

Supporting Information

Mechanistic Insight into the Pyridine Enhanced α -Selectivity in Alkyne Hydrothiolation Catalysed by Quinolinolate–Rhodium(I)–N-Heterocyclic Carbene Complexes

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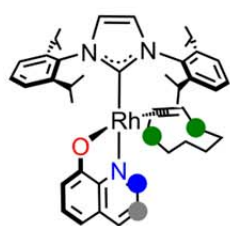
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General considerations. All reactions were carried out with rigorous exclusion of air using Schlenk-tube techniques. Organic products were purchased from commercial sources and were used as received, except for phenylacetylene that was distilled under argon and stored over molecular sieves. Organic solvents were dried by standard procedures and distilled under argon prior to use or obtained oxygen- and water-free from a Solvent Purification System (Innovative Technologies). The organometallic starting material $[\text{Rh}(\mu\text{-OH})(\text{IPr})(\eta^2\text{-olefin})]_2$ was prepared as previously described in the literature.¹ ^1H , $^{13}\text{C}\{^1\text{H}\}$ and HSQC ^1H - ^{15}N spectra were recorded either on a Varian Gemini 2000 300 MHz, a Bruker ARX 300 MHz, a Bruker Avance 400 MHz, or a Bruker Avance 500 MHz instruments. Chemical shifts (expressed in parts per million) are referenced to residual solvent peaks (^1H , $^{13}\text{C}\{^1\text{H}\}$), external liquid NH_3 (^{15}N). Coupling constants, J , are given in Hz. Spectral assignments were achieved by combination of ^1H - ^1H COSY, $^{13}\text{C}\{^1\text{H}\}$ -APT and ^1H - ^{13}C HSQC/HMBC experiments. GC-MS analysis were recorder on an Agilent 5973 mass selective detector interfaced to an Agilent 6890 series gas chromatograph system, using a HP-5MS 5% phenyl methyl siloxane column (30 m x 250 mm with a 0.25 mm film thickness). The nature of phenyl(1-phenylvinyl)sulfane was compared with previously reported data.²

- 1) L. Palacios, M. J. Artigas, V. Polo, F. J. Lahoz, R. Castarlenas, J. J. Pérez-Torrente, L. A. Oro, *ACS Catal.* **2013**, 3, 2910-2919.
- 2) C. C. Silveira, P. C. S. Santos, S. R. mendes, A. L. Braga. *J. Organomet. Chem.* **2008**, 693, 3787-3790.

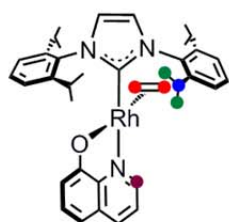
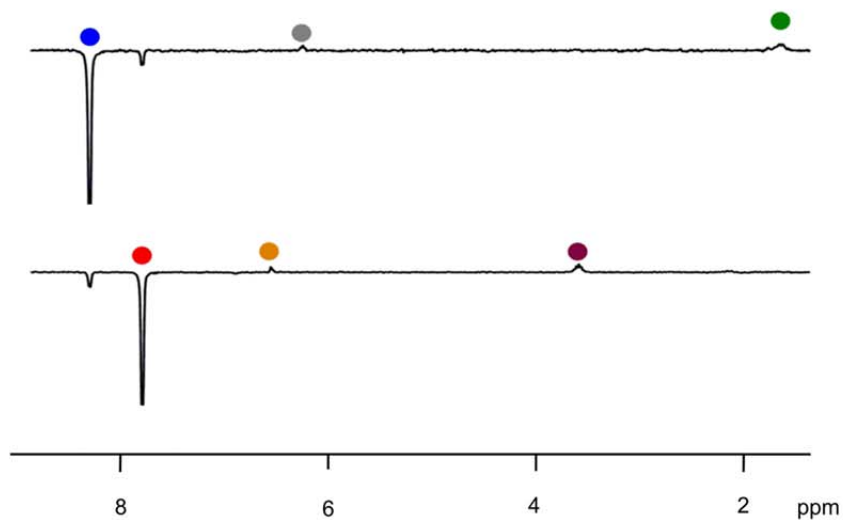
1-D NOESy experiments



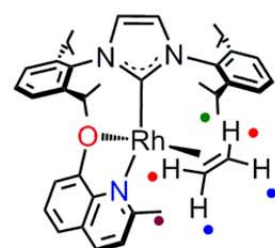
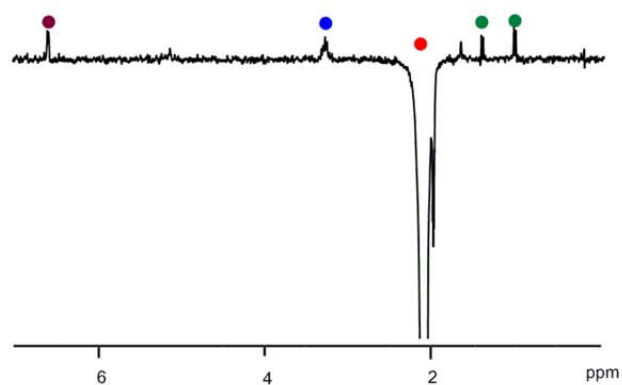
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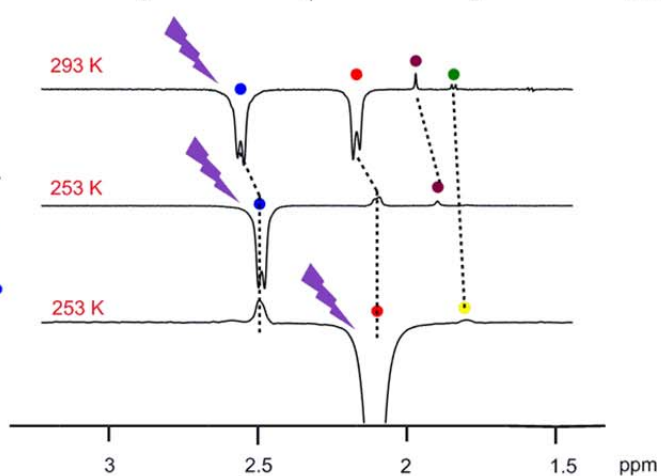
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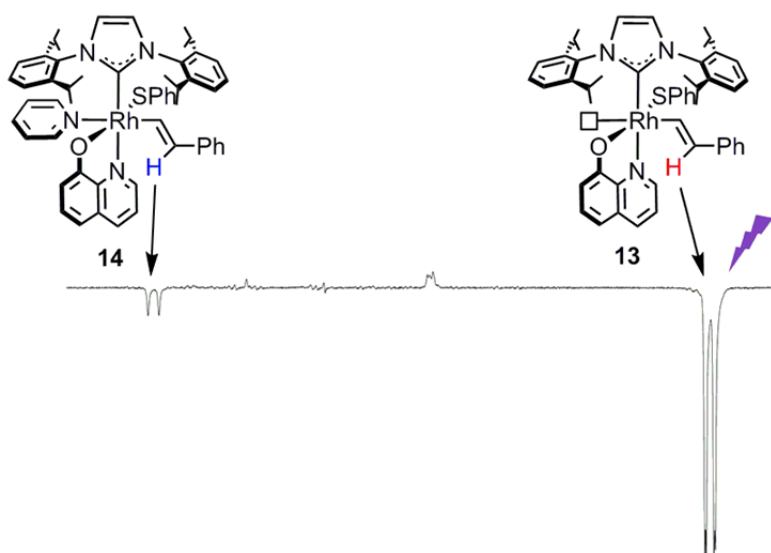


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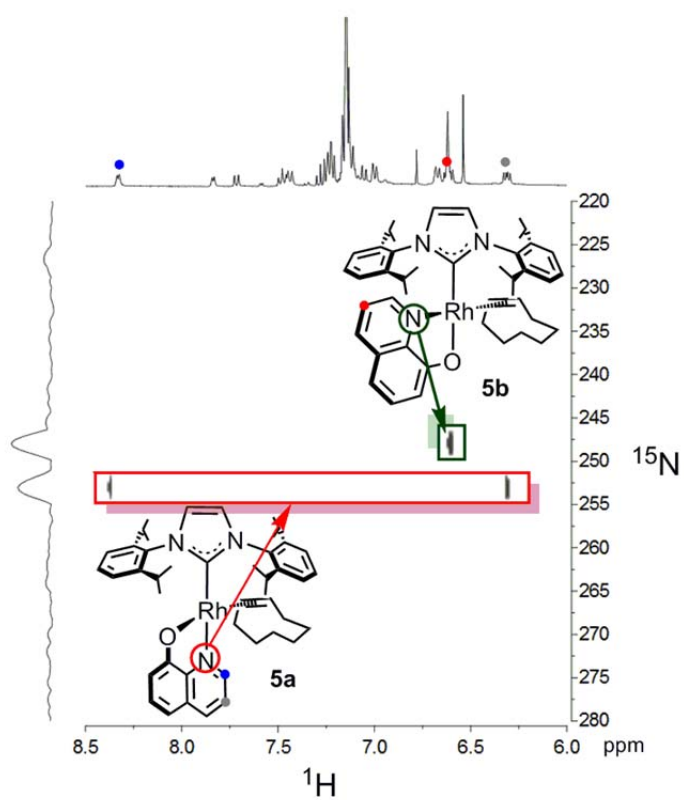


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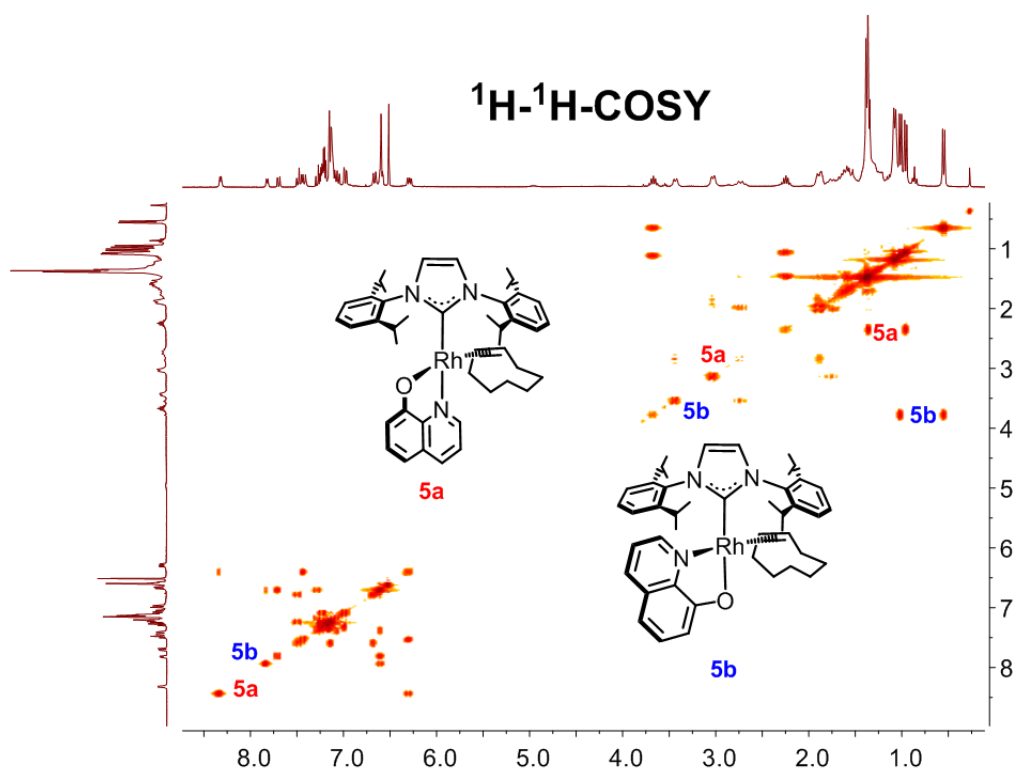
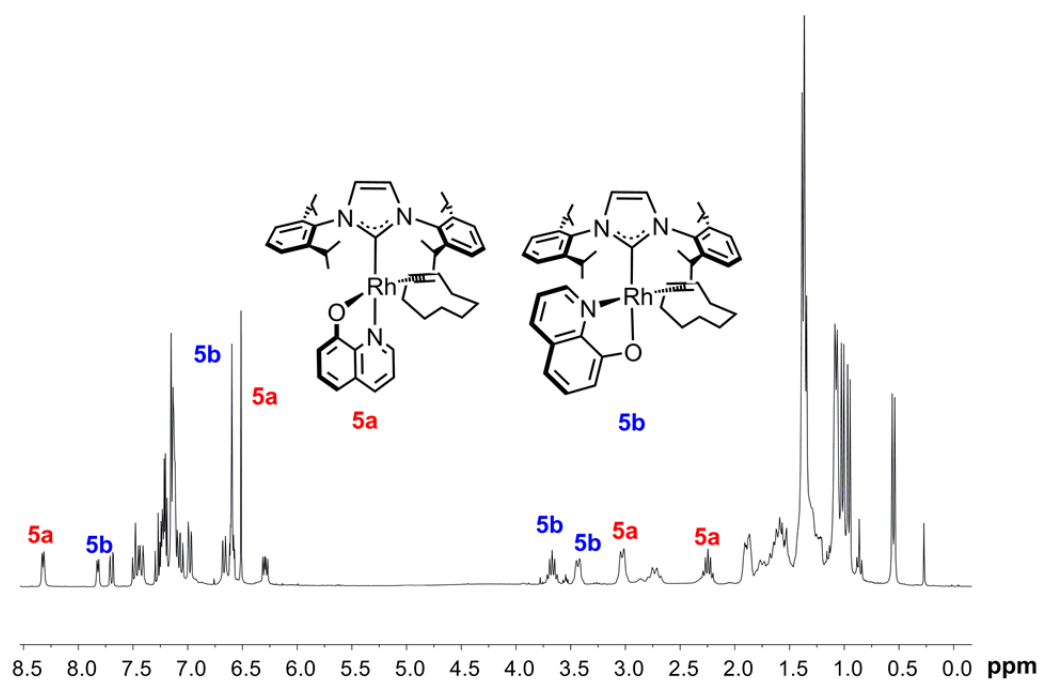


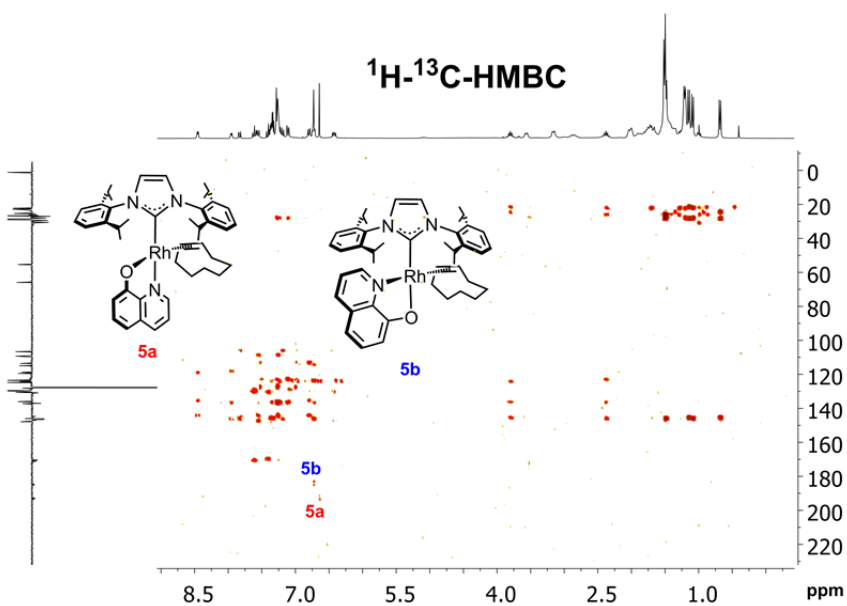
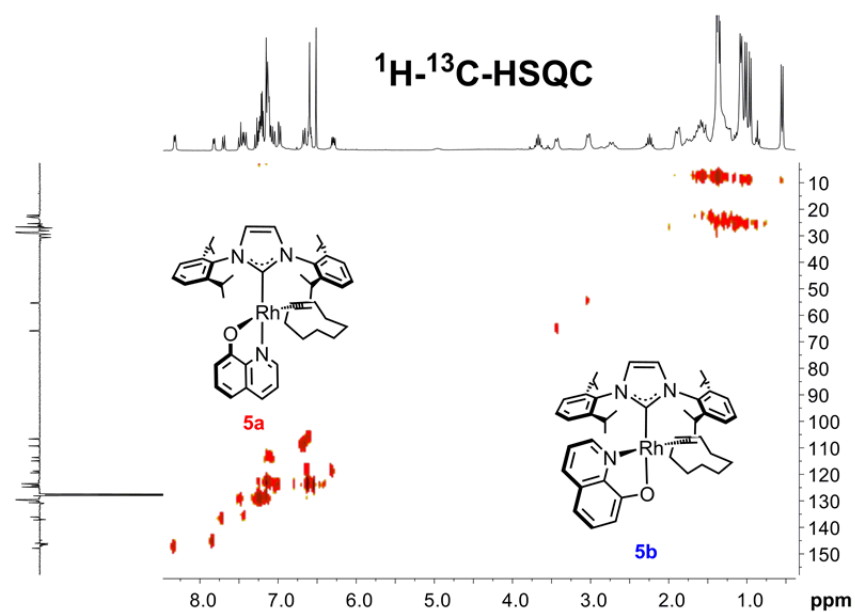
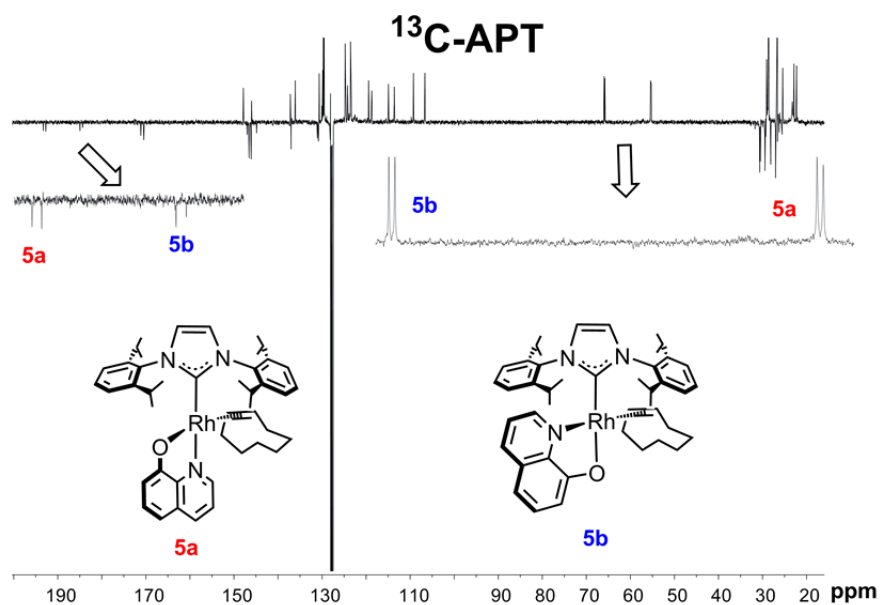


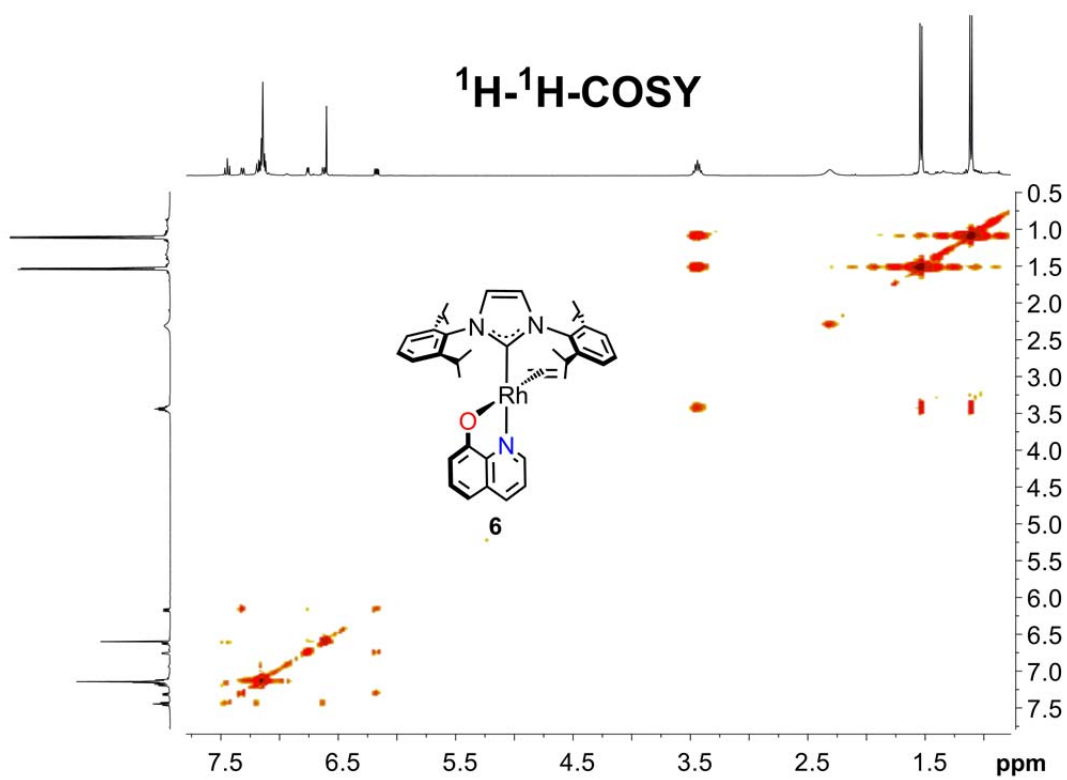
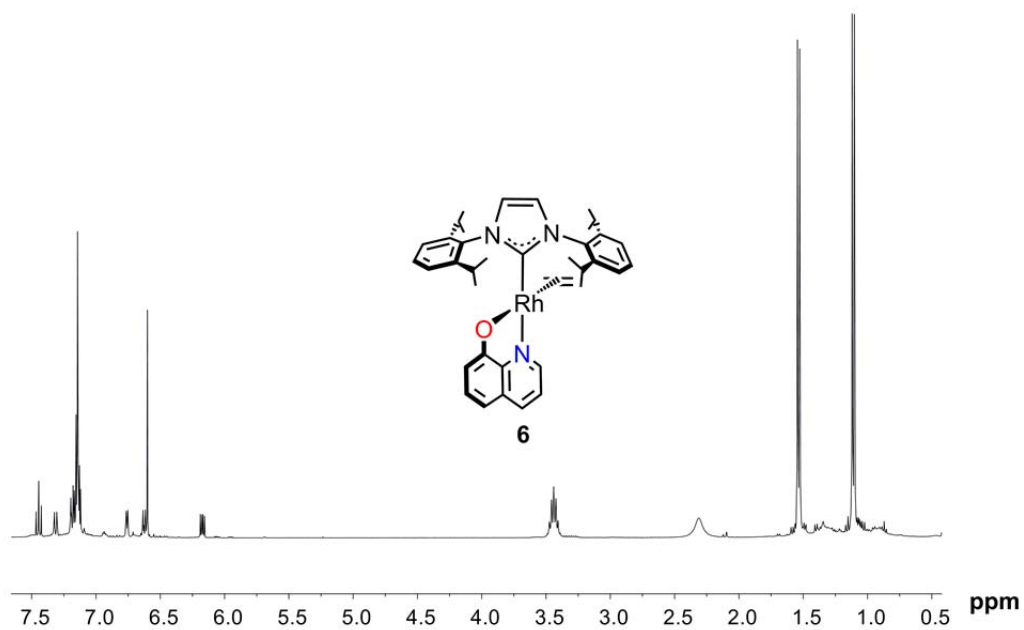
^1H - ^{15}N HMBC Correlation for 5a,b

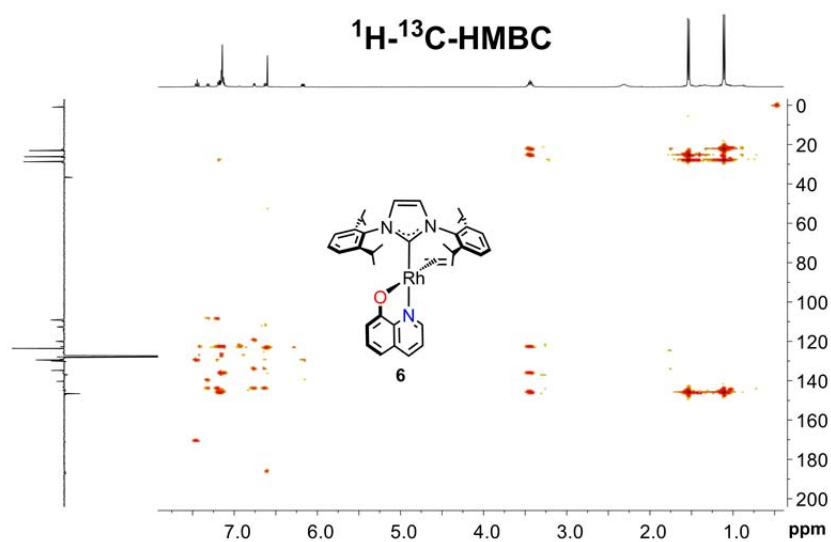
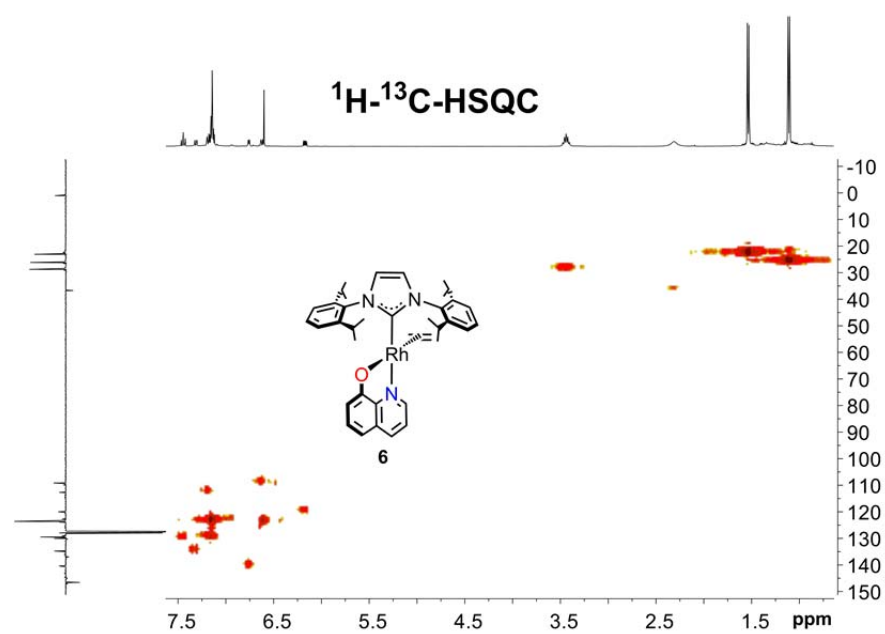
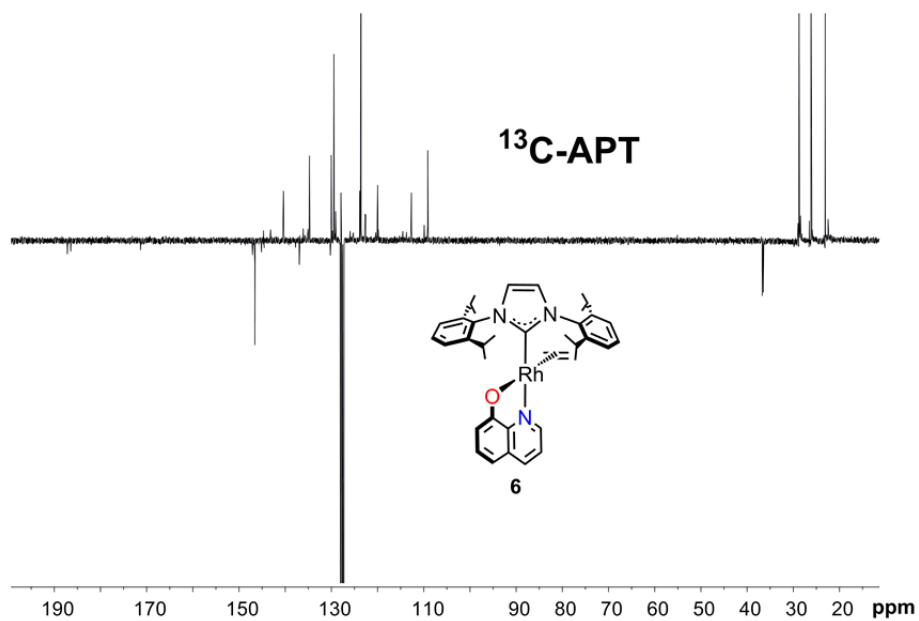


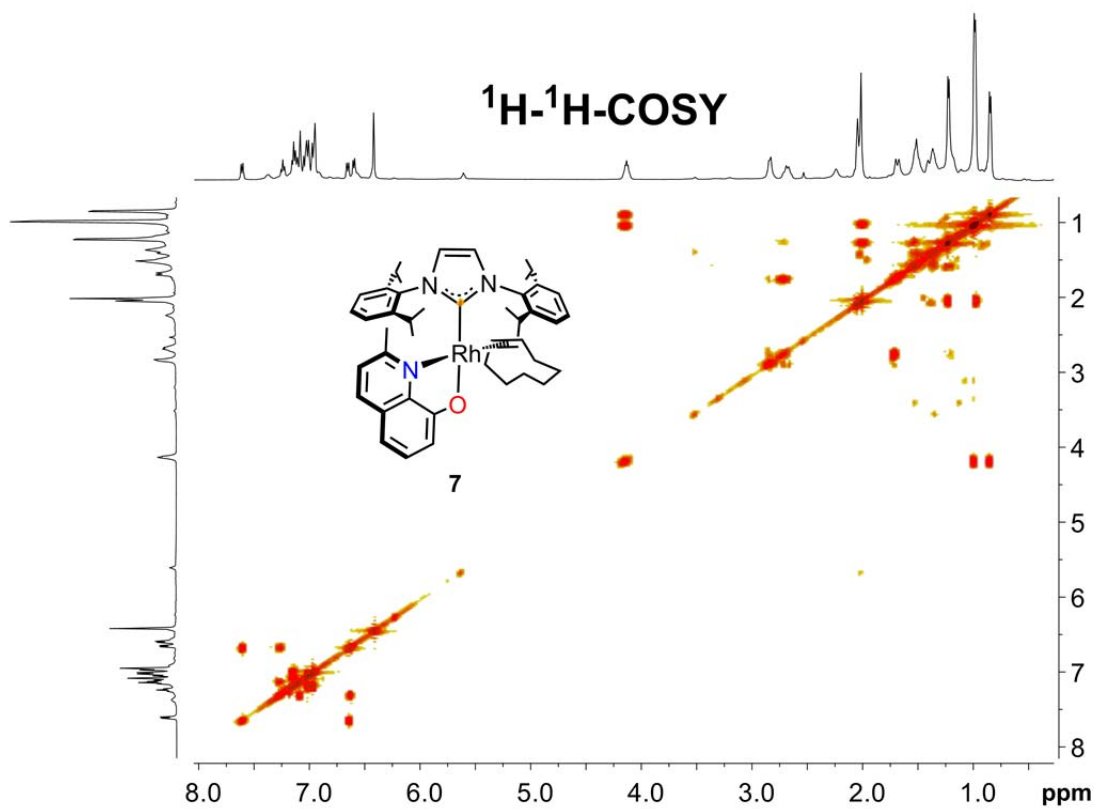
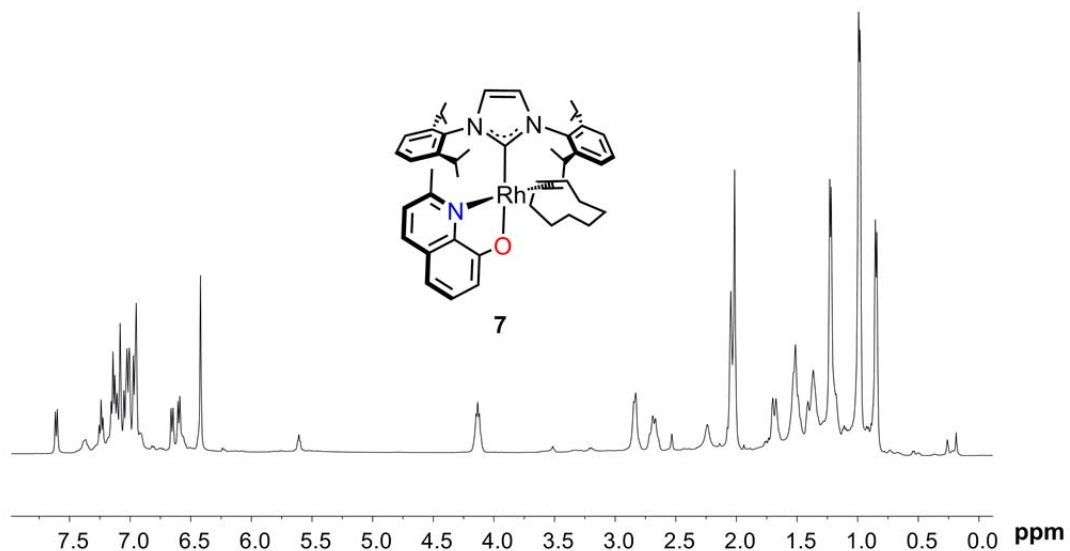
NMR Spectra of Complexes

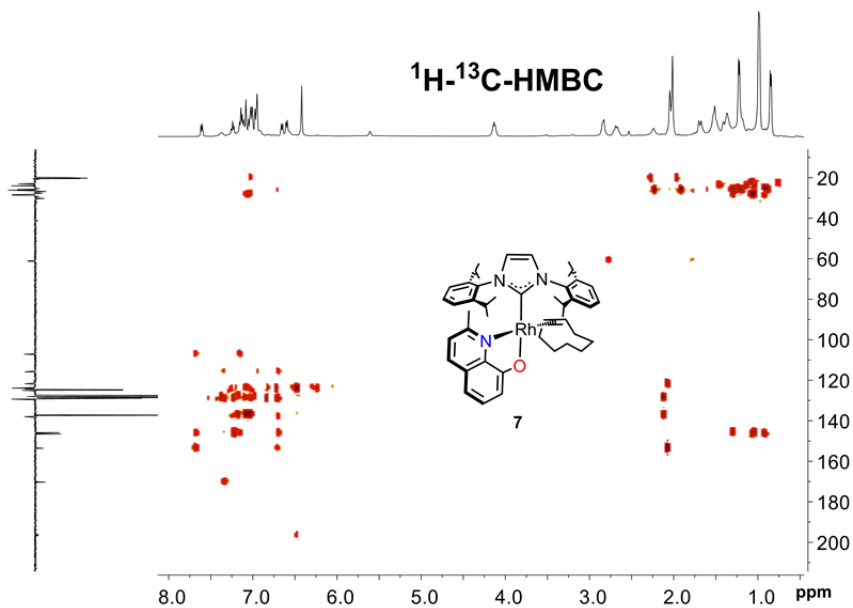
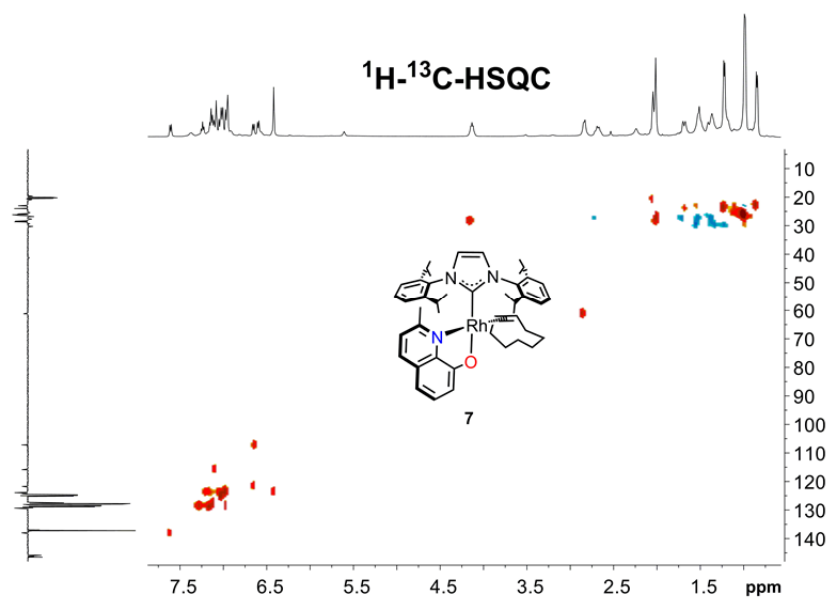
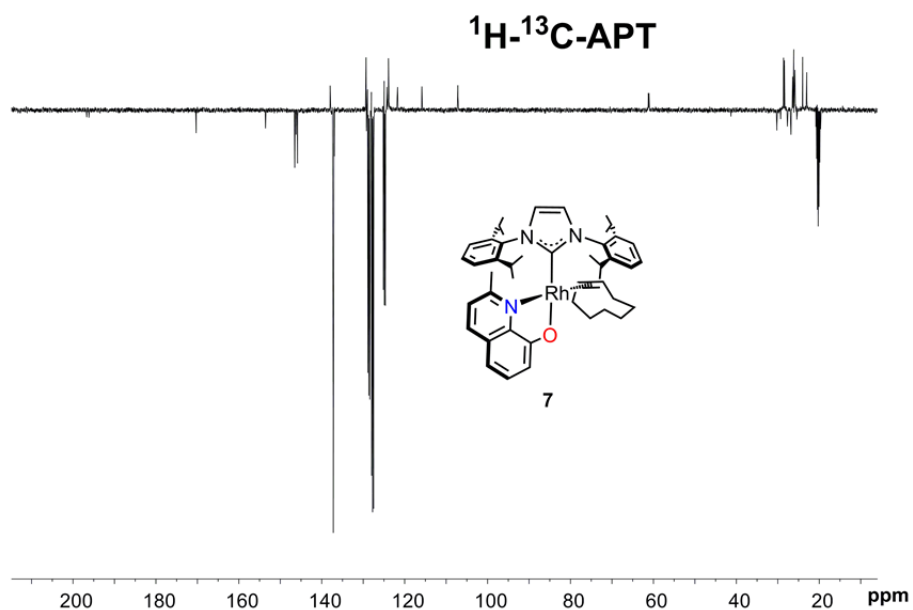


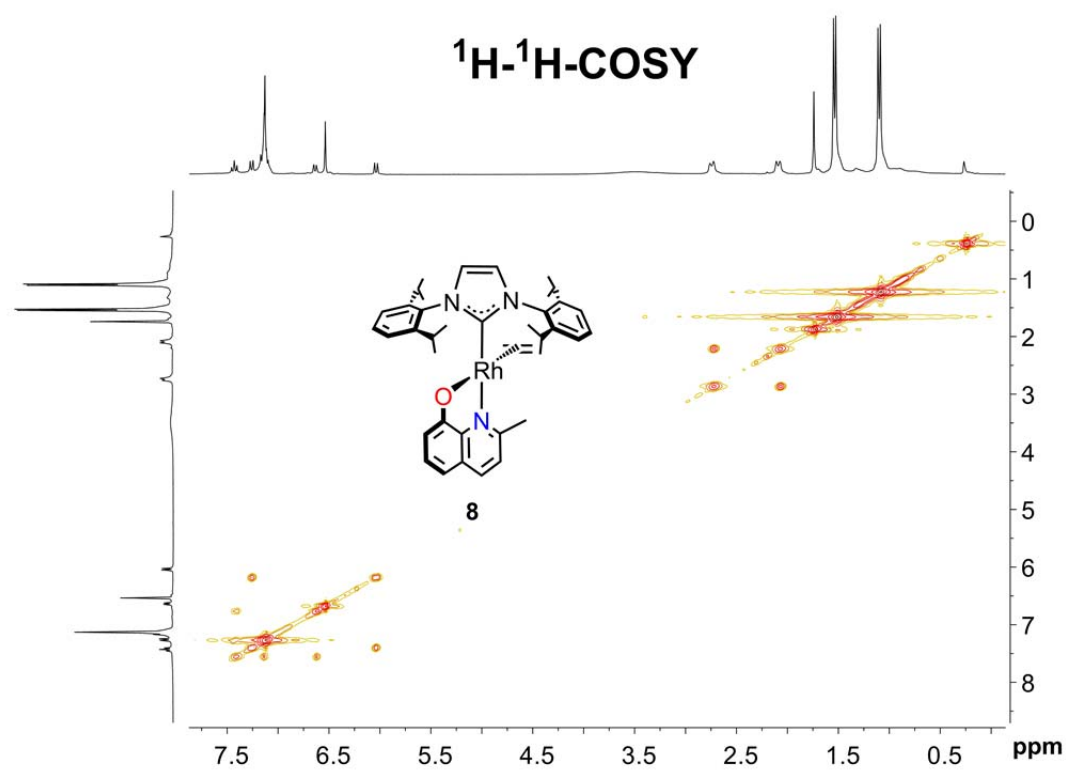
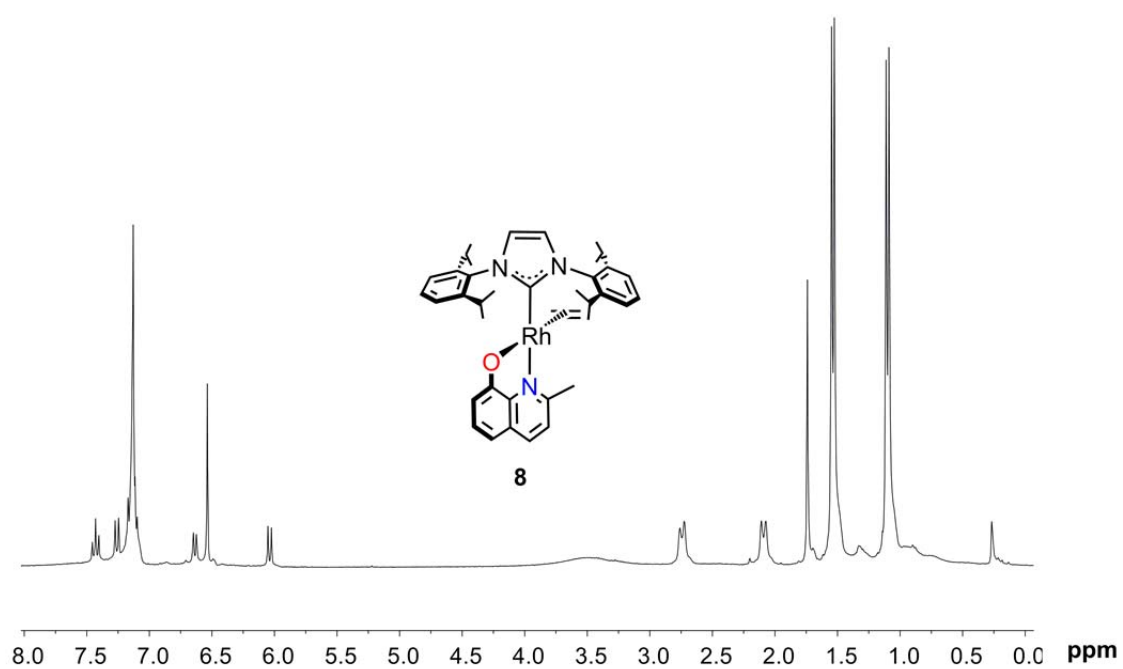


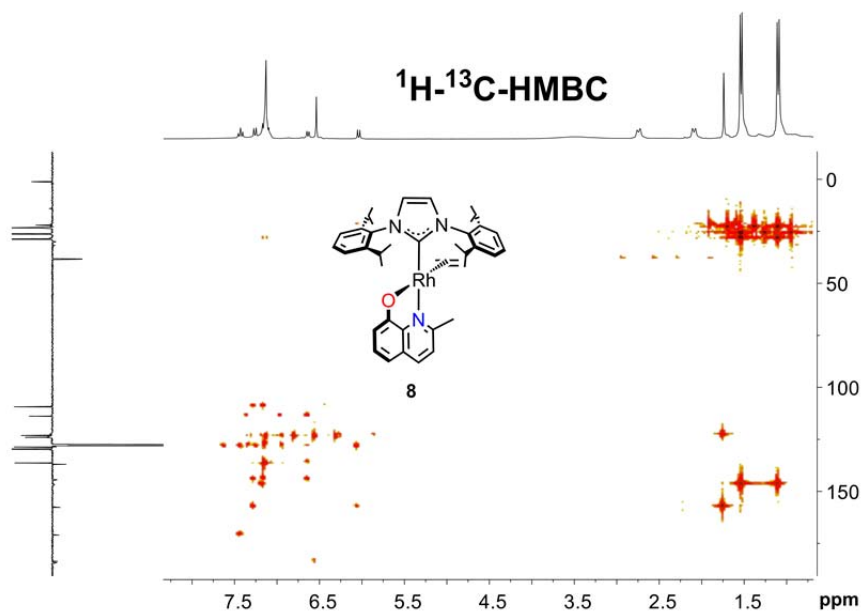
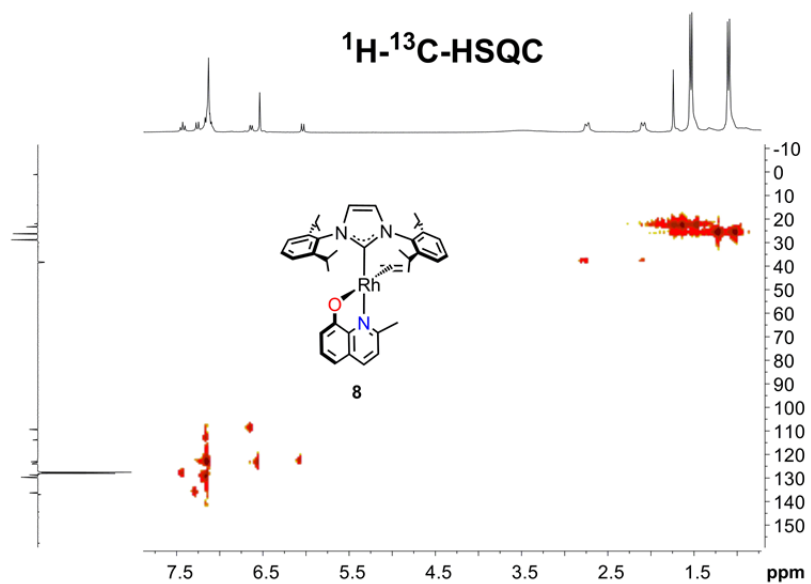
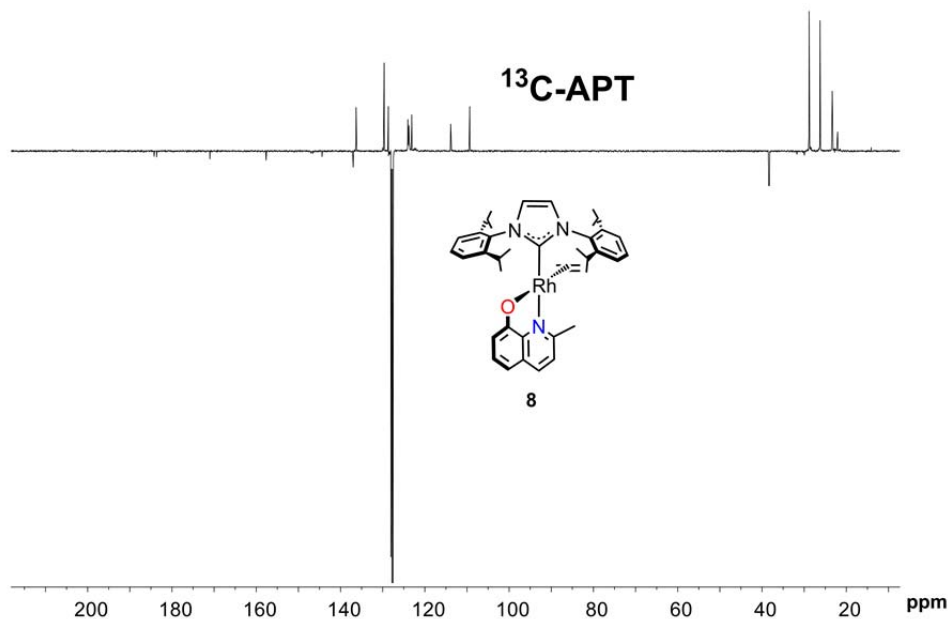


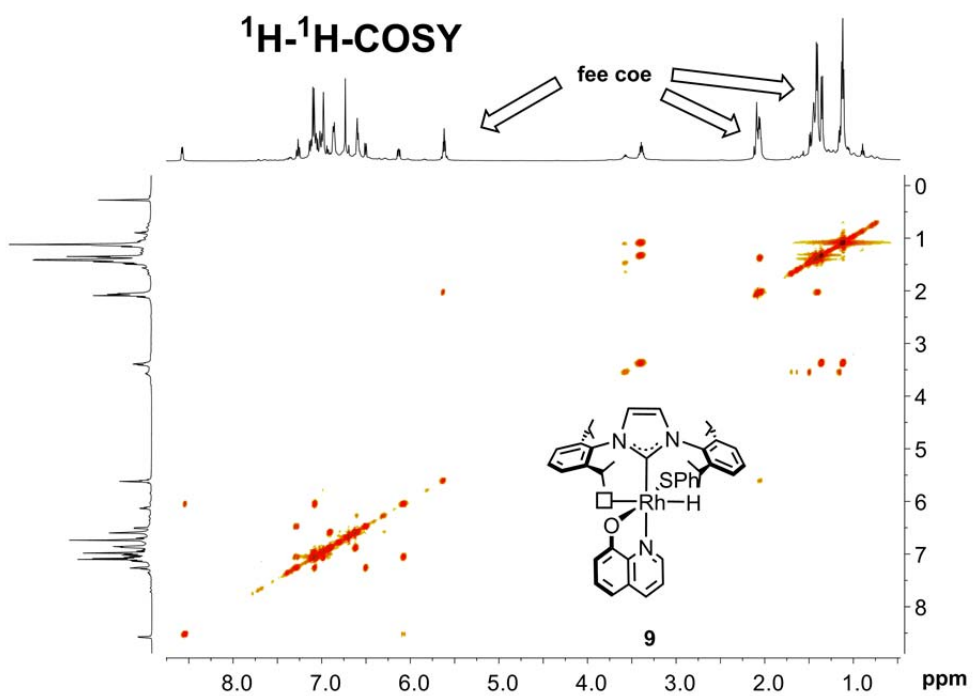
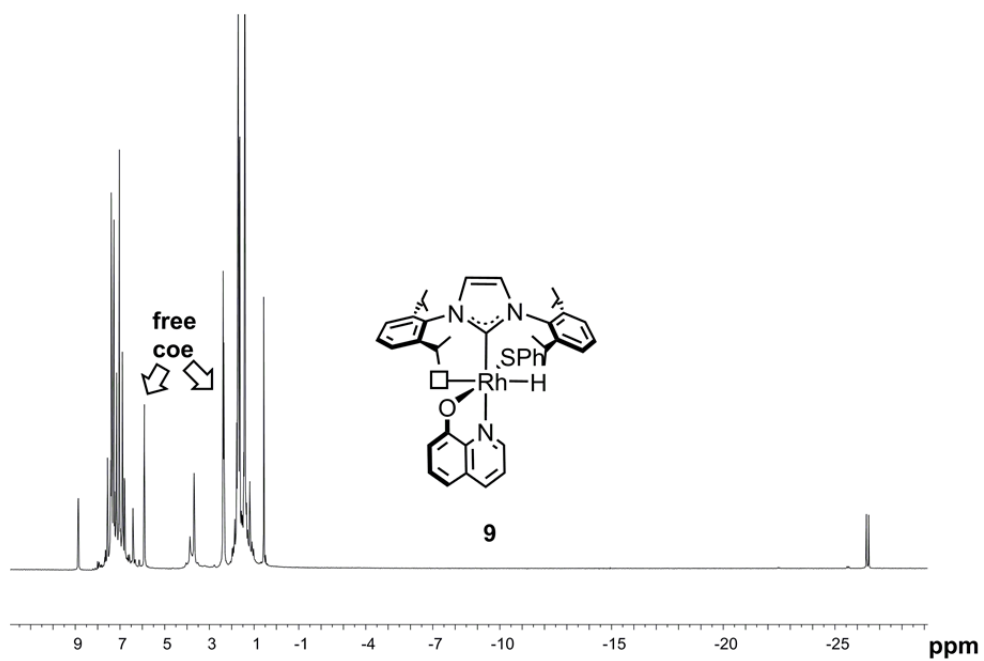


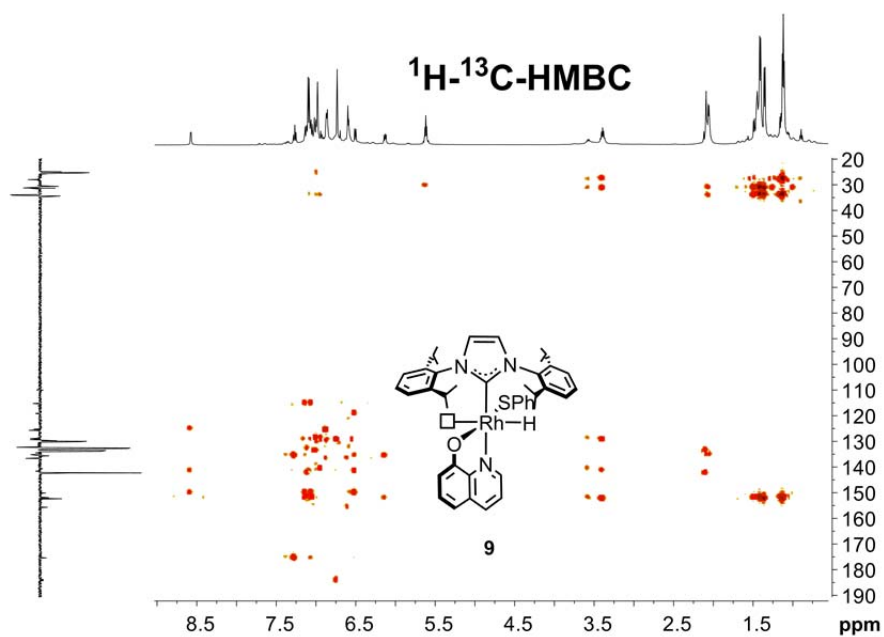
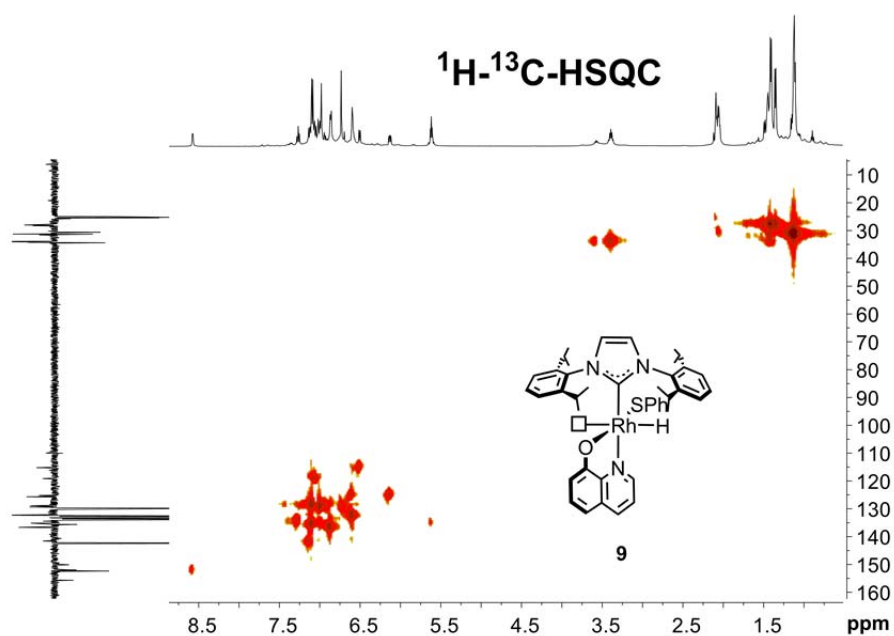
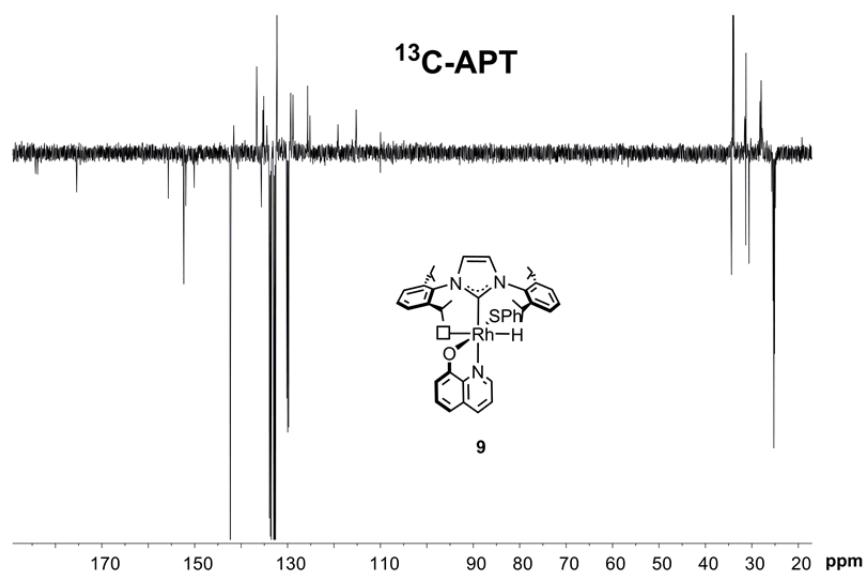


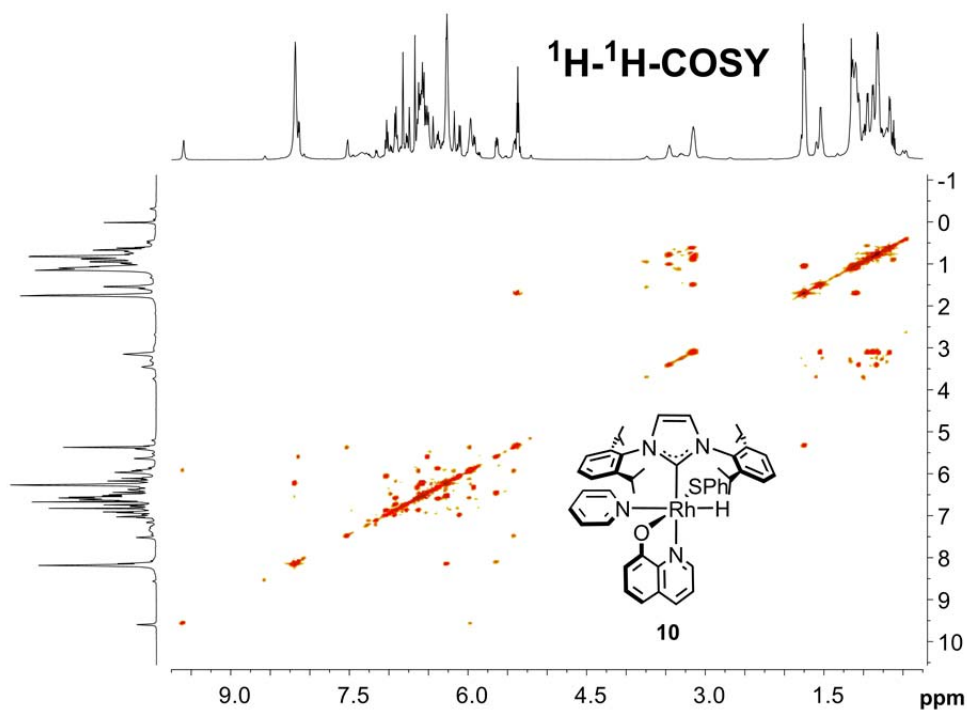
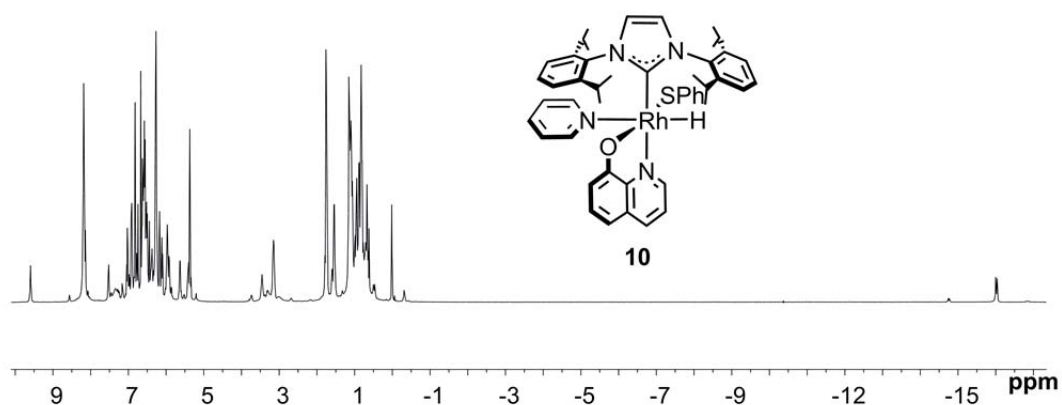


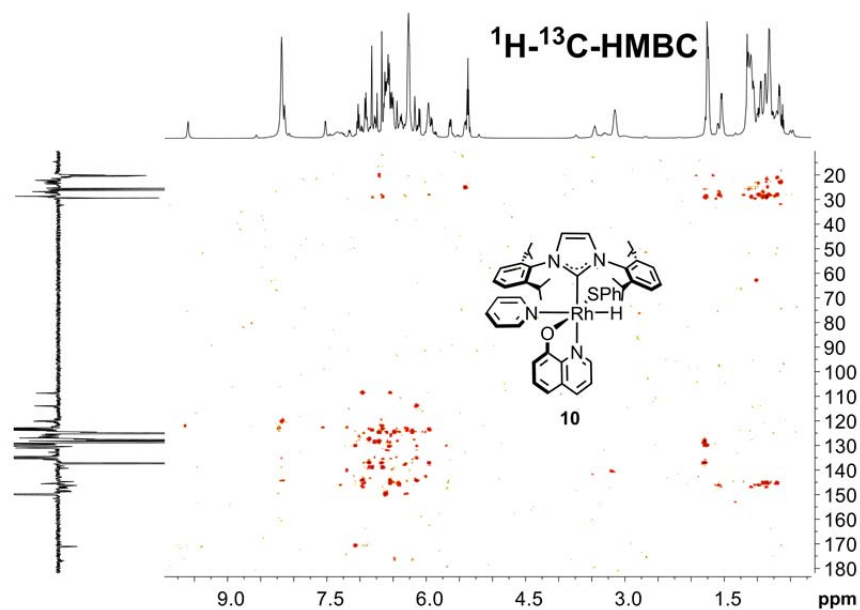
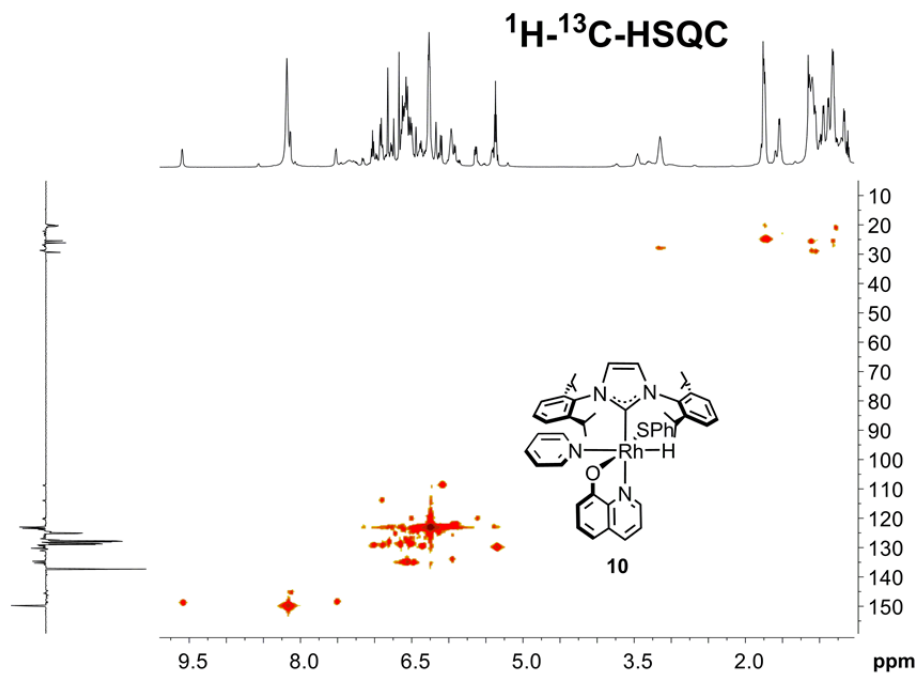
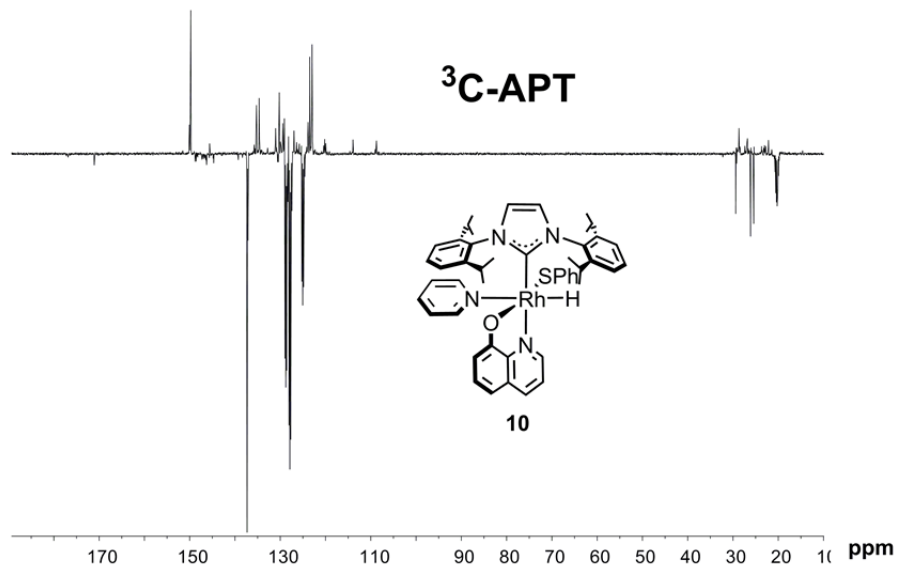


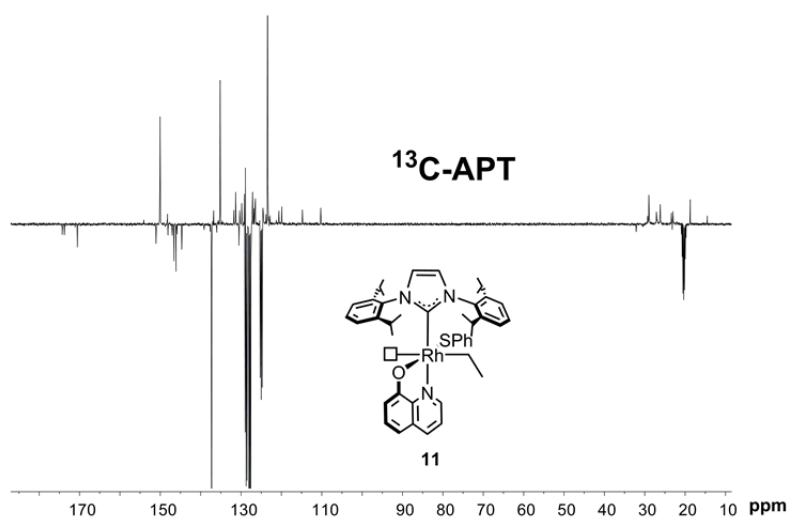
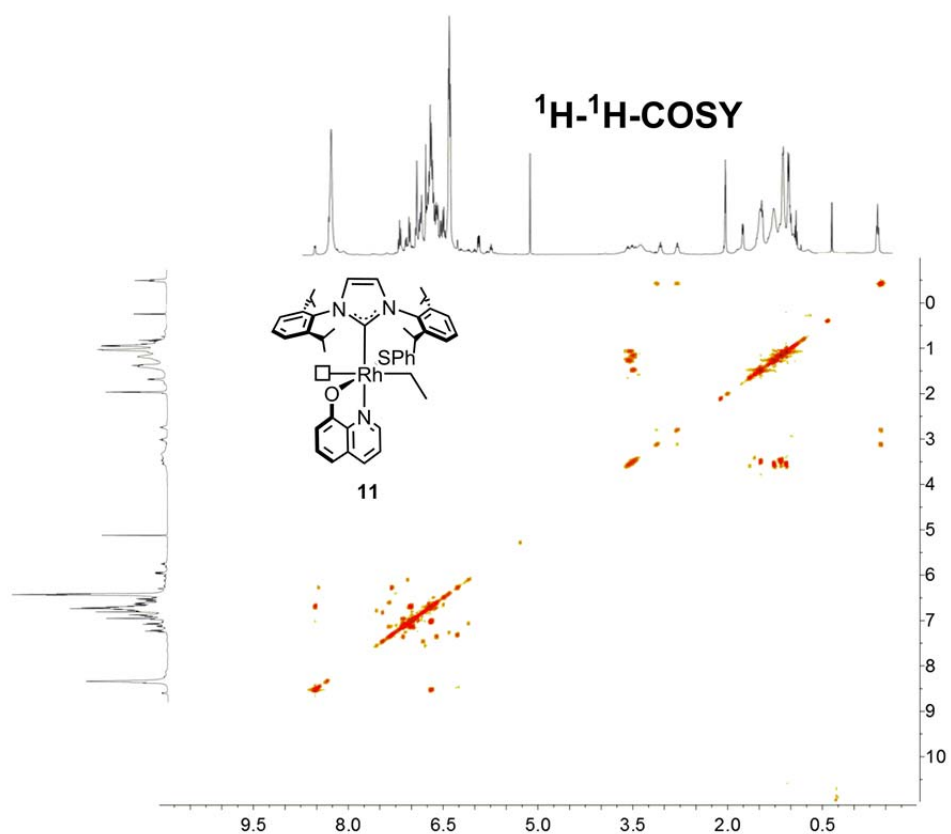
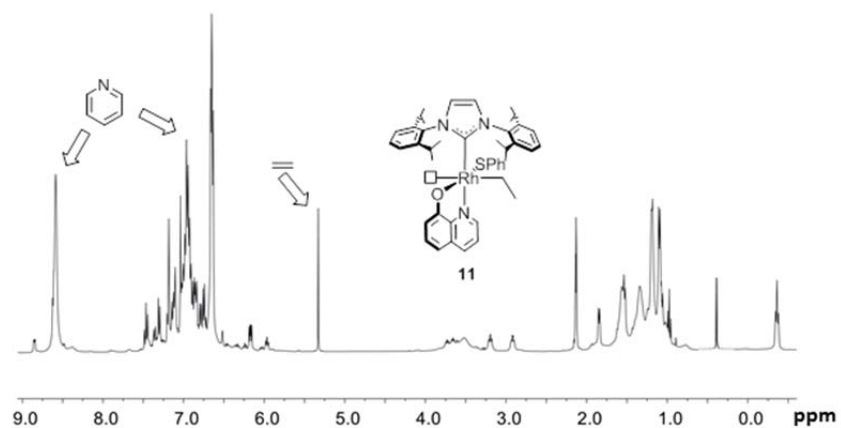


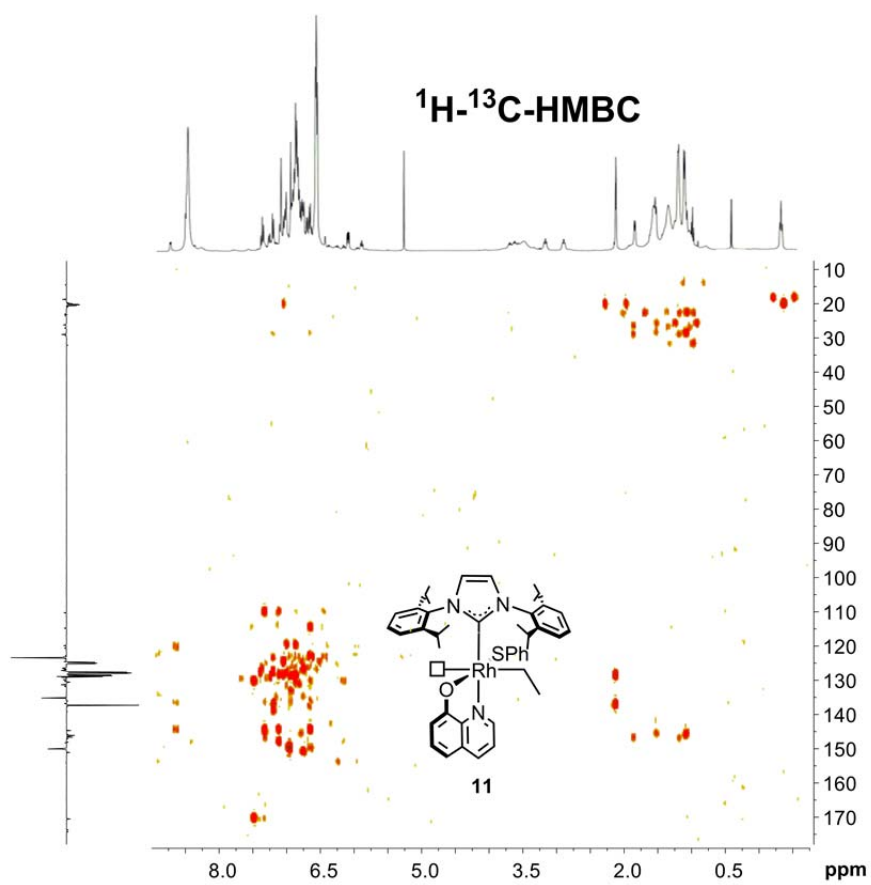
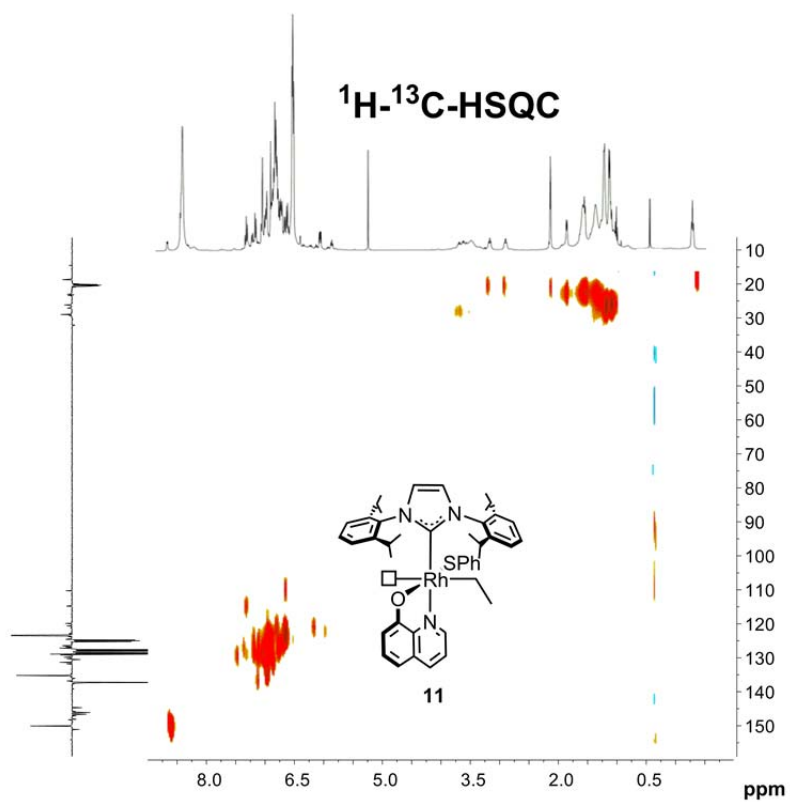


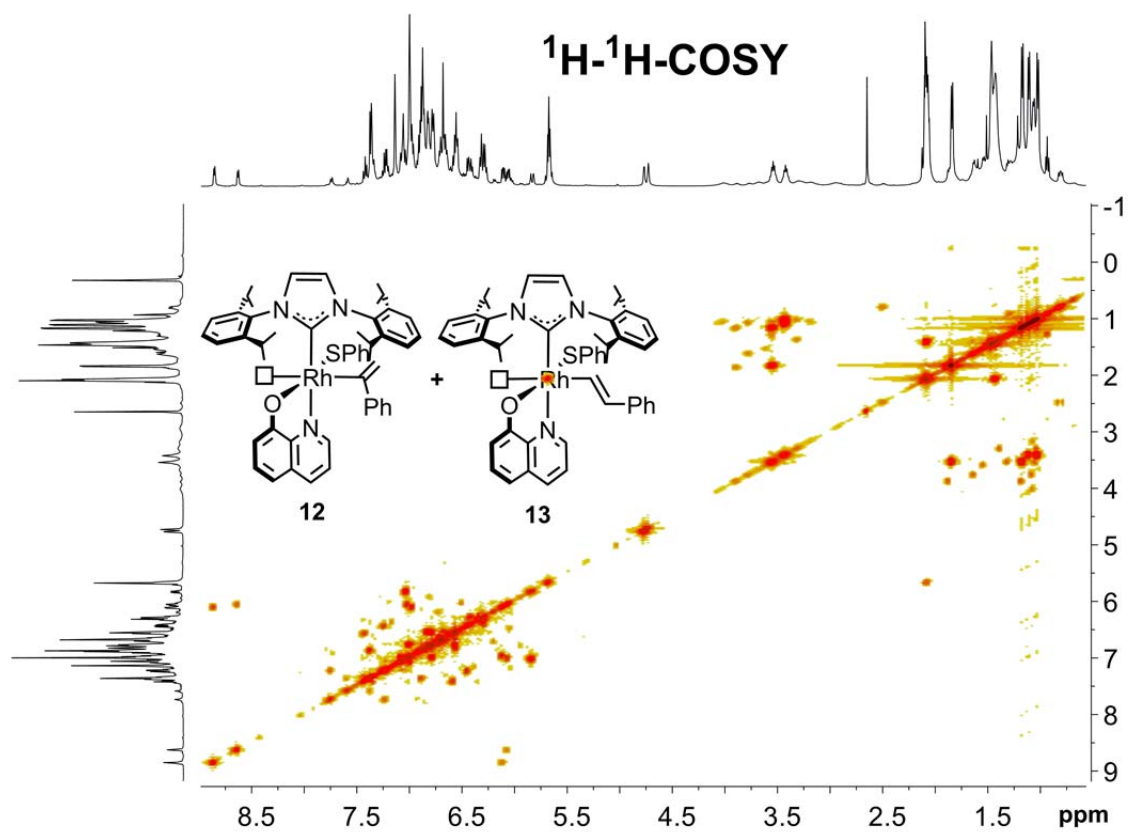
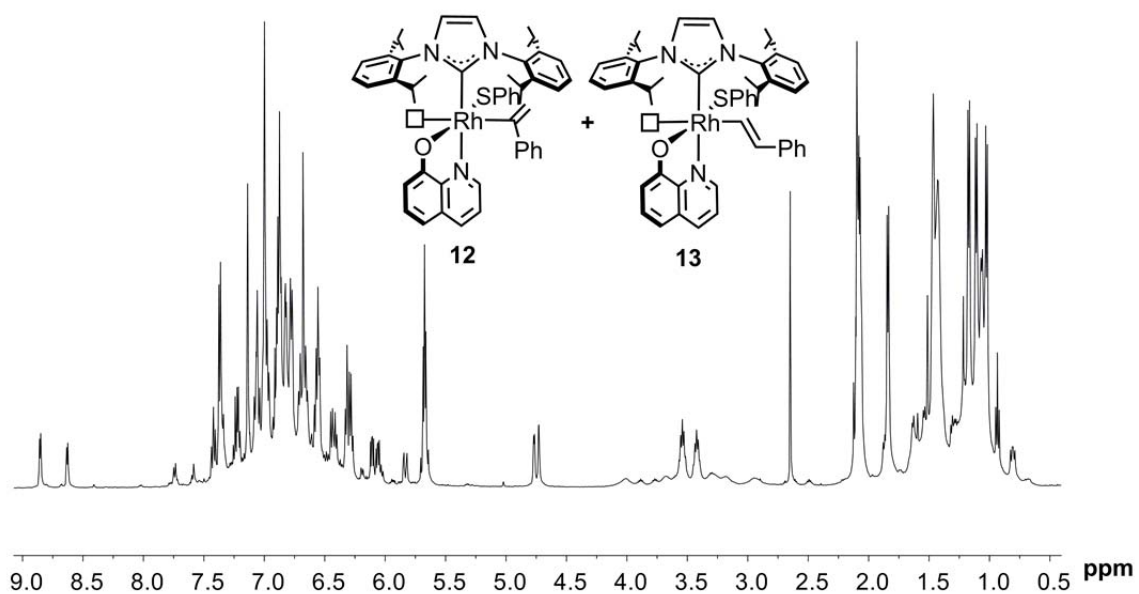


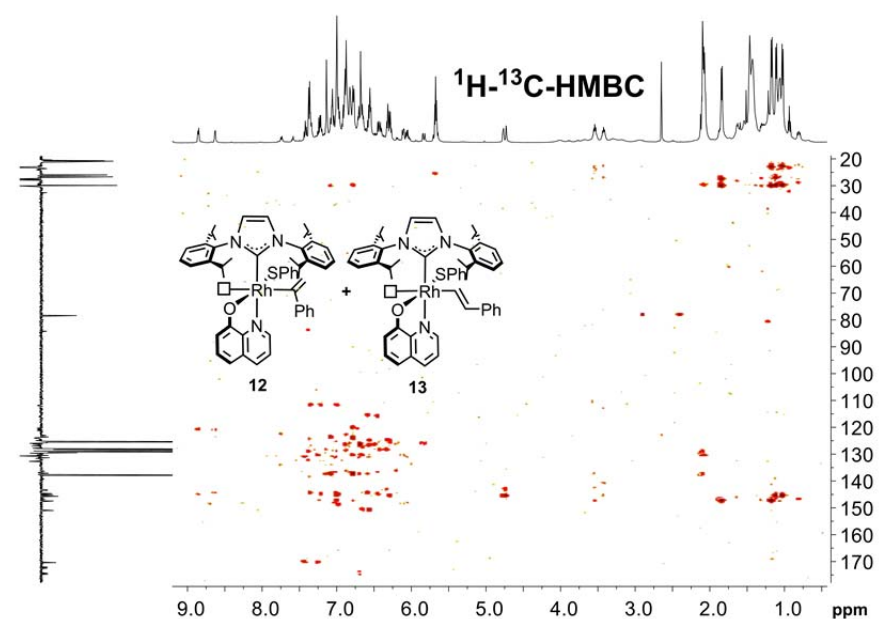
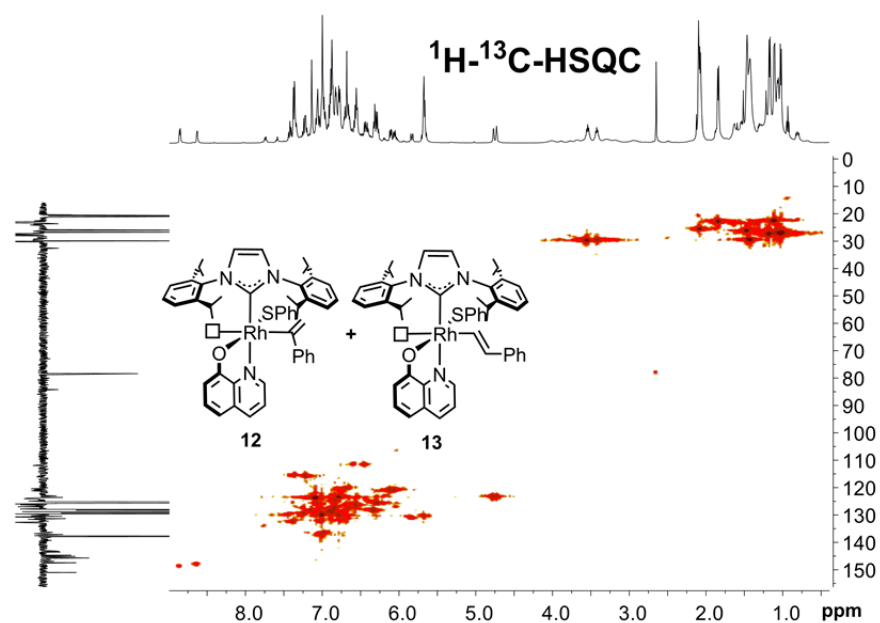
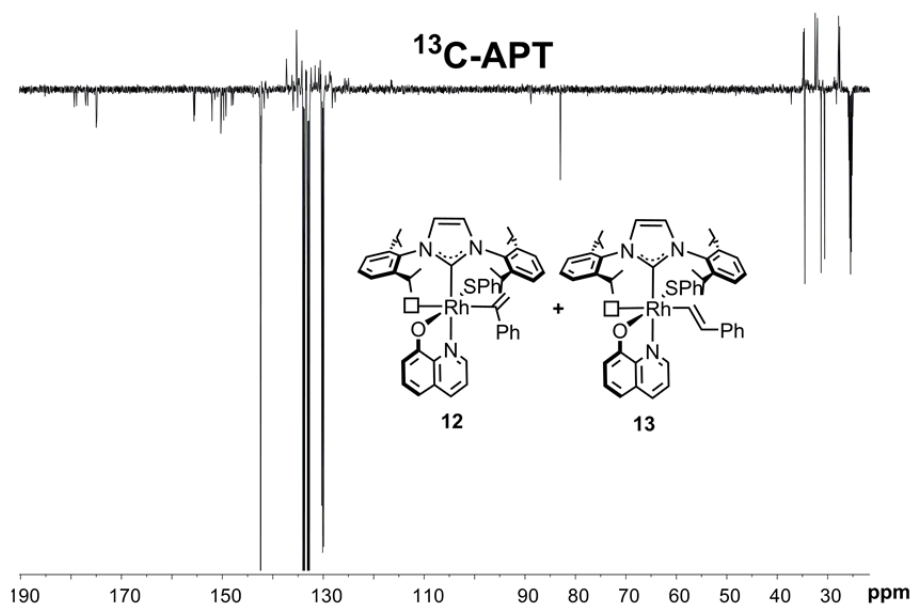


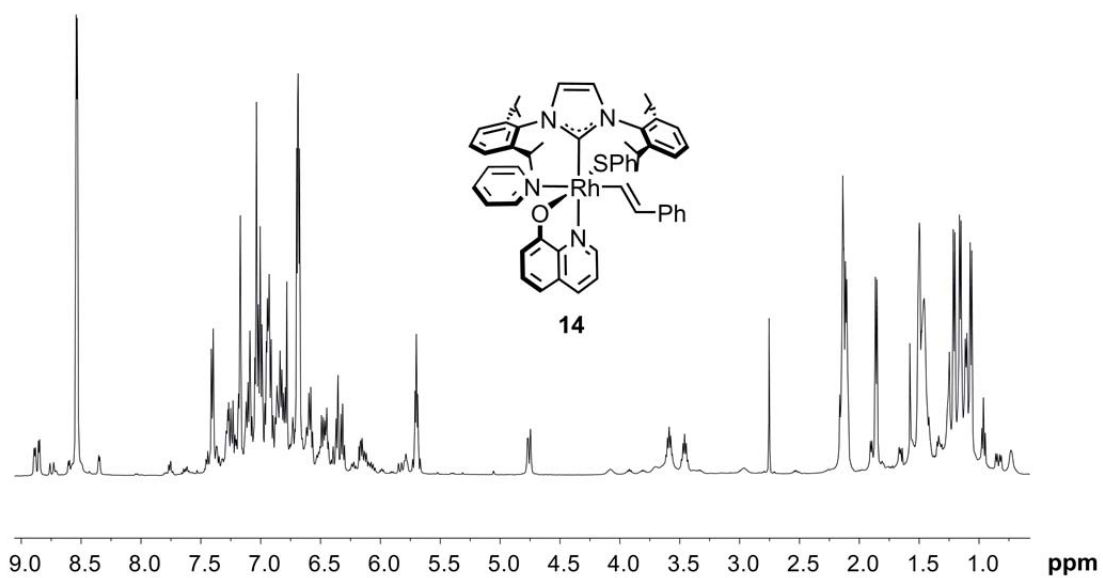












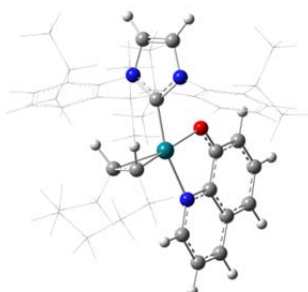
Computational details

Total energies and Cartesian coordinates (in Å) of calculated structures

Complex **5at**

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G= -2058,60744 a.u.



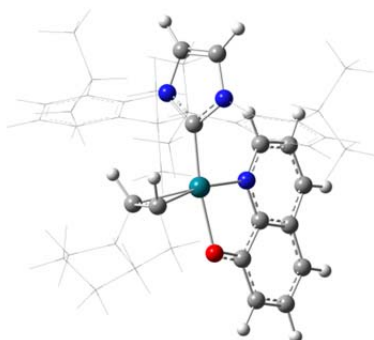
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N	-0.77749500	1.97321200	-1.08896500	H	0.83584400	-2.97326800	-4.81931700
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C	-1.56357800	-1.32441500	-2.11923800	H	1.70424900	-2.67888700	-1.09509500
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H	6.02465800	-2.11016500	2.41076000	N	2.44603300	-0.92712600	1.36076500
H	6.43784200	-0.15100200	-1.98935000	H	-0.92008700	-2.66583400	4.68460900
O	2.04718600	0.34007700	-0.98767400				

Complex **5bt**

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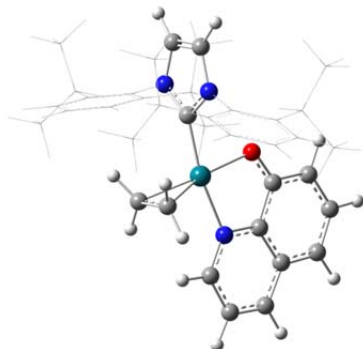
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N	-0.98066200	0.12011800	-2.02317700	H	5.94048700	-1.33682600	-1.69585700
N	-0.19415600	1.95496100	-1.17001800	H	6.53096000	-2.29709000	0.60197200
O	1.61427900	-1.21365600	2.13026000	H	5.77093200	-2.84529200	2.90902200
C	2.72136500	-0.22448200	-1.59663000	H	3.45324300	-2.34678200	3.65741300
C	3.99657400	-0.51234700	-2.12471700	H	-1.56578500	0.90771800	-3.96023600
C	4.94125900	-1.10850700	-1.31538800	H	-0.54398500	3.26181100	-2.86890700
C	4.61916100	-1.43927100	0.02742600	H	-1.26825900	-4.46280000	-2.60847800
C	5.51638600	-2.06034800	0.92805000	H	-3.71309200	-4.44233600	-2.19207000
C	5.07935200	-2.36423100	2.21129100	H	-4.87303500	-2.30147800	-1.72313000
C	3.77368900	-2.08567600	2.64707500	H	-3.09740100	0.99094100	-1.42073200
C	2.83397700	-1.47244400	1.79513800	H	-4.21752000	0.71286500	-3.62547300
C	3.29073700	-1.12967900	0.46658400	H	-5.55567300	-0.15930500	-2.84468200
C	-0.36756800	0.61253400	-0.88629300	H	-5.26617500	1.55462700	-2.45577500
C	-1.11985200	1.11410600	-2.99247900	H	-5.39575800	-0.66335000	-0.24152300
C	-0.62752400	2.26011300	-2.45960600	H	-5.06606800	1.05777300	0.03949800
C	-1.69683400	-1.13122100	-2.09696400	H	0.84462000	-1.37114300	-2.53784600
C	-1.02398200	-2.33404000	-2.37963600	H	0.23329300	-2.13065700	-4.83092200
C	-1.77449900	-3.51766300	-2.40283000	H	1.82235200	-2.76568800	-4.32433900
C	-3.14699600	-3.50813900	-2.17040400	H	0.39454400	-3.82711600	-4.32023700
C	-3.79720500	-2.30386500	-1.90885600	H	-2.91350200	-3.68067700	1.55112500
C	-3.08950600	-1.09690100	-1.85805000	H	2.29246600	-3.22500400	-1.83455300
C	-3.83603400	0.18915100	-1.53214600	H	-2.06185000	-4.24877000	2.98958600
C	-4.77084900	0.59654000	-2.68093200	H	1.00553200	-2.95733400	-0.63554800
C	-4.59539700	0.09178100	-0.20113100	H	0.90553000	-4.33784300	-1.76744800
C	0.46257600	-2.38661500	-2.66537300	H	2.76490400	4.86156300	0.87589000
C	0.74036500	-2.80038300	-4.11815100	H	1.01560800	5.69437800	2.42136200
C	1.20592700	-3.28261600	-1.66610800	H	-1.29354700	4.82112200	2.26411500
C	0.15394500	2.96136100	-0.19311200	H	-2.29443100	1.95884600	0.16568800
C	1.46464300	3.47189900	-0.13913000	H	-3.92043100	-0.17551500	0.62424700
C	1.75225800	4.45920200	0.81446700	H	-3.10949300	4.89249900	-0.20019700
C	0.77165300	4.93043600	1.67935900	H	-2.59431100	3.78879900	-1.49874100
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C	-0.86831600	3.45157100	0.65507900	H	-3.29057400	4.01297600	2.21105900
C	-2.31354800	2.99278200	0.53076200	H	-4.03199300	2.47137100	1.75057900
C	-3.07103200	3.83574000	-0.50994700	H	-2.50045400	2.47992300	2.65418500
C	-3.06921900	2.99109800	1.86511600	H	2.17640500	2.15094200	-1.63026200
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C	3.83682100	2.61280500	-0.36793900	H	3.62699100	1.85872000	0.40374500
C	2.83145200	4.11534000	-2.14903900	H	4.32453300	3.47261500	0.11770200
C	-1.23917900	-0.16622900	1.90983500	H	3.58919100	3.77073500	-2.87129900
C	-0.89748500	-0.00051900	3.37312000	H	3.20837000	5.03802400	-1.67892300
C	-2.06858100	-0.28910800	4.32953400	H	1.91982300	4.37663100	-2.70927500
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C	-2.30931700	-3.34035500	2.41145400	H	-0.03637800	-0.62948200	3.63641800
C	-0.99815900	-2.72249400	1.89323000	H	-2.95249800	0.29966400	4.01902300
C	-1.25942900	-1.39898200	1.22416400	H	-1.79068500	0.09227700	5.32793500

H	-3.17462400	-1.80859300	5.34976300	H	-3.61939000	-1.62596900	2.64091600
H	-0.27544900	-2.59852200	2.70905700	H	-4.03877000	-3.01293400	3.62975200
H	-0.53550700	-3.42124300	1.17724500	H	-1.60607100	-2.35808600	4.78294100
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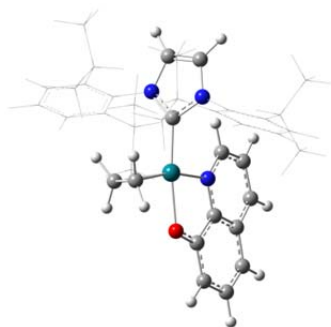


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C	-0.64605100	3.11000900	0.00000000	N	-1.03385900	-1.52024200	-1.07856100
C	1.08470400	4.91940300	0.00000000	N	-1.03385900	-1.52024200	1.07856100
C	3.40111200	4.20854300	0.00000000	C	-2.01585200	0.68640400	2.71147100
H	3.68062700	2.04611500	0.00000000	H	-1.95524200	0.68242000	1.61714000
C	-1.62467700	4.11476700	0.00000000	C	0.73754400	-3.57861900	2.05866000
C	0.05383600	5.89317800	0.00000000	H	0.61172300	-3.27622000	1.00950000
C	2.47133400	5.22693500	0.00000000	C	-2.01585200	0.68640400	-2.71147100
H	4.47236900	4.41792400	0.00000000	H	-1.95524200	0.68242000	-1.61714000
C	-1.26816500	5.47733400	0.00000000	C	0.73754400	-3.57861900	-2.05866000
H	-2.67324500	3.81060900	0.00000000	H	0.61172300	-3.27622000	-1.00950000
H	0.31512400	6.95317500	0.00000000	C	-3.45235200	0.31454200	-3.11367800
H	2.78667500	6.27366500	0.00000000	H	-4.16943300	1.04160300	-2.69967100
H	-2.06464400	6.22675500	0.00000000	H	-3.57088600	0.30514400	-4.21006900
N	1.67596500	2.54108500	0.00000000	H	-3.72957900	-0.68361100	-2.73926200
O	-0.91820300	1.83574300	0.00000000	C	-1.66108300	2.11139100	-3.14886600
Rh	0.78573000	0.62299300	0.00000000	H	-1.79717700	2.26384000	-4.23221700
C	2.48559000	-0.38429600	0.70595800	H	-2.30342600	2.83620100	-2.62788500
H	3.12974800	0.30307100	1.26649800	H	-0.61903100	2.35040300	-2.89166100
H	2.22254800	-1.28401200	1.26443500	C	-3.45235200	0.31454200	3.11367800
C	2.48559000	-0.38429600	-0.70595800	H	-3.57088600	0.30514400	4.21006900
H	2.22254800	-1.28401200	-1.26443500	H	-4.16943300	1.04160300	2.69967100
H	3.12974800	0.30307100	-1.26649800	H	-3.72957900	-0.68361100	2.73926200
C	-2.07324500	-2.35528200	-0.67867700	C	-1.66108300	2.11139100	3.14886600
C	-2.07324500	-2.35528200	0.67867700	H	-0.61903100	2.35040300	2.89166100
H	-2.71106200	-2.85978500	-1.39658500	H	-2.30342600	2.83620100	2.62788500
H	-2.71106200	-2.85978500	1.39658500	H	-1.79717700	2.26384000	4.23221700
C	-0.39828700	-0.96236000	0.00000000	C	-0.15601400	-4.80823100	-2.29595200
C	-0.58310400	-1.41159600	-2.44110700	H	-0.06243500	-5.16013500	-3.33612800
C	0.29202200	-2.40810200	-2.92646800	H	0.13550800	-5.63518400	-1.62818100
C	-1.03650300	-0.34671800	-3.24013000	H	-1.21585400	-4.58355900	-2.11204400
C	0.71359300	-2.31059800	-4.25796500	C	2.21363300	-3.95324800	-2.24585400
C	-0.58459200	-0.29563400	-4.56632900	H	2.50628700	-4.70923600	-1.50001700
C	0.28072100	-1.26369700	-5.07088500	H	2.40360300	-4.38747100	-3.24000400
H	1.39216300	-3.06238900	-4.66426200	H	2.87421900	-3.08291300	-2.12360900
H	-0.91602700	0.51920800	-5.21173900	C	-0.15601400	-4.80823100	2.29595200
H	0.62262600	-1.20239200	-6.10700800	H	0.13550800	-5.63518400	1.62818100
C	-0.58310400	-1.41159600	2.44110700	H	-0.06243500	-5.16013500	3.33612800
C	-1.03650300	-0.34671800	3.24013000	H	-1.21585400	-4.58355900	2.11204400
C	0.29202200	-2.40810200	2.92646800	C	2.21363300	-3.95324800	2.24585400
C	-0.58459200	-0.29563400	4.56632900	H	2.40360300	-4.38747100	3.24000400
C	0.71359300	-2.31059800	4.25796500	H	2.50628700	-4.70923600	1.50001700
C	0.28072100	-1.26369700	5.07088500	H	2.87421900	-3.08291300	2.12360900
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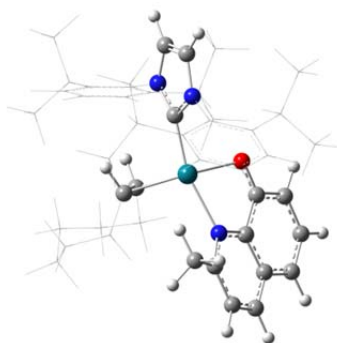


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N	0.86243800	1.36854000	1.03845000	H	-6.43325000	-1.34571400	-2.74321100
N	1.53033700	-0.69227500	1.14298600	O	-1.98929600	-0.48399900	-2.49706500
C	0.77899800	0.16407800	0.36394200	N	-2.16878100	-0.47402800	0.19068100
C	1.59540000	1.24014500	2.21733700	C	-0.12907900	-3.12343000	1.43384900
C	2.01259300	-0.04843200	2.28324300	H	-0.36713200	-2.08063800	1.65775300
C	0.45615000	2.64095900	0.49070300	C	-1.57707000	2.68053500	2.05726700
C	-0.71203000	3.27126800	0.95935600	H	-1.24036700	1.65110000	2.21824200
C	-1.05532300	4.51700500	0.41360000	C	2.61931700	2.63284600	-0.89438500
C	-0.26412100	5.11865500	-0.55778600	H	2.49891300	1.54416400	-0.83932400
C	0.90359200	4.49096600	-0.98984200	C	4.18060400	-0.73938700	-0.01473700
C	1.29465200	3.25128200	-0.47323100	H	3.55803800	0.12275300	0.24996800
C	2.04197600	-1.97111600	0.71600000	C	-1.37583700	3.43925800	3.37907700
C	1.27052500	-3.13935200	0.85429200	H	-1.96990400	2.97942800	4.18538700
C	1.83171100	-4.35085500	0.42799800	H	-1.69067500	4.49110300	3.28555400
C	3.11573500	-4.40320600	-0.10772400	H	-0.31918700	3.43622600	3.68955600
C	3.86371700	-3.23419900	-0.23355400	C	-0.20642700	-3.90451900	2.75348000
C	3.34323000	-1.99749300	0.16683900	H	0.00513000	-4.97575400	2.60420700
H	1.74993600	2.07825700	2.88930300	H	-1.21619000	-3.82167200	3.18695900
H	2.61370200	-0.57086600	3.02054700	H	0.51632000	-3.52066000	3.49106100
H	-1.96043500	5.01930000	0.75934600	C	-3.05926700	2.62856900	1.66400300
H	-0.55166500	6.08556200	-0.97742400	H	-3.48858100	3.63841200	1.56993900
H	1.52518200	4.97929100	-1.74049200	H	-3.64078500	2.09138400	2.42799100
H	1.24637900	-5.26806200	0.51853200	H	-3.19835300	2.10855500	0.70561100
H	3.53473500	-5.35824400	-0.43344600	C	-1.16613000	-3.61813100	0.41610400
H	4.86695300	-3.27944200	-0.66208900	H	-2.18437900	-3.49860400	0.81793100
C	0.88705100	0.02995900	-2.72138700	H	-1.02077100	-4.68423100	0.17828800
H	1.79625600	0.58227900	-2.48554600	H	-1.09898200	-3.03744900	-0.51513600
H	0.30422400	0.42715600	-3.55835600	C	3.74075700	3.02964700	0.08184700
C	0.77579300	-1.32698100	-2.36719700	H	4.69162500	2.55487100	-0.20854900
H	0.09647200	-1.98146600	-2.92233000	H	3.89024300	4.12137800	0.07789600
H	1.58458900	-1.84021500	-1.84274500	H	3.51397500	2.72189200	1.11209500
C	-3.30173800	-0.71219300	-0.54076200	C	5.38900000	-0.73011100	0.93326900
C	-2.22517200	-0.53630400	1.51339100	H	6.07347300	-1.56615400	0.71720000
C	-3.15541900	-0.69381500	-1.98015300	H	5.95741600	0.20774800	0.82701100
C	-4.56087600	-0.99651500	0.08141800	H	5.07409000	-0.81967900	1.98428200
C	-3.41285300	-0.83589700	2.21148700	C	3.02204200	2.97127600	-2.33402300
H	-1.30045800	-0.34642800	2.05659300	H	3.32682800	4.02465000	-2.43820500
C	-4.32296400	-0.92014200	-2.73516200	H	3.88097600	2.35381100	-2.63711500
C	-5.69728400	-1.21970800	-0.73142200	H	2.20080900	2.78117300	-3.03956700
C	-4.57413600	-1.05531500	1.50025200	C	4.61304700	-0.54711000	-1.47531600
H	-3.39518200	-0.88061400	3.30194300	H	5.14607000	0.40959700	-1.59213200
C	-5.55646500	-1.17219600	-2.11261200	H	5.29398900	-1.34623700	-1.80776900
H	-4.23843500	-0.90290700	-3.82334900	H	3.74529300	-0.54099600	-2.15024800
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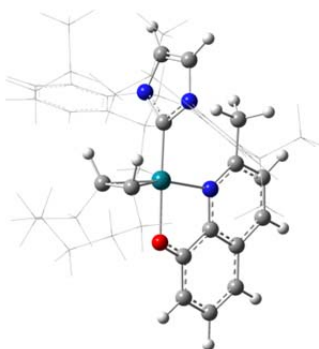


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N	0.64001600	2.26844200	0.94761600	H	-0.00479100	-3.24196200	2.56390100
C	0.85517000	0.92854100	0.74673600	H	0.88075500	-3.45293300	4.10376600
C	2.44143900	1.81550100	2.12309900	H	-3.66843100	3.82361100	0.43656800
C	1.59557300	2.82361700	1.78820700	H	-3.16303900	4.70797700	-1.81794500
C	2.69970500	-0.57949400	1.48852100	H	-0.89441400	4.46795500	-2.78123200
C	2.24782200	-1.62263500	2.32132800	H	1.79920500	2.45832900	-1.13801200
C	2.96093500	-2.82766200	2.28147600	H	3.69016600	-0.64143300	-2.11998000
C	4.07279300	-2.98250000	1.45322000	H	1.72104600	5.45464500	-1.80568900
C	4.49409400	-1.93463600	0.63776900	H	2.21147800	4.75624200	-0.24520000
C	3.81003200	-0.71195800	0.63109500	H	3.18888100	4.44658600	-1.70086500
C	4.25692400	0.41453300	-0.29047400	H	0.98914200	3.86449900	-3.73921900
C	5.47524600	1.15176100	0.28853800	H	2.35598100	2.76764900	-3.46985400
C	4.53939100	-0.07093400	-1.71871900	H	0.69207900	2.14491500	-3.37261300
C	1.03822400	-1.43971200	3.22332000	H	-1.30170600	1.71274000	2.38120600
C	1.44369800	-0.74984600	4.53708200	H	-3.49879600	1.47454700	3.28838700
C	0.28909100	-2.74478900	3.50039900	H	-3.63306500	1.30249100	1.53017500
C	-0.39252400	2.95974500	0.22437500	H	-4.15446200	2.81650400	2.32640000
C	-1.67576500	3.07683500	0.79487000	H	-1.88176300	3.26324300	4.25653000
C	-2.66189200	3.71833200	0.03049200	H	-2.34317000	4.52472500	3.08326400
C	-2.37775600	4.21454700	-1.23983200	H	-0.64947600	3.99373100	3.20113900
C	-1.09889700	4.08075800	-1.78203700	H	1.58857900	0.13046700	-1.88414300
C	-0.08006400	3.44496100	-1.06456300	H	0.02716200	0.22059900	-3.80728100
C	1.32232500	3.31158000	-1.63908200	H	-0.76722700	-1.26276100	-3.31058300
C	2.15883200	4.56376900	-1.32684400	H	2.19084000	-1.10332600	-4.10732500
C	1.33260000	3.00626200	-3.14008000	H	0.88223400	-1.38671900	-5.25052100
C	-1.97474900	2.55865300	2.19260600	H	1.84639100	-3.47376700	-4.82039600
C	-3.39939100	2.01313900	2.33433100	H	-0.82625800	-2.78272800	-1.87180000
C	-1.69355900	3.64802300	3.24139100	H	-0.52732100	-3.18645500	-0.18783400
C	0.69295800	-0.50142600	-1.89804500	H	1.49425500	-1.62111300	-0.22581100
C	0.20418800	-0.74612200	-3.31199100	H	2.63432500	-2.75485200	-2.30426400
C	1.18056300	-1.54332300	-4.19841400	H	2.57992200	-4.40992100	-2.88423200
C	1.27580700	-3.06121000	-3.97121400	C	-3.09368200	-1.46709400	0.06574500
C	1.94389700	-3.53606500	-2.66400800	C	-3.09889100	-0.51449600	-2.07337800
C	0.99336900	-3.93654000	-1.52768500	C	-2.56162300	-1.33352200	1.40500300
C	-0.03008300	-2.86389000	-1.11771200	C	-4.24402700	-2.26620100	-0.20327900
C	0.64084500	-1.53023600	-0.89931800	C	-4.24487600	-1.28157800	-2.41808400
H	3.31886200	1.79678800	2.76058200	C	-3.18756200	-2.09935800	2.40682600
H	1.58191700	3.87149100	2.06906400	C	-4.81040400	-3.04162800	0.83829800
H	2.63677700	-3.66287500	2.90228500	C	-4.77743000	-2.17625900	-1.51797500
H	4.60993300	-3.93390800	1.43744200	H	-4.69450400	-1.14208200	-3.40340000
H	5.35604100	-2.07326500	-0.01699800	C	-4.27203500	-2.94546400	2.11354600
H	3.43138000	1.13757400	-0.35402200	H	-2.81988000	-2.00290900	3.42968400
H	5.26484300	1.55935800	1.28829000	H	-5.67610500	-3.67419600	0.63217200
H	6.33701000	0.47080800	0.37949300	H	-5.64668800	-2.78385800	-1.78441000
H	5.77077100	1.98866100	-0.36456000	H	-4.71695200	-3.52597100	2.92691600
H	5.43402300	-0.71146400	-1.76553000	O	-1.59309500	-0.49935300	1.62686800
H	4.71799500	0.78943900	-2.38310400	N	-2.49622600	-0.70264800	-0.90268300
H	0.32184900	-0.79235600	2.70000000	H	0.26702500	-3.50565500	-4.05599600
H	1.91915000	0.22573300	4.35581500	C	-2.62956300	0.60404400	-2.95745400
H	0.55709200	-0.57734900	5.16787000	H	-2.55162500	0.30530900	-4.01293800
H	2.15426900	-1.37104600	5.10766900	H	-3.36229100	1.42689400	-2.89676600
H	1.60454800	-4.19793300	-0.64582600	H	-1.66869800	0.99367200	-2.60042300

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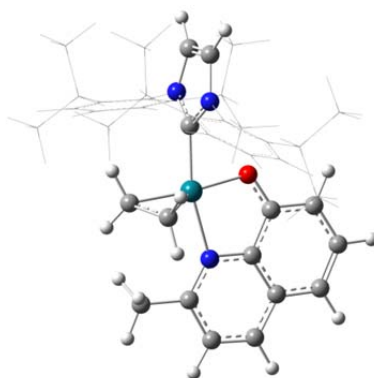


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N	1.10450700	0.89177800	1.78675000	H	-2.80425800	-4.14619700	0.12772800
C	0.56836200	-0.10783100	0.98941000	H	-0.06879500	5.24255000	0.67544800
C	1.54952900	-0.99777600	2.85348200	H	2.28381100	5.83735300	0.16306300
C	1.66072800	0.35082000	2.94666700	H	4.06456500	4.12812200	0.39670400
C	0.96656800	-2.59322800	1.03515200	H	3.45216200	0.57642400	1.36424300
C	-0.18030500	-3.40703900	0.97888200	H	3.50823800	-2.04104500	-1.70356700
C	-0.04970200	-4.70244000	0.45938400	H	5.32904900	2.87834800	2.11596800
C	1.17389600	-5.17723900	-0.00023700	H	4.30601100	1.97210000	3.24999300
C	2.29023500	-4.34476900	0.02675800	H	5.62256700	1.14212200	2.38133300
C	2.21164200	-3.03988000	0.52811300	H	5.12362900	2.36679900	-0.48165600
C	3.44963300	-2.15344100	0.48532900	H	5.42340400	0.65990400	-0.10069100
C	4.41780200	-2.46077800	1.63891400	H	3.96219000	1.12585400	-1.00696700
C	4.18548900	-2.23598000	-0.86048500	H	-1.17214900	1.83788100	1.66836400
C	-1.53812300	-2.93216500	1.45101500	H	-3.06846600	3.00486300	0.66846100
C	-1.95072000	-3.61890000	2.76029500	H	-1.75970400	2.83067500	-0.51970500
C	-2.60762900	-3.08803400	0.36198700	H	-2.05989800	4.40990900	0.26488800
C	1.38709900	2.24406900	1.34896500	H	-2.51554600	3.32289900	3.14773000
C	0.36390000	3.20434600	1.21498200	H	-1.39339700	4.66806100	2.83494600
C	0.71481100	4.49097700	0.78396400	H	-0.82209400	3.22645800	3.70622000
C	2.03338300	4.82761600	0.49663100	H	1.78014200	1.12488900	-1.04258400
C	3.03094500	3.86684700	0.63145100	H	0.43136600	2.77573400	-2.21335200
C	2.73374600	2.56258200	1.04651500	H	-0.35892700	1.55570900	-3.20761800
C	3.87724000	1.55983200	1.13836000	H	2.64758700	2.23140900	-3.33137800
C	4.83601700	1.90808100	2.28736700	H	1.42046800	2.96269100	-4.36264600
C	4.63571800	1.42397800	-0.19023900	H	2.48731400	1.31146900	-5.65725400
C	-1.08514900	2.91739600	1.55185400	H	-0.40573800	-0.59718500	-3.61681600
C	-2.04302100	3.32011100	0.42358300	H	-0.20459600	-2.18620700	-2.89602500
C	-1.47366700	3.57004200	2.88698600	H	1.51441800	-1.24988600	-1.30224500
C	0.97530100	0.78676900	-1.70141100	H	3.04992900	-0.19698500	-3.42471800
C	0.59791200	1.81951300	-2.73750600	H	3.21331100	-0.75979400	-5.07822600
C	1.67278900	2.03642600	-3.81722700	H	0.87284000	0.70371600	-5.32776800
C	1.84774600	0.91269600	-4.85186700	C	-4.43302200	0.07469900	2.21351700
C	2.47240900	-0.40507800	-4.34200400	C	-5.41821300	0.14207400	1.26242500
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C	0.32870200	-1.25008400	-3.13020200	C	-3.66561800	0.22202000	-0.41456900
C	0.82311300	-0.61221500	-1.85851100	C	-3.06146700	0.07820900	1.83761600
H	1.84933700	-1.78723700	3.53453500	H	-7.08958600	0.30794000	-0.88454700
H	2.08880300	0.97863700	3.72127200	H	-4.68135600	0.01750700	3.27530100
H	-0.93037000	-5.34565000	0.41392800	H	-6.47442300	0.13743100	1.54505000
H	1.25635200	-6.19201900	-0.39659600	C	-6.02827700	0.31050900	-1.14046800
H	3.24149500	-4.71054100	-0.36244200	C	-3.23572600	0.31840700	-1.79241900
H	3.10980500	-1.11642700	0.59891100	C	-4.23601400	0.40568700	-2.78187100
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H	4.80584100	-3.48895600	1.55739200	H	-3.90721900	0.47912700	-3.82020300
H	5.27745600	-1.77154300	1.61577800	H	-6.33559700	0.46794200	-3.26158100
H	4.64758300	-3.22300200	-1.01551900	O	-1.97869400	0.32833800	-2.08354600
H	4.99310600	-1.49012200	-0.89475700	N	-2.69120900	0.13968900	0.55754300
H	-1.44025200	-1.86536700	1.64871300	C	-2.07149900	0.01917700	2.97031600
H	-1.20881300	-3.44415400	3.55579700	H	-2.17651400	0.90876300	3.61003300
H	-2.92373100	-3.23444900	3.10680300	H	-2.27162900	-0.85677200	3.60534900
H	-2.05003300	-4.70875900	2.62933500	H	-1.04095600	-0.03250800	2.62805400
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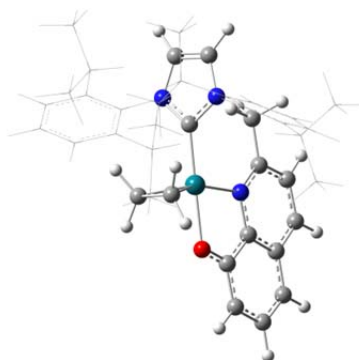


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C	2.91027300	-0.24127800	0.81203100	H	0.32984600	-1.60183500	1.94345500
C	4.82244300	-0.78102800	-0.68389300	C	-4.07361200	-1.46638400	-0.52203500
C	4.41061700	-0.71159800	-3.05911200	H	-3.64781900	-0.47233400	-0.32915900
C	3.78783400	-0.37788300	1.89828100	C	0.84285900	2.68673800	2.39293900
C	5.66608600	-0.92083500	0.44759200	H	0.68751900	1.60173500	2.35499300
C	5.27996400	-0.92364400	-2.01681300	C	-2.84573100	2.53440900	-1.15071400
H	4.75214500	-0.78032300	-4.09336700	H	-2.74115500	1.45711000	-0.96940000
C	5.13958400	-0.71943100	1.71153400	C	0.23684100	3.23216100	3.69726300
H	3.38516700	-0.21392700	2.89947700	H	0.72437600	2.77162500	4.57171300
H	6.71795000	-1.17449400	0.30195400	H	0.37097900	4.32422100	3.76978100
H	6.32712000	-1.17735100	-2.20209800	H	-0.84175100	3.02493300	3.76678300
H	5.78488800	-0.82113400	2.58851400	C	2.35889800	2.90872800	2.36360000
N	2.57021300	-0.31735300	-1.56987300	H	2.62754700	3.96730000	2.51335400
O	1.65669300	0.07518000	0.95857400	H	2.83856300	2.33323400	3.16952500
Rh	0.51698600	-0.10827100	-0.76625200	H	2.78929200	2.56822100	1.41223100
C	-0.35087600	-1.42595300	-2.13573900	C	0.05624000	-3.09797200	3.45627600
H	0.44483500	-1.93629600	-2.68890100	H	-0.03926400	-4.19116900	3.56566300
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C	-0.74907400	-0.11693600	-2.48540300	H	-0.84356900	-2.63811500	3.89542600
H	-1.76683700	0.20186300	-2.25699700	C	1.51760300	-3.26439000	1.38256800
H	-0.31633300	0.40319200	-3.34146300	H	1.61980000	-2.95493200	0.33185300
C	-2.28066600	1.16996700	2.03395800	H	2.39240900	-2.88212800	1.92768500
C	-2.55410400	-0.15739300	2.09153800	H	1.54635200	-4.36530300	1.42773000
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H	-3.21186700	-0.73094000	2.73612000	H	-4.29924900	4.07248000	-0.59754000
C	-1.02525300	0.14732600	0.42459900	H	-5.01252200	2.46123600	-0.87778600
C	-0.92542700	2.63554000	0.54141200	H	-4.11346300	2.79035000	0.62261600
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C	0.14020300	3.29020400	1.18788900	H	-3.72898200	2.08190900	-3.08308400
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C	0.50468800	4.55720700	0.71014100	H	-1.99348400	2.47379600	-3.16392300
C	-0.16520700	5.14498800	-0.35988000	C	-5.40002800	-1.55287500	0.24845500
H	-1.75314500	4.95754800	-1.80147900	H	-6.09881700	-0.77120600	-0.09059500
H	1.32987800	5.08944200	1.18533300	H	-5.88419900	-2.53066500	0.09327600
H	0.13994400	6.13115700	-0.71848400	H	-5.24586900	-1.42474200	1.33053100
C	-1.94724800	-2.14882600	0.74463000	C	-4.30373500	-1.56555500	-2.03693900
C	-0.99363700	-3.08920100	1.17259600	H	-4.81079000	-2.50369100	-2.31286300
C	-3.07648700	-2.50382400	-0.02259700	H	-4.94119000	-0.73425600	-2.37881700
C	-1.21499200	-4.43088900	0.83091800	H	-3.35364100	-1.51712200	-2.58785500
C	-3.25452100	-3.85781900	-0.33194600	C	2.15824400	-0.09193900	-3.98707800
C	-2.33372700	-4.81434600	0.09373500	H	1.39087600	-0.86397100	-4.13594200
H	-0.49439400	-5.18689200	1.14782600	H	1.63992100	0.86446600	-3.83464300
H	-4.11892300	-4.16549500	-0.92375800	H	2.75268500	-0.02508200	-4.90813900
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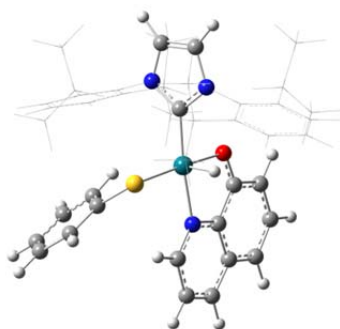


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N	1.28126700	1.17843100	1.00191900	C	0.65811700	-0.79167400	-2.46401200
N	1.45712700	-0.99292800	1.03251600	C	0.61660000	0.61668300	-2.51992800
N	-2.46671000	-0.16014800	0.40108700	H	5.12083000	3.34492300	0.45355600
O	-2.13767100	-0.15200100	-2.32621100	H	5.56767100	1.62567800	0.31075900
C	0.82722700	0.04153300	0.35932900	H	4.40009300	2.14257300	1.54810800
C	2.17551400	-0.50580800	2.12543300	H	-0.47745400	3.22394400	3.35952600
C	2.06637800	0.84576300	2.10617000	H	-2.24643200	3.06090300	3.18485800
C	1.24237700	2.52435200	0.46796600	H	-1.43218700	4.55370200	2.66283300
C	0.11593300	3.34829700	0.65065500	H	-2.60398900	4.15550900	0.29499100
C	0.18297200	4.67347600	0.19908000	H	-3.27296200	2.61463300	0.87554700
C	1.32461700	5.16802100	-0.42233000	H	-2.23933500	2.63643200	-0.57077100
C	2.41563300	4.32747200	-0.63024900	H	5.00736300	-2.34639900	-1.91131000
C	2.39643400	2.99333000	-0.20570400	H	5.38934400	-0.66008300	-1.50738500
C	3.59670000	2.10227400	-0.49777700	H	3.78029000	-1.07954500	-2.14647100
C	4.73284600	2.31534800	0.51561700	H	4.89640000	-2.12515500	1.92847600
C	4.12611400	2.27892200	-1.92878200	H	6.03048200	-1.23980200	0.87667700
H	3.32709700	2.15882000	-2.67447400	H	5.70579600	-2.96625000	0.58943300
H	4.90202800	1.52800900	-2.13865900	H	-1.68298700	-2.82713100	-0.92810100
H	4.58372600	3.26913400	-2.07721400	H	-2.83678300	-3.04353400	0.40531100
C	-1.15419900	2.85232700	1.30893000	H	-1.90055400	-4.43661900	-0.17797200
C	-1.33499700	3.45678200	2.70823900	H	2.70258900	-1.16947500	2.80320300
C	-2.38576100	3.08346300	0.42343100	H	2.46577700	1.60395500	2.77147200
C	1.66523700	-2.32859900	0.51301500	H	-0.68198300	5.32466100	0.33782700
C	0.63285300	-3.28819100	0.50725300	H	1.36015000	6.20598200	-0.76155100
C	0.92068200	-4.56659300	0.01035600	H	3.29781800	4.71159400	-1.14438300
C	2.18627000	-4.89434500	-0.46507700	H	3.25727800	1.06239000	-0.40894000
C	3.19138600	-3.93179300	-0.46068800	H	-1.04293500	1.77427600	1.42132400
C	2.95434000	-2.63560800	0.01432300	H	0.12998300	-5.31876300	0.00013800
C	4.09249300	-1.62499900	-0.04911100	H	2.38827300	-5.89844800	-0.84532200
C	4.59210200	-1.41933800	-1.48656800	H	4.18105800	-4.18501200	-0.84609400
C	5.24458800	-2.01199200	0.89021700	H	3.71228700	-0.65831300	0.29658100
C	-0.75776100	-3.00505400	1.03772600	H	-4.04993800	-0.24213300	3.37542500
C	-1.85306900	-3.35445500	0.02211400	H	-6.06989600	-0.27337400	1.91197200
C	-0.98590500	-3.70854700	2.38368100	H	-7.02500700	-0.28197500	-0.40939300
H	-0.92870000	-4.80421100	2.27881200	H	-6.61909500	-0.26325700	-2.87509300
H	-1.98369000	-3.46312400	2.78207600	H	-4.29577700	-0.20338900	-3.77429000
H	-0.23273500	-3.40519500	3.12828300	H	-0.53750100	-0.10972200	2.22014500
C	-2.65077600	-0.18499700	1.72205200	H	-1.52808500	-1.09423900	3.31165400
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C	-5.06461600	-0.24395400	1.48300000	H	-0.81659400	-1.93005100	1.20450600
C	-4.91114900	-0.22795300	0.07447200	H	1.53667200	-1.31560200	-2.07903100
C	-6.01138300	-0.25312300	-0.81384900	H	1.46317600	1.21525400	-2.17921000
C	-5.77454300	-0.24298600	-2.18046100	H	0.02753000	-1.38135500	-3.13665000
C	-4.47268600	-0.20881300	-2.69715100	H	-0.04471100	1.11444000	-3.23566300
C	-3.34069300	-0.18061700	-1.85756700				
C	-3.56920400	-0.18772600	-0.42835100				

Complex 9t

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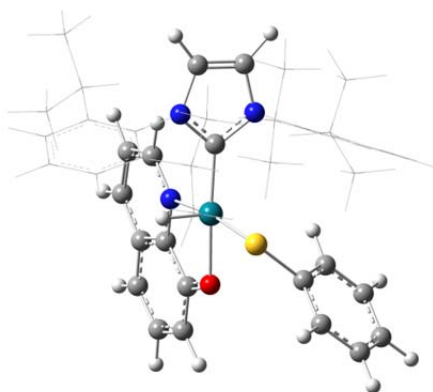


Rh	0.07670900	0.52063800	-0.43166700	H	5.83445700	-0.53718500	1.97958800
N	0.06893200	-1.84434600	1.41840700	H	4.70726100	-0.16328800	3.30956200
N	1.95305100	-1.69201700	0.38265600	H	4.47612200	-1.63032900	2.32947800
C	0.72405900	-1.11195700	0.47279800	C	4.26508600	1.72143500	1.35095700
C	2.06814700	-2.76207000	1.26468300	H	5.33104700	1.88942200	1.12698800
H	2.97736700	-3.34917500	1.33559500	H	3.65775200	2.29196900	0.63581000
C	0.88382300	-2.85353400	1.92266000	H	4.07375200	2.13216100	2.35432400
H	0.54421600	-3.52951900	2.69937600	C	1.90864700	-2.79724200	-2.27881100
C	-1.28721000	-1.60324300	1.83382100	H	1.02942600	-2.64088200	-1.63825600
C	-2.31175400	-2.41002400	1.29686800	C	2.37220100	-4.25089100	-2.08832300
C	-3.62004900	-2.15839800	1.72734200	H	3.25837600	-4.46444000	-2.70822500
H	-4.44030500	-2.75146900	1.32209200	H	1.57472900	-4.95321300	-2.37963700
C	-3.89349600	-1.14517300	2.64324500	H	2.63836700	-4.45719400	-1.04048900
H	-4.92403200	-0.95921200	2.95464000	C	1.44682700	-2.54468500	-3.71831300
C	-2.86249100	-0.35697700	3.15067300	H	1.14554100	-1.49658900	-3.85844400
H	-3.09168000	0.43658900	3.86270300	H	0.57230300	-3.17325000	-3.94484300
C	-1.53291300	-0.56826000	2.75994800	H	2.23093000	-2.78829000	-4.45330000
C	-0.40126300	0.25385500	3.35948600	C	0.03536600	3.42924200	-0.44824900
H	0.41820100	0.28733500	2.63207500	C	-1.16715100	2.69122600	-2.30655400
C	-0.78916500	1.71273700	3.61809700	C	0.82297700	3.03990100	0.69399300
H	-1.21917500	2.17747900	2.71907300	C	-0.20799500	4.80141600	-0.75756100
H	0.10438700	2.29347800	3.88968900	C	-1.45393400	4.02019200	-2.68757300
H	-1.51374900	1.81321700	4.44247000	H	-1.51760600	1.83587700	-2.88717400
C	0.12608400	-0.41820800	4.63833600	C	1.33262500	4.06923000	1.49753700
H	0.97069300	0.15398600	5.05471000	C	0.32995900	5.80247100	0.09096400
H	0.47756300	-1.44250400	4.44109200	C	-0.98313500	5.06413200	-1.91834800
H	-0.66117300	-0.47497400	5.40801000	H	-2.04745100	4.19937200	-3.58554300
C	-2.02174200	-3.53326900	0.31169600	C	1.08066200	5.42162400	1.19149500
H	-1.07304500	-3.29038000	-0.18767900	H	1.93217000	3.79695800	2.36760300
C	-3.08530200	-3.65933900	-0.78567400	H	0.14766100	6.85487400	-0.13483300
H	-3.27477000	-2.69494500	-1.27244100	H	-1.19548200	6.10078900	-2.19330900
H	-2.74281100	-4.36906300	-1.55472200	H	1.49772100	6.19114500	1.84695500
H	-4.03848900	-4.04454600	-0.38888800	O	1.02328500	1.77077200	0.93225300
C	-1.85872600	-4.87465300	1.04834800	N	-0.46099400	2.41550200	-1.22178900
H	-2.79342500	-5.14975600	1.56361900	C	-2.79590500	-0.14433200	-1.68018700
H	-1.06083100	-4.84113000	1.80377000	C	-3.76530700	-0.26478700	-2.69665600
H	-1.61477800	-5.67892800	0.33584600	C	-3.18138800	0.45276000	-0.46460600
C	2.99001500	-1.28305900	-0.52473400	C	-5.06579800	0.20081900	-2.50216100
C	2.98688700	-1.82430400	-1.82522200	H	-3.48075800	-0.72301600	-3.64695000
C	4.02397300	-1.43885700	-2.68399600	C	-4.47766800	0.93453000	-0.28209600
H	4.05684700	-1.83672300	-3.69927200	H	-2.46955500	0.52194800	0.36054000
C	5.00757500	-0.54507200	-2.26211500	C	-5.43101100	0.81137000	-1.29673400
H	5.80777700	-0.25545700	-2.94762800	H	-5.80011700	0.09463000	-3.30534800
C	4.96680600	-0.00452000	-0.97757700	H	-4.74500100	1.39335100	0.67305000
H	5.73084300	0.71090600	-0.67032100	H	-6.44802100	1.18198000	-1.14966600
C	3.95051800	-0.35552500	-0.07944000	S	-1.15743900	-0.75495400	-1.96819400
C	3.89592300	0.23494900	1.32115600	H	1.24628400	0.41316200	-1.36941600
H	2.85452100	0.17031600	1.66265200				
C	4.77688800	-0.57268900	2.28887100				

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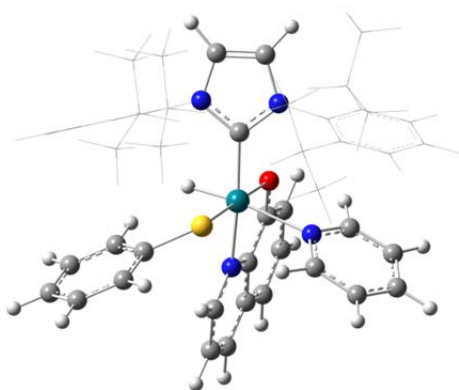


Rh	0.08033000	0.49161900	-0.70361900	H	-1.58966700	-4.25253000	-3.45913600
N	-1.92773000	-1.38546400	0.64762000	H	0.07727300	-4.07765500	-2.86763300
N	-0.06821200	-1.20060200	1.73847700	H	-0.75597700	-2.66776000	-3.54037800
C	-0.68734700	-0.80034300	0.58185600	C	-1.64277600	-4.50885200	-0.71121700
C	-0.91883100	-1.97137200	2.52479400	H	-1.91757100	-4.28751600	0.33015300
H	-0.61044300	-2.35673700	3.49047300	H	-0.73497800	-5.13282200	-0.69155900
C	-2.08163400	-2.09469100	1.83881300	H	-2.45625600	-5.10296500	-1.15867600
H	-3.00037100	-2.62146800	2.07298300	C	-4.44518700	0.12305300	0.87107200
C	1.33654800	-1.03506600	2.02668500	H	-3.54242700	0.21991200	1.48883800
C	2.21042900	-2.09537300	1.69306200	C	-4.90262000	1.53424600	0.47864300
C	3.56619900	-1.93379400	1.99829300	H	-4.17255000	2.02513400	-0.17988600
H	4.26953300	-2.72485500	1.73713600	H	-5.03110600	2.16099700	1.37495900
C	4.03677800	-0.77518700	2.61378400	H	-5.87093400	1.51167900	-0.04512100
H	5.10173000	-0.67002900	2.83257500	C	-5.50888100	-0.57925900	1.73173800
C	3.15560100	0.25249200	2.93414700	H	-5.73753600	0.01503300	2.63105600
H	3.53192500	1.15921300	3.41086600	H	-5.17437700	-1.57599100	2.05782100
C	1.78743400	0.14573400	2.64521700	H	-6.44542800	-0.71394200	1.16749600
C	0.84536500	1.27508800	3.01991900	H	-1.10502600	0.19787700	-1.58510500
H	-0.11379400	1.07479700	2.53071400	S	1.29852300	-1.17691000	-1.78511100
C	0.58672000	1.29713700	4.53417600	C	2.92958100	-0.48410600	-1.80152300
H	0.17361100	0.33757100	4.88310400	C	3.77859600	-0.74996800	-2.89136400
H	-0.12980800	2.09339400	4.79321000	C	3.43270300	0.27867800	-0.73188700
H	1.51729200	1.48395700	5.09408900	C	5.08814100	-0.26729500	-2.90668300
C	1.34367800	2.63460400	2.51167800	H	3.39438700	-1.33100800	-3.73268100
H	2.24894600	2.96162400	3.04670900	C	4.73386100	0.77790100	-0.76133700
H	0.57317900	3.40606500	2.65998200	H	2.80446300	0.47080200	0.13789100
H	1.58112500	2.59825300	1.43872400	C	5.57315200	0.50508100	-1.84603600
C	1.71755300	-3.39166400	1.06553000	H	5.73198000	-0.48555000	-3.76310900
H	0.76648600	-3.17225600	0.56382600	H	5.09736900	1.37302200	0.08061300
C	2.66920800	-3.94360200	-0.00276400	H	6.59584600	0.88932300	-1.86473000
H	2.91935300	-3.17373800	-0.74340500	C	-0.38305500	3.36281800	-0.58192100
H	2.18600200	-4.78085300	-0.53080200	C	-1.70737800	2.36180500	1.04995200
H	3.60031800	-4.33279900	0.43945900	C	-0.82462200	4.67515700	-0.21836300
C	1.45893900	-4.45709800	2.14558900	C	0.58465200	3.14857900	-1.62991400
H	2.39417100	-4.71500200	2.66848300	C	-2.19127900	3.61466700	1.48075100
H	1.06021200	-5.37712700	1.68895200	H	-2.03477600	1.44160900	1.53021000
H	0.73713200	-4.11776900	2.90190300	C	-0.30769400	5.78886400	-0.92082100
C	-2.88904500	-1.45900400	-0.42582300	C	-1.75663500	4.76172800	0.84968700
C	-4.08646400	-0.72458700	-0.33850600	C	1.06516500	4.29307900	-2.29245600
C	-5.00131800	-0.83405800	-1.39585000	H	-2.90506300	3.65448300	2.30509700
H	-5.93529600	-0.27079700	-1.35658400	C	0.61773900	5.57616800	-1.93555100
C	-4.73585200	-1.64815300	-2.49173300	H	-0.63698700	6.79497600	-0.65460500
H	-5.45521900	-1.71262900	-3.31150100	H	-2.11862500	5.74412600	1.16414600
C	-3.55823600	-2.39313100	-2.53967000	H	1.79916100	4.15360900	-3.08782800
H	-3.37024400	-3.04233200	-3.39460900	H	1.01929200	6.43722900	-2.47728800
C	-2.61585900	-2.32996000	-1.50692600	N	-0.83696000	2.24116500	0.05843400
C	-1.38828800	-3.22795100	-1.52589700	O	0.96858700	1.94072100	-1.89425700
H	-0.56828600	-2.68621400	-1.03920100				
C	-0.89798400	-3.57337900	-2.93425900				

Complex 10t

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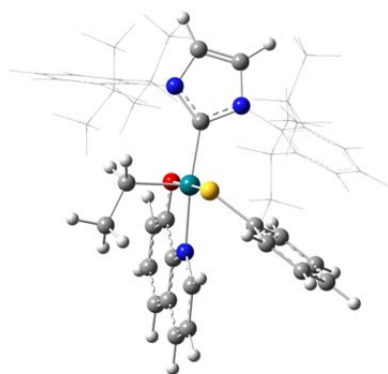


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O	1.24725200	1.21912800	1.37525600	C	-2.43850600	-0.47373200	2.56754000
N	-0.07706800	2.57754200	-0.55695200	C	-3.75850900	-0.05187700	2.77105200
N	-0.87293000	-1.92063400	1.36748200	H	-3.96877000	0.70150000	3.53212800
N	1.16522700	-2.17788600	0.72198100	C	-4.80276400	-0.57284000	2.00868000
C	-0.70734000	3.20384800	-1.53530300	H	-5.82429400	-0.22170500	2.17246400
H	-1.22384100	2.57553300	-2.26289100	C	-4.54920500	-1.52667400	1.02534100
C	-0.71714100	4.61450700	-1.62797100	H	-5.37386900	-1.90857800	0.42290600
H	-1.25641900	5.08931100	-2.44929200	C	-3.24861900	-1.98734000	0.78360800
C	-0.05546300	5.36088100	-0.67685700	C	-2.98120000	-3.06047600	-0.26328900
H	-0.05535700	6.45319900	-0.72368600	H	-1.93753300	-2.94346400	-0.58768000
C	0.63853700	4.71444800	0.38240000	C	-3.85700200	-2.91639100	-1.51277500
C	1.35009900	5.39431200	1.40244000	H	-4.90986700	-3.16774100	-1.30536900
H	1.38151800	6.48559200	1.40160600	H	-3.50607900	-3.60855400	-2.29434100
C	1.99097800	4.65605000	2.38520600	H	-3.81676900	-1.89735000	-1.91526000
H	2.53664200	5.17841300	3.17605300	C	-3.14979100	-4.46722100	0.33793300
C	1.96529000	3.24831400	2.40337100	H	-2.48470600	-4.63631700	1.19630600
H	2.47614600	2.69209800	3.19103700	H	-2.92528500	-5.23792600	-0.41715100
C	1.28081900	2.52262300	1.41530300	H	-4.18579200	-4.62025600	0.68182000
C	0.60117500	3.28680700	0.39611200	C	-1.30049000	0.08862800	3.40742900
C	0.09925500	-1.33064400	0.60223500	H	-0.35906500	-0.11670100	2.88313600
C	0.87457200	-3.24748600	1.56580700	C	-1.37733200	1.61234900	3.55809700
H	1.60203700	-4.02396200	1.77374800	H	-1.45419400	2.09937100	2.57538200
C	-0.40565200	-3.07922000	1.97533600	H	-0.46479200	1.99110900	4.04215300
H	-1.03032000	-3.66577100	2.63950100	H	-2.23726600	1.92747500	4.17103900
C	2.43266000	-2.06375200	0.05711000	C	-1.24148800	-0.61161800	4.77431700
C	2.51378900	-2.42414900	-1.30620200	H	-0.39467200	-0.23141100	5.36834000
C	3.77750600	-2.37493400	-1.90508900	H	-1.11591500	-1.70012800	4.66249300
H	3.88478200	-2.63284500	-2.95833400	H	-2.16577500	-0.43901200	5.34995300
C	4.90714900	-1.99953300	-1.17591900	H	-1.19157500	0.62569000	0.70829600
H	5.88361300	-1.97433800	-1.66569400	S	-1.34953900	-0.23679100	-1.93825300
C	4.79436900	-1.64449100	0.16479600	C	-2.91824300	0.58761300	-1.89632300
H	5.68323100	-1.33859300	0.71950300	C	-3.70945400	0.53395200	-3.06439100
C	3.54885400	-1.65572000	0.80962400	C	-3.44290900	1.25390200	-0.77392000
C	3.43250700	-1.25446500	2.27437200	C	-4.97691200	1.11448800	-3.10028100
H	2.36947500	-1.07554700	2.48506100	H	-3.31475100	0.02522100	-3.94739100
C	3.93109300	-2.38360900	3.19202800	C	-4.71000400	1.83699600	-0.81887400
H	3.38705400	-3.32395400	3.02060000	H	-2.85416400	1.30073200	0.14038100
H	3.80280800	-2.10767300	4.25090300	C	-5.48953500	1.77289600	-1.97682200
H	5.00154200	-2.58413100	3.02166600	H	-5.56860300	1.05468800	-4.01800900
C	4.16700900	0.05471600	2.59011700	H	-5.09237300	2.34074700	0.07299000
H	5.25651800	-0.03778800	2.45449300	H	-6.48143300	2.22989200	-2.00600700
H	3.99088700	0.33664500	3.64002100	N	1.85758500	0.66556800	-1.58530800
H	3.79865600	0.87793100	1.96502100	C	3.04558600	0.99337400	-1.06223900
C	1.27493200	-2.84934800	-2.08636300	C	1.70523600	0.70880600	-2.91637900
H	0.46212600	-2.16715200	-1.79848000	C	4.13967800	1.35129600	-1.84800400
C	1.43252100	-2.73562300	-3.60513800	H	3.10218200	0.96736700	0.02440300
H	1.81344500	-1.75059600	-3.90652900	C	2.74589000	1.05618200	-3.77734700
H	0.45307100	-2.87827300	-4.08561400	H	0.70500800	0.46149000	-3.28510000
H	2.11439100	-3.50369500	-4.00588300	C	3.99077500	1.37947700	-3.23459600
C	0.82856900	-4.27692400	-1.72190800	H	5.08843400	1.60044800	-1.37032700
H	1.60958700	-5.00861300	-1.98648200	H	2.57348800	1.07276100	-4.85517900
H	-0.08582800	-4.53785000	-2.27789700	H	4.82756700	1.65486200	-3.88120400
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Complex **11t**

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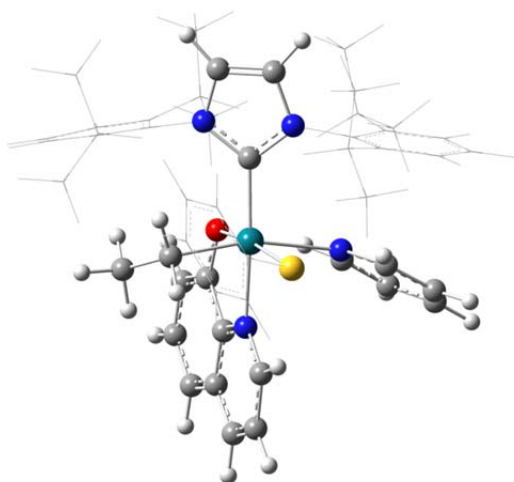


Rh	0.06857500	0.52784900	-0.46738300	H	-0.04257700	-5.69045500	1.02961200
O	-0.74056900	2.03226300	0.72309700	H	-0.17424800	-4.53848800	2.37651100
N	1.22699000	2.18502500	-1.11910400	C	-3.33399300	-0.80152500	-0.21175500
N	-2.28626200	-1.10774300	0.72186600	C	-4.17719300	0.29069700	0.05020300
N	-0.37671200	-1.46254200	1.64842200	C	-5.23472900	0.51436600	-0.84298300
C	2.18459900	2.22527500	-2.03071900	H	-5.91303400	1.35228200	-0.67286900
H	2.40826200	1.29122200	-2.54665600	C	-5.42079500	-0.30843100	-1.95164100
C	2.87449500	3.41905600	-2.33409600	H	-6.24922700	-0.11643100	-2.63787800
H	3.66140600	3.39986400	-3.08965300	C	-4.54431000	-1.36540600	-2.20333500
C	2.53932700	4.58267700	-1.67420900	H	-4.68780300	-1.98230300	-3.09118600
H	3.05742300	5.51976300	-1.89496600	C	-3.47579900	-1.63430300	-1.34058400
C	1.50779800	4.57643100	-0.69747600	C	-2.49028500	-2.76325300	-1.61872300
C	1.08675800	5.72090400	0.02609600	H	-1.52193100	-2.46621500	-1.19143800
H	1.57210700	6.68159100	-0.15612200	C	-2.24050000	-2.99430800	-3.11259700
C	0.06216200	5.59512700	0.95047600	H	-3.12069400	-3.41941300	-3.62141900
H	-0.26651300	6.47623700	1.50845800	H	-1.40778800	-3.70178000	-3.24234700
C	-0.57652000	4.36438100	1.19897000	H	-1.96181900	-2.05973700	-3.62164500
H	-1.37889100	4.29068700	1.93484300	C	-2.92253700	-4.06659900	-0.92641200
C	-0.19583000	3.20041000	0.51575400	H	-3.03263500	-3.93443200	0.15962200
C	0.86724500	3.32452400	-0.44999600	H	-2.17304500	-4.85685300	-1.09357300
C	-0.96019000	-0.81929600	0.59076900	H	-3.88746200	-4.42009600	-1.32522400
C	-1.32505500	-2.09893000	2.44101100	C	-3.95188600	1.20426900	1.24566900
H	-1.04738600	-2.63926900	3.33916300	H	-2.93015900	1.02956700	1.60799200
C	-2.52726200	-1.88319200	1.85400400	C	-4.02181100	2.68785400	0.86443600
H	-3.52879500	-2.20575500	2.11725900	H	-3.30933400	2.92207800	0.06148100
C	1.03719500	-1.56337300	1.90261400	H	-3.75695600	3.30967900	1.73339600
C	1.71355900	-2.71503800	1.44359500	H	-5.03172100	2.98707100	0.54082300
C	3.06779900	-2.83709400	1.77179300	C	-4.93506400	0.87488600	2.38030400
H	3.62864200	-3.70307200	1.41919500	H	-4.74480300	1.51517500	3.25657500
C	3.71643600	-1.86117100	2.52676400	H	-4.84669400	-0.17373300	2.70332800
H	4.77620000	-1.97657900	2.76505700	H	-5.97751100	1.03824200	2.06088000
C	3.02719900	-0.73111200	2.95762600	S	1.00225000	-1.12968800	-1.85544700
H	3.54890500	0.03058300	3.53891700	C	2.75687600	-1.06148300	-1.63938400
C	1.66965400	-0.55352100	2.65283800	C	3.57871700	-1.70906800	-2.58639600
C	0.91412200	0.66449300	3.16226300	C	3.38259300	-0.40898600	-0.56095600
H	0.01103200	0.78981100	2.55221400	C	4.96729500	-1.69903300	-2.45560400
C	0.47047500	0.45293800	4.61872200	H	3.11083800	-2.21707800	-3.43319000
H	-0.16802600	-0.43856600	4.71850700	C	4.77200800	-0.38986000	-0.44288600
H	-0.10347900	1.32220100	4.97773800	H	2.77491200	0.08155300	0.19890300
H	1.33996600	0.31928500	5.28323500	C	5.57774000	-1.03497800	-1.38522000
C	1.71909100	1.96038700	3.00632200	H	5.58006900	-2.20969800	-3.20358400
H	2.59029700	1.99270200	3.68016300	H	5.22523400	0.12520400	0.40800500
H	1.08618500	2.82951100	3.23639900	H	6.66568700	-1.02330400	-1.28747600
H	2.08132100	2.08358700	1.97488400	C	-1.34606000	0.86156700	-1.91541200
C	1.00151700	-3.80984900	0.66024500	H	-1.66533900	-0.12990200	-2.25023300
H	0.12982600	-3.34906400	0.17576400	H	-2.16403600	1.33654500	-1.36065600
C	1.86462300	-4.41185900	-0.45446500	C	-0.91556100	1.70249200	-3.09879700
H	2.28646300	-3.63107000	-1.09820600	H	-0.05824900	1.25998200	-3.62599100
H	1.24963800	-5.07771000	-1.08008800	H	-1.75605400	1.75375700	-3.81678800
H	2.69131900	-5.01797200	-0.05009300	H	-0.66522900	2.73593000	-2.82050500
C	0.50269600	-4.92160800	1.60035000				
H	1.35066900	-5.41138400	2.10613400				

Complex **11t-py**

E= -2703,29282972 a.u.

G= -2702,424417 a.u.



Rh	-0.55638300	0.07433600	-0.60588300	H	4.76590100	3.50686200	-1.30710400
O	-2.21636200	-0.72529500	0.40259700	C	5.13950200	1.86349000	0.81339900
N	-2.07844300	0.33082200	-2.07095600	H	5.54209900	2.86885500	1.01838800
N	1.11913100	-1.49822300	1.43264900	H	5.91722400	1.28714400	0.28733300
N	1.70432900	0.58736300	1.42504500	H	4.95970400	1.37630900	1.78259700
C	-1.97129400	0.87421600	-3.27080600	C	0.33835500	-2.71541100	1.42675800
H	-0.97378400	1.23140600	-3.54306900	C	-0.82462700	-2.75305500	2.22680700
C	-3.08068700	0.97823900	-4.14052400	C	-1.59505600	-3.92117400	2.19921200
H	-2.94677600	1.43803500	-5.12134600	H	-2.51305900	-3.96962700	2.78621000
C	-4.30557400	0.48994300	-3.73937200	C	-1.19118900	-5.03135100	1.46020700
H	-5.17596900	0.54998400	-4.39835500	H	-1.80913100	-5.93231500	1.44647800
C	-4.44735600	-0.11099700	-2.45939900	C	0.01625000	-5.00541200	0.76786800
C	-5.65494500	-0.66598700	-1.96739400	H	0.34781800	-5.89491700	0.22993900
H	-6.55396200	-0.63584700	-2.58602200	C	0.81193900	-3.85266100	0.74174900
C	-5.66315100	-1.25140400	-0.71109200	C	2.17495600	-3.89849100	0.06441600
H	-6.58932300	-1.69382900	-0.33346900	H	2.53314900	-2.86704300	-0.03542100
C	-4.51530900	-1.30258300	0.10278100	C	2.14563600	-4.50942100	-1.34239100
H	-4.55637700	-1.78238200	1.08113600	H	1.85198500	-5.57051200	-1.31951700
C	-3.29711800	-0.74883900	-0.32411400	H	3.14563100	-4.45294400	-1.79786400
C	-3.27868300	-0.15860100	-1.64039100	H	1.45012300	-3.97141200	-1.99942700
C	0.79818200	-0.28556800	0.85405300	C	3.17976900	-4.65363200	0.95306800
C	2.57795700	-0.08065100	2.27917800	H	3.24788900	-4.21697700	1.96105000
H	3.35505000	0.44669700	2.81938800	H	4.18599600	-4.63328100	0.50422800
C	2.21231300	-1.38138000	2.28485400	H	2.88275500	-5.70793000	1.07205000
H	2.60465400	-2.23457500	2.82611300	C	-1.12752200	-1.66070100	3.24158700
C	1.73367600	2.03523600	1.38977100	H	-0.68526000	-0.72872000	2.87484500
C	2.76522600	2.69078400	0.68442800	C	-2.61331400	-1.38275600	3.47228000
C	2.80748700	4.09163200	0.73588700	H	-3.09464900	-1.11616200	2.52576600
H	3.58680100	4.61849900	0.18359800	H	-2.72716000	-0.54009200	4.17332200
C	1.88551100	4.81394900	1.48551100	H	-3.13537400	-2.24426000	3.91906800
H	1.93503700	5.90530900	1.51255200	C	-0.43871500	-2.03071100	4.56983800
C	0.90772300	4.14352600	2.21648300	H	-0.61286600	-1.25434700	5.33054700
H	0.20206100	4.71980900	2.81333200	H	0.64819200	-2.14775200	4.44961100
C	0.81239500	2.74648100	2.19482000	H	-0.83722500	-2.98222800	4.95709400
C	-0.22735000	2.04378000	3.05893700	S	1.06009400	1.14163800	-1.96530300
H	-0.63042900	1.20967300	2.46732600	C	2.33357000	0.06792800	-2.56310500
C	0.41091600	1.47598600	4.33989400	C	2.75864200	0.21063400	-3.89820800
H	1.17022700	0.71275500	4.13213300	C	3.01912400	-0.85350200	-1.75121100
H	-0.35965800	1.01317500	4.97474500	C	3.83788800	-0.52443700	-4.39171400
H	0.88537000	2.28471600	4.91876700	H	2.23154300	0.91554800	-4.54488900
C	-1.40921400	2.93516800	3.45740800	C	4.09226900	-1.59308200	-2.24716600
H	-1.11835600	3.67482400	4.22082300	H	2.70866300	-0.98080900	-0.71719800
H	-2.20659800	2.31429900	3.89408800	C	4.51439700	-1.43220100	-3.57056900
H	-1.83433600	3.47766800	2.60456700	H	4.14911000	-0.39054800	-5.43124200
C	3.86761200	1.94725400	-0.04983600	H	4.60786000	-2.29705500	-1.58843500
H	3.51431300	0.92793200	-0.23040100	H	5.35667700	-2.00985500	-3.95811400
C	4.20924100	2.56139100	-1.41357400	C	-0.15610700	-1.70960300	-1.58198600
H	3.29980700	2.74946600	-1.99827600	H	0.06303200	-1.41334700	-2.61868200
H	4.84109400	1.86605800	-1.98617300	H	0.77431100	-2.10688200	-1.17284000

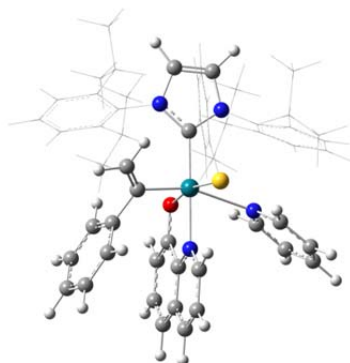
C	5.12356900	3.01104700	-0.77788800
H	3.92686000	3.51808200	0.95158200
H	6.05307200	2.28950000	-2.59557900
H	5.94781500	3.67831500	-0.51583900
S	1.69135400	0.18162400	-1.96600700
C	-1.15294900	-0.60855300	-2.88090500
C	-1.35683400	0.12740600	-1.78571900
H	-0.23916600	-1.17237500	-3.06909600
H	-1.93547900	-0.65813200	-3.64608900
C	-2.55884900	0.98455400	-1.64061600
C	-3.49386900	0.79457100	-0.61346900

C	-2.76542700	2.04484800	-2.54295400
C	-4.58917500	1.64565500	-0.47442600
H	-3.33910200	-0.02017500	0.08501100
C	-3.85668000	2.90283400	-2.40124700
H	-2.04157600	2.20238300	-3.34446600
C	-4.77055500	2.71113900	-1.36061700
H	-5.29957200	1.48103500	0.33946600
H	-3.98950000	3.73055200	-3.10251500
H	-5.61829400	3.38997000	-1.24038800

Complex **12t-py**

E= -2932,9767273 a.u.

G= -2932,055251 a.u.



C	3.00226000	0.16333100	2.09611400
H	3.78722500	-0.34194100	2.64451700
C	2.70063300	1.47412300	1.97881300
H	3.15327200	2.35673800	2.41602900
N	1.56482700	1.55712300	1.18072800
N	2.04917200	-0.54777400	1.37160500
C	1.14966300	0.30599300	0.76238800
C	-3.24771500	-0.67692700	-0.75494900
C	-2.42024400	-0.25964400	-2.89360500
C	-2.94431300	-0.75160200	0.65051900
C	-4.55229700	-0.97112400	-1.25152600
C	-3.68035100	-0.53013000	-3.47028400
H	-1.54777600	0.00431300	-3.49777500
C	-3.99652100	-1.07890200	1.51663400
C	-5.57539100	-1.31940500	-0.33451100
C	-4.73428900	-0.88791900	-2.65750300
H	-3.79587500	-0.46230800	-4.55333500
C	-5.28382200	-1.35985700	1.01911100
H	-3.78938600	-1.13369200	2.58632000
H	-6.57596700	-1.54796200	-0.70638000
H	-5.71671200	-1.11326300	-3.08082700
H	-6.07225800	-1.62450600	1.72919600
O	-1.72871800	-0.50761900	1.06014200
N	-2.22402100	-0.33140400	-1.59006300
Rh	-0.42456600	-0.00919100	-0.49468400
C	0.06107900	-1.91879100	-1.00761300
C	1.24531600	-2.29323100	-1.49640900
H	2.09424200	-1.62079900	-1.57377600
C	2.00590500	-1.99100200	1.51656300
C	1.03006900	-2.55033400	2.37161400
C	3.00821400	-2.77991700	0.91242500
C	0.98557000	-3.94647800	2.47686700
C	2.92473900	-4.16892800	1.06588300
C	1.90399200	-4.75232900	1.81006700
H	0.22268800	-4.41106700	3.10102100
H	3.67171400	-4.80304600	0.58626600
H	1.84043400	-5.83959500	1.89584600
C	0.79719800	2.78573400	1.20468100
C	0.99117100	3.78139200	0.22562300
C	-0.05090100	2.97889500	2.31537800
C	0.22473300	4.94845200	0.33155100

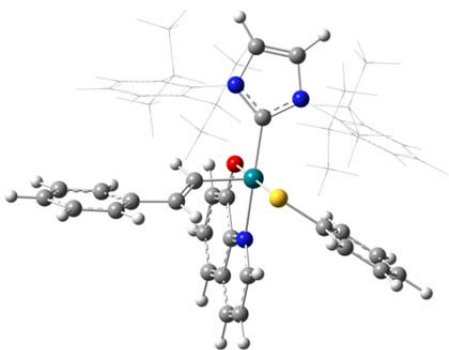
C	-0.79142400	4.16615500	2.37329700
C	-0.67288800	5.13401000	1.38112600
H	0.32923500	5.72495900	-0.42603800
H	-1.47131300	4.33163500	3.21142000
H	-1.27116400	6.04663800	1.43251600
C	4.20431200	-2.18503900	0.18150300
H	3.95400100	-1.15177200	-0.08398100
C	2.01379000	3.62064600	-0.88419300
H	1.99132400	2.56512000	-1.16760600
C	-0.11897400	2.00406600	3.48391000
H	0.47548800	1.12238200	3.22719700
C	0.14647500	-1.68840200	3.26590100
H	-0.15877600	-0.80816900	2.69069400
C	5.43448900	-2.15879700	1.10875500
H	5.75297700	-3.18405700	1.35686200
H	6.27910500	-1.65230500	0.61428200
H	5.23966400	-1.64270900	2.05990500
C	4.57840900	-2.90972800	-1.11879700
H	5.37451100	-2.35296000	-1.63496900
H	4.95832900	-3.92497100	-0.92346800
H	3.72969700	-2.98713000	-1.80771000
C	1.69444200	4.41231700	-2.15448800
H	0.66621200	4.23453900	-2.49672300
H	1.83125100	5.49747500	-2.01544800
H	2.37253100	4.09425200	-2.96069400
C	3.43022600	3.96702000	-0.39649700
H	3.74281600	3.34008000	0.44966300
H	4.15731000	3.80816000	-1.20809400
H	3.49058800	5.02096000	-0.07822300
C	0.52952300	2.63708400	4.72682700
H	-0.04310700	3.51101000	5.07660900
H	0.57326300	1.90878200	5.55191300
H	1.55598700	2.97471200	4.51575000
C	-1.53628500	1.50132800	3.78782600
H	-1.89868800	0.85978400	2.97364600
H	-1.53111000	0.89849800	4.70910900
H	-2.24530500	2.32981200	3.94269900
C	0.95626300	-1.24275900	4.49928200
H	1.28800400	-2.12037400	5.07724500
H	1.84820900	-0.66263900	4.22764200
H	0.33886700	-0.61595600	5.16117700

C	-1.14642200	-2.36136300	3.73511900	C	4.72169300	0.49995600	-2.12230300
H	-1.75088400	-2.73033200	2.89764700	H	3.12054000	0.90999000	-0.75351700
H	-0.95243400	-3.19881100	4.42451600	C	4.08814600	-0.00087600	-4.39133900
H	-1.75808200	-1.62755900	4.28080400	H	1.96471300	0.00083700	-4.79962700
H	1.40697900	-3.32929100	-1.81516500	C	5.08949400	0.17508200	-3.42999300
C	-1.06162100	-2.89439300	-1.04339800	H	5.48752100	0.63365200	-1.35348300
C	-1.65780500	-3.40653100	0.11732900	H	4.35563300	-0.26654200	-5.41752900
C	-1.56359800	-3.32467200	-2.28614300	H	6.14197600	0.05438500	-3.69649100
C	-2.72964400	-4.29643300	0.04760900	N	-1.67888800	2.17046200	-0.43986400
H	-1.27636300	-3.07978500	1.07792900	C	-2.64883400	2.35484000	0.46143900
C	-2.64151400	-4.20808800	-2.36151000	C	-1.70474300	2.91033300	-1.55505200
H	-1.10648500	-2.93339000	-3.19703100	C	-3.68636900	3.27235800	0.28526900
C	-3.23541800	-4.69396000	-1.19263900	H	-2.59548900	1.73734200	1.35380500
H	-3.18161400	-4.67003100	0.96993400	C	-2.69506500	3.85646600	-1.81610300
H	-3.02367400	-4.51445100	-3.33889800	H	-0.89701200	2.72103600	-2.26689000
H	-4.08672500	-5.37686800	-1.24861400	C	-3.71274200	4.03975700	-0.87792900
S	0.64214700	0.80847400	-2.44759100	H	-4.45566700	3.37098400	1.05301500
C	2.36022800	0.49248500	-2.73712900	H	-2.66425600	4.43067100	-2.74400000
C	3.37753300	0.65495200	-1.77754500	H	-4.51145900	4.76495000	-1.05244400
C	2.74437500	0.14990800	-4.04999300				

Complex 13t

E= -2684,8429739 a.u.

G= -2684,014402 a.u.



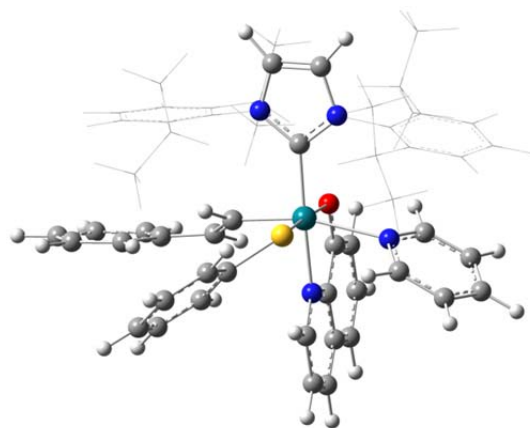
Rh	0.21903800	0.52542400	-0.09624700	C	-1.06856100	-4.58448600	-0.52489600
N	-0.76444000	-1.93719900	1.47618200	H	-1.92270900	-5.28109500	-0.53664600
N	1.37334000	-1.67491300	1.51184300	H	-0.66415600	-4.56195300	0.49669600
C	0.23554600	-1.19042900	0.93423300	H	-0.28588500	-4.99357400	-1.18385500
C	1.08225100	-2.67417300	2.43377800	C	2.71557600	-1.29637700	1.15212800
H	1.85980700	-3.16312600	3.01004200	C	3.39078800	-2.08649000	0.19595500
C	-0.26288400	-2.84438700	2.40656000	C	4.71051800	-1.73661500	-0.10733300
H	-0.91615400	-3.52342400	2.94377100	H	5.25820800	-2.30773600	-0.85742200
C	-2.15468100	-1.91698500	1.10637700	C	5.33250000	-0.66106900	0.52518500
C	-2.53590200	-2.56552300	-0.08663100	H	6.36152900	-0.40296400	0.26597700
C	-3.90058200	-2.58521600	-0.39289100	C	4.64337500	0.09745400	1.46709900
H	-4.24026400	-3.05415500	-1.31575900	H	5.13984800	0.94158500	1.94831700
C	-4.83599400	-1.98435400	0.44995700	C	3.31293600	-0.19710000	1.79699300
H	-5.89354800	-1.99910600	0.17912200	C	2.57350800	0.61887900	2.84638100
C	-4.42370400	-1.32560400	1.60450600	H	1.49800300	0.43883900	2.72723600
H	-5.16272400	-0.82843600	2.23541700	C	2.97076900	0.16367000	4.25973700
C	-3.06656000	-1.26466200	1.95239900	H	4.04699600	0.32013900	4.44008700
C	-2.60996700	-0.49774700	3.18513300	H	2.41098700	0.73073600	5.02068900
H	-1.52090100	-0.37219600	3.11558700	H	2.75852200	-0.90640400	4.41019800
C	-3.20236200	0.91671100	3.23584200	C	2.77686300	2.12823700	2.66692600
H	-2.95452900	1.48118500	2.32638500	H	3.81164600	2.43734200	2.88517800
H	-2.78302800	1.47014700	4.09041600	H	2.53564300	2.44598800	1.64176400
H	-4.29742000	0.90281500	3.35521100	H	2.11140700	2.68332000	3.34397600
C	-2.92544900	-1.27866100	4.47050700	C	2.74068400	-3.30884000	-0.43861800
H	-2.56037800	-0.73471300	5.35649900	H	1.65271200	-3.16603800	-0.38788100
H	-2.45449800	-2.27379100	4.46641800	C	3.09680400	-4.58182000	0.35013000
H	-4.01157000	-1.42615800	4.58717200	H	4.18206200	-4.76989200	0.31224800
C	-1.49821400	-3.18951600	-1.01118100	H	2.58409800	-5.45664100	-0.08086400
H	-0.61195500	-2.53938600	-0.98733500	H	2.80746900	-4.51104500	1.40791000
C	-1.94313600	-3.24882900	-2.47437300	C	3.09716700	-3.49059500	-1.91746600
H	-2.30305200	-2.27113600	-2.82006300	H	2.89111900	-2.57810800	-2.48841200
H	-1.09043600	-3.53881200	-3.10666600	H	2.49508200	-4.30765800	-2.34525300
H	-2.74381100	-3.98905600	-2.63489200	H	4.15651900	-3.76048800	-2.05487200

C	-0.08491400	3.39353600	0.16358500	H	2.69970400	-0.83059400	-4.30178000
C	0.46719100	2.92363300	-2.05721500	C	5.09035500	1.23714200	-3.00523600
C	-0.36512800	2.84177100	1.46457200	H	4.92336600	2.25867100	-1.10485800
C	-0.16289700	4.79594900	-0.08815700	H	4.94301700	0.07876100	-4.82816900
C	0.41219200	4.29419700	-2.39304500	H	6.07670000	1.64382600	-3.23950400
H	0.69207000	2.15297200	-2.79741900	S	0.94015700	-0.52407400	-2.08124600
C	-0.70720200	3.74482000	2.47953600	C	-2.22830000	0.40175900	-1.81577700
C	-0.50775400	5.66595200	0.97726300	C	-1.67310800	0.50495500	-0.60090200
C	0.10611600	5.21993900	-1.41722600	H	-1.60003500	0.20301800	-2.68807700
H	0.61211900	4.59821600	-3.42162800	H	-2.28026500	0.68307000	0.28989800
C	-0.76990900	5.13041100	2.22780100	C	-3.68205000	0.44630200	-2.05211300
H	-0.92412300	3.34742500	3.47249100	C	-4.20984400	-0.12077300	-3.22724700
H	-0.56777900	6.74087400	0.79682300	C	-4.58723900	1.00726000	-1.12972400
H	0.05740400	6.28583100	-1.65529700	C	-5.58683400	-0.16548400	-3.45478500
H	-1.03966400	5.79849800	3.05021600	H	-3.52406500	-0.54375600	-3.96599900
O	-0.28408700	1.54806100	1.64522600	C	-5.96052600	0.96587200	-1.35620900
N	0.24514200	2.50531600	-0.82306800	H	-4.20537900	1.47996700	-0.22343900
C	2.53350000	0.18157900	-2.39645300	C	-6.47182500	0.37113600	-2.51617200
C	3.18574800	1.06053300	-1.51342400	H	-5.97011100	-0.62019700	-4.37198900
C	3.19341200	-0.15740400	-3.59670400	H	-6.64167600	1.40587900	-0.62303700
C	4.44255400	1.58345000	-1.81718400	H	-7.54977400	0.34071100	-2.69231500
H	2.71587200	1.33374300	-0.56848900				
C	4.45403100	0.36003500	-3.89149800				

Complex 14t

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G= -2932,080088 a.u.



Rh	-0.36238900	0.44004800	0.29820300	C	-5.06063500	-1.43227200	0.87579100
O	-0.66365500	1.41316900	-1.52020400	H	-5.60821700	-1.53178400	1.81346900
N	-0.20684300	2.45301600	0.92956400	C	-5.69153600	-0.86321000	-0.23046100
N	0.39270900	-2.27826400	-1.01782200	H	-6.72328000	-0.51372000	-0.14618200
N	-1.71041300	-2.16879800	-0.56848600	C	-5.01852800	-0.75315000	-1.44496300
C	-0.05378100	2.92390700	2.15451200	H	-5.53149300	-0.32989300	-2.31101000
H	0.01076000	2.18795500	2.95703500	C	-3.68730100	-1.17095100	-1.56985400
C	0.01982900	4.31143800	2.41227400	C	-2.99436400	-1.12468600	-2.92669800
H	0.15838700	4.65450200	3.43876900	H	-1.94146100	-1.39148500	-2.78070400
C	-0.07469800	5.20110500	1.36356400	C	-3.60638500	-2.18132100	-3.86180900
H	-0.01095200	6.27856400	1.53711300	H	-3.57319600	-3.18515400	-3.41107700
C	-0.26652400	4.72408800	0.03870600	H	-3.05445200	-2.21774000	-4.81430200
C	-0.40299200	5.55759600	-1.09960000	H	-4.66020600	-1.95177500	-4.08829200
H	-0.34651100	6.64153300	-0.98313700	C	-3.00073500	0.26610200	-3.57388000
C	-0.60766800	4.97690200	-2.34133600	H	-4.02006400	0.66918700	-3.68477000
H	-0.70987900	5.61790300	-3.22131000	H	-2.55756000	0.21061200	-4.58081800
C	-0.69283600	3.58124700	-2.51269600	H	-2.38951300	0.96304100	-2.98547800
H	-0.85562900	3.14980700	-3.50177100	C	-3.07742900	-2.60502900	1.96446000
C	-0.56656300	2.71087400	-1.42038400	H	-1.99751000	-2.40847200	1.90867500
C	-0.33604600	3.30809700	-0.12835200	C	-3.55409100	-2.13024500	3.34062500
C	-0.55113600	-1.43391000	-0.49173100	H	-3.50411400	-1.03838100	3.43601200
C	-1.48507500	-3.42827400	-1.11309200	H	-2.91321400	-2.56344100	4.12318200
H	-2.29453800	-4.13133700	-1.27300400	H	-4.58935900	-2.44637200	3.54929000
C	-0.16538500	-3.49577900	-1.39394800	C	-3.28666100	-4.12553900	1.84025500
H	0.43849800	-4.27534900	-1.84407100	H	-4.35989600	-4.37585900	1.86885100
C	-3.06303500	-1.69982400	-0.42289400	H	-2.79164000	-4.64820000	2.67420400
C	-3.73706100	-1.88302000	0.79960000	H	-2.87161200	-4.52556700	0.90505700

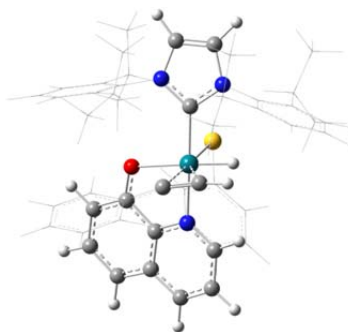
C	1.77320800	-2.03946900	-1.37071600	H	2.10305300	1.35741600	2.21412600
C	2.04420200	-1.37162900	-2.58105500	C	2.70572300	-1.03896800	5.20263900
C	3.38335000	-1.28037000	-2.97568800	H	0.85849300	-1.99568400	4.62345400
H	3.63774800	-0.75096100	-3.89396900	C	3.63736200	-0.03321500	4.92023100
C	4.40178600	-1.83580600	-2.20288000	H	4.11373300	1.61430100	3.60101400
H	5.44131400	-1.73337400	-2.52036500	H	2.87222600	-1.72035500	6.04146600
C	4.10285300	-2.47097700	-1.00130500	H	4.53540100	0.07941400	5.53183300
H	4.91273800	-2.86511100	-0.38625400	C	1.60600600	0.42441000	0.04580000
C	2.77988900	-2.58137100	-0.55202500	C	2.33514500	1.31967200	-0.64257500
C	2.45893900	-3.24424000	0.78175300	H	2.13515500	-0.36098500	0.58488500
H	1.45635800	-2.90741400	1.08704600	H	1.84675800	2.09917500	-1.23227000
C	3.42780800	-2.82403700	1.89507900	C	3.80171500	1.29535300	-0.75123400
H	4.44903700	-3.19410000	1.71158700	C	4.42723700	1.92262700	-1.84627700
H	3.09404800	-3.23386400	2.85921500	C	4.62494500	0.63761200	0.18430500
H	3.47094000	-1.73277000	2.00662100	C	5.80900500	1.85401700	-2.02852200
C	2.43226100	-4.77640000	0.65157000	H	3.80863000	2.45303400	-2.57527800
H	1.69150700	-5.11581400	-0.08688500	C	6.00498400	0.57303400	0.00699800
H	2.18032500	-5.24177300	1.61804300	H	4.17403200	0.17174500	1.05982400
H	3.41761200	-5.15808300	0.33751600	C	6.60732600	1.16991800	-1.10661900
C	0.92951400	-0.76995300	-3.42543700	H	6.26649400	2.33789200	-2.89572200
H	0.11405700	-0.49382400	-2.74576500	H	6.61859600	0.05209800	0.74698800
C	1.33455200	0.52940000	-4.12685900	H	7.68999100	1.11630100	-1.24534100
H	1.74452300	1.25099800	-3.40894300	N	-2.58406200	1.04433800	0.81548800
H	0.44884000	0.98643200	-4.59412300	C	-3.33138200	1.65545400	-0.11142300
H	2.07884500	0.36224300	-4.92225100	C	-2.93102500	1.18075500	2.10404900
C	0.39497400	-1.79216800	-4.44290600	C	-4.45538200	2.41818300	0.20717000
H	-0.43436600	-1.35956400	-5.02545800	H	-3.00451500	1.53734500	-1.14127500
H	0.02053200	-2.70273600	-3.95297400	C	-4.04180600	1.91511600	2.51261200
H	1.18667600	-2.09076700	-5.14938000	H	-2.26809500	0.68950300	2.82172400
S	-0.17078200	-0.64771900	2.40712100	C	-4.82254500	2.55054700	1.54484200
C	1.32179700	-0.33734000	3.31677500	H	-5.02448900	2.89664700	-0.59146700
C	2.25374500	0.68378400	3.05408500	H	-4.27884500	1.98952400	3.57552700
C	1.56944800	-1.19350100	4.41122600	H	-5.69623500	3.14175100	1.82977200
C	3.39917500	0.82320300	3.84307900				

Complex A correspond to **9t**

Complex B

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G= -2683,952164 a.u.



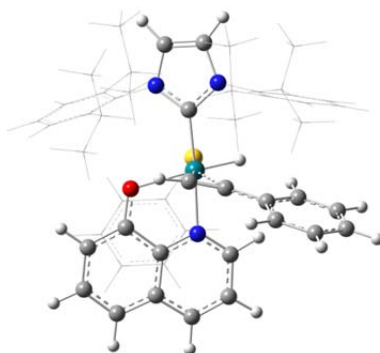
Rh	-0.20168400	0.38444900	-0.46015800	C	4.23467400	0.30081600	-1.27685200
N	2.43993100	1.30237500	0.74662200	H	3.60981900	-0.31010800	-0.61503500
N	1.71752000	-0.46092200	1.76698400	C	4.33231000	-0.44448200	-2.61263600
C	1.44870300	0.35301700	0.70349800	H	3.35453900	-0.53608800	-3.10400000
C	2.79988000	0.01802600	2.49960600	H	4.71297700	-1.46317000	-2.43942600
H	3.14344700	-0.48604800	3.39598000	H	5.02885400	0.04654200	-3.31047200
C	3.25675600	1.12035900	1.85724300	C	5.62954400	0.41257500	-0.63383600
H	4.08614100	1.78503600	2.07188400	H	6.08154900	-0.58396300	-0.51165400
C	2.78943900	2.19769000	-0.32887900	H	5.58465100	0.88638000	0.35678900
C	2.35602300	3.53576000	-0.30130900	H	6.29910200	1.01809800	-1.26566900
C	2.69072200	4.34677400	-1.39562300	C	1.61845000	4.11391300	0.89262100
H	2.35783400	5.38550200	-1.40993400	H	1.15907400	3.27832800	1.43533600
C	3.43855000	3.84922600	-2.46007700	C	0.47653200	5.05303600	0.49600600
H	3.67895700	4.49639400	-3.30711300	H	-0.20252900	4.55902600	-0.21157300
C	3.90469900	2.53455700	-2.43572400	H	-0.11491700	5.31724500	1.38533300
H	4.52329900	2.16691800	-3.25595100	H	0.84426900	5.99042100	0.04727400
C	3.60380400	1.68448100	-1.36464300	C	2.61099600	4.81497800	1.83608200

H	3.10329000	5.66469600	1.33484900	C	-3.67313800	-1.89888200	0.69488900
H	3.40116200	4.12973100	2.18002800	C	-5.31354900	-1.09735400	-0.93463700
H	2.08791000	5.20048200	2.72561500	C	-4.53121600	0.49220700	-2.70674400
C	1.11548900	-1.74190500	2.06751300	H	-3.63855700	1.84312900	-4.13394600
C	0.11311900	-1.80099500	3.04971000	C	-4.97572800	-1.86908600	0.16826400
C	-0.40953700	-3.06085200	3.36869400	H	-3.43176700	-2.52628800	1.55473600
H	-1.19370500	-3.13822900	4.12307500	H	-6.32948200	-1.09190000	-1.33379900
C	0.04720400	-4.20864800	2.72905600	H	-5.52938800	0.52594600	-3.15082400
H	-0.37818400	-5.18241100	2.98449900	H	-5.74586700	-2.48258500	0.64484900
C	1.04606900	-4.12269600	1.76020000	O	-1.43108400	-1.10302100	0.58949000
H	1.38638300	-5.03060700	1.26374600	N	-2.00079800	0.44675400	-1.55324100
C	1.61034400	-2.89064300	1.40756600	C	-2.74622000	2.25681200	0.75623200
C	2.72837000	-2.82441600	0.36941400	C	-3.79607200	1.62850000	1.44885800
H	2.52532600	-1.94587800	0.26200400	C	-3.06701400	3.16754000	-0.26545900
C	4.10979500	-2.64407300	1.02670200	C	-5.12644800	1.89186700	1.11909900
H	4.31912700	-3.48678600	1.70498700	H	-3.55636000	0.91531100	2.23492300
H	4.89696200	-2.62909200	0.25639600	C	-4.39811500	3.42386100	-0.59847500
H	4.19354100	-1.71465400	1.60115700	H	-2.25889400	3.66247400	-0.80628700
C	2.79695600	-4.04271600	-0.55964200	C	-5.43401500	2.78637000	0.09031100
H	3.17282900	-4.93157000	-0.02744500	H	-5.92604800	1.37950100	1.65914000
H	1.82709000	-4.29244100	-1.00209200	H	-4.62740100	4.12450700	-1.40578000
H	3.49958800	-3.83625500	-1.38147800	H	-6.47533700	2.98345900	-0.17597300
C	-0.37621800	-0.55885700	3.77214800	S	-1.05479800	1.92138000	1.19776400
H	-0.13082200	0.30959100	3.14772800	H	0.35817200	1.69858000	-1.01567600
C	0.32914400	-0.40100900	5.12930900	C	0.90370300	-0.01381700	-2.25060200
H	0.10755700	-1.25404000	5.79193700	H	1.45997600	0.71975400	-2.80982200
H	-0.00921400	0.51812200	5.63414100	C	0.43740300	-1.13662500	-1.94248700
H	1.42293500	-0.34082600	5.02121500	C	0.13050200	-2.52914600	-2.15248300
C	-1.89795000	-0.54262800	3.93887600	C	0.54098500	-3.12777100	-3.36396300
H	-2.38176400	-0.72720700	2.97206300	C	-0.55125900	-3.30744100	-1.20076900
H	-2.22182000	0.44312600	4.30599300	C	0.27301600	-4.47136100	-3.61266800
H	-2.24643100	-1.29745300	4.66275400	H	1.07276300	-2.52478700	-4.10283800
C	-2.99158800	-0.31801100	-1.01610000	C	-0.82203700	-4.65080300	-1.46283600
C	-2.22821600	1.18205000	-2.63053900	H	-0.84393400	-2.84241600	-0.26156600
C	-2.64356200	-1.11805200	0.13707900	C	-0.41345500	-5.23813100	-2.66266200
C	-4.31441500	-0.31352100	-1.55825400	H	0.59800700	-4.92455500	-4.55235700
C	-3.49367900	1.21938100	-3.25041300	H	-1.35092700	-5.24313500	-0.71278000
H	-1.39133800	1.77083600	-3.00960500	H	-0.62631000	-6.29146600	-2.86088600

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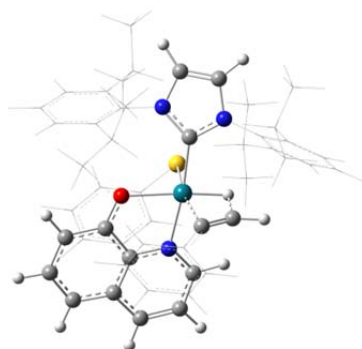
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N	-1.89222900	1.94196700	0.35016300	H	-5.83167500	-0.00353500	-1.00871200
N	0.09886100	2.63528400	-0.09988900	C	-3.95459900	0.92159500	-0.47983900
C	-0.63708700	1.48936800	0.05002600	C	-3.69011200	1.48466700	-1.87027400
C	-0.68416400	3.76440500	0.11072700	H	-2.60480900	1.63875300	-1.95975700
H	-0.27231500	4.76308400	0.02498300	C	-4.11175600	0.53937200	-3.00084900
C	-1.93325700	3.33115400	0.40477900	H	-3.68101000	-0.46076300	-2.87202900
H	-2.84351000	3.86580000	0.65172000	H	-3.77202400	0.93899700	-3.96916800
C	-3.06595600	1.14809300	0.59025000	H	-5.20679700	0.43534600	-3.05985100
C	-3.31347500	0.69538900	1.89978300	C	-4.37830900	2.85028700	-2.04466800
C	-4.50775300	-0.00105000	2.12507100	H	-4.15552900	3.27076500	-3.03846900
H	-4.73416000	-0.36565500	3.12862900	H	-4.04785500	3.57798400	-1.29100400
C	-5.40269000	-0.24615400	1.08524400	H	-5.47178800	2.74633800	-1.95569200
H	-6.32057100	-0.80586400	1.27804700	C	-2.35053500	0.98449300	3.04225600

H	-1.39441300	1.30251600	2.60633000	C	1.06379300	-4.65119800	0.67146800
C	-2.04888000	-0.25445600	3.89308400	H	-0.45912900	-3.23719600	1.34163600
H	-1.61958400	-1.05713800	3.27673300	C	3.48294000	-1.44237700	-2.35571900
H	-1.30082000	-0.00734300	4.66096600	C	3.78336200	-3.79490400	-1.75803400
H	-2.94676300	-0.63493700	4.40606800	C	2.17118500	-4.81081500	-0.13356300
C	-2.87603600	2.14479200	3.90320200	H	0.68462100	-5.46872200	1.28689600
H	-3.83655200	1.88439700	4.37730500	C	4.16996600	-2.66321800	-2.46137100
H	-3.03594600	3.05169500	3.29947300	H	3.83300300	-0.55681100	-2.88924900
H	-2.15731300	2.39009900	4.70112500	H	4.33825500	-4.73153000	-1.83811200
C	1.48195800	2.75011900	-0.49673600	H	2.69905900	-5.76728000	-0.17441900
C	2.44857000	3.09061000	0.46983400	H	5.04809100	-2.71421900	-3.11188100
C	3.77500500	3.21617700	0.03391000	O	1.72497000	-0.19351300	-1.34794300
H	4.55315000	3.46263800	0.75736300	N	0.82588100	-2.37517900	-0.01802900
C	4.11531800	3.02766500	-1.30360300	C	2.68234000	-0.88163000	1.85398400
H	5.15767300	3.12109300	-1.61805600	C	3.71913000	-0.41590300	1.02804700
C	3.13027800	2.73195100	-2.24339000	C	2.86302600	-2.08480500	2.55744600
H	3.40722400	2.60146300	-3.29002000	C	4.89495700	-1.15471300	0.88847000
C	1.79239200	2.59305400	-1.86112300	H	3.57608400	0.50438800	0.46482700
C	0.70457600	2.36031100	-2.89807900	C	4.04227300	-2.81819700	2.41784300
H	-0.12027400	1.84248400	-2.39282300	H	2.05622100	-2.44716200	3.19709800
C	0.15589100	3.70405800	-3.40972400	C	5.06031900	-2.35967300	1.57602700
H	0.94660600	4.27948100	-3.91779000	H	5.67846300	-0.79345800	0.21838700
H	-0.66345800	3.54143800	-4.12926600	H	4.16071500	-3.76087800	2.95861200
H	-0.23503200	4.32303400	-2.58858000	H	5.97548400	-2.94319600	1.45061100
C	1.14893400	1.47175900	-4.06356200	S	1.15351800	0.01820300	2.01172100
H	1.88388600	1.97668500	-4.71042700	H	-1.11964000	-0.66591100	1.00997700
H	1.59518900	0.54124200	-3.68831200	C	-0.91608400	-0.71544000	-2.01434800
H	0.28443700	1.22533300	-4.70216900	H	-0.43792000	-0.28826900	-2.87666800
C	2.09257700	3.39830000	1.91778900	C	-1.63164100	-1.36662100	-1.23314200
H	1.12182600	2.92792200	2.12533700	C	-2.66075100	-2.29059500	-0.82523400
C	1.96242800	4.91822700	2.12757600	C	-3.36690800	-2.97827600	-1.83588300
H	2.92477500	5.42076900	1.93802800	C	-2.99415600	-2.53781600	0.51540000
H	1.66304700	5.14055000	3.16458600	C	-4.38371900	-3.87151400	-1.50748200
H	1.21805600	5.37283300	1.45781700	H	-3.10192500	-2.80590100	-2.88046600
C	3.09596500	2.81949800	2.92277100	C	-4.01105800	-3.43434100	0.83937200
H	3.25671900	1.74801600	2.75283800	H	-2.45957100	-2.00258000	1.29703500
H	2.71331700	2.94798500	3.94741800	C	-4.71180400	-4.10279000	-0.16681400
H	4.06879900	3.33463700	2.87174700	H	-4.92068300	-4.39491100	-2.30209700
C	1.92601700	-2.49498500	-0.81633400	H	-4.26156800	-3.60399900	1.88897800
C	0.41028300	-3.40173400	0.70628100	H	-5.50822800	-4.80516500	0.09009900
C	2.35622900	-1.30694900	-1.52228200				
C	2.64856200	-3.72593200	-0.91483200				

Complex C-TS

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G= -2683,950999 a.u.



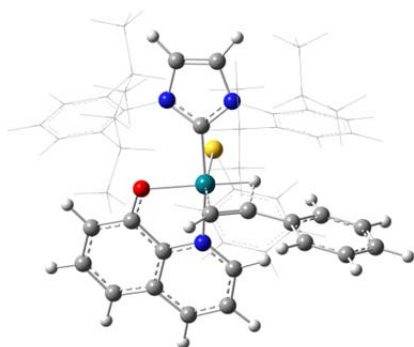
Rh	-0.03785300	0.27221600	-0.64175600	H	-4.24412300	-0.93232400	-4.18289200
N	-2.56287300	-1.29358800	0.08088200	C	-5.10191200	0.45136300	-2.77171100
N	-0.95889000	-1.81201800	1.42401200	H	-5.77121500	0.89893500	-3.51051700
C	-1.26718800	-0.96643500	0.38847900	C	-5.10768900	0.92052300	-1.45748000
C	-2.03123200	-2.64317200	1.72934000	H	-5.77395300	1.73883300	-1.18191600
H	-1.97071900	-3.36903100	2.53093900	C	-4.25265500	0.37054600	-0.49468000
C	-3.03627900	-2.32657900	0.88209700	C	-4.21999400	0.90332100	0.93121600
H	-4.03776300	-2.72523900	0.76559600	H	-3.21336500	0.70162200	1.32696800
C	-3.40889000	-0.68235700	-0.90372100	C	-4.44123100	2.41788400	1.00879600
C	-3.37932700	-1.17671100	-2.22014100	H	-3.77942700	2.95847300	0.32097800
C	-4.24281700	-0.58023300	-3.15001500	H	-4.22831700	2.77676000	2.02734000

H	-5.48299200	2.69211200	0.77718400	C	1.50277500	1.72420900	-2.90824100
C	-5.23520300	0.17390500	1.82816800	C	2.40530800	1.23067400	0.55538500
H	-5.17263600	0.55062700	2.86140400	C	3.66053800	2.38910700	-1.27700500
H	-5.05825900	-0.90964400	1.85693600	C	2.60323200	2.41374200	-3.46082200
H	-6.26245500	0.34096700	1.46547500	H	0.64091900	1.44468300	-3.51703900
C	-2.46256500	-2.32119500	-2.62308800	C	3.45459900	1.56819500	1.42427500
H	-1.68337200	-2.41586500	-1.85566100	C	4.70015900	2.68546100	-0.36248900
C	-1.73878500	-2.06250800	-3.94891300	C	3.67123800	2.74215200	-2.65223400
H	-1.18989200	-1.10999000	-3.91813100	H	2.59425900	2.67151600	-4.52118600
H	-0.99667000	-2.85392200	-4.12768400	C	4.57438300	2.28054200	0.95822800
H	-2.43292600	-2.04553500	-4.80476500	H	3.39593900	1.22717000	2.45919500
C	-3.24095200	-3.64652100	-2.65697200	H	5.58401900	3.22443300	-0.70854300
H	-4.04169800	-3.61740200	-3.41418000	H	4.53624200	3.27246800	-3.05882000
H	-3.70720000	-3.86412800	-1.68360400	H	5.37748500	2.51039500	1.66429500
H	-2.56670300	-4.48158400	-2.90424100	O	1.36431700	0.54306900	0.91876000
C	0.26382100	-1.91469300	2.18658700	N	1.46882900	1.37932700	-1.63259900
C	1.08101500	-3.04866000	2.00597100	C	2.71504900	-1.41518000	-1.55348500
C	2.23840100	-3.14059800	2.79341300	C	3.50762300	-1.39898700	-0.39172300
H	2.90217600	-3.99684900	2.66684100	C	3.32418600	-1.12576100	-2.78768900
C	2.54989000	-2.16156100	3.73054200	C	4.86496300	-1.08256000	-0.46415400
H	3.45909600	-2.24983600	4.33034800	H	3.03877800	-1.60053600	0.57029200
C	1.69899100	-1.07292000	3.91632500	C	4.68260200	-0.81169600	-2.85598200
H	1.95298900	-0.32353900	4.66483800	H	2.71045900	-1.13477700	-3.69041400
C	0.53567100	-0.92464700	3.15399300	C	5.45866600	-0.78353100	-1.69317900
C	-0.41003700	0.24868000	3.38282000	H	5.45703700	-1.04936900	0.45344900
H	-0.69737900	0.62203000	2.38979100	H	5.13540700	-0.57633900	-3.82295700
C	-1.69121000	-0.18082000	4.12109600	H	6.51833600	-0.52194400	-1.74353600
H	-1.45077600	-0.57735200	5.12109000	S	0.97842400	-1.78603700	-1.48325100
H	-2.36142900	0.68429500	4.25270700	H	-0.97693900	0.12175000	-1.90665800
H	-2.25246500	-0.95262000	3.57792100	C	-1.57163500	1.54673900	-1.48846500
C	0.24172100	1.41341200	4.13228300	H	-2.29776700	1.51563100	-2.29035000
H	0.45847800	1.15203300	5.18063000	C	-1.06009600	2.14109100	-0.48358700
H	1.18064100	1.72691300	3.65460500	C	-0.93528300	3.35036800	0.29337800
H	-0.43907200	2.27708900	4.14468800	C	-0.09177700	3.39496900	1.41609100
C	0.72482700	-4.19807100	1.07083500	C	-1.63531700	4.51779900	-0.08157600
H	-0.01882400	-3.82674100	0.35330500	C	0.03652100	4.57033200	2.15677700
C	0.11633600	-5.36910200	1.86509800	H	0.46109500	2.49640500	1.67746700
H	0.85293500	-5.78272400	2.57277300	C	-1.50323800	5.68859600	0.66078800
H	-0.18831600	-6.17963400	1.18348000	H	-2.27689800	4.49511800	-0.96513300
H	-0.76594600	-5.07274900	2.45086300	C	-0.66906700	5.71779000	1.78568500
C	1.91972000	-4.70251200	0.25144000	H	0.69893300	4.58889100	3.02517800
H	2.40887900	-3.88217900	-0.28599500	H	-2.04984600	6.58620300	0.36130900
H	1.57538100	-5.43762400	-0.49284600	H	-0.56524500	6.63829800	2.36523400
H	2.66693800	-5.20640100	0.88554500				
C	2.51094200	1.68369400	-0.80787200				

Complex C'-TS

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Rh	0.22491700	-0.25837200	-0.38606800	C	-2.79314000	1.22454500	0.83933900
N	-1.51069900	1.85777500	1.01911500	C	-3.24761900	0.29155300	1.79242800
N	0.52019000	2.54457800	0.76880900	C	-4.54228000	-0.21687600	1.62171900
C	-0.30379400	1.48846400	0.48650400	H	-4.92838500	-0.94825500	2.33148000
C	-0.15791000	3.53708300	1.46832100	C	-5.33883700	0.17670100	0.54863600
H	0.33916500	4.45200200	1.77097400	H	-6.33659900	-0.25029800	0.42725000
C	-1.43057300	3.10692900	1.62852700	C	-4.86009300	1.09607300	-0.38091600
H	-2.29099800	3.56102900	2.10643200	H	-5.48974200	1.38837000	-1.22234500

C	-3.58032200	1.64954300	-0.25097900	H	3.76653600	0.27194100	2.23239300
C	-3.09543500	2.71231100	-1.22892400	H	3.52120000	0.62502900	3.95491300
H	-2.00133200	2.76287200	-1.15154500	H	4.79326800	1.48810700	3.06048600
C	-3.42439700	2.39138400	-2.69146200	C	2.37028700	-1.88145600	-1.47424100
H	-3.05370500	1.39867500	-2.97490700	C	0.45816700	-3.20724600	-1.34273900
H	-2.95126200	3.13441600	-3.35265900	C	2.92280200	-0.57001100	-1.26214600
H	-4.50762600	2.42415500	-2.88753900	C	3.17113900	-2.97194300	-1.92953900
C	-3.65583900	4.09515300	-0.85327800	C	1.17125600	-4.33706400	-1.79990900
H	-3.25899100	4.86870700	-1.52996400	H	-0.59909500	-3.27643500	-1.08990900
H	-3.39019900	4.37922100	0.17430100	C	4.29757200	-0.40698900	-1.49976200
H	-4.75506100	4.10326600	-0.93118400	C	4.55045300	-2.75191100	-2.16438900
C	-2.37367600	-0.13728300	2.96134300	C	2.51267700	-4.22027100	-2.09090800
H	-1.33337500	-0.18373500	2.60114700	H	0.64907700	-5.28962100	-1.89651000
C	-2.71414600	-1.53407900	3.49078800	C	5.08152400	-1.48806000	-1.94300800
H	-2.78790000	-2.27272900	2.7932700	H	4.73378400	0.57821800	-1.32731100
H	-1.92395600	-1.87019900	4.17803900	H	5.17720100	-3.57806300	-2.50581900
H	-3.66687000	-1.54934100	4.04513900	H	3.08726900	-5.08589800	-2.43073600
C	-2.42884300	0.88017400	4.11387400	H	6.14874300	-1.32179600	-2.11562900
H	-3.45565600	0.97895200	4.50376700	O	2.14300300	0.39209500	-0.87189500
H	-2.08467600	1.87612300	3.80394000	N	1.04215700	-2.03011700	-1.19250100
H	-1.77907000	0.55005200	4.93966500	C	1.24852600	-2.65409700	1.75298900
C	1.86379600	2.80030000	0.30451700	C	2.51027100	-3.21840400	1.49231000
C	2.93378800	2.66446300	1.20166600	C	0.16015400	-3.52261500	1.95319400
C	4.20923800	3.02000200	0.74048800	C	2.67298900	-4.60316700	1.42577700
H	5.06527500	2.92304400	1.41021000	H	3.35857700	-2.55372200	1.32116000
C	4.40079800	3.48522300	-0.55775400	C	0.32465000	-4.90791600	1.88859100
H	5.40313900	3.75848800	-0.89685300	H	-0.81898600	-3.09559000	2.16871700
C	3.31861200	3.59085500	-1.43128000	C	1.58276000	-5.45630400	1.62202800
H	3.48394800	3.93610100	-2.45308000	H	3.66084200	-5.01752200	1.20802500
C	2.02875800	3.24271400	-1.02109800	H	-0.53641000	-5.56302800	2.04800400
C	0.85788500	3.32615300	-1.98805400	H	1.71255900	-6.53992200	1.56687800
H	0.06753000	2.67228700	-1.60057600	S	1.06109600	-0.88831000	1.83726900
C	0.28591600	4.75048500	-2.05617000	H	-1.20983300	-0.82567200	0.02148900
H	1.03793300	5.46041300	-2.43728700	C	-1.61637800	-0.63406000	-1.48641200
H	-0.58906400	4.78879800	-2.72613300	C	-0.80730800	0.08448800	-2.17144900
H	-0.03420100	5.10059400	-1.06272300	H	-0.61157300	0.54883300	-3.12964000
C	1.21060500	2.78530200	-3.37780100	C	-2.81054400	-1.45920100	-1.43966500
H	1.92951600	3.43115700	-3.90622600	C	-3.72855700	-1.41232400	-2.50807600
H	1.64551300	1.77869700	-3.29606500	C	-3.06430700	-2.33386400	-0.37116000
H	0.30538000	2.73227300	-4.00511000	C	-4.87281500	-2.20529400	-2.48956700
C	2.74667700	2.15389900	2.62134100	H	-3.53530500	-0.74666200	-3.35040400
H	1.75750300	1.67844200	2.67727400	C	-4.20622100	-3.13357300	-0.36016200
C	2.77957500	3.30877700	3.63582300	H	-2.35094300	-2.38073900	0.45309600
H	3.75388900	3.82410600	3.61516900	C	-5.11945600	-3.06780900	-1.41442400
H	2.61816200	2.93061700	4.65813200	H	-5.57872700	-2.15308300	-3.32191200
H	2.00268000	4.06079100	3.42832000	H	-4.38500500	-3.80595500	0.48205300
C	3.77475200	1.07418700	2.98218100	H	-6.01734500	-3.68990300	-1.40444700

Complex **D** correspond to **12t**

Complex **D'** correspond to **13t**

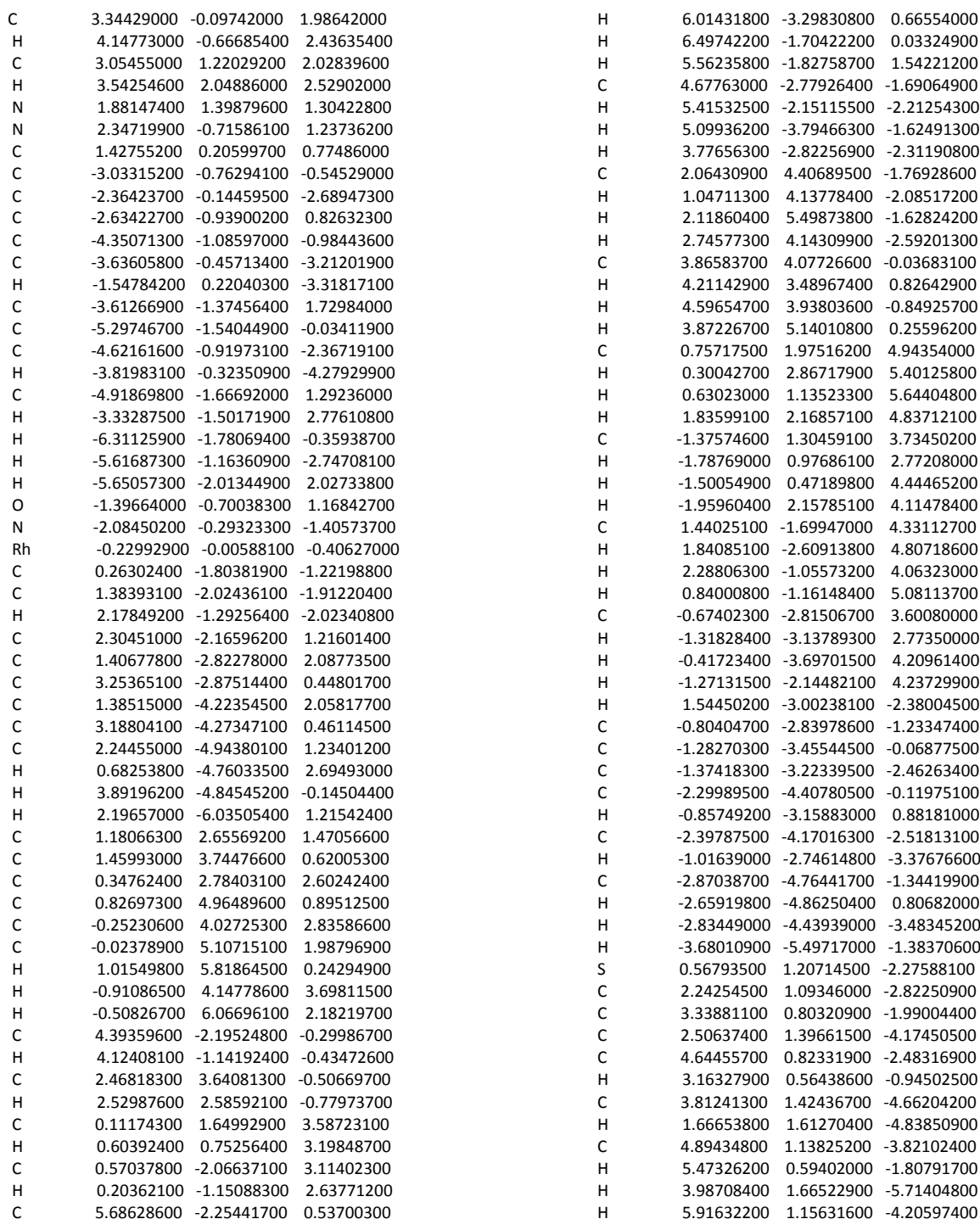
Complex **D-py** correspond to **12t-py**

Complex **D'-py** correspond to **14t**

Complex **D-HSPH**

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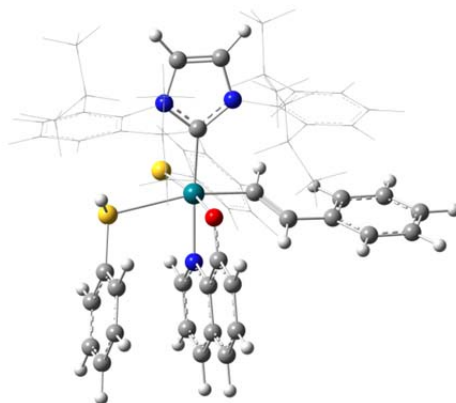


S	-1.58147900	2.53403000	0.01406100	C	-5.24222100	2.44849900	-1.78298600
H	-1.18911100	2.88739000	-1.22934000	H	-3.22136900	2.88086600	-2.41893700
C	-3.31907800	2.37689600	-0.31641500	C	-6.07281900	2.07023400	-0.72681600
C	-4.15342100	2.00637300	0.75039600	H	-6.15890100	1.53901100	1.36997800
C	-3.86797200	2.60148700	-1.58490900	H	-5.66132300	2.61784600	-2.77773100
C	-5.52156100	1.84854100	0.53942600	H	-7.14503400	1.94088200	-0.88934300
H	-3.72529300	1.82203600	1.73652100				

Complex D'-HSPb

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G= -3314,136607 a.u.



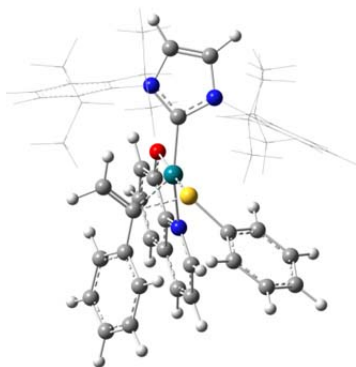
Rh	-0.37384400	0.14159200	0.29164900	C	-1.89895200	-3.66967300	2.01088200
O	-0.99003700	0.94442100	-1.52889400	H	-0.92548300	-3.18439000	1.85649000
N	-0.76966800	2.12326200	0.88705900	C	-2.41738400	-3.19112800	3.37164100
N	1.16739400	-2.21721600	-1.03998900	H	-2.61938100	-2.11129100	3.35961500
N	-0.85367500	-2.77359100	-0.55519100	H	-1.65593400	-3.37774600	4.14389600
C	-0.67078700	2.65647100	2.09376900	H	-3.33554300	-3.72068300	3.67471200
H	-0.40794500	1.97479300	2.90404800	C	-1.67954300	-5.19185000	2.00605000
C	-0.90824300	4.02978200	2.31688700	H	-2.63135900	-5.72999500	2.14771900
H	-0.80061200	4.42997100	3.32621600	H	-0.99959100	-5.48284100	2.82240700
C	-1.28550800	4.83280100	1.26228800	H	-1.23548600	-5.53773900	1.06049200
H	-1.48534400	5.89673600	1.41291100	C	2.40798800	-1.57230700	-1.40864700
C	-1.43239400	4.27972100	-0.03761600	C	2.44952400	-0.84443000	-2.61396700
C	-1.85108700	5.01087000	-1.17614700	C	3.69779800	-0.37192200	-3.03356500
H	-2.07954100	6.07374500	-1.07856100	H	3.76932300	0.21525100	-3.94907000
C	-1.96080100	4.36056800	-2.39568500	C	4.85059700	-0.62284200	-2.29122100
H	-2.28076600	4.92565500	-3.27556900	H	5.81087700	-0.22892800	-2.62967300
C	-1.67053900	2.99105800	-2.54572400	C	4.77253900	-1.32536800	-1.09272500
H	-1.75946800	2.50350300	-3.51784300	H	5.67549500	-1.47862900	-0.50073000
C	-1.25916000	2.21803500	-1.44985900	C	3.54643800	-1.81088000	-0.61780100
C	-1.14506600	2.88950100	-0.17820800	C	3.46128800	-2.55023900	0.71244600
C	0.01718900	-1.71147200	-0.48671700	H	2.41316100	-2.50907200	1.04816800
C	-0.25673300	-3.89817400	-1.11508400	C	4.30957300	-1.89052300	1.80716500
H	-0.80705200	-4.82164800	-1.25679200	H	5.38614600	-1.94940600	1.58201100
C	1.01051200	-3.54630600	-1.42045900	H	4.14339200	-2.39738100	2.76799100
H	1.81875500	-4.09430700	-1.89071800	H	4.04369200	-0.83530500	1.94976700
C	-2.27728800	-2.79033500	-0.35886500	C	3.85933100	-4.02824800	0.55937400
C	-2.80211100	-3.25972700	0.86024400	H	3.22161000	-4.55838100	-0.16209700
C	-4.19695000	-3.37492300	0.96283000	H	3.77840600	-4.55112000	1.52579400
H	-4.63529500	-3.72582000	1.89785300	H	4.90213700	-4.11508200	0.21287700
C	-5.02641400	-3.04043900	-0.10407900	C	1.19028000	-0.57610300	-3.42566300
H	-6.11012600	-3.13326600	-0.00173600	H	0.34889300	-0.52586700	-2.72372900
C	-4.47865800	-2.57957900	-1.30301200	C	1.20663800	0.77946000	-4.13736800
H	-5.13811400	-2.32134200	-2.13356900	H	1.43340500	1.59092000	-3.43407000
C	-3.09186500	-2.45204200	-1.46121500	H	0.21484800	0.97936500	-4.57058500
C	-2.51196100	-1.99862200	-2.79300000	H	1.93977200	0.81336400	-4.95960600
H	-1.44610700	-1.78993700	-2.64525700	C	0.92458000	-1.71010800	-4.42996900
C	-2.62869300	-3.12215500	-3.83553900	H	-0.00030500	-1.51350700	-4.99575900
H	-2.12776400	-4.04085500	-3.49408500	H	0.81045400	-2.68391100	-3.93212200
H	-2.16283400	-2.81633000	-4.78509500	H	1.75268400	-1.79477100	-5.15258900
H	-3.68356000	-3.36903600	-4.03796400	S	0.02897300	-0.74158600	2.46548500
C	-3.14221600	-0.69410700	-3.29529900	C	1.50478900	-0.19144000	3.28433400
H	-4.21979800	-0.80312000	-3.49731500	C	2.16456500	1.03131900	3.05536300
H	-2.65819200	-0.38375700	-4.23443900	C	2.00916900	-1.03380500	4.29793300
H	-2.97963900	0.11042000	-2.56685100	C	3.29626900	1.38108100	3.79680300

H	1.80813200	1.70713000	2.28137600	C	6.06846800	2.86649600	-1.14344300
C	3.12540100	-0.66903000	5.04872800	H	5.37365800	3.93263800	-2.89330400
H	1.51191700	-1.98906000	4.48207500	H	6.43491300	1.75054700	0.67481600
C	3.78626500	0.53846900	4.79773900	H	7.11785700	3.13177200	-1.29386800
H	3.79699900	2.32887600	3.58246400	S	-3.01606600	-0.08290300	1.03110700
H	3.49271500	-1.34310700	5.82739900	C	-3.78071400	1.52747300	0.93094800
H	4.67068100	0.81776700	5.37483900	C	-3.87610900	2.29181000	2.09862000
C	1.51103700	0.69668100	0.05153100	C	-4.25608800	2.03938700	-0.28533100
C	1.94409400	1.76613200	-0.63523400	C	-4.43245800	3.57240300	2.04485700
H	2.23196400	0.08239200	0.58951800	H	-3.51203800	1.88460800	3.04364600
H	1.24477500	2.37437100	-1.21332800	C	-4.82100700	3.31314200	-0.32633700
C	3.35379800	2.16667900	-0.75812600	H	-4.16367900	1.45186100	-1.19902200
C	3.75152200	2.97605300	-1.83997700	C	-4.90664100	4.08533900	0.83640000
C	4.34772400	1.74987200	0.14893900	H	-4.49416400	4.17004000	2.95722900
C	5.09076500	3.31446300	-2.03707800	H	-5.17564400	3.71164100	-1.27883500
H	2.99332300	3.32530700	-2.54597200	H	-5.33748900	5.08818100	0.79681400
C	5.68412900	2.09197300	-0.04288800	H	-3.67141900	-0.60092300	-0.02721900
H	4.06671700	1.14972200	1.01303800				

Complex E-TS

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G= -2683,951841 a.u.



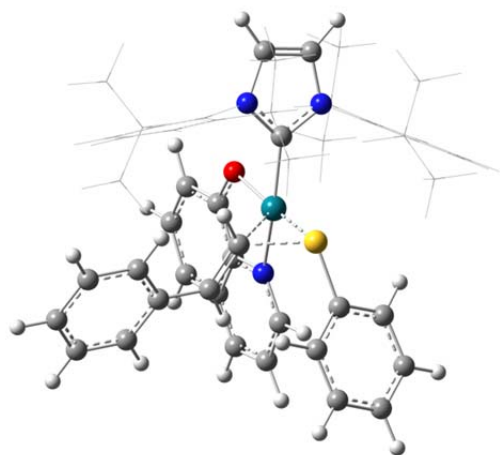
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N	2.70109500	0.85985500	-0.68611600	H	6.28071100	0.25368100	0.38549100
N	1.89119800	-0.92325500	-1.58978800	H	6.23584000	-1.27132700	1.30776300
C	1.60921900	0.03419700	-0.64692400	C	1.11707900	-2.11670300	-1.82121400
C	3.09539700	-0.66320800	-2.23538700	C	1.38315400	-3.24929400	-1.01916600
H	3.46755800	-1.29927400	-3.03144300	C	0.66749400	-4.42025500	-1.29445700
C	3.60605200	0.45693600	-1.66619000	H	0.83813500	-5.30930800	-0.68717100
H	4.52890400	0.99960700	-1.84358200	C	-0.27324400	-4.46374900	-2.32235900
C	3.07875100	1.80668500	0.32915400	H	-0.82209800	-5.38814200	-2.51804400
C	3.92720700	1.33729700	1.35602200	C	-0.52614200	-3.32856000	-3.08814700
C	4.32207300	2.24857900	2.34256300	H	-1.27346300	-3.36866200	-3.88203800
H	4.97054100	1.91323600	3.15473100	C	0.16260200	-2.12903800	-2.85514300
C	3.88698400	3.57290300	2.30854100	C	-0.11084600	-0.90225000	-3.70877600
H	4.19996300	4.26963000	3.09000500	H	0.24386200	-0.02347800	-3.15577600
C	3.05157300	4.00752300	1.28257500	C	0.65937500	-0.97956600	-5.03680200
H	2.71340300	5.04538100	1.26581500	H	0.34205300	-1.85274800	-5.63083500
C	2.62868400	3.13578200	0.26867000	H	0.47971900	-0.07465300	-5.63911500
C	1.72498600	3.63555300	-0.84217100	H	1.74459800	-1.06412100	-4.87198100
H	1.40853200	2.77355500	-1.43993500	C	-1.61023900	-0.68809400	-3.95060000
C	0.43980600	4.25514600	-0.27887200	H	-2.03780400	-1.45505100	-4.61696400
H	-0.07162700	3.53072700	0.36974200	H	-2.16708500	-0.70519100	-3.00299100
H	-0.24664300	4.51967700	-1.09659800	H	-1.78262300	0.29261200	-4.41710200
H	0.64097800	5.16799600	0.30564300	C	2.41111000	-3.21180000	0.10366700
C	2.47349600	4.60994900	-1.76380800	H	2.42208700	-2.18465200	0.49105400
H	1.82124000	4.93032500	-2.59213700	C	3.82248700	-3.53737300	-0.41411700
H	3.37027000	4.14090500	-2.19974900	H	3.86082700	-4.56095800	-0.82095200
H	2.79907000	5.51442400	-1.22328600	H	4.55729500	-3.46855800	0.40429900
C	4.39411300	-0.11095200	1.43568900	H	4.13964000	-2.84549000	-1.20622600
H	3.97042000	-0.65449000	0.58306600	C	2.05550900	-4.12499600	1.28242000
C	3.87936800	-0.80774400	2.70396200	H	1.02321200	-3.96577900	1.62252100
H	2.78098700	-0.79905500	2.74770200	H	2.72764300	-3.91739400	2.12902900
H	4.20838000	-1.85910700	2.71993800	H	2.17251100	-5.19038500	1.02680400
H	4.26163100	-0.32365200	3.61665600	C	-2.72435200	1.41520700	-1.21724300
C	5.92133600	-0.21538500	1.31463400	C	-3.42269900	-0.10500300	0.38878400

C	-1.61286900	1.97277100	-1.93925300	C	-3.07552900	-4.53773600	1.68253500
C	-4.06546000	1.80758400	-1.51457300	H	-3.11476300	-4.23147900	-0.46195400
C	-4.77718300	0.21024000	0.15459100	H	-2.79708700	-4.62281000	3.82768900
H	-3.16109300	-0.83269100	1.15033000	H	-3.78749000	-5.36621100	1.66171300
C	-1.88992100	2.93111500	-2.92594100	S	0.04210600	-1.17393100	1.76317700
C	-4.29386400	2.78546100	-2.51656800	C	-0.41733200	0.72500600	2.20233200
C	-5.09941400	1.16747200	-0.78170700	C	0.62215200	1.48652200	2.61355200
H	-5.54459000	-0.30311100	0.73547800	H	0.42565400	2.37031600	3.22529400
C	-3.21377700	3.32617600	-3.19614900	H	1.65525900	1.26194600	2.36742100
H	-1.05231000	3.35459300	-3.48351600	C	-1.79335600	1.05102000	2.65468800
H	-5.31698200	3.09254500	-2.74225600	C	-2.50307000	0.24126400	3.55189300
H	-6.14034000	1.43999400	-0.97490900	C	-2.38674400	2.24660600	2.21282700
H	-3.38956200	4.07771700	-3.97096700	C	-3.78704200	0.59895000	3.97201800
O	-0.41272800	1.55405100	-1.66247700	H	-2.04705200	-0.67417800	3.92362700
N	-2.42468000	0.47785300	-0.26050300	C	-3.66413800	2.60774300	2.63675100
C	-1.25655700	-2.40625600	1.73652600	H	-1.84434100	2.87175300	1.50300700
C	-1.79681900	-2.84111200	0.51561200	C	-4.37534800	1.77902700	3.51112800
C	-1.60954800	-3.06363500	2.92563400	H	-4.32739200	-0.04836400	4.66737200
C	-2.70398700	-3.89979700	0.49434700	H	-4.11399600	3.53265300	2.26833100
H	-1.49637300	-2.33891800	-0.40427200	H	-5.38259800	2.05423100	3.83314200
C	-2.52187100	-4.12021200	2.89723200				
H	-1.15623200	-2.75194800	3.86906900				

Complex E'-TS

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G= -2683,969615 a.u.



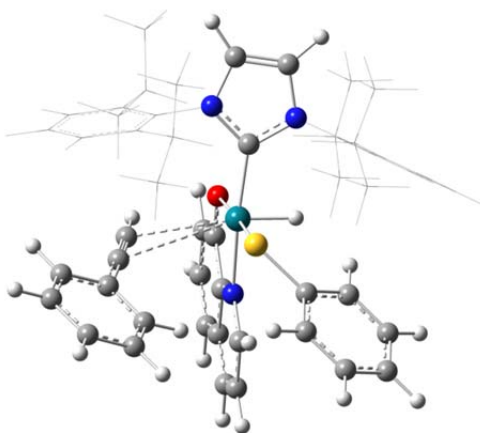
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N	-0.35689100	-2.29099600	-1.33893200	C	0.11520500	-4.22948100	0.74074200
N	-2.29722500	-1.42399400	-0.96294600	H	-0.77415600	-3.61083100	0.56649100
C	-0.96363600	-1.23366000	-0.72306200	C	0.48246300	-4.06645600	2.22273400
C	-2.51278600	-2.54809500	-1.75191000	H	0.72908400	-3.02118500	2.45810000
H	-3.50717600	-2.84639100	-2.06645200	H	-0.36726300	-4.36261700	2.85872100
C	-1.29295400	-3.09424500	-1.98809700	H	1.34180900	-4.69633700	2.50198300
H	-0.99354400	-3.97728600	-2.54288800	C	-0.27182100	-5.67986100	0.41536000
C	1.00249400	-2.73604700	-1.15677800	H	0.57311000	-6.36615000	0.58657200
C	1.22290000	-3.72945500	-0.17734300	H	-0.58202100	-5.78645300	-0.63530100
C	2.51483600	-4.25830700	-0.06480300	H	-1.10872100	-6.00899700	1.05205300
H	2.71535800	-5.03157600	0.67956700	C	-3.34612200	-0.63414500	-0.36919800
C	3.54634000	-3.80575200	-0.88615900	C	-3.78805200	-0.98451200	0.92611700
H	4.54936700	-4.22632500	-0.78409800	C	-4.80914400	-0.21145600	1.49047500
C	3.30918500	-2.79432000	-1.81257300	H	-5.17185000	-0.44815100	2.49127900
H	4.13297300	-2.41842700	-2.42125200	C	-5.37021300	0.85853500	0.79240200
C	2.03338400	-2.23365000	-1.97015000	H	-6.16687700	1.44907600	1.25157200
C	1.81261700	-1.11965700	-2.97604100	C	-4.91795700	1.17718000	-0.48509400
H	0.78161100	-0.76194600	-2.87499300	H	-5.36165800	2.01815600	-1.01985500
C	2.71856100	0.08146400	-2.66626800	C	-3.89230600	0.44008000	-1.09473400
H	2.55299500	0.43848100	-1.64037100	C	-3.41805700	0.78518800	-2.49659600
H	2.49501600	0.91072300	-3.35357100	H	-2.41287200	0.36424500	-2.62272500
H	3.78611800	-0.17014200	-2.77105700	C	-4.34359100	0.15613200	-3.55091800
C	2.00145500	-1.62309200	-4.41449800	H	-5.37120300	0.54537000	-3.46007500
H	1.79333200	-0.81316400	-5.13179900	H	-3.98226100	0.38352500	-4.56667800
H	1.32151700	-2.46048100	-4.64031700	H	-4.39179100	-0.93892700	-3.44796400

C	-3.28344500	2.29738100	-2.71165900	N	0.17496700	2.62770200	0.02720300
H	-4.26307400	2.80169500	-2.74309900	C	-0.15361200	0.96697500	3.33439600
H	-2.68323300	2.75831900	-1.91445600	C	-1.28791100	1.75925300	3.56712600
H	-2.77489600	2.49973200	-3.66552100	C	0.99795100	1.13462000	4.11461200
C	-3.20217700	-2.17176200	1.67805200	C	-1.26540100	2.72302300	4.57713100
H	-2.15734100	-2.27285400	1.35654300	H	-2.17077700	1.62572500	2.93774500
C	-3.93281700	-3.47578200	1.31427000	C	1.01569700	2.11122900	5.11393500
H	-4.99094200	-3.42732200	1.61848600	H	1.87495900	0.51482900	3.92382600
H	-3.46870200	-4.33307500	1.82840100	C	-0.11161300	2.90562100	5.34718800
H	-3.90041000	-3.67625500	0.23440600	H	-2.14904700	3.34005900	4.75663100
C	-3.17752200	-1.98060100	3.19789800	H	1.91628600	2.24868500	5.71732300
H	-2.71070800	-1.02528600	3.47623800	H	-0.09205400	3.66547000	6.13200100
H	-2.59358900	-2.78839100	3.66537500	S	-0.24866300	-0.31380300	2.10084600
H	-4.18859100	-2.01356500	3.63448600	C	2.42824500	0.69533900	1.23327300
C	0.33379400	3.14816800	-1.23182900	C	1.39371400	-0.18088200	1.01970800
C	0.34512600	3.42276900	1.07441400	H	2.21380500	1.73183800	1.49108600
C	0.08404100	2.25739000	-2.33173100	H	1.64354700	-1.21456800	0.77863100
C	0.70885700	4.50900300	-1.45644300	C	3.83484500	0.37045000	1.06322600
C	0.71096600	4.78030600	0.94789300	C	4.78626800	1.41549600	0.99603300
H	0.20469500	2.98132900	2.05794500	C	4.31990600	-0.95225100	0.94082800
C	0.24467800	2.76273600	-3.62924100	C	6.14066300	1.15491800	0.79817500
C	0.86004300	4.97245700	-2.78778400	H	4.43905800	2.44853400	1.08781300
C	0.90098600	5.31918100	-0.30632600	C	5.67285100	-1.20889700	0.73731800
H	0.84104200	5.37770700	1.85184100	H	3.62562500	-1.78945100	1.01020100
C	0.63032600	4.10012200	-3.84001400	C	6.59801900	-0.16058600	0.66152000
H	0.05853200	2.09252500	-4.47055800	H	6.84792100	1.98721600	0.74518000
H	1.15412100	6.00877300	-2.96479000	H	6.01196900	-2.24433500	0.64255700
H	1.19164800	6.36557000	-0.43131600	H	7.65942100	-0.36627300	0.50455400
H	0.74742700	4.45656700	-4.86710000				
O	-0.29194200	1.03432300	-2.08001000				

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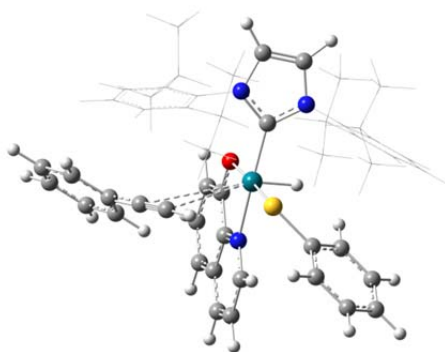
Rh	0.16539300	0.20379900	-0.51457400	C	2.33214300	-2.79335900	3.26134500
N	1.39459200	1.17208500	2.05718100	H	2.16761500	-3.12063200	2.22766700
N	-0.71388300	1.61559200	2.02166000	H	1.56189600	-3.26132700	3.89403700
C	0.26603700	0.99706600	1.30437600	H	3.30824000	-3.17754200	3.59918500
C	-0.20723900	2.18164600	3.18774000	C	2.59334600	-0.83286800	4.82137200
H	-0.84135700	2.71561500	3.88672100	H	1.93680600	-1.33978000	5.54677100
C	1.12159100	1.90845200	3.20453200	H	2.48121700	0.25094300	4.96703800
H	1.89892500	2.16864900	3.91406900	H	3.63551300	-1.09592900	5.06551600
C	2.69975300	0.65239200	1.74585200	C	3.02059800	2.64155000	0.16785100
C	3.49724500	1.35013700	0.81594300	H	1.92411100	2.64240400	0.18148100
C	4.76127100	0.82037300	0.52621000	C	3.42225800	2.75181500	-1.30637900
H	5.40389700	1.33046100	-0.19262000	H	3.11745200	1.85617800	-1.86686200
C	5.20620000	-0.35043600	1.13896800	H	2.92073500	3.61447000	-1.76888700
H	6.19301700	-0.75105100	0.89474700	H	4.50814300	2.88938900	-1.43499300
C	4.39385900	-1.01972000	2.05160200	C	3.50390400	3.85649300	0.97646100
H	4.74706800	-1.94485300	2.50808200	H	4.60505500	3.90635700	0.99712700
C	3.11878400	-0.53687100	2.37480400	H	3.15081500	3.81228100	2.01856400
C	2.24688300	-1.26746300	3.38639400	H	3.12812700	4.79175500	0.53112300
H	1.20456400	-0.98792000	3.17821200	C	-2.11139300	1.61107700	1.68497800

C	-2.64131300	2.70301600	0.97152400	H	0.53145800	-2.76909200	-4.88008900
C	-4.01596100	2.68626000	0.70262800	C	0.48452700	3.06946900	-4.92409900
H	-4.46598700	3.51221200	0.15014600	H	0.29672000	4.16169300	-3.04781800
C	-4.81466300	1.62358300	1.12132900	H	0.65468300	1.76844100	-6.64507700
H	-5.88426100	1.62858900	0.89688600	H	0.65198400	-0.78319000	-6.40720200
C	-4.25742700	0.54982200	1.81346700	H	0.53136900	3.98478300	-5.52049800
H	-4.89227100	-0.28022000	2.12468900	O	0.14259700	2.09304000	-1.41492600
C	-2.88972300	0.51701800	2.11182100	N	0.30531700	-0.34653600	-2.56201300
C	-2.28740500	-0.62524400	2.91902500	C	1.33975300	-2.95210200	-0.22150800
H	-1.21619500	-0.67589600	2.67882100	C	2.59388100	-2.48216000	-0.65899200
C	-2.41756400	-0.33978500	4.42553900	C	1.08711600	-4.33803300	-0.29388800
H	-3.47799500	-0.28863600	4.72226700	C	3.55158000	-3.36641200	-1.15511700
H	-1.93761500	-1.13972000	5.01185300	H	2.81543200	-1.41722400	-0.60357200
H	-1.94450900	0.61312200	4.70486400	C	2.05395100	-5.21805500	-0.78324900
C	-2.87443700	-1.99726800	2.57361100	H	0.11789500	-4.71515400	0.04171900
H	-3.93416400	-2.08088400	2.86304400	C	3.29282100	-4.73948000	-1.22185200
H	-2.78733200	-2.21153100	1.50185300	H	4.51655000	-2.97331500	-1.48626900
H	-2.32131900	-2.78026400	3.11425700	H	1.83332400	-6.28813200	-0.82805800
C	-1.76430800	3.87148800	0.54322800	H	4.04699900	-5.42791800	-1.60997300
H	-0.73678200	3.49493500	0.45303900	S	0.08231200	-1.91782000	0.47478700
C	-1.78732500	4.98260800	1.60729800	H	1.66050400	0.18348100	-0.43718500
H	-2.80559300	5.38705700	1.72856500	C	-2.49972500	0.55638300	-1.49888700
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H	-1.45436000	4.61645700	2.58917000	C	-2.94339200	-0.55652500	-1.29483500
C	-2.13882400	4.44144600	-0.82888900	C	-3.49344400	-1.85080300	-1.04583200
H	-2.14200900	3.66534800	-1.60590500	C	-2.72076400	-3.01226800	-1.23751600
H	-1.39939300	5.19928100	-1.12986100	C	-4.81891700	-1.97538000	-0.58322400
H	-3.12533700	4.93203300	-0.82128900	C	-3.26011400	-4.26595500	-0.95326600
C	0.36565300	0.76019300	-3.36602200	H	-1.69361800	-2.91424900	-1.57941100
C	0.36379900	-1.55447000	-3.09680500	C	-5.35136500	-3.23278300	-0.30591300
C	0.28652200	2.04258700	-2.71195000	H	-5.41410100	-1.07342300	-0.43707900
C	0.49487600	0.65545700	-4.78455800	C	-4.57179400	-4.38109900	-0.48353800
C	0.48633600	-1.75094800	-4.49040700	H	-2.64743500	-5.15930400	-1.09532600
H	0.32982200	-2.39911100	-2.40928000	H	-6.37886400	-3.31908200	0.05548300
C	0.35250200	3.18250500	-3.52650000	H	-4.98867600	-5.36563700	-0.25825400
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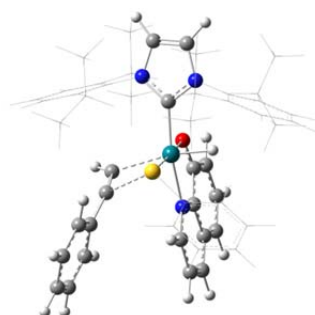
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N	-0.06588600	2.51323300	0.69500800	C	-4.26206800	1.79818000	-0.03348000
C	-0.74034000	1.33123600	0.66805100	H	-3.26660100	2.12083600	-0.36971100
C	-0.68603800	3.42801700	1.54143800	C	-5.02148700	1.32667200	-1.27920000
H	-0.28821300	4.42518500	1.69505600	H	-4.57072600	0.42207300	-1.70507500
C	-1.78128100	2.80635000	2.04766900	H	-4.99784700	2.11417700	-2.04856200
H	-2.53709600	3.14140200	2.74920400	H	-6.08106500	1.11929200	-1.05849300
C	-2.86161600	0.57934700	1.73500400	C	-4.97576100	3.00488000	0.60072500
C	-2.64530400	-0.43570500	2.68856900	H	-5.09191900	3.81537000	-0.13670500
C	-3.68356900	-1.35267900	2.89891700	H	-4.42339000	3.40960000	1.46073900
H	-3.55062900	-2.15469900	3.62631000	H	-5.98049300	2.71997200	0.95319400
C	-4.87944100	-1.25770800	2.18846000	C	-1.34750300	-0.52459400	3.47726100
H	-5.67475500	-1.98648400	2.36241200	H	-0.56395000	-0.02198200	2.89752600
C	-5.06042900	-0.24798500	1.24555400	C	-0.86779800	-1.96677000	3.67095100

H	-0.82009000	-2.49966600	2.71016000	H	-0.53674000	-2.60189000	-2.45106400
H	0.14518500	-1.97159800	4.09936600	C	2.65467200	-2.37595900	2.25470500
H	-1.52043800	-2.53675900	4.35198300	C	2.92659600	-4.49993000	1.06998600
C	-1.48544100	0.20922200	4.82104600	C	1.60537400	-4.84663900	-1.03778600
H	-2.26391900	-0.25527600	5.44849100	H	0.40116000	-4.90493800	-2.82755400
H	-1.75864400	1.26604600	4.67578100	C	3.23396600	-3.65198700	2.12409800
H	-0.53498000	0.17884300	5.37767000	H	2.92574800	-1.72140600	3.08417400
C	1.08191900	2.82919500	-0.11242100	H	3.38863200	-5.48492900	0.98126200
C	2.36511500	2.69717300	0.44951900	H	2.03333000	-5.84342400	-1.17342200
C	3.45202600	3.10621600	-0.33346900	H	3.95373500	-3.97843500	2.87984600
H	4.46186500	3.01999300	0.06806000	O	1.20031600	-0.71307600	1.35739500
C	3.26202300	3.60497000	-1.61997900	N	0.50458700	-2.30632700	-0.70172800
H	4.12385500	3.92077700	-2.21341600	C	-2.74669900	-1.36943200	-2.13430900
C	1.98176600	3.68863100	-2.16423500	C	-3.17785100	-2.16478200	-1.05554200
H	1.85265000	4.05972600	-3.18147400	C	-3.28647300	-1.63260400	-3.41028300
C	0.85924600	3.30254600	-1.42231900	C	-4.11076300	-3.18391200	-1.24969200
C	-0.54472600	3.43151700	-1.99746100	H	-2.78633900	-1.97560000	-0.05720600
H	-1.17707800	2.67829900	-1.50698200	C	-4.22441700	-2.64889300	-3.59602000
C	-1.14055600	4.81574600	-1.68831000	H	-2.95878400	-1.02629400	-4.25806300
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H	-2.17083700	4.88567200	-2.07289500	H	-4.42898200	-3.78193300	-0.39159100
H	-1.17182900	5.01543300	-0.60760000	H	-4.62746800	-2.83103000	-4.59598900
C	-0.61097300	3.14101800	-3.50049200	H	-5.37409200	-4.23373300	-2.66453600
H	-0.12604200	3.93125800	-4.09609500	S	-1.62672900	-0.00196800	-1.97617900
H	-0.13721500	2.18045600	-3.74591900	H	-1.30356100	-0.97931600	0.60064200
H	-1.66209600	3.08122700	-3.82031900	C	1.85531000	0.02977800	-2.44108200
C	2.57302100	2.17430700	1.86255400	H	0.87146900	0.13359100	-2.86633800
H	1.68209400	1.59293100	2.13327100	C	2.96384600	-0.13881400	-1.97125400
C	2.71615900	3.34034100	2.85506200	C	4.26832300	-0.33590300	-1.41813700
H	3.60200800	3.95224100	2.61779300	C	4.55606500	-1.48166800	-0.65152200
H	2.83117500	2.96123100	3.88330100	C	5.28356900	0.62054700	-1.62053700
H	1.83823700	4.00372700	2.83729300	C	5.81283200	-1.64466500	-0.07145500
C	3.76289100	1.21427000	1.96624800	H	3.78636600	-2.23491300	-0.50356400
H	3.66604600	0.38730400	1.25275800	C	6.53992900	0.44777700	-1.04317800
H	3.80519500	0.78311300	2.97847300	H	5.06710500	1.49951100	-2.22667200
H	4.72500300	1.71925300	1.78490600	C	6.80644700	-0.67975500	-0.25840300
C	1.39619500	-2.78422400	0.21976500	H	6.00850400	-2.53225500	0.53402600
C	0.17244000	-3.04186400	-1.74896800	H	7.31729700	1.19883400	-1.20368000
C	1.73445500	-1.90096300	1.30825000	H	7.78977800	-0.80766700	0.20049300
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C	0.70836100	-4.33401900	-1.94998800				

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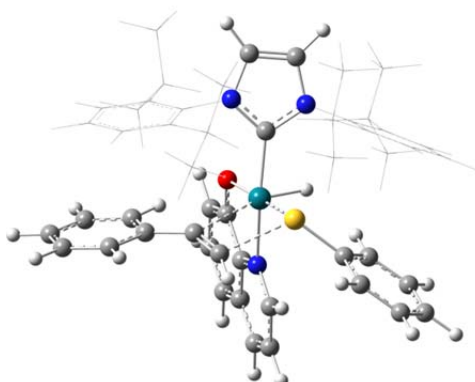
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N	2.07944000	-1.63803000	0.92222100	H	3.00489300	4.90940400	1.16795800
C	1.52537800	-0.39183900	0.81371500	C	2.73356300	2.77158100	1.29297500
C	3.19157800	-1.62465900	1.75596700	C	3.74205200	2.45367200	0.20021600
H	3.77857800	-2.51768200	1.93999400	H	3.49655200	1.45950900	-0.19442600
C	3.32441300	-0.35234600	2.20760000	C	3.65189000	3.42238900	-0.98321400
H	4.04287300	0.10028100	2.88205400	H	2.62782400	3.46623700	-1.37721200
C	2.03613700	1.75969900	1.97514500	H	4.30902500	3.07939700	-1.79704500
C	1.10223200	2.02660100	2.99865000	H	3.97441900	4.44096900	-0.71273400
C	0.89248600	3.36638600	3.34460000	C	5.16941500	2.42006700	0.77213200
H	0.17322900	3.61518600	4.12496900	H	5.89546000	2.15868600	-0.01455500
C	1.57783100	4.39161600	2.69299300	H	5.27003600	1.68063100	1.58064800

H	5.45266000	3.40334800	1.18264800	C	-0.70872800	1.63726500	-4.44745300
C	0.34612600	0.90400200	3.69673200	C	-2.90655000	1.04419400	-3.61096600
H	0.16145600	0.12441700	2.94410300	H	-2.91230600	0.27248700	-1.56802700
C	-1.02463500	1.33648000	4.22469500	C	2.05604000	1.81439000	-3.87787600
H	-1.59904500	1.86405600	3.45247000	C	0.18942400	2.12239800	-5.42993300
H	-1.59907600	0.44978600	4.53448800	C	-2.11378500	1.52190200	-4.63195400
H	-0.93831000	1.99434000	5.10463700	H	-3.98784700	0.95077000	-3.72453100
C	1.17675500	0.27911200	4.83112900	C	1.54186600	2.19575000	-5.13084500
H	1.38967600	1.02645400	5.61285800	H	3.12402100	1.88658900	-3.66802800
H	2.13510100	-0.11947900	4.47214800	H	-0.19323200	2.42919000	-6.40529400
H	0.62357100	-0.55265600	5.29674200	H	-2.55122400	1.81866800	-5.58898000
C	1.58815100	-2.82821300	0.28292800	H	2.23763400	2.56498800	-5.88954100
C	0.68692800	-3.64684800	0.99040300	O	1.62941800	0.99634900	-1.67911300
C	0.21845100	-4.79726900	0.34169100	N	-1.00484800	0.74231500	-2.19188000
H	-0.49106900	-5.45006100	0.85095600	C	-1.89846100	1.75270200	0.75126200
C	0.63428400	-5.11083800	-0.95110800	C	-0.70854100	2.07070500	0.40804000
H	0.25325500	-6.01092000	-1.43981700	S	-1.60992300	-0.53425300	0.92538000
C	1.52288600	-4.27642200	-1.62862400	C	-2.68291800	-1.65281800	0.05386000
H	1.82913500	-4.52602400	-2.64578700	C	-2.22560000	-2.41938400	-1.03067900
C	2.01390000	-3.11004100	-1.02936400	C	-4.00434600	-1.81899800	0.50678500
C	2.96821600	-2.18671600	-1.77156700	C	-3.07148700	-3.34901900	-1.63540800
H	2.92862300	-1.20410900	-1.28509700	H	-1.20380100	-2.27581500	-1.38628300
C	4.41095200	-2.70769200	-1.67498600	C	-4.84951700	-2.73777100	-0.11769100
H	4.50792600	-3.69869100	-2.14836200	H	-4.36417300	-1.22707200	1.34975100
H	5.10610500	-2.01910000	-2.18178000	C	-4.38709900	-3.50996000	-1.18846600
H	4.73466100	-2.80492600	-0.62680400	H	-2.69732000	-3.94786900	-2.46958400
C	2.54849000	-1.95477500	-3.22740300	H	-5.87630600	-2.85359300	0.23872400
H	2.66166900	-2.86145500	-3.84382000	H	-5.04988900	-4.23055800	-1.67338800
H	1.50181300	-1.62285400	-3.28173200	H	0.40506900	-1.18418300	-1.17301600
H	3.16885900	-1.16569300	-3.67800500	H	-0.23278300	3.04884500	0.32727300
C	0.25292500	-3.31727000	2.41271100	C	-3.30406300	2.02881300	0.92013400
H	0.32330300	-2.22643200	2.52956400	C	-3.93257700	2.88189400	-0.01127100
C	1.19584200	-3.96720600	3.44039400	C	-4.07137400	1.49700800	1.97570400
H	1.16494200	-5.06562000	3.35464700	C	-5.28380000	3.20390600	0.12217700
H	0.89483300	-3.69670900	4.46546700	H	-3.34403700	3.27993800	-0.83975300
H	2.23864100	-3.64901400	3.30261700	C	-5.41931900	1.82172000	2.10333100
C	-1.19994100	-3.70813500	2.70746800	H	-3.59319100	0.81912400	2.68315800
H	-1.88543500	-3.32871900	1.93903900	C	-6.03178300	2.67605000	1.17801100
H	-1.50930600	-3.28871200	3.67756200	H	-5.75697500	3.86489400	-0.60811000
H	-1.32376900	-4.80125800	2.77155000	H	-6.00085800	1.40428700	2.92897700
C	-0.19422700	1.23501300	-3.17654400	H	-7.09132600	2.92322000	1.27787300
C	-2.30949700	0.65694000	-2.38953400				
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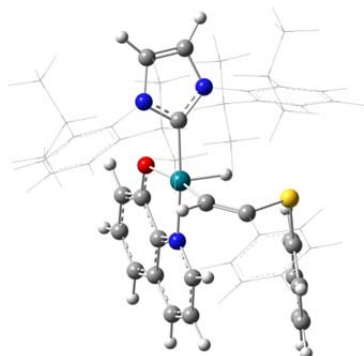
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N	-0.85423700	-2.21990700	0.91960700	C	-2.29518900	-2.67095400	-1.00590800
N	1.20460400	-1.85068100	1.43943000	C	-3.58629900	-2.70132800	-1.54297600
C	0.16124600	-1.33282600	0.71770700	H	-3.73740100	-3.05366200	-2.56288300
C	0.82844300	-3.01167900	2.10439300	C	-4.68624600	-2.27218500	-0.80077800
H	1.51536700	-3.54951600	2.74796400	H	-5.68222800	-2.29093100	-1.24762300
C	-0.46474000	-3.24820900	1.77366700	C	-4.51627500	-1.78928100	0.49208900
H	-1.14359000	-4.04751200	2.04863200	H	-5.38275800	-1.43467500	1.05146100

C	-3.24459200	-1.72696200	1.07822600	H	3.70842400	-3.59015500	-2.29166200
C	-3.06970900	-1.22344300	2.50447400	H	5.13801500	-2.98143500	-1.43877600
H	-2.01217600	-0.95628500	2.63330200	C	-0.53595100	3.24194400	0.39628100
C	-3.87840300	0.04628700	2.79335600	C	0.61873500	3.17488300	-1.62530700
H	-3.62669100	0.84286600	2.08404100	C	-1.12858600	2.47154500	1.45844900
H	-3.64760400	0.41188100	3.80639700	C	-0.59714900	4.66822500	0.38559700
H	-4.96427000	-0.13534800	2.75179600	C	0.60051000	4.58469000	-1.72117700
C	-3.42658900	-2.32531200	3.51716600	H	1.08257100	2.56194000	-2.39786500
H	-3.26197700	-1.97312000	4.54832800	C	-1.75434600	3.18026400	2.49361500
H	-2.82169800	-3.23210200	3.37111900	C	-1.24307500	5.33603200	1.45638000
H	-4.48604200	-2.61463100	3.42262900	C	0.00402500	5.32411900	-0.72257400
C	-1.09176200	-3.16174100	-1.80233800	H	1.06504500	5.06452000	-2.58411900
H	-0.25191800	-2.49404900	-1.56389000	C	-1.80126700	4.58813000	2.48077300
C	-1.29383400	-3.09334500	-3.31881800	H	-2.20612800	2.61448500	3.30947500
H	-1.64891900	-2.10258000	-3.63119000	H	-1.29281800	6.42659400	1.45868100
H	-0.33632000	-3.28468300	-3.82713200	H	-0.01711700	6.41606800	-0.77106000
H	-2.01143400	-3.85178600	-3.67188000	H	-2.29878900	5.10137200	3.30830700
C	-0.68542500	-4.58943300	-1.39529100	O	-1.08585300	1.16620700	1.40265900
H	-1.50024000	-5.30058200	-1.60831900	N	0.07970900	2.53682000	-0.60144000
H	-0.44005400	-4.66447000	-0.32749800	C	-0.59387200	0.29633200	-2.95668700
H	0.20296200	-4.90935400	-1.96359500	C	-1.46801700	0.37190100	-2.04757800
C	2.52367100	-1.28682700	1.53505100	H	-0.19340800	0.36515000	-3.95613900
C	3.53537800	-1.78808600	0.69254700	C	-2.90313700	0.60880300	-1.94500000
C	4.80708000	-1.20954100	0.80108600	C	-3.48059900	1.11012400	-0.76792700
H	5.61211800	-1.55752500	0.15324200	C	-3.74691000	0.35302900	-3.04805900
C	5.05522000	-0.18673900	1.71400700	C	-4.84881200	1.37884600	-0.70257900
H	6.05274000	0.25489600	1.77506800	H	-2.84107000	1.26352400	0.09727000
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H	4.24478300	1.08235400	3.25415800	H	-3.31118700	-0.04788300	-3.96569900
C	2.74573200	-0.25672500	2.47130100	C	-5.67265100	1.12264400	-1.79980000
C	1.63920700	0.23789600	3.39233200	H	-5.27356500	1.77478600	0.22294300
H	0.67723200	-0.02975800	2.93761800	H	-5.75237700	0.39017400	-3.83652400
C	1.72595900	-0.46258500	4.75804700	H	-6.74532700	1.32429100	-1.74380400
H	2.67796300	-0.23058700	5.26316500	S	1.41304500	-0.37465800	-1.93404500
H	0.90332000	-0.13496100	5.41388400	C	2.85757500	0.63644100	-2.14576500
H	1.66049700	-1.55680300	4.65339400	C	3.38498700	1.43144700	-1.11460600
C	1.63108300	1.76305500	3.54362500	C	3.53023800	0.58837900	-3.38202800
H	2.50631500	2.13092900	4.10316600	C	4.56410200	2.14976900	-1.31446500
H	1.61475000	2.25548200	2.56056600	H	2.86588500	1.47338400	-0.15708700
H	0.72970100	2.08428800	4.08622500	C	4.70250300	1.31960400	-3.57769400
C	3.28532000	-2.94727800	-0.26348900	H	3.13079900	-0.03645800	-4.18467500
H	2.21398100	-2.94277200	-0.51067200	C	5.22708600	2.10387900	-2.54457100
C	3.61658100	-4.28992700	0.41271000	H	4.96538600	2.75349000	-0.49654100
H	4.68386100	-4.33387200	0.68412000	H	5.21173500	1.27374600	-4.54386400
H	3.40415600	-5.12823000	-0.27021000	H	6.14511800	2.67561300	-2.69895500
H	3.03237100	-4.44838400	1.32980300	H	1.30012900	0.72692900	0.76056700
C	4.05696700	-2.82330200	-1.58236800				
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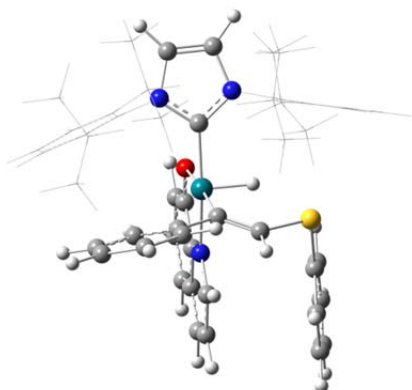
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N	-0.57818100	-1.81708100	2.00685400	H	-1.82444200	-4.66508500	0.95940100
C	-0.71430800	-1.57611600	0.67138600	C	-1.32352000	-2.97105200	-1.25250400
C	-1.02389800	-3.09684100	2.32878800	C	-0.16066100	-3.36239800	-1.95681000

C	-0.29015500	-3.58162700	-3.33293100	H	1.65242100	-3.85861800	4.19032500
H	0.58198400	-3.88191300	-3.91422800	C	3.38652000	-2.15988000	1.66514400
C	-1.51811100	-3.41342600	-3.97543400	H	3.09754100	-1.49506500	0.84105300
H	-1.59513600	-3.59046900	-5.05102000	H	3.83252300	-3.06711100	1.22677100
C	-2.64075900	-3.00818500	-3.25835200	H	4.16849000	-1.65461900	2.25298400
H	-3.58960000	-2.86471100	-3.77713700	C	-2.30961800	2.46315900	-1.00150200
C	-2.56794900	-2.76945600	-1.87778400	C	-0.18488800	2.74397800	-1.92664800
C	-3.79276600	-2.33158300	-1.09040200	C	-3.18849200	1.58762500	-0.26031600
H	-3.44005800	-1.82520000	-0.18276100	C	-2.74216800	3.74411600	-1.46244900
C	-4.64478500	-1.30590300	-1.84618000	C	-0.53024000	4.01981000	-2.41950500
H	-4.03349200	-0.46164000	-2.19403500	H	0.81253400	2.32947300	-2.07264500
H	-5.41773300	-0.89734800	-1.17832200	C	-4.49035300	2.05541000	-0.01858300
H	-5.15810600	-1.74937900	-2.71500500	C	-4.06633300	4.16582300	-1.18101300
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H	-5.50180100	-3.23471600	-0.07579700	H	0.21768800	4.59748900	-2.96272600
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H	-5.00783700	-4.09223200	-1.55922900	H	-5.17187500	1.40875100	0.53769000
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C	2.39251600	-3.31428500	-2.15085400	H	-5.92952700	3.64392200	-0.25616900
H	2.33216800	-2.35826500	-2.68792800	O	-2.74777900	0.43115200	0.13703400
H	3.30793100	-3.28701100	-1.54109800	N	-1.04371900	2.00074600	-1.24445000
H	2.51536100	-4.11997600	-2.89256400	C	2.32997300	0.44995700	-0.64198800
C	1.27372200	-4.93795500	-0.59224400	C	1.14285000	-0.06939900	-1.03968700
H	1.23612000	-5.73070500	-1.35689900	S	2.41841100	1.29293800	0.96088200
H	0.45952500	-5.11721300	0.12253400	C	2.10532300	2.98804800	0.48701400
H	2.22571500	-5.03614600	-0.04641800	C	1.08616200	3.68482800	1.15130700
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C	1.65223400	0.65023600	4.57895200	H	3.64791600	3.09479100	-1.02595200
H	2.24243200	1.29827300	5.23121100	C	1.54247000	5.65172100	-0.18698000
C	0.31773200	0.95827100	4.31778600	H	0.00518700	5.54257500	1.33143600
H	-0.12946900	1.84211500	4.77557100	H	3.14025700	5.45167500	-1.63321400
C	-0.46281100	0.15068100	3.48007500	H	1.31842100	6.68654100	-0.45624800
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H	-2.25270800	-0.06311000	2.33563500	H	1.18423700	-0.63581000	-1.98640900
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H	-2.50387100	0.41103100	5.36418900	C	4.85203200	0.31719500	-0.79732800
H	-3.84710700	0.09482500	4.23319900	C	3.55573900	0.22549300	-2.82687000
H	-2.62771200	-1.16577900	4.54965500	C	6.02308900	0.16166500	-1.54053600
C	-2.20071800	1.94339300	2.99834900	H	4.90354600	0.43479700	0.28593500
H	-1.98791400	2.56310100	3.88466500	C	4.72607700	0.07102700	-3.56965700
H	-1.59380300	2.31266000	2.15964300	H	2.59565600	0.28202800	-3.34344900
H	-3.25551300	2.09702400	2.72860800	C	5.96945700	0.03200400	-2.93109200
C	2.17120200	-2.52979400	2.52522600	H	6.98774400	0.14459600	-1.02657500
H	1.44691000	-3.00698100	1.85296100	H	4.66719100	-0.00548600	-4.65856800
C	2.53500200	-3.56535800	3.60042200	H	6.88705100	-0.08306400	-3.51287000
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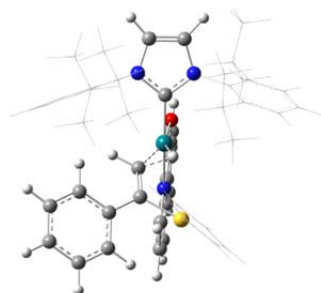


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N	-1.11124900	-1.83988600	1.55913300	C	-2.99205200	-4.12636400	-0.10601800
C	-1.20787400	-0.62108900	0.95291300	H	-2.87011900	-5.22027900	-0.05058500
C	-2.12654200	-2.02033200	2.49408600	H	-3.88291800	-3.91472100	-0.71877400
H	-2.19467100	-2.92177300	3.09386100	H	-3.18950100	-3.75559000	0.90872800
C	-2.90183100	-0.90770400	2.44876400	C	-1.58669600	-3.93389700	-2.18374800
H	-3.79857900	-0.63259900	2.99360000	H	-0.66589000	-3.54067200	-2.63624000
C	-3.03929300	1.06360300	0.93403300	H	-2.44042000	-3.57201600	-2.77780000
C	-4.06382500	0.79711500	-0.00203800	H	-1.57103900	-5.03231200	-2.27063800
C	-4.75510600	1.88890000	-0.53665400	C	2.57186900	2.03904000	0.66915900
H	-5.54358000	1.71764300	-1.27129400	C	2.36651800	1.88282400	-1.65071300
C	-4.44570800	3.19158800	-0.14890100	C	2.00515800	1.68614200	1.95029800
H	-4.99350000	4.03191500	-0.58204600	C	3.74842900	2.84258600	0.56777100
C	-3.44050300	3.42522500	0.78531500	C	3.51353400	2.68149200	-1.84021700
H	-3.21282100	4.44878400	1.08827100	H	1.81486500	1.47234500	-2.49616800
C	-2.71362300	2.36676300	1.35044600	C	2.67331800	2.16196100	3.09118500
C	-1.66554100	2.63672500	2.41594800	C	4.38419800	3.28755300	1.75426000
H	-1.06159400	1.73137100	2.54646000	C	4.20076900	3.15136300	-0.74237900
C	-0.68916400	3.74689000	2.00841500	H	3.84674400	2.89750500	-2.85552800
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H	0.12036000	3.82996200	2.74785000	H	2.25883500	1.90957600	4.06928200
H	-1.18140000	4.73018600	1.93473100	H	5.28590100	3.89906700	1.68484500
C	-2.34103200	2.94859600	3.76093300	H	5.09931800	3.76195900	-0.86484700
H	-1.58275400	3.10165600	4.54539000	H	4.32622300	3.28732100	3.89843600
H	-2.99648700	2.12231100	4.07906500	O	0.92239300	0.97089200	1.99295200
H	-2.95812500	3.86049400	3.70045500	N	1.91796300	1.57656500	-0.44229300
C	-4.46876300	-0.62391000	-0.37177500	C	0.47595400	-0.95774700	-2.61342800
H	-3.67601300	-1.30001200	-0.02944400	C	-0.18359300	-0.04141700	-1.86279100
C	-4.61127000	-0.84047600	-1.88128500	S	1.65755000	-2.12023500	-1.94047700
H	-3.69164500	-0.56021400	-2.40819900	C	3.20898400	-1.24228700	-2.13101100
H	-4.82510400	-1.90077000	-2.09045700	C	4.01467400	-1.05125800	-1.00071400
H	-5.43670900	-0.24881900	-2.30786400	C	3.64324100	-0.77188500	-3.37864700
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H	-6.60487700	-0.39177600	0.03706700	H	3.66530300	-1.40390600	-0.02950300
H	-5.66241900	-0.91027000	1.45140700	C	4.86607500	-0.10759700	-3.48767900
H	-6.01808700	-2.07173900	0.14878000	H	3.01858000	-0.92724000	-4.26058700
C	-0.17583700	-2.87394200	1.20512600	C	5.66933900	0.08291200	-2.35836500
C	-0.50065200	-3.71666300	0.11998200	H	5.85300300	-0.23240500	-0.22566800
C	0.37820100	-4.76793500	-0.16125100	H	5.19684300	0.25936600	-4.46286400
H	0.16673700	-5.43874000	-0.99405400	H	6.62369900	0.60737300	-2.44594700
C	1.54290400	-4.94907200	0.58390800	H	1.03918800	-0.89793400	-0.00879000
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C	1.00595800	-3.01066700	1.95133700	C	-2.21822700	3.06226800	-2.65816300
C	1.35401800	-2.05608800	3.08153300	H	-0.80288500	2.48903000	-1.14610100
H	0.70300000	-1.17699300	2.99630400	C	-2.74542200	1.38841000	-4.31362700
C	1.10412300	-2.71200500	4.44841600	H	-1.76196000	-0.51489900	-4.08658600
H	1.74321100	-3.59943600	4.58937200	C	-2.92218600	2.67773200	-3.80204400
H	1.32271000	-2.00356600	5.26353900	H	-2.35117900	4.06181800	-2.23994400
H	0.05683500	-3.03653900	4.55418200	H	-3.30139600	1.07091100	-5.19968500
C	2.78863200	-1.52855500	2.96457700	H	-3.60972000	3.37457300	-4.28748400
H	3.53941000	-2.32538100	3.09050800	H	0.31978100	-1.04442200	-3.69419900
H	2.94418600	-1.05084500	1.98769100				
H	2.97678900	-0.76458000	3.73299600				

Complex J-TS

E= -2684,78601775 a.u.

G= -2683,959038 a.u.

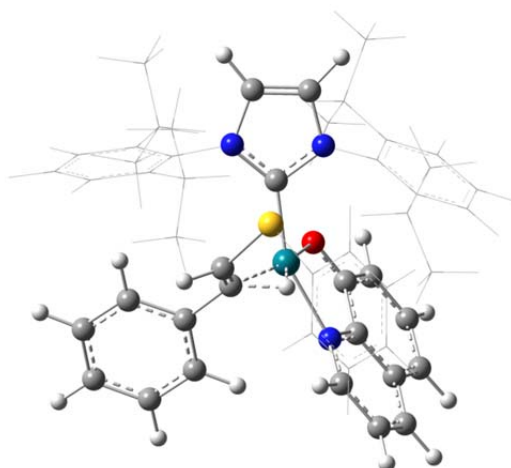


Rh	-0.85803000	0.40898400	0.36000400	C	0.60146900	-3.37553200	0.02736200
N	-0.98637900	-0.60229600	-2.49678400	H	0.67102000	-2.39549300	-0.46343700
N	-1.71142800	-2.06432800	-1.08951200	C	0.75522300	-4.44988800	-1.06294200
C	-1.09985700	-0.84609000	-1.15785700	H	0.69585800	-5.45972100	-0.62551000
C	-1.99615600	-2.55676400	-2.35992300	H	1.73200600	-4.35303300	-1.56387800
H	-2.48259200	-3.51484600	-2.50690300	H	-0.02752400	-4.36841100	-1.83128300
C	-1.54410900	-1.63426900	-3.24739000	C	1.75614200	-3.44568100	1.02973000
H	-1.55026500	-1.61308300	-4.33241600	H	1.63593200	-2.70033000	1.82837500
C	-0.21218300	0.46563200	-3.06208600	H	2.71023200	-3.23787200	0.52414500
C	1.08511300	0.15658300	-3.52135200	H	1.84428200	-4.44215800	1.49120100
C	1.84199700	1.19792300	-4.07467200	C	-2.45126200	2.20915900	2.02362800
H	2.85188400	0.99407800	-4.43654700	C	-0.24607300	2.40656200	2.73210300
C	1.33220600	2.49373600	-4.14535500	C	-3.36281000	1.57251300	1.10967700
H	1.94131700	3.29601300	-4.56845900	C	-2.90210100	3.19161000	2.95714400
C	0.05226200	2.77162500	-3.66749800	C	-0.60517900	3.37216900	3.69782300
H	-0.33305400	3.79123600	-3.72192200	H	0.79366200	2.10602600	2.61805000
C	-0.75270700	1.76383900	-3.11805100	C	-4.70487000	1.97391700	1.15545700
C	-2.16017000	2.07445500	-2.63528600	C	-4.27493900	3.54747800	2.97561700
H	-2.51506100	1.22519000	-2.03965200	C	-1.92189000	3.76302500	3.81023900
C	-2.19869700	3.29356400	-1.70545200	H	0.17218500	3.79768500	4.33461500
H	-1.49492600	3.16544800	-0.86981000	C	-5.14152300	2.94329500	2.07989800
H	-3.20550200	3.40946600	-1.27748600	H	-5.40503900	1.51482000	0.45615300
H	-1.94743000	4.22815700	-2.23285100	H	-4.62599900	4.29686300	3.68766200
C	-3.11166700	2.24003400	-3.83092000	H	-2.22432100	4.51463700	4.54423700
H	-4.13983300	2.42382800	-3.48056000	H	-6.19866500	3.22299700	2.08483300
H	-3.12319300	1.33646500	-4.46114100	O	-2.90492600	0.67366300	0.28095500
H	-2.81290800	3.08892600	-4.46805100	N	-1.13405400	1.83755700	1.93030500
C	1.68532800	-1.23881300	-3.39372200	C	2.27507400	0.97040100	0.79457400
H	0.91029100	-1.91035600	-3.00282400	C	1.10755900	0.87191800	0.10404100
C	2.83627900	-1.25982300	-2.37722900	S	2.39803200	0.15395600	2.39081800
H	2.49792200	-0.90195000	-1.39560700	C	3.87059400	-0.83965500	2.25097900
H	3.22014900	-2.28463100	-2.25165500	C	4.35896600	-1.40827200	3.43833700
H	3.67505900	-0.62158800	-2.69692600	C	4.51867100	-1.11307700	1.03844600
C	2.11995200	-1.80034500	-4.75434900	C	5.47180100	-2.24933600	3.40792500
H	2.93326400	-1.20494400	-5.19906400	H	3.86038500	-1.19129400	4.38646100
H	1.28279500	-1.80935300	-5.46985300	C	5.63925900	-1.94592200	1.02029800
H	2.48710900	-2.83301800	-4.64373000	H	4.14926500	-0.68070800	0.11104000
C	-1.89823500	-2.81308800	0.12552100	C	6.12026700	-2.52152700	2.19919900
C	-0.77216700	-3.45870800	0.68121200	H	5.83813600	-2.68974000	4.33865200
C	-0.97113400	-4.21351100	1.84262300	H	6.13741800	-2.14762700	0.06860400
H	-0.12451000	-4.72097100	2.30555400	H	6.99542300	-3.17471300	2.17772200
C	-2.23661300	-4.32524400	2.41863900	H	0.53816900	-0.30250500	0.62682800
H	-2.37010800	-4.92106400	3.32490700	H	1.08871000	1.37143800	-0.87173700
C	-3.32751900	-3.67373300	1.84976400	C	3.41354000	1.80989600	0.34119300
H	-4.30956000	-3.76036200	2.31698500	C	4.36479700	2.31338100	1.24772200
C	-3.18241500	-2.89494800	0.69278600	C	3.57549400	2.12737100	-1.02259700
C	-4.38096600	-2.19064800	0.07640400	C	5.42473800	3.10986500	0.81173000
H	-3.99439500	-1.37837700	-0.55329100	H	4.26447700	2.07498900	2.30722800
C	-5.19516500	-3.15821200	-0.79908800	C	4.63487400	2.92137700	-1.45674800
H	-5.59963100	-3.98772800	-0.19595200	H	2.86960700	1.74284300	-1.75629500
H	-6.04404200	-2.63547500	-1.26872700	C	5.56885100	3.41973200	-0.54250400
H	-4.58704900	-3.60002900	-1.60250800	H	6.14608200	3.48872600	1.54008900
C	-5.27810100	-1.53548200	1.13254200	H	4.73287700	3.14763300	-2.52183500
H	-5.79532400	-2.28201500	1.75673200	H	6.40227800	4.03841100	-0.88353500
H	-4.69835700	-0.87150600	1.78722100				
H	-6.05493600	-0.92933300	0.64160600				

Complex J'-TS

E= -2684,77960475 a.u.

G= -2683,950406 a.u.



Rh	0.45552600	0.09594800	-0.63239200	H	3.35624500	4.27832500	1.86498500
N	-1.70116600	1.13496400	1.40405400	H	2.15325200	3.75776000	0.64973300
N	0.22617000	0.58827200	2.22744700	H	1.75437200	5.04099100	1.83107600
C	-0.46147900	0.66882400	1.04166400	C	1.46270500	-2.05961000	2.10596000
C	-0.57621000	0.95210600	3.30056200	H	0.51547300	-1.79883000	1.62002600
H	-0.20502900	0.94610200	4.31982500	C	1.12491700	-2.59630500	3.50629000
C	-1.77868300	1.30682900	2.78915200	H	2.04094000	-2.84926700	4.06551200
H	-2.67249900	1.68395400	3.26944600	H	0.50790300	-3.50500900	3.43058500
C	-2.72787300	1.63351400	0.52590500	H	0.56555500	-1.85243100	4.09504200
C	-4.04536400	1.12966700	0.64459400	C	2.12626100	-3.13560300	1.24149200
C	-5.04284100	1.70222500	-0.15609700	H	2.40173900	-2.73136400	0.25630800
H	-6.06506800	1.32789400	-0.08018300	H	1.43273400	-3.97398300	1.08520400
C	-4.75448500	2.73490300	-1.04466200	H	3.03542900	-3.54533300	1.71061700
H	-5.54639000	3.16372300	-1.66334300	C	3.11926900	0.14581800	-1.79371700
C	-3.45430200	3.21853700	-1.13833100	C	2.10844300	-1.84464300	-2.45656100
H	-3.23197400	4.03162300	-1.83104800	C	2.97036500	1.37103000	-1.04913600
C	-2.41648400	2.69546400	-0.35427400	C	4.36259400	-0.21851800	-2.39896700
C	-1.04693600	3.35428300	-0.44784200	C	3.30186300	-2.29627200	-3.05821600
H	-0.32826100	2.77065800	0.13475800	H	1.21172500	-2.46768000	-2.46283700
C	-0.51240400	3.37070900	-1.88600300	C	4.08337600	2.22526800	-1.00414500
H	-0.49638600	2.35552300	-2.30636900	C	5.45690900	0.67606500	-2.30964500
H	0.51927700	3.75139800	-1.89455000	C	4.41668200	-1.48398600	-3.04104500
H	-1.12116100	4.01025800	-2.54537500	H	3.32135200	-3.27928900	-3.53181900
C	-1.08933200	4.76481200	0.16084800	C	5.29412900	1.87275600	-1.62840800
H	-0.08951600	5.22359400	0.12367000	H	3.99978300	3.16204900	-0.45477000
H	-1.41222400	4.73590200	1.21394700	H	6.40990500	0.40977600	-2.77075800
H	-1.78493900	5.42290300	-0.38493400	H	5.35111300	-1.80610000	-3.50798300
C	-4.44379100	0.03387300	1.62599200	H	6.13675200	2.56639500	-1.55848300
H	-3.52680300	-0.43407600	2.00790600	O	1.84070300	1.61641900	-0.44577700
C	-5.27983200	-1.07492800	0.96866300	N	2.01571900	-0.66071400	-1.86164800
H	-4.80431400	-1.45413600	0.05580400	C	-2.19405600	-1.70205600	-0.67039000
H	-5.39608100	-1.92094900	1.66273300	C	-1.27045700	-0.90087200	-1.26515400
H	-6.28848400	-0.71948600	0.70486700	S	-1.99512000	-2.40324900	0.94129500
C	-5.22039000	0.61611700	2.82101100	C	-1.37542000	-4.04146100	0.60390800
H	-6.17668300	1.05035300	2.48804900	C	-0.91353000	-4.44803700	-0.65523200
H	-4.66761900	1.41474100	3.33741000	C	-1.29755700	-4.92979100	1.68930600
H	-5.44553300	-0.17202400	3.55712100	C	-0.36373000	-5.72218300	-0.81716100
C	1.66273600	0.47344700	2.32734300	H	-0.98128000	-3.76459900	-1.50267500
C	2.28076100	-0.78526100	2.21573200	C	-0.73858700	-6.19618900	1.51914800
C	3.68055100	-0.82517000	2.25758100	H	-1.67090600	-4.62047500	2.66858700
H	4.19165100	-1.78353800	2.16143100	C	-0.26499800	-6.59928600	0.26584700
C	4.42955700	0.33931700	2.41483000	H	-0.00446700	-6.02829200	-1.80306800
H	5.52072400	0.28725300	2.43243900	H	-0.67517100	-6.87492700	2.37331800
C	3.79088700	1.57017400	2.54087600	H	0.17236600	-7.59136500	0.13479300
H	4.38718500	2.47683000	2.65795800	H	-0.15725400	-1.37826800	-0.74054300
C	2.39503500	1.66713600	2.49203400	C	-1.60724600	-0.31414600	-2.59221600
C	1.72556800	3.02787600	2.64442100	C	-0.73500500	-0.31404900	-3.69718200
H	0.66314700	2.91738000	2.39192700	C	-2.86721300	0.29514800	-2.74715700
C	1.80640000	3.50331300	4.10476500	C	-1.10970200	0.27406300	-4.90484700
H	2.85379700	3.65895600	4.41006700	H	0.24690500	-0.76992800	-3.61404000
H	1.27071700	4.45759700	4.23466600	C	-3.23501100	0.89330000	-3.95239200
H	1.36791200	2.76846900	4.79743000	H	-3.54911000	0.33101100	-1.89995300
C	2.28585500	4.08698500	1.68780900	C	-2.35890700	0.88798900	-5.03957200

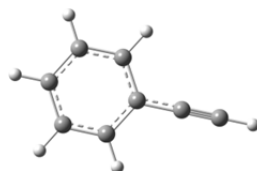
H	-0.41242400	0.25868900	-5.74605800
H	-4.21084000	1.37841000	-4.03153600

H	-2.64237100	1.36213800	-5.98219800
H	-3.13082800	-1.93309900	-1.18488300

Phenylacetylene

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G= -308,119925 a.u.



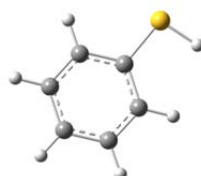
C	0.00000000	0.00000000	3.24038600
H	0.00000000	0.00000000	4.31380000
C	0.00000000	0.00000000	2.02644400
C	0.00000000	0.00000000	0.59481600
C	0.00000000	1.21445300	-0.12062300
C	0.00000000	-1.21445300	-0.12062300
C	0.00000000	1.20993700	-1.51475300

H	0.00000000	2.15634300	0.43090500
C	0.00000000	-1.20993700	-1.51475300
H	0.00000000	-2.15634300	0.43090500
C	0.00000000	0.00000000	-2.21583700
H	0.00000000	2.15740300	-2.05878900
H	0.00000000	-2.15740300	-2.05878900
H	0.00000000	0.00000000	-3.30837100

Thiophenol

E= -630,18978115 a.u.

G= -630,120946 a.u.



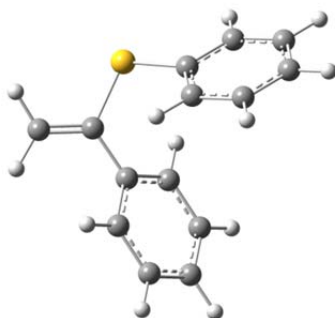
C	0.51289900	0.00085200	-0.00028400
C	-0.19460500	1.21276400	-0.00004400
C	-0.19842800	-1.21033900	-0.00022600
C	-1.59106300	1.20863400	-0.00000100
H	0.34520600	2.16269300	0.00022900
C	-1.59360100	-1.20349800	0.00009100
H	0.34352600	-2.15921000	-0.00062600

C	-2.29850200	0.00385700	0.00008700
H	-2.12836800	2.16026900	-0.00012400
H	-2.13376400	-2.15344500	0.00038200
H	-3.39056300	0.00540900	0.00034900
S	2.28951700	-0.08366300	0.00018600
H	2.51148900	1.24926600	-0.00093100

Phenyl(1-phenylvinyl)sulfane

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G= -938,226333 a.u.

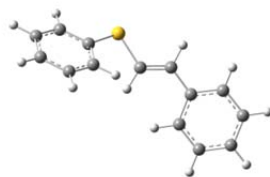


S	0.66580900	1.98530500	-0.59505100	H	-2.60473100	2.63824000	1.03777900
C	1.59323300	0.54827900	-0.08400300	H	-1.04331100	3.66258400	0.89677500
C	2.56163600	0.04196800	-0.96242900	C	-1.57072600	0.35148300	-0.06777600
C	1.40741700	-0.05362400	1.16843800	C	-1.34583500	-0.40674100	-1.22932400
C	3.34064300	-1.05448500	-0.58676700	C	-2.40741100	-0.17992600	0.92948300
H	2.69452100	0.50349100	-1.94374800	C	-1.95765100	-1.64847700	-1.39764800
C	2.17431800	-1.16311100	1.52666300	H	-0.68600900	-0.00894900	-2.00176200
H	0.66094400	0.34400900	1.85757900	C	-3.01831000	-1.42305800	0.76106400
C	3.14550700	-1.66536500	0.65500900	H	-2.55927800	0.38059100	1.85433200
H	4.09449600	-1.44187000	-1.27653700	C	-2.79687400	-2.16206800	-0.40444300
H	2.01585900	-1.63399000	2.49998300	H	-1.77522100	-2.22116800	-2.31010500
H	3.74651800	-2.53111400	0.94214600	H	-3.66041600	-1.82249300	1.54987000
C	-0.94464900	1.68416900	0.12070800	H	-3.26860400	-3.13903900	-0.53389300
C	-1.55925000	2.71509300	0.72909300				

(E)-phenyl(styryl)sulfane

E= -938,45605328 a.u.

G= -938,282962 a.u.

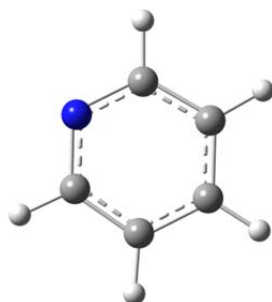


S	1.29303700	-1.61982600	-0.18507500	H	-1.36547000	-1.92740800	0.81585300
C	2.57710800	-0.39700400	-0.00924600	H	-0.03805000	0.30608800	-0.85977100
C	3.84873600	-0.70609700	-0.51748700	C	-2.61951300	-0.31943800	0.05577100
C	2.36932400	0.82681500	0.64488500	C	-3.72817800	-0.75898900	0.80509900
C	4.89933300	0.20009400	-0.36870900	C	-2.80037400	0.77901400	-0.80955700
H	4.00678900	-1.65363100	-1.03788700	C	-4.96463000	-0.11991600	0.70842600
C	3.42224600	1.73602700	0.76943500	H	-3.60942100	-1.61361500	1.47641500
H	1.38983900	1.06099800	1.06585900	C	-4.03372900	1.41944700	-0.90325000
C	4.68987500	1.42718100	0.26852500	H	-1.96930400	1.12806100	-1.42567600
H	5.88596500	-0.04970300	-0.76653800	C	-5.12313300	0.97505600	-0.14455400
H	3.25077700	2.68925100	1.27572300	H	-5.80883800	-0.47938000	1.30184300
H	5.51151800	2.13896800	0.37469700	H	-4.15101500	2.26850700	-1.58116200
C	-0.15055200	-0.62217200	-0.29105400	H	-6.09042000	1.47644100	-0.22462800
C	-1.33667200	-1.01124300	0.21613000				

Pyridine

E= -248,1224197 a.u.

G= -248,028443 a.u.



C	-1.22436800	-0.57713800	0.00000000	H	2.09356300	-1.32765300	0.00000000
C	-0.07473600	-1.37352100	0.00000000	H	-2.21662000	-1.04346700	0.00000000
C	1.17062500	-0.74234300	0.00000000	H	-0.15846800	-2.46246200	0.00000000
C	1.21054500	0.65325000	0.00000000	H	2.15981800	1.19333000	0.00000000
C	0.00000000	1.35356200	0.00000000	H	-0.00126700	2.44992800	0.00000000
N	-1.19563300	0.75820900	0.00000000				