35794500	-2.83153500	4.65356900
C	1.21280700	-3.95369000	3.53736300
H	1.58837400	-4.71255800	2.84085700
H	2.00290000	-3.77729800	4.27668400
H	0.35364900	-4.37448000	4.05986600
C	6.20484400	-0.22720400	-0.32430800
H	6.69702000	-0.27943500	0.65821300
H	6.25466100	-1.23904900	-0.75041600
H	6.80938600	0.42416200	-0.95728900
C	5.28519700	2.40371400	-1.51401300
H	6.12350700	2.70838700	-0.87551400
H	5.71513200	1.91158100	-2.39542900
H	4.77536900	3.31021300	-1.85343200
C	1.59361700	-2.76347100	-3.49689700
H	2.51356300	-2.19555900	-3.33391700
H	1.76635500	-3.78764900	-3.14805900
H	1.41478000	-2.80911300	-4.57684900
C	-1.20280800	-3.90297300	-3.56648900
H	-1.61794900	-4.66417900	-2.89567600
H	-1.96075300	-3.69731900	-4.33154200
H	-0.33408400	-4.33341100	-4.06386200
C	-5.31042300	2.32510200	1.55927300

H	-5.77602300	1.78768400	2.39274500
H	-4.76475000	3.17676800	1.97397000
H	-6.11624000	2.71801300	0.92955300
C	-6.26576700	-0.18144400	0.17209600
H	-6.69414100	-0.22062800	-0.83655100
H	-6.34298300	-1.18966700	0.59548300
H	-6.88634600	0.48225900	0.77332000

1 3 1.0 30 1.0 31 1.0
2 6 1.5 10 1.5
3 11 1.0 15 1.0
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 42 1.0
8 9 1.5 46 1.0
9 10 1.5 36 1.5
10 11 1.5
11 12 1.5
12 13 1.5 34 1.5
13 14 1.5 50 1.0
14 15 2.0 54 1.0
15 27 1.0
16 17 1.5 28 1.0
17 18 1.5 58 1.0
18 19 1.5 62 1.0
19 20 1.5 38 1.5
20 21 1.5
21 22 1.5
22 23 1.5 40 1.5
23 24 1.5 70 1.0
24 25 1.5 66 1.0
25 29 1.0
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Optimized T_1 geometry of **2**

Re	0.02872100	1.34847500	0.01513300
N	0.51446500	-0.32464600	1.33898000
N	2.01850500	1.04275800	-0.39448700
N	-0.51389700	-0.34479700	-1.28320300
N	-2.07704100	1.03566700	0.38971600
C	-0.26752400	-0.96803800	2.19941700
C	0.13168800	-2.13568600	2.86678200
C	1.39598900	-2.67833400	2.64855200
C	2.25963900	-2.00868300	1.74345700
C	1.78324700	-0.82159200	1.09915600
C	2.58140400	-0.10341400	0.19051900
C	3.90037000	-0.53049500	-0.10048300
C	4.70038400	0.24131000	-0.99206100
C	4.12942700	1.44652400	-1.50182400
C	2.85456100	1.82282400	-1.19360100
C	0.29038500	-0.99364300	-2.12344900
C	-0.11503900	-2.14840100	-2.80613400
C	-1.38930300	-2.66766000	-2.63085400
C	-2.26430200	-1.97714800	-1.74025100
C	-1.77868300	-0.81989600	-1.09033600
C	-2.61726700	-0.08360800	-0.19144900
C	-3.94248400	-0.50771100	0.05584600
C	-4.74638400	0.26162500	0.94809700
C	-4.17338600	1.39800600	1.50285000
C	-2.85614100	1.75957000	1.20314900
H	-1.25219100	-0.54474500	2.36708300
H	-0.56180000	-2.60779400	3.55386500
H	4.72183900	2.08782400	-2.14714100
H	2.41241000	2.73517800	-1.57241400
H	1.28436100	-0.58218000	-2.25129000
H	0.58979400	-2.63168300	-3.47379200
H	-4.74129000	2.02777900	2.17889900
H	-2.41086700	2.64880300	1.63239000
C	-0.29331700	2.72081400	-1.29403400
C	0.32002000	2.80307100	1.26922800

O	0.46170600	3.68511300	2.00858800
O	-0.47577600	3.55211100	-2.08688400
C	4.36066900	-1.72536000	0.54407200
H	5.36493000	-2.07548500	0.33165000
C	3.57854500	-2.43407800	1.42562600
H	3.97702500	-3.32950800	1.89005900
C	-3.60863100	-2.39160200	-1.46501200
H	-3.99638900	-3.27910100	-1.95138900
C	-4.40844300	-1.69097900	-0.60774500
H	-5.42081800	-2.03147700	-0.42460000
C	-1.83215500	-3.90911700	-3.35408500
H	-2.12425900	-4.69198900	-2.64454100
H	-2.70291200	-3.70331300	-3.98748300
H	-1.03311300	-4.30116500	-3.98734100
C	-6.16017200	-0.13484500	1.26856300
H	-6.77602000	-0.15546100	0.36173400
H	-6.19565400	-1.13874500	1.70774900
H	-6.61426700	0.56405700	1.97449000
C	1.82841200	-3.93440600	3.35732900
H	2.08914100	-4.72086500	2.63938200
H	2.71722700	-3.75222800	3.97278200
H	1.03544700	-4.31366900	4.00672600
C	6.10068600	-0.16663000	-1.34985300
H	6.75046800	-0.21602300	-0.46446500
H	6.12929900	-1.16170300	-1.81532400
H	6.54875400	0.54270900	-2.05154800

1 3 1.0 34 1.0 35 1.0
2 6 1.5 10 1.0
3 11 1.0 15 1.0
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 54 1.0
9 10 1.5 40 1.5
10 11 1.5
11 12 1.5
12 13 1.5 38 1.5
13 14 1.5 58 1.0
14 15 2.0 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 1.5 31 1.0

18 19 1.5 46 1.0
19 20 1.5 42 1.5
20 21 1.5
21 22 1.5
22 23 1.5 44 1.5
23 24 1.5 50 1.0
24 25 1.5 32 1.0
25 33 1.0
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34 37 2.0
35 36 2.0
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38 39 1.0 40 2.0
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40 41 1.0
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42 43 1.0 44 2.0
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44 45 1.0
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46 47 1.0 48 1.0 49 1.0
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Optimized T_1 geometry of **3**

Re	0.02227500	1.42556000	0.00790400
N	0.65947900	-0.22966900	1.27034900
N	1.96220300	1.12221000	-0.64091100
N	-0.65645300	-0.27886400	-1.21553000
N	-2.02638400	1.11999600	0.60980200
C	-0.02408700	-0.86470700	2.22961000
C	0.45915300	-2.00894100	2.86039300
C	1.70732000	-2.52177600	2.48736600
C	2.46578700	-1.88809500	1.49460100
C	1.90115800	-0.71938900	0.89484000
C	2.58836800	-0.01869800	-0.09965700
C	3.87421100	-0.44656900	-0.52209000
C	4.53358700	0.33135600	-1.48721500
C	3.92392500	1.52147200	-1.97535000
C	2.68122000	1.88674300	-1.53566300
C	0.06031200	-0.92863600	-2.13185000
C	-0.42236100	-2.08724600	-2.75586000
C	-1.67129700	-2.57438600	-2.41821300
C	-2.46063900	-1.90273500	-1.45286100
C	-1.89242300	-0.74512400	-0.87877000
C	-2.62487200	-0.00136100	0.09667500
C	-3.91507800	-0.42847100	0.47805700
C	-4.58497600	0.36866500	1.43743700
C	-3.98060900	1.50915100	1.93619300
C	-2.70181000	1.86420600	1.49636900
H	-0.98407600	-0.43735600	2.49819100
H	-0.13394900	-2.48549700	3.63219800
H	4.44100900	2.14762800	-2.69384300
H	2.18655100	2.78492400	-1.88384200
H	1.03298600	-0.51435500	-2.36638300
H	0.19245200	-2.58819300	-3.49465400
H	-4.48348900	2.13711000	2.66246200
H	-2.20454500	2.75420000	1.86091500
H	2.08009700	-3.41128100	2.98114700
H	5.51552400	0.05668100	-1.84942200

H	-5.57540400	0.09950700	1.78218200
H	-2.03936100	-3.47108200	-2.90114800
C	-0.47239900	2.80619000	-1.24982200
C	0.49279800	2.88974800	1.19618200
O	0.75283600	3.77616600	1.89530000
O	-0.76252500	3.64072000	-2.00403900
C	4.44878500	-1.64957400	0.07061500
C	3.76862700	-2.34571300	1.05094200
C	-3.78227300	-2.34740000	-1.04641300
C	-4.49147100	-1.62853600	-0.10541600
C	4.30805100	-3.58966300	1.72259500
H	4.40212300	-3.43593200	2.80434000
H	3.62865600	-4.43787300	1.57562500
H	5.28671900	-3.88885800	1.35271700
C	5.81012200	-2.05402600	-0.44820600
H	6.54953700	-1.26761100	-0.25196300
H	6.18674100	-2.97344400	-0.00409600
H	5.78203800	-2.20279700	-1.53456100
C	-4.29892800	-3.60475500	-1.70707500
H	-4.35479000	-3.47717700	-2.79448000
H	-3.62747100	-4.44928500	-1.51207900
H	-5.29008300	-3.89249400	-1.36371800
C	-5.87278100	-2.01033300	0.37555900
H	-6.59282500	-1.21071600	0.16470100
H	-6.25176400	-2.91713400	-0.09053800
H	-5.87620800	-2.17518700	1.45955800

1 3 1.0 38 1.0 39 1.0
2 6 1.5 10 1.0
3 11 1.0 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 34 1.0
9 10 1.5 43 1.0
10 11 1.5
11 12 1.5

12 13 1.5 42 1.0
13 14 1.5 35 1.0
14 15 2.0 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 2.0 31 1.0
18 19 1.5 37 1.0
19 20 1.5 44 1.0
20 21 1.5
21 22 1.5
22 23 1.5 45 1.0
23 24 2.0 36 1.0
24 25 1.5 32 1.0
25 33 1.0
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38 41 2.0
39 40 2.0
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42 43 2.0 50 1.0
43 46 1.0
44 45 2.0 54 1.0
45 58 1.0
46 47 1.0 48 1.0 49 1.0
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50 51 1.0 52 1.0 53 1.0
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54 55 1.0 56 1.0 57 1.0
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58 59 1.0 60 1.0 61 1.0
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Optimized T_1 geometry of **4**

Re	0.02303200	-1.10167100	-0.01256200
N	-0.56230200	0.60354000	1.26382200
N	-2.06620200	-0.79718300	-0.47622900
N	0.56243900	0.56119300	-1.32023500
N	2.00183300	-0.80018600	0.50139900
C	0.21030000	1.26422600	2.12576800
C	-0.23278800	2.41915800	2.79254800
C	-1.50919000	2.89340000	2.55704000
C	-2.35177900	2.20724600	1.65315200
C	-1.82561700	1.05606700	1.02348100
C	-2.62594600	0.31430100	0.09857300
C	-3.94745900	0.73007200	-0.18141500
C	-4.69729600	-0.04621200	-1.09308400
C	-4.12554300	-1.17241000	-1.65679300
C	-2.81062100	-1.52421800	-1.32126600
C	-0.18030700	1.20940100	-2.22334300
C	0.26009500	2.35880000	-2.88671000
C	1.53224800	2.86389500	-2.60572300
C	2.34748900	2.21289800	-1.67261700
C	1.83013100	1.04193700	-1.03237100
C	2.58615200	0.33617600	-0.08817500
C	3.90198100	0.75610200	0.24199900
C	4.64168600	-0.00851800	1.15777900

C	4.06677400	-1.19597700	1.69205200
C	2.79366600	-1.56155500	1.34458700
H	1.20319600	0.86219100	2.28524500
H	0.43673200	2.92094900	3.48140900
H	-4.67475800	-1.79513600	-2.35326200
H	-2.34057600	-2.40444800	-1.74200000
H	-1.16168600	0.79278800	-2.42327900
H	-0.39060100	2.83814300	-3.60859400
H	4.63109300	-1.82390000	2.37254800
H	2.32710200	-2.45903900	1.73091200
H	-1.87334000	3.78432300	3.05918100
H	-5.71475300	0.24360400	-1.33629200
H	5.64879400	0.29118600	1.42802400
H	1.89712200	3.75491300	-3.10860100
C	0.39546000	-2.56656900	-1.23421500
C	-0.37278500	-2.47925800	1.28079700
O	-0.60414600	-3.31165800	2.05704200
O	0.59726900	-3.45332400	-1.95149400
C	-4.45775900	1.90581200	0.46547800
H	-5.47219700	2.21829700	0.23912400
C	-3.69251700	2.61496100	1.34525300
H	-4.08758700	3.50201500	1.83025700
C	3.66697000	2.63797200	-1.31529300
H	4.07310200	3.52616800	-1.79084100
C	4.40743400	1.94094700	-0.40106200
H	5.41093700	2.26962400	-0.14594900

1 5 1.0 38 1.0 39 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.0
5 21 1.0 25 1.0
6 7 1.5 26 1.0
7 8 2.0 27 1.0
8 9 1.5 34 1.0
9 10 1.5 44 1.5
10 11 1.5
11 12 1.5

12 13 1.5 42 1.5
13 14 2.0 35 1.0
14 15 1.5 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 1.5 31 1.0
18 19 1.5 37 1.0
19 20 1.5 46 1.5
20 21 1.5
21 22 1.5
22 23 1.5 48 1.5
23 24 1.5 36 1.0
24 25 2.0 32 1.0
25 33 1.0
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38 41 3.0
39 40 2.0
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42 43 1.0 44 2.0
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44 45 1.0
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46 47 1.0 48 2.0
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48 49 1.0
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Optimized T_1 geometry of **5**

Re	-0.02779400	2.18834300	-0.06339600
N	0.43037800	0.51280100	1.28480000
N	2.09490100	1.87715300	-0.28994800
N	-0.43797200	0.49280700	-1.37635200
N	-2.04637400	1.89237300	0.21761200
C	-0.43237600	-0.12508400	2.07599800
C	-0.09656600	-1.30475200	2.74757800
C	1.16816900	-1.86794200	2.61015700
C	2.12257200	-1.16216200	1.81261600
C	1.69652300	0.02012100	1.16238600
C	2.60221300	0.76900500	0.33901200
C	3.95256600	0.36545100	0.21167300
C	4.82248400	1.16602800	-0.59217900
C	4.26642200	2.27211500	-1.22997500
C	2.92212000	2.60255000	-1.05489900
C	0.40143400	-0.16007600	-2.17845900
C	0.07137500	-1.36450000	-2.80478700
C	-1.18362300	-1.94955000	-2.60030800
C	-2.12041600	-1.24947800	-1.79419600
C	-1.70906000	-0.01928100	-1.18926500
C	-2.57764600	0.73313700	-0.37350300
C	-3.92335200	0.32799000	-0.18231800
C	-4.79167600	1.15050500	0.60299900
C	-4.21158000	2.32698300	1.19008100
C	-2.91326100	2.67180800	0.96976100
H	-1.42304300	0.30538500	2.15571100
H	-0.85242400	-1.79883000	3.34719900
H	4.88497000	2.91698800	-1.84362700
H	2.49855100	3.47857100	-1.53001600
H	1.38307700	0.28154500	-2.31258900
H	0.81518900	-1.86216200	-3.41599200
H	-4.83496500	2.99373200	1.77536300
H	-2.48517200	3.57807400	1.37888000
C	-0.24526800	3.62119700	-1.35705600
C	0.21219400	3.58275800	1.24146900

O	0.34152600	4.42603800	2.03181900
O	-0.34551700	4.48959800	-2.11869800
C	4.35754200	-0.83721600	0.88091900
H	5.37943700	-1.17676800	0.76926400
C	3.48936700	-1.56137500	1.64558900
H	3.83873900	-2.45461300	2.14815600
C	-3.46138100	-1.66657000	-1.55066900
H	-3.81849700	-2.58855700	-1.99328900
C	-4.31110700	-0.91929300	-0.77650400
H	-5.31472200	-1.28611200	-0.60113900
C	6.26458400	0.87361200	-0.76085600
C	6.81942700	0.82645300	-2.05120800
C	7.10536000	0.69352600	0.35173300
C	8.18153100	0.58367400	-2.22505900
H	6.17601800	0.95981000	-2.91631800
C	8.46899300	0.46234600	0.17378800
H	6.69435000	0.76259600	1.35454600
C	9.00912100	0.40111400	-1.11377600
H	8.59573800	0.53648900	-3.22788700
H	9.10970300	0.33567000	1.04142400
H	10.07054300	0.21577600	-1.25022000
C	1.47427900	-3.15241200	3.28241100
C	2.00408900	-4.23904900	2.56480300
C	1.18331600	-3.31168200	4.64768600
C	2.24408400	-5.45516300	3.20395400
H	2.20170000	-4.13793100	1.50170300
C	1.43504500	-4.52592700	5.28564800
H	0.77897600	-2.47501200	5.21021100
C	1.96569100	-5.59987500	4.56583300
H	2.64370400	-6.29049000	2.63653700
H	1.21783400	-4.63242000	6.34439400
H	2.15830800	-6.54615700	5.06289700
C	-6.22187800	0.88340900	0.81001000
C	-6.79495800	1.06697900	2.08755000
C	-7.07709100	0.50172000	-0.24694500
C	-8.15436600	0.85268500	2.30339100
H	-6.15817900	1.35427500	2.91964800
C	-8.43742000	0.29243400	-0.02887400

H	-6.67678000	0.40858300	-1.25172600
C	-8.98357700	0.46107500	1.24733600
H	-8.56736300	0.98703600	3.29945200
H	-9.07581000	0.01023800	-0.86165100
H	-10.04396600	0.29626300	1.41548500
C	-1.48171300	-3.26061100	-3.22602800
C	-1.95722000	-4.34117700	-2.46252200
C	-1.23889500	-3.45349900	-4.59668900
C	-2.19426800	-5.57948000	-3.05959300
H	-2.11847600	-4.21390500	-1.39614200
C	-1.48502500	-4.69013000	-5.19303700
H	-0.87489700	-2.62349900	-5.19574600
C	-1.96367200	-5.75634600	-4.42654200
H	-2.55397100	-6.40733600	-2.45523700
H	-1.30468900	-4.82025100	-6.25630800
H	-2.15259500	-6.72001200	-4.89085700

1 5 1.0 34 1.0 35 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.0
5 21 1.0 25 1.0
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 57 1.0
9 10 1.5 40 1.5
10 11 1.5
11 12 1.5
12 13 1.5 38 1.5
13 14 1.5 46 1.0
14 15 1.5 28 1.0
15 29 1.0
16 17 1.5 30 1.0
17 18 1.5 31 1.0
18 19 1.5 79 1.0
19 20 1.5 42 1.5
20 21 1.5
21 22 1.5

22 23 1.5 44 1.5
23 24 1.5 68 1.0
24 25 2.0 32 1.0
25 33 1.0
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34 37 2.0
35 36 2.0
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38 39 1.0 40 2.0
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40 41 1.0
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42 43 1.0 44 2.0
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44 45 1.0
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46 47 1.5 48 1.5
47 49 1.5 50 1.0
48 51 1.5 52 1.0
49 53 1.5 54 1.0
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51 53 1.5 55 1.0
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53 56 1.0
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57 58 1.5 59 1.5
58 60 1.5 61 1.0
59 62 1.5 63 1.0

60 64 1.5 65 1.0
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62 64 1.5 66 1.0
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64 67 1.0
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68 69 1.5 70 1.5
69 71 1.5 72 1.0
70 73 1.5 74 1.0
71 75 1.5 76 1.0
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73 75 1.5 77 1.0
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75 78 1.0
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79 80 1.5 81 1.5
80 82 1.5 83 1.0
81 84 1.5 85 1.0
82 86 1.5 87 1.0
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84 86 1.5 88 1.0
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86 89 1.0
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Optimized T_1 geometry of **6**

Re	0.01305600	0.91435500	0.01981500
N	-0.01680300	-0.75415800	-1.41229000
N	-2.07041600	0.62381400	-0.43893800
N	-0.01596500	-0.73100200	1.41710700
N	2.03712900	0.61040500	0.36876700

C	1.08305000	-1.36753600	-1.87982800
C	1.03802300	-2.49091000	-2.70610900
C	-1.37328700	-2.33595800	-2.57822500
C	-1.24642600	-1.21891000	-1.74755800
C	-2.38508100	-0.46671200	-1.19449800
C	-3.72251900	-0.80605400	-1.41259100
C	-4.41426600	1.10425200	-0.09989300
C	-3.06131300	1.38759500	0.07139500
C	-1.11385100	-1.34746100	1.91395200
C	-1.07288900	-2.46588100	2.72448300
C	1.34687700	-2.36761700	2.55655700
C	1.24376100	-1.22136900	1.72374800
C	2.34564600	-0.51457000	1.16386500
C	3.70791400	-0.84859700	1.35992400
C	4.39237200	1.09708900	0.06296800
C	3.06455400	1.38543900	-0.11323900
H	2.02821900	-0.93378500	-1.57690800
H	-2.35081000	-2.70805700	-2.85775400
H	-3.97639200	-1.67443400	-2.00728100
H	-2.74413500	2.25303000	0.64044100
H	-2.06441800	-0.90041900	1.64279600
H	2.32469600	-2.75918100	2.81194900
H	3.95930200	-1.72329700	1.94896400
H	2.75387700	2.25786800	-0.67654200
C	-0.08459700	2.36738900	1.30968200
C	0.14705500	2.31906700	-1.31055200
O	0.23034800	3.16622000	-2.10029700
O	-0.14972900	3.24871300	2.05808700
C	-4.73275500	-0.02895500	-0.86108700
H	-5.77180700	-0.29601600	-1.02849600
C	0.21654500	-2.97800100	3.04290700
H	0.30406100	-3.85329300	3.68074300
C	4.70915600	-0.07963800	0.82135200
H	5.74901900	-0.34963800	0.98118000
C	-0.23145800	-2.97095700	-3.05177200
H	-0.32660300	-3.84016800	-3.69579200
C	2.30149400	-3.15232200	-3.18659900
H	3.18558500	-2.56000600	-2.93505500

H	2.41493600	-4.14243000	-2.72912000
H	2.27845700	-3.29519600	-4.27230300
C	-5.47762500	1.98125400	0.50360000
H	-6.08635300	1.41313000	1.21632500
H	-5.04498900	2.83660500	1.02935800
H	-6.15190500	2.35954600	-0.27276400
C	5.48077900	1.96764700	-0.50420900
H	6.12110000	1.40179100	-1.19336200
H	5.06955500	2.82236400	-1.05040800
H	6.13145200	2.35489000	0.29041700
C	-2.32733100	-3.10768500	3.25364800
H	-3.22349200	-2.57858500	2.91407800
H	-2.40753800	-4.15214500	2.92603000
H	-2.33657800	-3.11569600	4.35104000

1 5 1.0 30 1.0 31 1.0
2 6 1.5 9 1.5
3 10 1.5 13 1.5
4 14 1.5 17 1.0
5 18 1.0 21 1.5
6 7 1.5 22 1.0
7 40 1.5 42 1.0
8 9 1.5 23 1.0 40 1.5
9 10 1.0
10 11 1.5
11 24 1.0 34 1.5
12 13 1.5 34 1.5 46 1.0
13 25 1.0
14 15 2.0 26 1.0
15 36 1.5 54 1.0
16 17 1.5 27 1.0 36 2.0
17 18 1.5
18 19 1.5
19 28 1.0 38 2.0
20 21 2.0 38 1.5 50 1.0
21 29 1.0
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30 33 3.0
31 32 2.0
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34 35 1.0
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36 37 1.0
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38 39 1.0
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40 41 1.0
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42 43 1.0 44 1.0 45 1.0
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46 47 1.0 48 1.0 49 1.0
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50 51 1.0 52 1.0 53 1.0
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54 55 1.0 56 1.0 57 1.0
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Optimized T_1 geometry of **7**

Re 0.00171700 -1.88681800 0.04474900

N	0.30758000	-0.19233900	-1.32906700
N	2.11782700	-1.54869700	0.05010000
N	-0.29413000	-0.19613000	1.36160500
N	-2.05245300	-1.60092500	-0.04485400
C	-0.66420000	0.42780700	-2.01344200
C	-0.48416100	1.67265100	-2.60771300
C	0.74638300	2.32855800	-2.49908900
C	1.76466900	1.64124300	-1.81858200
C	1.53114300	0.39398500	-1.24793000
C	2.55277000	-0.38194500	-0.51549100
C	3.88166700	0.01009200	-0.40281000
C	4.82109300	-0.76877800	0.29018300
C	4.35048000	-1.97270800	0.83112600
C	3.01709400	-2.32716300	0.68612200
C	0.64700500	0.45303500	2.07596400
C	0.44283600	1.68312800	2.66730400
C	-0.81918000	2.32564600	2.52961500
C	-1.79909600	1.63855800	1.83472800
C	-1.55663400	0.37073600	1.24899700
C	-2.51281700	-0.38695200	0.51013400
C	-3.86044300	-0.01428000	0.30794000
C	-4.76189200	-0.81360200	-0.37139700
C	-4.27504300	-2.07498400	-0.85066600
C	-2.96154700	-2.41295300	-0.66266300
H	-1.61408700	-0.08875200	-2.06756800
H	-1.32179600	2.11466300	-3.13061400
H	2.74145400	2.09587800	-1.71933100
H	4.19398900	0.93799800	-0.86272100
H	5.00174300	-2.65087500	1.36628600
H	2.63784200	-3.25560400	1.09437000
H	1.60519500	-0.04835000	2.15876500
H	1.25697400	2.13215600	3.21962100
H	-2.77981700	2.08230000	1.71261400
H	-4.19005600	0.93486200	0.71307000
H	-4.91939600	-2.77540100	-1.36400700
H	-2.56824500	-3.35607800	-1.02379100
C	-0.12084300	-3.32075700	1.34616800
C	0.14683900	-3.31181800	-1.26370000

O	0.21974300	-4.17088500	-2.04112600
O	-0.17492300	-4.19265700	2.10762000
C	6.26815000	-0.28952400	0.42403400
C	1.00690900	3.73079100	-3.05592000
C	7.14447400	-1.29945500	1.18648400
H	7.19214000	-2.26619200	0.67277900
H	8.16545000	-0.91121100	1.25737300
H	6.78230600	-1.46387100	2.20748900
C	6.27174200	1.05278900	1.19647000
H	5.69666400	1.82661400	0.67736100
H	5.84951600	0.92876400	2.19981500
H	7.30090400	1.41331600	1.30014500
C	6.86776600	-0.07957400	-0.98722200
H	7.90546600	0.25936500	-0.89630200
H	6.86086900	-1.01388200	-1.55905200
H	6.32125000	0.67649800	-1.56028700
C	1.35106300	4.66892600	-1.87292500
H	2.24750100	4.33936800	-1.33727800
H	1.53754100	5.68138500	-2.24748600
H	0.52297600	4.71494000	-1.15633700
C	2.19768900	3.67700400	-4.04219300
H	2.38715400	4.67790400	-4.44497600
H	3.11794900	3.33459400	-3.55787400
H	1.98276900	3.00534600	-4.88055100
C	-0.21962400	4.29714000	-3.79350000
H	-0.50464200	3.67255100	-4.64761200
H	-1.08511000	4.39443000	-3.12849300
H	0.01599000	5.29526700	-4.17628200
C	-1.10454100	3.72609700	3.09156600
C	0.09901300	4.29812100	3.86351300
H	0.36956600	3.66860200	4.71886000
H	0.97998100	4.40489800	3.22036400
H	-0.15155600	5.29242500	4.24854900
C	-1.42522300	4.67778900	1.91392700
H	-0.57982100	4.73378200	1.21768600
H	-2.30452600	4.34501300	1.35234500
H	-1.62695800	5.68817300	2.28881900
C	-2.31545300	3.66490300	4.05145300

H	-2.11418000	2.98974000	4.89084600
H	-2.52455800	4.66188700	4.45661100
H	-3.22077400	3.31446600	3.54517200
C	-6.20821800	-0.34757300	-0.58144300
C	-6.87396400	-0.09408800	0.79243400
H	-6.35164800	0.68147300	1.36217700
H	-7.91005000	0.23557100	0.65116700
H	-6.88530000	-1.00889100	1.39555300
C	-6.19942000	0.96706600	-1.39871600
H	-5.65249400	1.76263800	-0.88183800
H	-5.73150300	0.81415900	-2.37803000
H	-7.22617400	1.31565200	-1.56089900
C	-7.05017900	-1.38775200	-1.34383200
H	-7.11478300	-2.33647000	-0.79916700
H	-8.06984000	-1.00914100	-1.47234000
H	-6.64283700	-1.58861000	-2.34118700

1 5 1.0 38 1.0 39 1.0
2 6 1.5 10 1.5
3 11 1.5 15 1.5
4 16 1.5 20 1.0
5 21 1.0 25 1.5
6 7 1.5 26 1.0
7 8 1.5 27 1.0
8 9 1.5 43 1.0
9 10 1.5 28 1.0
10 11 1.0
11 12 1.5
12 13 1.5 29 1.0
13 14 1.5 42 1.0
14 15 1.5 30 1.0
15 31 1.0
16 17 2.0 32 1.0
17 18 1.5 33 1.0
18 19 2.0 68 1.0
19 20 1.5 34 1.0
20 21 1.5
21 22 1.5

22 23 2.0 35 1.0
23 24 1.5 81 1.0
24 25 2.0 36 1.0
25 37 1.0
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38 41 2.0
39 40 2.0
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42 44 1.0 48 1.0 52 1.0
43 56 1.0 60 1.0 64 1.0
44 45 1.0 46 1.0 47 1.0
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48 49 1.0 50 1.0 51 1.0
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52 53 1.0 54 1.0 55 1.0
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56 57 1.0 58 1.0 59 1.0
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60 61 1.0 62 1.0 63 1.0
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64 65 1.0 66 1.0 67 1.0
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68 69 1.0 73 1.0 77 1.0
69 70 1.0 71 1.0 72 1.0
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77 78 1.0 79 1.0 80 1.0
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81 82 1.0 86 1.0 90 1.0
82 83 1.0 84 1.0 85 1.0
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86 87 1.0 88 1.0 89 1.0
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90 91 1.0 92 1.0 93 1.0
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Optimized T_1 geometry of **8**

Re 0.01670400 -0.84438400 -0.01814800

N	0.40541900	0.79821400	-1.36554500
N	2.06054200	-0.55139000	0.22990100
N	-0.42993800	0.83192700	1.33315700
N	-2.10917600	-0.56270200	-0.18044400
C	-0.49465000	1.41500100	-2.16355200
C	-0.20024500	2.53858200	-2.90825000
C	1.11260100	3.06662700	-2.83291300
C	2.04718400	2.44963400	-2.03431500
C	1.70029800	1.29457500	-1.28148100
C	2.59071300	0.57984600	-0.43010900
C	3.95359700	0.91156500	-0.22324900
C	4.75888000	0.13140000	0.57128000
C	4.22032300	-1.04112700	1.18199400
C	2.89967400	-1.33727500	0.97551700
C	0.48427800	1.45264600	2.09798500
C	0.17650900	2.57717400	2.85601200
C	-1.12617300	3.07113800	2.81922100
C	-2.07668700	2.42396700	2.03363800
C	-1.70512900	1.29938100	1.29226300
C	-2.63616600	0.53342700	0.44228700
C	-3.98203900	0.86566800	0.27658300
C	-4.79757300	0.07363000	-0.52693900
C	-4.25414500	-1.05444700	-1.14160100
C	-2.91215700	-1.34322000	-0.93697700
H	-1.48167000	0.96738400	-2.19427600
H	-0.96135700	2.99024000	-3.53351300
H	3.05549200	2.84254000	-1.97880300
H	4.36335900	1.79000400	-0.70794000
H	4.83248300	-1.69294900	1.79386600
H	2.44175500	-2.21542000	1.41459400
H	1.47865800	1.02511600	2.09218600
H	0.94659800	3.04705200	3.45660000
H	-3.09343500	2.79365600	2.00459200
H	-4.39525800	1.73633600	0.76907500
H	-4.85299500	-1.70801600	-1.76491700
H	-2.44768600	-2.21284100	-1.38367000
H	1.38287300	3.94792000	-3.40623900
H	5.80073500	0.39632600	0.71944600

H	-5.84291400	0.32984700	-0.66124900
H	-1.40422600	3.94610800	3.39715200
C	-0.24028300	-2.25049600	1.29726100
C	0.29751000	-2.30811900	-1.26908200
O	0.45289900	-3.19700000	-1.99377200
O	-0.38553900	-3.09853600	2.07518500

1 3 1.0 42 1.0 43 1.0
2 6 1.5 10 1.0
3 11 1.0 15 1.5
4 16 1.5 20 1.5
5 21 1.5 25 1.5
6 7 2.0 26 1.0
7 8 1.5 27 1.0
8 9 2.0 38 1.0
9 10 1.5 28 1.0
10 11 1.5
11 12 1.5
12 13 2.0 29 1.0
13 14 1.5 39 1.0
14 15 2.0 30 1.0
15 31 1.0
16 17 1.5 32 1.0
17 18 1.5 33 1.0
18 19 1.5 41 1.0
19 20 1.5 34 1.0
20 21 1.0
21 22 1.5
22 23 1.5 35 1.0
23 24 1.5 40 1.0
24 25 1.5 36 1.0
25 37 1.0
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42 45 2.0
43 44 3.0
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Optimized T_1 geometry of **9**

Re	-0.02047700	-1.12845100	0.01733800
N	0.41740200	0.55130700	-1.33027800
N	2.10165400	-0.83549300	0.17384100
N	-0.39724700	0.51680000	1.36656400
N	-2.06114500	-0.82931400	-0.21450300
C	-0.49310000	1.17401700	-2.09997100
C	-0.18832000	2.30323300	-2.84483900
C	2.04869800	2.16586600	-2.01439500
C	1.68487000	1.03438500	-1.28169000
C	2.62054200	0.27230500	-0.43193300
C	3.95920500	0.62141700	-0.25338900
C	4.25168700	-1.30086300	1.13498200
C	2.91945100	-1.60910800	0.92345800
C	0.50093500	1.13366100	2.16509400
C	0.21288300	2.26601800	2.89549300
C	-2.01913300	2.19560800	2.01511600
C	-1.68318600	1.02938900	1.27456000
C	-2.57998900	0.31713600	0.42750800
C	-3.93719200	0.66510700	0.21129200
C	-4.22912900	-1.29731600	-1.15548400
C	-2.91499100	-1.61005700	-0.94679000

H	-1.48545500	0.74143300	-2.10698100
H	-0.96189300	2.76747900	-3.44721300
H	3.06499700	2.53770900	-1.97357900
H	4.35472100	1.50654500	-0.73592800
H	4.85515100	-1.95522900	1.75479300
H	2.47024800	-2.49113100	1.36170700
H	1.48447100	0.67873100	2.20728200
H	0.97722600	2.71395100	3.52124500
H	-3.02483700	2.59520800	1.94741400
H	-4.32975600	1.55901000	0.68328600
H	-4.85030700	-1.95090600	-1.75792600
H	-2.47276900	-2.50142200	-1.37566700
C	-0.27582300	-2.59249600	1.27076800
C	0.21560200	-2.52819700	-1.30401400
O	0.34533200	-3.37390000	-2.08888000
O	-0.41251200	-3.48313000	1.99863000
C	1.11037600	2.82897200	-2.81010000
C	4.80438400	-0.15525300	0.54336900
C	-4.77122200	-0.10420700	-0.56969600
C	-1.09375800	2.82608200	2.81991800
C	-1.43201500	4.06319200	3.60834700
H	-0.77733600	4.89655400	3.32368500
H	-2.46932500	4.37334100	3.45246600
H	-1.28158300	3.89349900	4.68185200
C	-6.21075400	0.25635000	-0.80415000
H	-6.48572500	1.18715700	-0.29975200
H	-6.41246100	0.37166100	-1.87707900
H	-6.87395700	-0.54075900	-0.44346700
C	6.25018700	0.20178400	0.74666300
H	6.49717000	1.16637800	0.29626500
H	6.49057500	0.24150700	1.81483100
H	6.89587800	-0.56317600	0.29892500
C	1.47106100	4.05887900	-3.59763100
H	0.92084900	4.92764300	-3.21712000
H	2.54018200	4.27850600	-3.54079700
H	1.19491800	3.93784000	-4.65088200

1 5 1.0 34 1.0 35 1.0

2 6 1.5 9 1.5
3 10 1.5 13 1.5
4 14 1.5 17 1.0
5 18 1.0 21 1.5
6 7 1.5 22 1.0
7 23 1.0 38 1.5
8 9 1.5 24 1.0 38 1.5
9 10 1.0
10 11 1.5
11 25 1.0 39 1.5
12 13 2.0 26 1.0 39 1.5
13 27 1.0
14 15 2.0 28 1.0
15 29 1.0 41 1.5
16 17 1.5 30 1.0 41 2.0
17 18 1.5
18 19 1.5
19 31 1.0 40 2.0
20 21 2.0 32 1.0 40 1.5
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Reference for the Electronic Supplementary Information

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