

Pyridine versus Acetonitrile Coordination in Rhodium–N-Heterocyclic Carbene Square-Planar Complexes

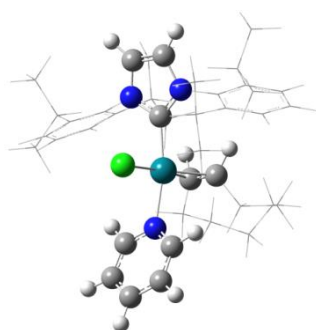
Laura Palacios, Andrea Di Giuseppe, Ricardo Castarlenas,* Fernando J. Lahoz, Jesús J. Pérez-Torrente, Luis A. Oro

Cartesian Coordinates and Energy Values for DFT Calculated Complexes

Complex **3at**

E= -2291.09544366 a.u.

G= -2290.302111 a.u.



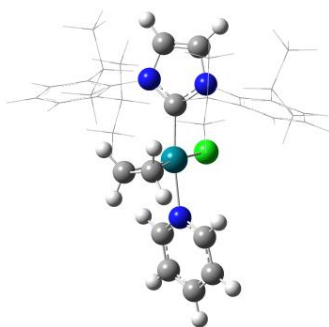
Rh	-0.30238400	0.90892200	-0.25902500	C	4.83281600	-0.40574300	-1.45786500
Cl	-1.44119100	0.97637300	-2.39506900	H	5.85674700	-0.03662200	-1.49827000
N	-0.88474200	2.98232600	-0.22059800	C	3.92755700	-0.04575700	-2.44676800
N	0.86494000	-1.74928600	-1.22231100	H	4.25142400	0.59690700	-3.26470600
N	-1.10972300	-1.98082500	-0.39166300	C	2.60585500	-0.49611100	-2.41838100
C	-2.11175000	3.25069700	0.25192500	C	1.65728100	-0.16704000	-3.54712000
H	-2.60522900	2.43160200	0.77683100	H	0.63016100	-0.35291100	-3.20465400
C	-2.73003300	4.47981900	0.07960900	C	1.71213500	1.29759300	-3.96364000
H	-3.72614500	4.64347100	0.48355200	H	1.52821200	1.95281300	-3.10172200
C	-2.05648100	5.47637700	-0.61711500	H	0.92456900	1.50058300	-4.70045800
H	-2.51348800	6.45239100	-0.77028300	H	2.67652300	1.56788300	-4.41929700
C	-0.79359100	5.19769600	-1.12388400	C	1.94355700	-1.08314000	-4.73768300
H	-0.23301000	5.93832900	-1.68893700	H	1.23055100	-0.88997400	-5.55028000
C	-0.24981300	3.93901500	-0.90901700	H	1.86257100	-2.14416500	-4.46207200
H	0.72708600	3.66905600	-1.30629200	H	2.95841400	-0.91923300	-5.13086200
C	1.43654800	1.12105400	0.93163900	C	2.74276500	-2.66701500	0.77402700
H	2.08552900	0.27380700	0.68841600	H	1.66408100	-2.86715400	0.70253100
C	0.34463400	0.87991600	1.79057000	C	2.99423900	-2.06990300	2.15666100
H	0.23061800	-0.14176500	2.16119000	H	2.43533900	-1.13463100	2.29864000
C	-0.23613800	1.89782800	2.73824400	H	2.67320100	-2.77700800	2.93576900
H	-0.31391400	2.88738200	2.26375500	H	4.05934000	-1.85450100	2.32487400
H	-1.27152100	1.59654800	2.97647700	C	3.45989800	-4.00888700	0.62743700
C	0.54449600	2.04292600	4.05020100	H	4.54746700	-3.89304300	0.73848700
H	-0.09043700	2.59042900	4.76452200	H	3.27516900	-4.46055000	-0.35650200
H	0.70580700	1.04344900	4.49254500	H	3.11858900	-4.71551200	1.39659700
C	1.89402500	2.76114100	3.96461500	C	-2.26709000	-1.81241500	0.44731100
C	3.03277100	1.97551100	3.29628700	C	-2.10894300	-2.00542100	1.83398100
C	3.37422600	2.37789600	1.86147900	C	-3.22633200	-1.81807000	2.64570700
H	4.12036300	1.66549000	1.46942800	H	-3.13552000	-1.95212100	3.72264400
H	3.86193600	3.36640300	1.86657900	C	-4.45803100	-1.47564500	2.10120700
C	2.18741000	2.41985900	0.89351600	H	-5.31881100	-1.33281500	2.75308200
H	1.52984000	3.26564200	1.14334300	C	-4.59665100	-1.34182800	0.72870200
H	2.57389200	2.60820000	-0.12219700	H	-5.57156400	-1.10423200	0.30478500
C	-0.10666000	-1.05563500	-0.54793300	C	-3.50829900	-1.51337800	-0.13108500
C	-0.78402800	-3.18642400	-1.00158400	C	-3.71529200	-1.46046800	-1.62809100
H	-1.47210000	-4.02226600	-1.00400200	H	-2.73909400	-1.29991800	-2.10537200
C	0.45309100	-3.04219200	-1.52132900	C	-4.29121300	-2.79247000	-2.11264400
H	1.09044400	-3.72553300	-2.06720700	H	-5.27558500	-2.98216600	-1.65859900
C	2.22986400	-1.31724300	-1.34757200	H	-4.41919800	-2.78315500	-3.20344800
C	3.13352000	-1.72922300	-0.35229100	H	-3.64160900	-3.64111200	-1.85570200
C	4.44263900	-1.25254500	-0.42874000	C	-4.61229100	-0.30588400	-2.06071800
H	5.16592000	-1.54528900	0.33287900	H	-5.65624400	-0.45268100	-1.74529400

H	-4.24642800	0.64737100	-1.65940000	C	-0.57585500	-1.99088900	3.86619600
H	-4.60702200	-0.22358800	-3.15526400	H	-0.79772300	-0.92141800	3.97665000
C	-0.80283400	-2.48270100	2.43895500	H	0.47149100	-2.15267000	4.15775800
H	0.01987000	-2.09766900	1.81772700	H	-1.19831000	-2.53910500	4.58783900
C	-0.72180400	-4.01074700	2.40891600	H	3.95057300	2.08464200	3.89310800
H	-1.53524300	-4.44961300	3.00504500	H	2.79096300	0.90141500	3.33003900
H	0.23317000	-4.35403000	2.83417400	H	1.75929000	3.73416400	3.46093200
H	-0.79760200	-4.40842000	1.38870800	H	2.19367400	3.00819900	4.99389000

Complex **3bt**

E= -2056.60914873 a.u.

G= -2055.959966 a.u.

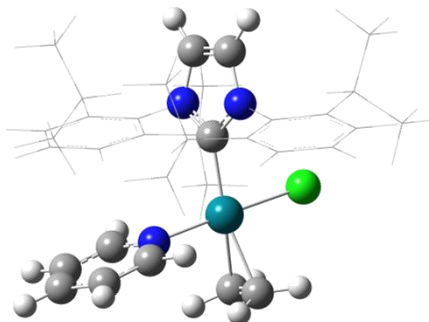


Rh	0.39057200	1.05871800	-0.46699500	C	1.74063000	-1.99964500	0.34605500
Cl	1.24337500	1.63209100	1.70537400	C	1.93834700	-2.54886500	-0.93490100
N	-1.59189800	-0.87403300	0.84403200	C	3.24324800	-2.86145200	-1.31185100
N	0.39224600	-1.69759900	0.74691600	H	3.43003900	-3.28588200	-2.29734700
C	-1.05127700	1.43186500	-1.95718500	C	4.30650600	-2.65618600	-0.44187700
H	-2.04218100	1.06848000	-1.67922300	H	5.31964100	-2.90747500	-0.75314500
C	-0.07719100	0.56714000	-2.48986700	C	4.07760000	-2.15425300	0.82979500
H	-0.31457800	-0.48544500	-2.64911000	H	4.91469500	-2.01952900	1.51338300
C	-0.34538800	-0.61225400	0.34281800	C	2.79073200	-1.81898600	1.25827200
C	-0.37590300	-2.58277600	1.49362400	C	2.56858300	-1.36299900	2.68409500
H	0.04482000	-3.49461000	1.89702800	H	1.59178300	-0.86160200	2.73423100
C	-1.61971900	-2.06570600	1.55734000	C	2.56112900	-2.57195300	3.62262500
H	-2.52691100	-2.41600700	2.03227600	H	3.53107400	-3.09055600	3.59777600
C	-2.79164100	-0.16903000	0.49863100	H	2.37741100	-2.25376300	4.65781900
C	-3.56226900	-0.67940900	-0.55915100	H	1.78973700	-3.30710100	3.35505900
C	-4.74004700	-0.00424100	-0.88183200	C	3.60976400	-0.35038600	3.15116200
H	-5.36565300	-0.37202200	-1.69528300	H	4.60387500	-0.80676700	3.26973800
C	-5.11791200	1.13809200	-0.18843300	H	3.68007000	0.49083800	2.45242600
H	-6.03627200	1.65746700	-0.45887600	H	3.31688600	0.05367400	4.12914700
C	-4.33175700	1.62010700	0.85047700	C	0.77955900	-2.89271400	-1.84770800
H	-4.64231800	2.51333500	1.39147300	H	-0.04746700	-2.20807200	-1.61593800
C	-3.15266300	0.97268300	1.22374000	C	0.28659700	-4.31402200	-1.56795700
C	-2.33901400	1.44835600	2.40534000	H	1.08494600	-5.04563400	-1.76127200
H	-1.31800900	1.05409900	2.30627000	H	-0.56653700	-4.56384700	-2.21609300
C	-2.21154400	2.96510700	2.47047600	H	-0.03798400	-4.43556200	-0.52571900
H	-1.85553200	3.37191500	1.51433400	C	1.10133300	-2.73212400	-3.32982400
H	-1.48048200	3.24061600	3.24099300	H	1.56798900	-1.76091800	-3.54153800
H	-3.16391100	3.45416500	2.72391200	H	0.17890000	-2.80432600	-3.92322900
C	-2.94268700	0.89656300	3.69726300	H	1.77807300	-3.52018000	-3.69001500
H	-2.34440500	1.20391600	4.56541500	H	-1.02932000	2.49849300	-2.20067500
H	-2.98305900	-0.20174200	3.68607300	H	0.69234000	0.95143600	-3.16663500
H	-3.96854700	1.26812700	3.84147600	N	1.38998700	2.83088800	-1.13341500
C	-3.15067800	-1.91081000	-1.34230800	C	2.52700800	2.73555800	-1.83519200
H	-2.12181400	-2.17348200	-1.05189700	C	0.98803200	4.04326900	-0.72798500
C	-3.14474000	-1.66734600	-2.85026200	C	3.29466000	3.84248300	-2.16935700
H	-2.54309000	-0.78918700	-3.11965600	H	2.82411200	1.72586700	-2.11771400
H	-2.72705600	-2.54048400	-3.37222300	C	1.69320900	5.20078800	-1.02371100
H	-4.16006100	-1.51177000	-3.24210500	H	0.07657500	4.06167800	-0.13213100
C	-4.04255500	-3.10383200	-0.99977700	C	2.86798000	5.09985400	-1.75897600
H	-5.08663800	-2.90809000	-1.28412100	H	4.21318300	3.71214300	-2.73624400
H	-4.02914300	-3.32979800	0.07453200	H	1.32557900	6.16111800	-0.67056300
H	-3.71068300	-4.00188200	-1.53930000	H	3.44687100	5.98845700	-2.00399500

Complex **3ct**

E= -2056.60090097 a.u.

G= -2055.951951 a.u.

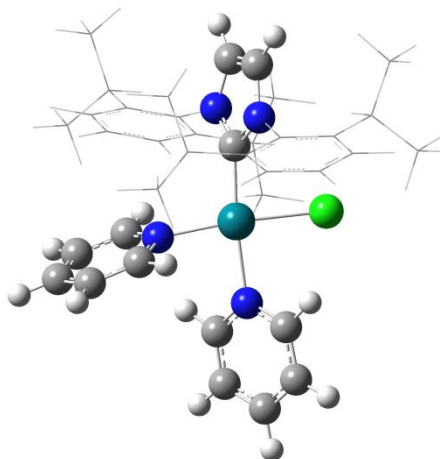


Rh	0.01031600	-0.50066100	-1.52548200	C	-4.88254100	1.87489000	-0.33675800
Cl	-1.30429500	-2.48481600	-1.38405400	H	-5.76501300	2.38682700	-0.71765200
N	0.52564600	-0.77964700	1.48462000	C	-4.92915500	0.51723300	-0.07100000
N	-1.48281400	-0.08203300	1.17039400	H	-5.85140100	-0.03579500	-0.24481400
C	-0.31520300	-0.32980000	0.50599100	C	-3.81004800	-0.16555600	0.41338300
C	-1.37582700	-0.41270000	2.51822000	C	-3.91649700	-1.63801900	0.74414700
H	-2.20795100	-0.28899700	3.19894500	H	-2.89710300	-2.03620800	0.84454000
C	-0.11608100	-0.85293700	2.71602400	C	-4.66438000	-1.83221900	2.06461500
H	0.39641600	-1.20195900	3.60316700	H	-5.69166200	-1.44500800	1.99289000
C	1.95312600	-0.85275700	1.34687800	H	-4.72580500	-2.89929300	2.31749500
C	2.69805000	0.27438200	1.73758600	H	-4.17865200	-1.31539100	2.90394900
C	4.08756500	0.20369900	1.62634200	C	-4.59906400	-2.43532900	-0.36317100
H	4.69379700	1.05857800	1.92763800	H	-5.66752400	-2.18795700	-0.44866200
C	4.70645700	-0.93947200	1.13752900	H	-4.11149800	-2.26237200	-1.32909100
H	5.79219300	-0.97957300	1.05972800	H	-4.52842000	-3.50862500	-0.14283700
C	3.94381700	-2.03565200	0.75438000	C	-1.33429200	2.77495800	0.73050400
H	4.43753600	-2.93079600	0.37717400	H	-0.44840700	2.17824500	0.45591000
C	2.55026300	-2.02043400	0.85323200	C	-1.28614300	3.05115000	2.23690600
C	1.73884800	-3.23958100	0.48116500	H	-2.16333600	3.64197800	2.53955900
H	0.69066300	-2.93540300	0.35306900	H	-0.38531600	3.62665800	2.49858500
C	2.17843000	-3.84806400	-0.84660000	H	-1.28000600	2.12949600	2.83331700
H	2.20190200	-3.08574400	-1.63864100	C	-1.23491200	4.10323600	-0.01362500
H	1.46204800	-4.62031800	-1.15415000	H	-1.39012100	3.99232000	-1.09542600
H	3.17151700	-4.31876400	-0.78197500	H	-0.24021900	4.54355200	0.14402800
C	1.80457700	-4.27109900	1.60726300	H	-1.97131300	4.83204700	0.35453400
H	1.19423600	-5.14906800	1.35757700	N	1.28815400	1.12322800	-1.72304000
H	1.43194100	-3.85829500	2.55578700	C	0.85089600	2.34239200	-2.08509700
H	2.83757100	-4.61290500	1.77436700	C	2.61682600	0.93905400	-1.60459800
C	2.04645400	1.52578100	2.29334200	C	1.70827900	3.40391500	-2.33904700
H	0.95837200	1.42305900	2.18675600	H	-0.23053600	2.44532700	-2.16787600
C	2.44246600	2.78937300	1.53436700	C	3.53739700	1.94787500	-1.84761500
H	2.10170400	2.75419200	0.49076900	H	2.92689400	-0.06041200	-1.29944700
H	1.98635100	3.67092600	2.00793600	C	3.07986200	3.20594400	-2.22365100
H	3.53003500	2.94965600	1.52943900	H	1.29448600	4.36870300	-2.62477000
C	2.34078200	1.67513300	3.78561200	H	4.59851000	1.73874900	-1.73083200
H	3.41115400	1.85005100	3.96688700	H	3.77832800	4.01750600	-2.41792900
H	2.05144900	0.77624100	4.34638900	C	0.73143100	-1.20904700	-3.46095600
H	1.78654800	2.52816800	4.20185400	H	1.73102100	-0.80488200	-3.64474800
C	-2.63938200	0.57537900	0.62124900	H	0.65485000	-2.29649100	-3.43472000
C	-2.56926100	1.96365600	0.38361300	C	-0.39765400	-0.42839200	-3.66004400
C	-3.71273000	2.59034700	-0.10715000	H	-1.37933600	-0.88592500	-3.78469800
H	-3.69777000	3.66066000	-0.30381000	H	-0.31037200	0.60397800	-4.00663200

Complex 6t

E= -2226.17065022 a.u.

G= -2225.489352 a.u.



Rh	-0.09806700	1.06348700	0.12938500	C	-2.40522300	-2.76784600	-2.27618500
Cl	1.38627200	1.62247100	1.91533000	H	-2.23621800	-1.69824800	-2.45574300
N	-0.53593800	3.16876500	-0.02723200	H	-1.94292400	-3.32453100	-3.10367300
N	-0.23843300	-1.81641300	1.02462500	H	-3.48820600	-2.95179800	-2.32342400
N	1.70843100	-1.37418000	0.22479000	C	-1.87983200	-4.73271800	-0.80367600
C	0.49160700	4.03350100	-0.08236100	H	-2.92295400	-5.08017200	-0.82608900
H	1.48115700	3.58507900	-0.02415700	H	-1.43679500	-5.07584200	0.14075300
C	0.30990500	5.40602100	-0.18141100	H	-1.34498100	-5.22505400	-1.62818600
H	1.17838400	6.05893700	-0.22469100	C	2.79359900	-0.81139800	-0.52933600
C	-0.98170200	5.91697200	-0.21282500	C	2.67730200	-0.77206700	-1.93278700
H	-1.15437900	6.98937800	-0.28455600	C	3.76157100	-0.28329700	-2.65845500
C	-2.04827000	5.02875400	-0.14314500	H	3.70604500	-0.23715900	-3.74470600
H	-3.07884400	5.37584000	-0.15250600	C	4.92274900	0.13520900	-2.01899400
C	-1.77966400	3.67050000	-0.05351800	H	5.76133400	0.50833000	-2.60550000
H	-2.58962900	2.94324100	0.00436300	C	5.01715700	0.06692700	-0.63917000
C	0.46351700	-0.81752000	0.39646400	H	5.93304200	0.38896900	-0.14459700
C	1.77192400	-2.65486300	0.76432700	C	3.95682600	-0.40541500	0.13942500
H	2.68080300	-3.24044500	0.72236000	C	4.12483500	-0.50552600	1.64126300
C	0.55314700	-2.93227200	1.26961000	H	3.12950800	-0.64678900	2.08601100
H	0.16233000	-3.80520500	1.77618200	C	5.01196500	-1.69983000	1.99892200
C	-1.65835100	-1.82477900	1.19680200	H	6.02232900	-1.57349600	1.58209800
C	-2.42749600	-2.52048600	0.24811100	H	5.11018100	-1.79528800	3.08886400
C	-3.80926800	-2.56681700	0.44239700	H	4.61872300	-2.64961700	1.61161800
H	-4.43372200	-3.10830600	-0.26901400	C	4.70361900	0.76836500	2.25138100
C	-4.39849600	-1.92493700	1.52434200	H	5.75020600	0.92961100	1.95365100
H	-5.47821200	-1.97139200	1.66173100	H	4.10727600	1.64248000	1.96578500
C	-3.61384200	-1.22445200	2.43314700	H	4.68555500	0.69306700	3.34697700
H	-4.08541400	-0.72388200	3.27868200	C	1.45170600	-1.31542300	-2.64467200
C	-2.22541300	-1.16092300	2.29352300	H	0.56815600	-1.03442300	-2.04918100
C	-1.37856600	-0.43704300	3.31604300	C	1.51847700	-2.84339800	-2.72734400
H	-0.37063100	-0.29891700	2.89993400	H	2.40325200	-3.15334200	-3.30362500
C	-1.90563100	0.96082900	3.62064500	H	0.62929800	-3.24632500	-3.23541900
H	-1.97547600	1.55519900	2.69750400	H	1.58231900	-3.31217000	-1.73589400
H	-1.20617700	1.48161900	4.28677200	C	1.25092100	-0.74410000	-4.04366000
H	-2.89006700	0.94069800	4.11218600	H	1.31951800	0.35247200	-4.05437300
C	-1.26434400	-1.28246100	4.58345800	H	0.25983500	-1.03053500	-4.42409500
H	-0.61705300	-0.78654800	5.31874600	H	1.99371500	-1.13189400	-4.75609900
H	-0.83509000	-2.27100500	4.36527700	N	-1.57085500	0.77221700	-1.31017700
H	-2.24867000	-1.44007800	5.05021000	C	-1.36049700	1.11868400	-2.59542500
C	-1.80045200	-3.21332000	-0.94694000	C	-2.83851500	0.49887800	-0.93993500
H	-0.73668200	-2.94055400	-0.97927400	C	-2.38053600	1.20676500	-3.53204600

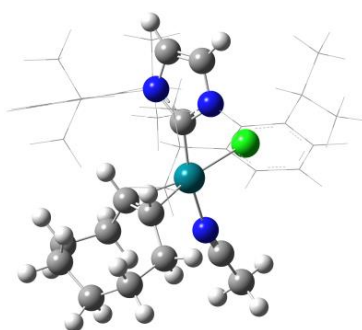
H	-0.32707700	1.34212300	-2.85406200
C	-3.91261500	0.57088500	-1.81579600
H	-2.97576200	0.22377500	0.10494100
C	-3.68601800	0.93012500	-3.13984200

H	-2.14283000	1.49195800	-4.55455300
H	-4.91071200	0.33726300	-1.45082800
H	-4.50706700	0.99218700	-3.85140900

Complex 4at

E= -2175.65340400 a.u.

G= -2174.903430 a.u.



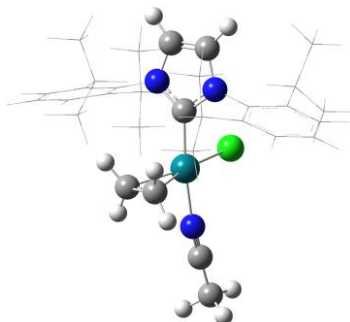
Rh	0.07933900	1.14598100	-0.18268800
Cl	-0.83478500	0.88351100	-2.29759100
O	1.55251600	1.26660700	1.14705000
N	0.18530700	3.30908100	-0.42705300
N	0.99043500	-1.71645200	0.11495300
C	1.02523800	3.99835000	0.36019100
H	1.64921900	3.38954300	1.01289900
C	1.10107400	5.38352300	0.32832000
H	1.80150900	5.89778700	0.98185400
C	0.27406400	6.08390900	-0.54066600
H	0.30852400	7.17105700	-0.58470800
C	-0.59668000	5.36948500	-1.35430500
H	-1.26316200	5.87072100	-2.05183800
C	-0.60927400	3.98481400	-1.26931400
H	-1.25968300	3.37566500	-1.89541300
C	-0.03623600	-0.82781600	0.09997100
C	0.53079000	-2.99861800	0.38118600
H	1.20787200	-3.84157300	0.41962700
C	2.37878200	-1.41374600	-0.11310100
C	2.83837600	-1.34115500	-1.43450100
C	4.19779700	-1.08692000	-1.62484500
H	4.59237700	-1.02735800	-2.63853000
C	5.05042700	-0.91425000	-0.54389100
H	6.10838400	-0.71884800	-0.71398700
C	4.56117200	-0.98823100	0.75418400
H	5.23969700	-0.84473200	1.59417900
C	3.21098300	-1.23234600	1.00105600
C	2.69431700	-1.33850300	2.41981500
H	1.60464500	-1.18612800	2.39605900
C	3.27399700	-0.27294100	3.34485500
H	2.76530500	-0.30925900	4.31744100
H	3.14046400	0.72977300	2.92353900
H	4.34471300	-0.43497900	3.53628200
C	2.98169100	-2.73145800	2.98352300
H	4.06526500	-2.91737200	3.01667300
H	2.52940100	-3.52666100	2.37599100
H	2.59209000	-2.82605600	4.00638500
C	1.93107400	-1.59337000	-2.61972400
H	0.89057500	-1.44113600	-2.29863000
C	2.17695600	-0.62274500	-3.76925500

H	3.15438600	-0.78522300	-4.24627500
H	2.12384600	0.41852800	-3.42717400
H	1.40836200	-0.75857800	-4.54132500
C	2.07793200	-3.04141800	-3.08796200
H	1.40833200	-3.24637100	-3.93423100
H	1.83954800	-3.75381100	-2.28580100
H	3.10873600	-3.24221000	-3.41534400
O	0.37276800	1.45246100	1.78332000
N	-1.14347500	-1.57327500	0.35840900
C	-0.80667700	-2.90715000	0.54443900
H	-1.55858600	-3.64949900	0.77712500
C	-2.49379900	-1.08800200	0.47599200
C	-3.37125100	-1.27849200	-0.60277100
C	-4.68689200	-0.84440800	-0.43981600
H	-5.39618000	-0.97573000	-1.25605200
C	-5.10479000	-0.24870500	0.74202500
H	-6.13647000	0.08440100	0.84623300
C	-4.21470700	-0.08160900	1.79373700
H	-4.55634500	0.37629000	2.72125600
C	-2.88815500	-0.50161900	1.68800600
C	-1.95420100	-0.39485700	2.87410700
H	-0.91954100	-0.45199900	2.51052500
C	-2.07358800	0.94017600	3.60001300
H	-1.28845000	1.01931400	4.36314100
H	-1.94427900	1.77834000	2.90352900
H	-3.04138700	1.05133800	4.11023400
C	-2.19869100	-1.56260800	3.83016700
H	-3.22626600	-1.53861100	4.22243700
H	-2.05488800	-2.53214000	3.33278900
H	-1.50968400	-1.51495500	4.68455400
C	-2.95324100	-1.97186100	-1.88241400
H	-1.85510300	-1.94535200	-1.94061700
C	-3.48905000	-1.27788600	-3.13104200
H	-4.57977800	-1.38455000	-3.22087300
H	-3.23851500	-0.21064600	-3.13011300
H	-3.04532700	-1.73067700	-4.02759800
C	-3.40187200	-3.43434500	-1.86437800
H	-3.09490800	-3.94540400	-2.78699400
H	-2.97813100	-3.98795600	-1.01601000
H	-4.49697300	-3.50299700	-1.78998400

Complex **4bt**

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G= -1940,559443 a.u.

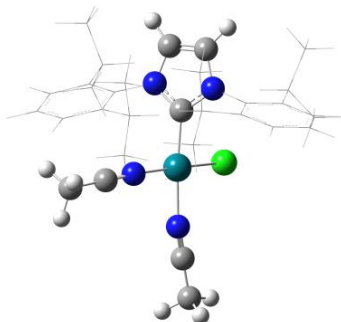


Rh	0.01419900	1.17661500	-0.97855700	H	-2.70271500	-3.92602300	1.46948200
Cl	0.76126400	2.58903800	0.81353700	H	-2.21520700	-4.96977700	0.11543700
N	-1.10349900	-0.75021300	1.09802500	C	2.38359100	-0.95102900	0.43645900
N	1.03344400	-0.93538400	0.93552000	C	2.67769000	-1.81800500	-0.63268400
C	-1.47914000	0.51258200	-2.32605000	C	3.99327300	-1.85905300	-1.09116800
H	-2.24853900	-0.08101900	-1.83013800	H	4.25250000	-2.51742100	-1.91907100
C	-0.25069900	-0.05293400	-2.70559200	C	4.98145800	-1.08446800	-0.49781700
H	-0.05808800	-1.10970200	-2.52028500	H	6.00410900	-1.13023900	-0.86977600
C	-0.04184400	-0.31044600	0.35634600	C	4.67171600	-0.26996700	0.57973700
C	0.64157800	-1.71077700	2.01971800	H	5.45835800	0.31503200	1.05441900
H	1.36075900	-2.27400700	2.59965000	C	3.36932400	-0.18651300	1.07849900
C	-0.69763300	-1.59187700	2.12537200	C	3.09324900	0.63650700	2.31887900
H	-1.40963300	-2.01684900	2.82065000	H	2.01244900	0.82708500	2.36994600
C	-2.48646100	-0.58569400	0.75231300	C	3.52689900	-0.13607900	3.56651900
C	-3.09781700	-1.61934700	0.02197400	H	4.60922400	-0.33310900	3.54889200
C	-4.44557500	-1.46833000	-0.30447700	H	3.30629700	0.44468100	4.47245500
H	-4.95356100	-2.25096300	-0.86793600	H	3.01899800	-1.10622000	3.65791200
C	-5.14569900	-0.32938400	0.07212800	C	3.77825900	1.99946800	2.28823200
H	-6.19629400	-0.22571500	-0.19565000	H	4.87189700	1.91342200	2.37143600
C	-4.51312200	0.67385200	0.79331400	H	3.52834500	2.54544800	1.37132400
H	-5.07480600	1.55879500	1.09123000	H	3.43364900	2.60348200	3.13808500
C	-3.16853000	0.56847000	1.15542500	C	1.64465400	-2.76412400	-1.21095200
C	-2.51506300	1.63967600	1.99798000	H	0.65164800	-2.31328700	-1.07092500
H	-1.42730700	1.48716300	1.97737900	C	1.65797400	-4.09010700	-0.44703000
C	-2.76120000	3.04192100	1.45167800	H	2.64329600	-4.57199900	-0.52998800
H	-2.43138800	3.11592100	0.40675100	H	0.90742700	-4.78308900	-0.85485300
H	-2.17900800	3.77053600	2.03036100	H	1.43973600	-3.94852200	0.61992700
H	-3.82070700	3.33263500	1.51235300	C	1.81979700	-3.01826700	-2.70481400
C	-2.98665000	1.51841800	3.44653600	H	1.92973500	-2.08103300	-3.26607800
H	-2.48610200	2.26542000	4.07678600	H	0.94300300	-3.55108000	-3.09893100
H	-2.76630700	0.52328900	3.85864300	H	2.69708500	-3.64632900	-2.91495700
H	-4.07205400	1.68005600	3.52826100	C	0.39722500	3.85488700	-2.72661100
C	-2.34648800	-2.86457800	-0.40931100	C	0.63722200	5.12378100	-3.38341200
H	-1.27855400	-2.71497200	-0.19183100	H	1.36826700	5.00660600	-4.19095000
C	-2.46365700	-3.13121000	-1.90866900	H	-0.29262800	5.52081800	-3.80530500
H	-2.14334600	-2.26548300	-2.50351100	H	1.02913900	5.84590500	-2.65851600
H	-1.83615900	-3.98913300	-2.19030200	N	0.21853700	2.85153700	-2.17885100
H	-3.49492900	-3.37642700	-2.19984600	H	-1.86902100	1.38909700	-2.84872500
C	-2.80658100	-4.08454900	0.38806200	H	0.32730300	0.36932700	-3.53118600
H	-3.86318100	-4.31215400	0.18593500				

Complex 7t

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G= -1994.691978 a.u.

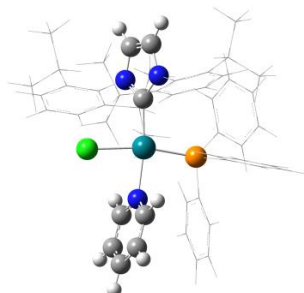


Rh	0.01644400	1.19808000	0.78931900	C	-3.64526600	-1.86095000	1.78594300
Cl	-1.39482200	2.47786500	-0.64295000	H	-3.65197000	-2.41025500	2.72697900
N	0.79305700	-0.69196100	-1.42531500	C	-4.82510300	-1.30459200	1.30941100
N	-1.28002000	-0.95529600	-0.90929900	H	-5.74636200	-1.41195900	1.88060800
C	-0.15734700	-0.27008000	-0.53439100	C	-4.83327000	-0.61728500	0.10541600
C	-1.03386600	-1.75641900	-2.01902400	H	-5.76442800	-0.18668500	-0.26119400
H	-1.81067000	-2.37115500	-2.45409800	C	-3.66732600	-0.45881500	-0.64689700
C	0.26376500	-1.58593800	-2.34886300	C	-3.71563900	0.27195500	-1.97188600
H	0.86918000	-2.01182300	-3.13854800	H	-2.68569600	0.54669100	-2.24201000
C	2.19574100	-0.47209200	-1.23301100	C	-4.30220300	-0.63021600	-3.05927400
C	2.94323000	-1.50552900	-0.64350200	H	-5.33832800	-0.90926600	-2.81615100
C	4.30163200	-1.27300900	-0.41893700	H	-4.31439400	-0.11068000	-4.02715600
H	4.91589300	-2.05918100	0.02282800	H	-3.73477500	-1.56302200	-3.18524500
C	4.88191700	-0.05626000	-0.75404900	C	-4.50690200	1.57394900	-1.89105400
H	5.94328500	0.10866300	-0.57138600	H	-5.58137000	1.39523400	-1.73739200
C	4.11590600	0.94525800	-1.33652100	H	-4.12735400	2.20755800	-1.08128500
H	4.58226700	1.89233300	-1.60605500	H	-4.40096700	2.12911200	-2.83268700
C	2.75599000	0.76124200	-1.59037000	C	-1.20662500	-2.45197400	1.56036600
C	1.94844400	1.83567300	-2.28273800	H	-0.33116400	-1.97245600	1.09916900
H	0.88300900	1.63603300	-2.10907200	C	-1.23584100	-3.91486800	1.11461400
C	2.21528600	3.22943900	-1.72702000	H	-2.09249100	-4.44030600	1.56214000
H	2.06677800	3.24562300	-0.63845000	H	-0.31923300	-4.43854800	1.42469500
H	1.50384900	3.94074700	-2.16558800	H	-1.32420100	-4.00290900	0.02269500
H	3.23113100	3.58539400	-1.95630700	C	-1.00746600	-2.34880500	3.06848900
C	2.20661900	1.77781600	-3.78827100	H	-1.05329700	-1.30452600	3.40318800
H	1.60153200	2.53004400	-4.31168400	H	-0.02310500	-2.75672000	3.34288400
H	1.95277800	0.79083100	-4.20109700	H	-1.75943700	-2.92391800	3.62787100
H	3.26508600	1.97423300	-4.01734200	C	2.26675100	-0.06457900	2.55815500
C	2.33735900	-2.85131600	-0.28529100	C	-0.06387500	3.87680700	2.56170000
H	1.24715100	-2.79142700	-0.41642300	C	3.39563000	-0.51864800	3.34602500
C	2.57492800	-3.24831200	1.16860400	H	4.23737400	-0.77059600	2.68789900
H	2.10177800	-2.53027300	1.85234600	H	3.72130200	0.26722000	4.03774000
H	2.13765500	-4.23744200	1.36585600	H	3.13415800	-1.40864000	3.93260600
H	3.64490100	-3.31097900	1.41426100	C	-0.23296700	5.14969100	3.23296500
C	2.85576900	-3.93715300	-1.22831600	H	-0.70750400	5.01054500	4.21094400
H	3.93809600	-4.08655900	-1.10411500	H	0.73482600	5.64230000	3.37975500
H	2.67941600	-3.67576100	-2.28009600	H	-0.86947300	5.80384900	2.62660700
H	2.35971600	-4.89660700	-1.02712300	N	1.37709500	0.31051100	1.90917400
C	-2.49166400	-1.03078700	-0.14169800	N	0.05034900	2.86658400	2.00826300
C	-2.45465900	-1.74268100	1.07117000				

Complex **12at**

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G= -3012.946705 a.u.



Rh	0.14725400	-0.65798800	-0.73090200	C	-1.09595700	1.01019400	4.18256400
Cl	2.00122300	-1.44323000	-2.05578100	H	-0.28862500	1.55193800	4.67616300
P	-1.82247700	-0.27583800	0.33956700	C	-2.21833300	0.60816000	4.89846900
C	1.35768300	0.53557800	0.33628600	H	-2.30334700	0.83600400	5.95985000
N	2.37472700	0.11774000	1.16992400	C	-3.22972900	-0.09650200	4.25095800
N	1.42999700	1.91287500	0.42252300	H	-4.10893600	-0.42182100	4.80535800
C	3.00280400	1.19527100	1.78362400	C	-3.12495500	-0.38681100	2.89468900
H	3.80345000	1.04646700	2.49571000	H	-3.92242300	-0.94652300	2.40616200
C	2.42703900	2.31505200	1.30927800	C	-2.93984200	-1.73271300	0.12669500
H	2.62289700	3.36201200	1.50113100	C	-3.93348900	-1.77570200	-0.85375900
C	2.97192200	-1.19731800	1.21456500	H	-4.14247800	-0.89163500	-1.45678700
C	2.37986300	-2.20103300	1.99338300	C	-4.65970900	-2.94296400	-1.07871300
C	2.99639000	-3.45113400	2.02552400	H	-5.42437300	-2.95927000	-1.85431300
H	2.55567800	-4.25206100	2.61724900	C	-4.41532900	-4.07936200	-0.31560000
C	4.17180000	-3.68430800	1.32425400	H	-4.98815000	-4.98922000	-0.48844700
C	4.75097600	-2.66751400	0.58155700	C	-3.43276500	-4.04605600	0.67091400
H	5.67125900	-2.86127500	0.03208500	H	-3.23215900	-4.92961200	1.27559700
C	4.16392500	-1.40430700	0.49767500	C	-2.69486300	-2.88697200	0.87954200
C	1.16052800	-1.90955900	2.83538900	H	-1.91377800	-2.87624800	1.64086500
H	0.52643500	-1.21744200	2.26282300	N	-0.89604200	-1.99828000	-2.03301900
C	4.83931600	-0.32424200	-0.32665500	C	-0.77973600	-3.31776100	-1.83561800
H	4.09252500	0.45123300	-0.54867900	C	-1.49044000	-1.56999800	-3.15353200
C	0.79699700	2.87334700	-0.44429600	C	-1.28097900	-4.25231600	-2.72965300
C	-0.07900300	3.82774200	0.09947400	H	-0.25056000	-3.61415900	-0.93080700
C	-0.61092300	4.79129500	-0.76139400	C	-2.01148500	-2.43659500	-4.10351900
H	-1.30116800	5.53570400	-0.36438400	H	-1.54212200	-0.48878000	-3.27872900
C	-0.28063400	4.81486400	-2.10576900	C	-1.91277200	-3.80504300	-3.88325400
C	0.61827900	3.88564500	-2.61344500	H	-1.16773800	-5.31306000	-2.51973800
H	0.90604900	3.93549300	-3.66243500	H	-2.48178600	-2.03728000	-4.99892700
C	1.19490100	2.91207300	-1.79743800	H	-2.31415300	-4.51359000	-4.60578900
C	-0.41660100	3.91724900	1.57361400	H	4.64230400	-4.66592400	1.36305400
H	0.01542500	3.04663500	2.08320200	H	-0.70915100	5.57300400	-2.76062300
C	2.30782700	2.04123800	-2.34013900	C	-1.91993500	3.90016100	1.83722400
H	2.32738200	1.09694400	-1.78578000	H	-2.39555900	3.00424000	1.41937100
C	-2.87541000	1.07870600	-0.34972900	H	-2.11513200	3.91357900	2.91856100
C	-4.12904300	1.41064500	0.17906900	H	-2.41993100	4.77641900	1.40014300
H	-4.50789800	0.88221700	1.05416100	C	0.21344500	5.16750900	2.19088300
C	-4.89246300	2.41992500	-0.39332400	H	-0.21584900	6.08207900	1.75784000
H	-5.86298400	2.67249800	0.03156400	H	0.03234000	5.19570600	3.27406600
C	-4.41703500	3.10716100	-1.50925200	H	1.29867600	5.20801300	2.02478100
H	-5.01705900	3.89752000	-1.95822200	C	1.57786500	-1.23253800	4.14176600
C	-3.17676700	2.78266200	-2.04534000	H	0.69870500	-1.02353300	4.76766500
H	-2.79399700	3.32069000	-2.91134400	H	2.25719900	-1.88623200	4.70916500
C	-2.40624700	1.77750500	-1.46337500	H	2.09627100	-0.27974800	3.96416900
H	-1.41268400	1.53910700	-1.85479100	C	0.31047000	-3.13315700	3.14694400
C	-2.00182300	0.01541400	2.16046200	H	-0.63304100	-2.81175500	3.61423000
C	-0.98898700	0.70407700	2.82932000	H	0.07431900	-3.70493600	2.23831400
H	-0.09497700	0.99423000	2.27965300	H	0.80405200	-3.81287200	3.85708000

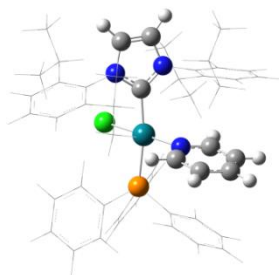
C	3.64951100	2.74825900	-2.13079700
H	4.47390200	2.11567300	-2.49160200
H	3.68343200	3.69944500	-2.68376600
H	3.83536300	2.96815200	-1.06853100
C	2.13010200	1.64386400	-3.79914500
H	2.26017300	2.49101100	-4.48942100
H	2.87864400	0.88367800	-4.05709100
H	1.14218000	1.19372600	-3.96977500

C	5.36511600	-0.82773000	-1.66928300
H	5.71905400	0.02475200	-2.26733600
H	6.22237000	-1.50565300	-1.54729100
H	4.57855400	-1.34252500	-2.23151100
C	5.99116200	0.32002700	0.44894600
H	6.77977900	-0.42027500	0.64919300
H	6.43783500	1.13524200	-0.13843300
H	5.67694400	0.73567400	1.41448000

Complex **12bt**

E= -3013.79540418 a.u.

G= -3012.943425 a.u.



Cl	0.28608900	1.66227000	1.91625400
C	-3.95973500	1.21398100	0.40505900
C	-4.09341300	-0.05336800	0.84447700
H	-4.68005300	2.01228800	0.28597400
H	-4.95002000	-0.60716800	1.20677300
C	-1.89469200	0.24518700	0.29115600
N	-2.83147100	-0.63319400	0.76360600
N	-2.62173100	1.38757600	0.07188000
Rh	0.14112900	0.01206200	0.18132500
N	0.12434400	-1.55787000	-1.19059900
C	0.21913900	-1.34820700	-2.51613800
C	0.19698300	-2.82971200	-0.75497400
C	0.38149400	-2.37297500	-3.43669800
H	0.18711900	-0.30610700	-2.82582300
C	0.37754100	-3.90752700	-1.60993000
H	0.11706300	-2.96356900	0.32383600
C	0.47133400	-3.68175400	-2.97826300
H	0.45271600	-2.13273900	-4.49573600
H	0.44201900	-4.90961900	-1.19199500
H	0.61480300	-4.50757000	-3.67233700
P	2.47526600	0.09611100	0.10053700
C	-2.11815400	2.61128100	-0.48958600
C	-1.98649000	3.74048500	0.33261000
C	-1.82634400	2.64012500	-1.86557900
C	-1.50526300	4.91187400	-0.25740800
C	-1.33955900	3.83243100	-2.40014600
C	-1.17383300	4.95785400	-1.60221400
H	-1.38488600	5.80328600	0.35633800
H	-1.09190500	3.88795200	-3.45881400
H	-0.79462700	5.88196200	-2.03779700
C	-2.61792400	-2.02964600	1.00888300
C	-3.11706600	-2.94078800	0.06723300
C	-1.95426000	-2.43320200	2.18261300
C	-2.94521900	-4.30352400	0.32729100
C	-1.80739000	-3.80472500	2.39016800
C	-2.29967700	-4.73184000	1.47624700
H	-3.32467600	-5.03548700	-0.38640900
H	-1.29833300	-4.15712300	3.28535200
H	-2.17693700	-5.79736500	1.66686900
C	-2.11632200	1.45327600	-2.76331000
H	-1.88538000	0.53750700	-2.19672700
C	-3.84611400	-2.50652300	-1.19011700
H	-3.82851100	-1.40812900	-1.24205900
C	-1.41366700	-1.41331000	3.16044000
H	-0.91556100	-0.63239600	2.56440100
C	-2.40457300	3.75482300	1.78851200
H	-2.43404000	2.71401700	2.14354500
C	-3.79872400	4.37227100	1.93276400
H	-4.10899500	4.37604800	2.98668300

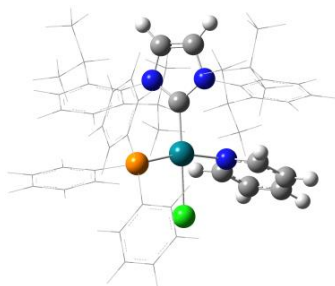
H	-3.79779500	5.41447400	1.58093600
H	-4.56654500	3.83542900	1.35974400
C	-1.42619400	4.51278000	2.68247000
H	-1.68607500	4.34825400	3.73658600
H	-0.39901600	4.16515700	2.52684300
H	-1.46887600	5.59759900	2.50539500
C	-3.60161200	1.42294200	-3.13317200
H	-3.87110400	2.32528600	-3.70192600
H	-3.82917000	0.54691900	-3.75755900
H	-4.24747200	1.38064100	-2.24651900
C	-1.27941000	1.43287400	-4.03759300
H	-0.20926500	1.58315300	-3.83347700
H	-1.40418700	0.46802200	-4.55040000
H	-1.59477400	2.21346700	-4.74483000
C	-5.30988900	-2.94406600	-1.13903500
H	-5.85612500	-2.57651400	-2.01807100
H	-5.39565400	-4.04001800	-1.12743700
H	-5.81592700	-2.56539300	-0.24076700
C	-3.17507000	-3.01745600	-2.46199700
H	-3.76248100	-2.72113700	-3.34244500
H	-2.16470500	-2.60403100	-2.57629400
H	-3.09351800	-4.11394200	-2.47381000
C	-0.36475300	-1.97116600	4.11161200
H	0.44130100	-2.49440500	3.57508700
H	0.08843500	-1.14088700	4.67026700
H	-0.79397200	-2.66879500	4.84728200
C	-2.52863400	-0.74143600	3.96279700
H	-3.26535600	-0.24509900	3.31840000
H	-3.05919700	-1.47398800	4.59036300
H	-2.09959200	0.02703000	4.62004200
C	3.07405200	1.54208500	-0.86326300
C	2.17067900	2.58205700	-1.10961300
C	4.37231200	1.63452200	-1.38076900
C	2.56144000	3.69200400	-1.85368300
H	1.15555300	2.50788900	-0.71213600
C	4.76088400	2.74558000	-2.12090400
H	5.08019300	0.82015300	-1.22030500
C	3.85469500	3.77637400	-2.35842100
H	1.84353400	4.49079300	-2.03730000
H	5.77299400	2.80464900	-2.51916000
H	4.15839700	4.64431900	-2.94251600
C	3.33830000	-1.31365300	-0.72503500
C	3.77095800	-2.41866700	0.01626100
C	3.42628700	-1.37283000	-2.12028500
C	4.28118300	-3.54628300	-0.61861500
H	3.71579000	-2.39190700	1.10493700
C	3.93639800	-2.50013300	-2.75566300
H	3.10332000	-0.51912800	-2.71809900
C	4.36316800	-3.59249900	-2.00698000

H	4.62120100	-4.39219500	-0.02239400	H	5.05042900	1.36459700	1.07270300
H	3.99929200	-2.52375800	-3.84337000	C	3.43749400	-0.58358000	4.00596200
H	4.76648000	-4.47412300	-2.50331700	H	1.80704200	-0.97104600	2.64292200
C	3.36560300	0.17165700	1.70592800	C	4.66618300	0.04747000	4.17883500
C	4.59405500	0.80666600	1.88954500	H	6.19484600	1.25203100	3.25541500
C	2.78708500	-0.51062000	2.77999000	H	2.97495100	-1.12109000	4.83326400
C	5.23876100	0.74756000	3.12191300	H	5.17368500	0.00115500	5.14145400

Complex 12ct

E= -3013.79472466 a.u.

G= -3012.939576 a.u.



Rh	0.37802100	-0.50659800	-0.86155800	C	-2.11211700	-0.81852800	3.81146800
Cl	-0.09935700	-1.68677600	-2.93875100	H	-1.52356800	-0.40262500	4.62972100
P	-1.80460900	-0.92885000	-0.32042900	C	-3.28635300	-1.51520800	4.07053500
C	0.84209700	0.65066800	0.70113800	H	-3.62977200	-1.65297600	5.09472300
N	1.80887300	0.41984400	1.66612200	C	-4.01452500	-2.04892100	3.00988300
N	0.30775400	1.86776800	1.10548600	H	-4.92746500	-2.61067300	3.20226900
C	1.82798500	1.41899100	2.63481100	C	-3.57275000	-1.88160800	1.70253800
H	2.51033300	1.37640100	3.47371900	H	-4.13547500	-2.33422600	0.88597200
C	0.89980000	2.32535100	2.28001000	C	-2.40655900	-2.53439200	-0.99868000
H	0.59856100	3.25721300	2.73958200	C	-3.44146800	-2.63474400	-1.92621700
C	2.89376700	-0.51925600	1.58489500	H	-3.92366200	-1.73580400	-2.30949400
C	2.70262200	-1.84628200	1.99733400	C	-3.85430100	-3.88418300	-2.38406300
C	3.80825500	-2.69689500	1.98630900	H	-4.65857300	-3.94962900	-3.11566100
H	3.68776500	-3.73220100	2.30241500	C	-3.24089900	-5.04022500	-1.91791800
C	5.05852000	-2.24155500	1.58498700	H	-3.56502600	-6.01519200	-2.27922900
C	5.21990200	-0.92747200	1.17068000	C	-2.20429600	-4.94570200	-0.99183600
H	6.20123200	-0.58331800	0.84428400	H	-1.71101000	-5.84629200	-0.62844000
C	4.14188500	-0.03910900	1.15161000	C	-1.78922400	-3.70127000	-0.53997800
C	1.35332800	-2.31991000	2.47945500	H	-0.96071000	-3.62592400	0.16612500
H	0.59726300	-1.73640700	1.93566500	N	2.34187800	-0.55256800	-1.75423700
C	4.35131000	1.39171200	0.69192600	C	2.54361500	0.12718400	-2.89325200
H	3.36309400	1.85101100	0.54354700	C	3.16209200	-1.57897000	-1.48666400
C	-0.60508600	2.69198400	0.35717900	C	3.57749300	-0.15579100	-3.77311300
C	-1.86671900	3.00338200	0.89450600	H	1.82035300	0.90807200	-3.10902800
C	-2.72265600	3.79373700	0.12221300	C	4.21401000	-1.93855600	-2.31829300
H	-3.71537500	4.03016100	0.50346300	H	2.95587200	-2.13513500	-0.57349600
C	-2.32594600	4.29783500	-1.10278600	C	4.43263600	-1.21182900	-3.48120600
C	-1.03765700	4.06089000	-1.56569200	H	3.68810500	0.43424700	-4.67980200
H	-0.72130700	4.50946200	-2.50526400	H	4.84299000	-2.78314600	-2.04587400
C	-0.14699400	3.26711400	-0.84701000	H	5.24952400	-1.46909000	-4.15311100
C	-2.27502800	2.67753900	2.32038100	H	5.91200500	-2.91813300	1.59281700
H	-1.57790200	1.93185200	2.72708700	H	-3.01301200	4.90381700	-1.69212000
C	1.30214200	3.15966300	-1.28487200	C	-3.68085700	2.10499300	2.46052100
H	1.65153400	2.13530700	-1.08024700	H	-3.78821200	1.15837800	1.92053800
C	-3.00538200	0.26516100	-1.05053000	H	-3.90059400	1.91468300	3.52009800
C	-4.31301300	0.44556300	-0.58918300	H	-4.44673200	2.79887400	2.08609700
H	-4.66093700	-0.09128500	0.29314600	C	-2.15972900	3.94732400	3.17190900
C	-5.18777100	1.29927700	-1.25366000	H	-2.89990600	4.69493500	2.85266500
H	-6.20144500	1.43291100	-0.87751000	H	-2.34594600	3.72340700	4.23123200
C	-4.76986400	1.97038700	-2.39909600	H	-1.17242600	4.42252700	3.08916900
H	-5.45621400	2.63362400	-2.92449200	C	1.20825900	-2.04490100	3.97580000
C	-3.47407600	1.78879900	-2.87155600	H	0.22040100	-2.36685200	4.33394700
H	-3.13952800	2.31198800	-3.76686100	H	1.97512000	-2.59222000	4.54448700
C	-2.59369800	0.94668800	-2.19960000	H	1.31876100	-0.97492100	4.20505900
H	-1.57603700	0.79505400	-2.56615300	C	1.07233200	-3.78558500	2.17773500
C	-2.40289100	-1.15909900	1.42229100	H	0.01945200	-4.00838400	2.40384300
C	-1.67872900	-0.64621600	2.49858000	H	1.25102200	-4.02031500	1.11846800
H	-0.75309900	-0.10866300	2.30796400	H	1.68411400	-4.46427400	2.79010500

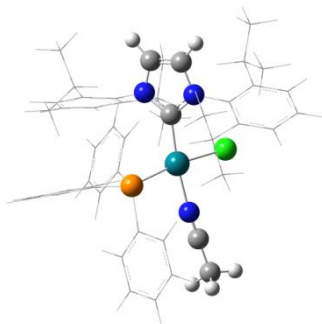
C	2.15643700	4.13865300	-0.47188800
H	3.21010600	4.08665400	-0.78411000
H	1.80880400	5.17004000	-0.63267900
H	2.11622500	3.93456600	0.60699300
C	1.51509100	3.42535400	-2.77064200
H	1.35583600	4.48298800	-3.02584100
H	2.55220200	3.18442700	-3.04514200
H	0.84182600	2.82209400	-3.39686800

C	5.09242100	1.48898500	-0.63938100
H	5.18105200	2.54279300	-0.93992100
H	6.11438700	1.09017500	-0.57243000
H	4.57030700	0.95320200	-1.44116700
C	5.08995000	2.20669600	1.75482000
H	6.10075900	1.80665700	1.92157100
H	5.19189200	3.25294800	1.43397400
H	4.56656500	2.20041100	2.71954600

Complex **13at**

E= -2898.36088165 a.u.

G= -2897.545775 a.u.



Rh	0.27786100	-0.68320800	-0.95136600
Cl	2.24838300	-0.85771000	-2.32420200
P	-1.76509100	-0.67159400	0.06194600
C	1.25525800	0.53246400	0.31672800
N	2.36103600	0.19467000	1.06689900
N	1.03274700	1.84984200	0.65600800
C	2.76422600	1.25285800	1.87307800
H	3.60806000	1.15548700	2.54287200
C	1.94986700	2.29068100	1.60623900
H	1.93026300	3.30371300	1.98466100
C	3.22656100	-0.94818500	0.88589000
C	2.84664200	-2.20085800	1.38521100
C	3.73325200	-3.26351900	1.22167500
H	3.46305500	-4.24867600	1.59891900
C	4.95818900	-3.08407700	0.59424400
C	5.31420300	-1.83265700	0.11644300
H	6.27379000	-1.69935700	-0.38226600
C	4.45630500	-0.73924000	0.23821400
C	1.55354000	-2.38163200	2.14440700
H	0.83109900	-1.66686600	1.72644500
C	4.89760000	0.60679400	-0.30558900
H	4.02217200	1.27218000	-0.32947700
C	0.12255000	2.75729400	0.00728600
C	-0.90872900	3.35893000	0.75015400
C	-1.75131800	4.25365500	0.08519000
H	-2.56581900	4.72425400	0.63507300
C	-1.56196100	4.56218700	-1.25108300
C	-0.49479800	4.00772900	-1.94443500
H	-0.32289400	4.28848800	-2.98267100
C	0.37690300	3.10618700	-1.33530800
C	-1.06540000	3.20366700	2.25197800
H	-0.42362900	2.37820500	2.58882400
C	1.61812800	2.64601100	-2.07112500
H	1.90981500	1.65567500	-1.70211800
C	-2.90544500	0.65918900	-0.51888300
C	-4.09222100	1.01738900	0.12832800
H	-4.34970800	0.56787000	1.08742900
C	-4.95925400	1.94070600	-0.44629600
H	-5.87722200	2.21471300	0.07225800
C	-4.66056100	2.50322000	-1.68448100
H	-5.34373000	3.22161100	-2.13586100
C	-3.48509600	2.14903000	-2.33840500
H	-3.23621900	2.59504400	-3.30081900
C	-2.61005300	1.23664400	-1.75651400
H	-1.67457500	0.96474900	-2.25215900
C	-2.02946200	-0.70790900	1.89057000
C	-1.05059200	-0.18555600	2.73807100

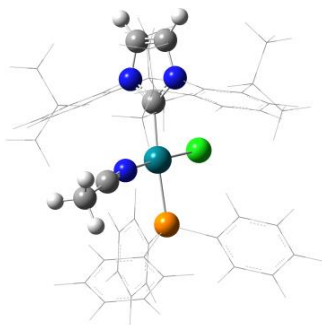
H	-0.12677200	0.20314000	2.31320400
C	-1.23489900	-0.15382900	4.11752300
H	-0.45327200	0.26102400	4.75399700
C	-2.40817600	-0.65004000	4.67394600
H	-2.55707300	-0.62634600	5.75229000
C	-3.38774900	-1.19068500	3.84448600
H	-4.30473900	-1.59334700	4.27234300
C	-3.19720900	-1.22642800	2.46744000
H	-3.96393200	-1.66928500	1.83112900
C	-2.74359600	-2.16681000	-0.42758900
C	-3.79803200	-2.11729800	-1.34096700
H	-4.14700700	-1.15795800	-1.72327100
C	-4.41000400	-3.29062600	-1.78060700
H	-5.23229100	-3.23329500	-2.49298100
C	-3.98201200	-4.52575000	-1.30677900
H	-4.46450700	-5.44134900	-1.64654200
C	-2.93602000	-4.58418600	-0.38649700
H	-2.59537600	-5.54554400	-0.00401600
C	-2.32224800	-3.41493900	0.04464600
H	-1.49241200	-3.46781300	0.75046900
H	5.63985000	-3.92559500	0.47875300
H	-2.23679500	5.25687700	-1.75030100
C	-2.48895600	2.88193900	2.69603000
H	-2.84216100	1.93342600	2.27479300
H	-2.52889500	2.79798600	3.79100500
H	-3.19826000	3.66805300	2.40064700
C	-0.58905200	4.48091100	2.95114400
H	-1.24365700	5.32827400	2.70261600
H	-0.60480300	4.35531100	4.04242900
H	0.42956900	4.76637700	2.65459600
C	1.76536900	-2.06896200	3.62539600
H	0.82183700	-2.16589400	4.18182400
H	2.49611700	-2.76578000	4.06306000
H	2.14634400	-1.04894900	3.77985900
C	0.93568200	-3.76343800	1.98203600
H	-0.06282900	-3.77458300	2.44457600
H	0.83614700	-4.02938100	0.92035700
H	1.52265400	-4.54783300	2.48146600
C	2.76019300	3.62509400	-1.78815200
H	3.68274700	3.28801900	-2.28228400
H	2.51767000	4.62924200	-2.16864100
H	2.96653800	3.71576600	-0.71160500
C	1.42599500	2.47649600	-3.57248400
H	1.29530500	3.43766000	-4.09252100
H	2.31401500	1.98718900	-3.99297600
H	0.56586600	1.83120100	-3.79537200
C	5.43130200	0.52395100	-1.73359000

H	5.65538600	1.53491800	-2.10338500	C	-0.84765200	-2.75043800	-3.12885700
H	6.36616700	-0.05214800	-1.78805900	C	-1.28337300	-3.73765000	-4.09404900
H	4.69245600	0.06238000	-2.39900600	H	-0.43332900	-4.07971100	-4.69448700
C	5.95400800	1.24085900	0.60201300	H	-1.72228500	-4.59563900	-3.57171500
H	6.86497600	0.62494800	0.62608400	H	-2.04102000	-3.31365500	-4.76275900
H	6.23413400	2.23590500	0.22874800	N	-0.50099500	-1.97888400	-2.34006400
H	5.60832700	1.35423200	1.63832900				

Complex **13bt**

E= -2898.35914127 a.u.

G= -2897.550326 a.u.



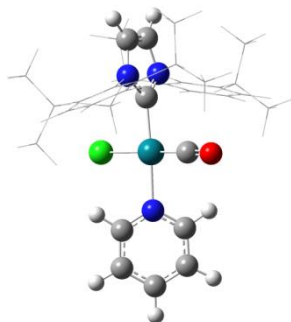
Cl	0.04043000	0.36434600	-2.31782400	H	4.07074000	2.41655700	2.72129700
C	4.03445300	1.00297000	0.01538100	C	0.73032900	2.40388500	3.68458400
C	4.15184700	-0.33998000	-0.07301600	H	-0.23238400	2.21923000	3.18652400
H	4.77724200	1.78942800	0.03517900	H	0.84144600	1.68355000	4.50840100
H	5.01808400	-0.98206300	-0.16585300	H	0.69951000	3.40445700	4.13859800
C	1.93227000	0.13680700	0.07345300	C	4.19906200	-2.49262900	2.81440800
N	2.86091800	-0.85560900	-0.03449800	H	4.40148900	-2.03059300	3.79072100
N	2.67492900	1.28119300	0.09607900	H	4.46849500	-3.55708300	2.88010200
Rh	-0.09411700	-0.00958800	0.04485300	H	4.86249300	-2.02441700	2.07619400
P	-2.40072600	-0.12365400	-0.25750200	C	1.84458900	-2.89732700	3.54848000
C	2.12409600	2.60612500	0.19226600	H	1.94733900	-2.27871000	4.45177900
C	2.00554700	3.37765900	-0.97501500	H	0.78768800	-2.91724300	3.24992900
C	1.72113900	3.07578600	1.45242300	H	2.13562500	-3.91956800	3.82928400
C	1.48517300	4.66637600	-0.84162400	C	1.50904100	-2.44652400	-3.71664400
C	1.20009100	4.36687400	1.52735100	H	0.48596800	-2.38506200	-3.32497300
C	1.08507200	5.15779100	0.39218600	H	1.57839600	-1.74365000	-4.55685100
H	1.38590400	5.29284800	-1.72692300	H	1.68344200	-3.45687200	-4.11671200
H	0.88179600	4.76241500	2.49103900	C	3.95366000	-2.24958600	-3.17896900
H	0.67849400	6.16524000	0.47136400	H	4.70772600	-1.90174000	-2.45909700
C	2.54712900	-2.25581200	-0.10476400	H	4.15854800	-3.30984000	-3.39100700
C	2.45509100	-2.98288000	1.09203200	H	4.09384700	-1.68642600	-4.11163100
C	2.35709400	-2.84326900	-1.36384100	C	-3.22834800	1.41151900	-0.83054900
C	2.15380800	-4.34159400	1.00328600	C	-2.43217500	2.50036000	-1.19651900
C	2.05507800	-4.20627300	-1.39715600	C	-4.62156900	1.55359500	-0.83639600
C	1.95065600	-4.94825800	-0.22950900	C	-3.01994700	3.69902200	-1.59010300
H	2.07931200	-4.93542400	1.91343600	H	-1.34731500	2.39471300	-1.16896800
H	1.90278700	-4.69161500	-2.36040300	C	-5.20675500	2.74944400	-1.23607700
H	1.71540100	-6.01068000	-0.27902400	H	-5.25317600	0.72768900	-0.50517600
C	1.89136200	2.24845900	2.70817500	C	-4.40493500	3.82286600	-1.61749600
H	1.92048700	1.18981200	2.41442700	H	-2.38676100	4.53902800	-1.87305500
C	2.72506300	-2.33987200	2.43515300	H	-6.29138000	2.84795100	-1.24033900
H	2.50493300	-1.26542500	2.34386400	H	-4.86389300	4.76098800	-1.92715000
C	2.52993200	-2.06644000	-2.65003300	C	-3.41093100	-0.49944500	1.23820600
H	2.36867300	-1.00110700	-2.43133100	C	-4.00088300	-1.74144900	1.47587000
C	2.43658400	2.86907200	-2.33494300	C	-3.50735700	0.49249900	2.22356800
H	2.39983900	1.76894000	-2.31028600	C	-4.68827500	-1.98207300	2.66556400
C	3.86145900	3.32683300	-2.65279800	H	-3.93504100	-2.52527200	0.72117400
H	4.17395000	2.95939500	-3.63980300	C	-4.20093000	0.25722400	3.40387600
H	3.91914100	4.42558800	-2.66989300	H	-3.03594300	1.46325000	2.05217200
H	4.59313300	2.96993700	-1.91611500	C	-4.79605300	-0.98447600	3.62836300
C	1.49550100	3.30901100	-3.45333000	H	-5.15333600	-2.95327000	2.83053300
H	1.74643200	2.77130800	-4.37700300	H	-4.28053400	1.04485800	4.15273800
H	0.45130700	3.07668500	-3.21091200	H	-5.34562000	-1.17014100	4.55029000
H	1.58406500	4.38444100	-3.66786300	C	-2.86876200	-1.46464800	-1.41812400
C	3.21638500	2.59383300	3.38830300	C	-3.96547400	-1.42246600	-2.27935100
H	3.23596300	3.65395500	3.68122300	C	-2.05393500	-2.60371300	-1.40553800
H	3.36274600	1.98975400	4.29471300	C	-4.25464000	-2.50768100	-3.10220100

H	-4.59059900	-0.53139000	-2.32432700	C	-0.60100500	-0.60155200	3.07274000
C	-2.35044600	-3.69005800	-2.22053900	C	-1.05144200	-0.86507000	4.42471100
H	-1.16672200	-2.61841500	-0.76497300	H	-0.32896700	-1.48736100	4.96662700
C	-3.45288800	-3.64375200	-3.07005000	H	-1.18894500	0.07616900	4.97318400
H	-5.10922700	-2.46144300	-3.77583500	H	-2.01903600	-1.38430500	4.39477600
H	-1.70667400	-4.56856400	-2.20341900	N	-0.30089100	-0.37768400	1.97094100
H	-3.68128300	-4.49053100	-3.71589500				

Complex 17at

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G= -2090.769681 a.u.

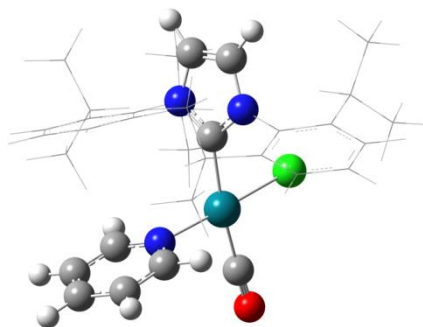


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Cl	0.86196800	1.62976300	1.91847300	H	4.17691200	-2.11103800	-2.42908500
N	-1.38013800	-1.26010200	0.69117300	C	4.79916700	-1.77730600	-0.40340700
N	0.71592400	-1.72025400	0.55576800	H	5.85911800	-1.81026200	-0.65171000
C	-0.18811800	-0.73615500	0.29404700	C	4.40174700	-1.56683400	0.90748600
C	0.09817400	-2.82679000	1.12600100	H	5.15368300	-1.43175300	1.68406600
H	0.66265800	-3.70798800	1.40103700	C	3.04970600	-1.51520500	1.25358800
C	-1.21611300	-2.53482600	1.21781300	C	2.64582400	-1.30577200	2.69698500
H	-2.05519900	-3.09830700	1.60286800	H	1.59112600	-0.99330700	2.71078400
C	-2.67353600	-0.68947000	0.43139600	C	2.79355500	-2.60542500	3.49020900
C	-3.34108700	-1.09990100	-0.73583800	H	3.84062500	-2.94272700	3.49227300
C	-4.61626700	-0.58343800	-0.96071400	H	2.48817100	-2.45587500	4.53466300
H	-5.16369000	-0.88011000	-1.85462000	H	2.18655700	-3.42187400	3.07617200
C	-5.19458800	0.30612000	-0.06396600	C	3.44463000	-0.19217900	3.36827200
H	-6.19157100	0.69965300	-0.25718600	H	4.49457700	-0.47883600	3.52768600
C	-4.50772400	0.69420100	1.07718100	H	3.41133800	0.72870600	2.77501900
H	-4.97170000	1.38982100	1.77562800	H	3.01310800	0.02861700	4.35345200
C	-3.22944300	0.20449800	1.35383000	C	1.45796000	-2.16786300	-2.19853600
C	-2.51924300	0.59440300	2.63098700	H	0.54198700	-1.62189400	-1.93299700
H	-1.45860100	0.31761400	2.54119400	C	1.10834500	-3.65519200	-2.26994200
C	-2.55276300	2.09897600	2.87508800	H	1.99865000	-4.25105300	-2.52000100
H	-2.14725600	2.64140200	2.01133700	H	0.35074600	-3.83670500	-3.04634500
H	-1.93292100	2.34988700	3.74540800	H	0.70841600	-4.02831200	-1.31653900
H	-3.57123200	2.46471900	3.07308500	C	1.88389000	-1.65507900	-3.56880400
C	-3.11919900	-0.16161700	3.81660300	H	2.20320400	-0.60470300	-3.52508700
H	-2.58402100	0.08819600	4.74251000	H	1.04254800	-1.72275400	-4.27087100
H	-3.06461200	-1.25029500	3.67724100	H	2.70820500	-2.24651100	-3.99266200
H	-4.17842600	0.10044800	3.95804900	N	0.76130600	3.15851100	-0.84047300
C	-2.73625300	-2.09671400	-1.70489000	C	1.51720000	3.42558800	-1.91639300
H	-1.64387900	-2.09209900	-1.56201800	C	0.38182000	4.18103400	-0.05954600
C	-3.00802700	-1.75415600	-3.16699100	C	1.91423600	4.71043900	-2.25447200
H	-2.76796800	-0.70981400	-3.39584000	H	1.81119600	2.56602100	-2.51695200
H	-2.39512900	-2.39332600	-3.81758400	C	0.72861700	5.49652800	-0.33409200
H	-4.05826000	-1.93593800	-3.43692900	H	-0.19956600	3.91098000	0.81975500
C	-3.23311700	-3.51331300	-1.40794100	C	1.50851300	5.76880900	-1.45048100
H	-4.32582200	-3.56861600	-1.52024700	H	2.53028300	4.86996400	-3.13579900
H	-2.98470700	-3.83514100	-0.38865300	H	0.39080900	6.28917500	0.32881900
H	-2.78425800	-4.23296400	-2.10688200	H	1.79747800	6.79044500	-1.69011900
C	2.11594500	-1.69672300	0.22476800	C	-0.35291700	0.79364400	-2.03893400
C	2.48644800	-1.91398600	-1.11417900	O	-0.70142900	0.61593100	-3.13549100

Complex **17bt**

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G= -2090.754067 a.u.

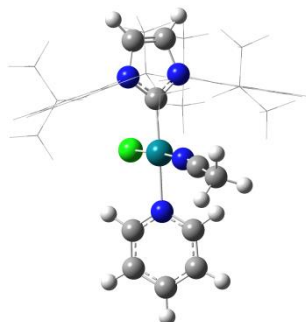


Rh	-0.04260600	-0.51037800	1.55273900	C	3.72957600	2.58918400	0.10712300
Cl	1.22162400	-2.51862900	1.34153300	H	3.72401400	3.66218500	0.28836900
N	-0.52075400	-0.75831700	-1.48870400	C	4.88577400	1.86338200	0.37083100
N	1.48880900	-0.07707600	-1.16500500	H	5.76600400	2.37018600	0.76365100
C	0.31464400	-0.30627200	-0.51102300	C	4.92188300	0.50202400	0.12455900
C	1.39289800	-0.42462900	-2.50776600	H	5.83340600	-0.05948000	0.32526700
H	2.23427900	-0.32022900	-3.18050300	C	3.80454400	-0.17468400	-0.37263300
C	0.12891400	-0.85383100	-2.71203500	C	3.90281500	-1.65217200	-0.68216500
H	-0.37841700	-1.20994200	-3.59915400	H	2.88350000	-2.03785200	-0.82202200
C	-1.94776100	-0.84847400	-1.34618400	C	4.70051600	-1.87199900	-1.96892900
C	-2.70195600	0.28821400	-1.68799600	H	5.73019600	-1.50012500	-1.86131600
C	-4.08836500	0.20919200	-1.55166100	H	4.75518600	-2.94259800	-2.20781300
H	-4.70292700	1.07076900	-1.81420500	H	4.25627500	-1.35664400	-2.83213000
C	-4.69452700	-0.95536800	-1.09696300	C	4.52409100	-2.44366600	0.46507900
H	-5.77845800	-1.00179800	-1.00024400	H	5.58875700	-2.20300800	0.60122400
C	-3.92324200	-2.06520900	-0.77742800	H	3.98911300	-2.25648000	1.40328500
H	-4.40837400	-2.97800700	-0.43308500	H	4.45539300	-3.51867100	0.25244700
C	-2.53129900	-2.04051200	-0.89714400	C	1.36953100	2.79158700	-0.77613800
C	-1.71293300	-3.27661100	-0.60500900	H	0.46990000	2.21797200	-0.49776400
H	-0.65856000	-2.98173300	-0.51347700	C	1.33735600	3.03199200	-2.28916100
C	-2.09432000	-3.93156300	0.71794900	H	2.23411100	3.58724300	-2.60128300
H	-2.02351100	-3.21239200	1.54523300	H	0.45709200	3.62978700	-2.56983800
H	-1.39836200	-4.75048900	0.93889800	H	1.30286000	2.09719600	-2.86292600
H	-3.11093900	-4.35186400	0.69639600	C	1.28464500	4.13998900	-0.06678000
C	-1.83814900	-4.26463300	-1.76482800	H	1.42904000	4.05660200	1.01912300
H	-1.21627000	-5.15049500	-1.58041200	H	0.29815200	4.59009800	-0.24533300
H	-1.51659700	-3.81675200	-2.71589300	H	2.03526100	4.84723600	-0.44768100
H	-2.87793800	-4.60229300	-1.89030800	C	-0.23948800	-0.91302000	3.37671800
C	-2.06290900	1.54813800	-2.23934500	O	-0.33228300	-1.19237800	4.49355200
H	-0.97480300	1.46519800	-2.11441000	N	-1.28041300	1.18000100	1.73823000
C	-2.49309600	2.81344000	-1.50432000	C	-0.77896200	2.39018800	2.03246100
H	-2.20929400	2.78040700	-0.44443900	C	-2.61613000	1.03810000	1.69192100
H	-2.01339000	3.69338400	-1.95649100	C	-1.58335200	3.49103900	2.29278100
H	-3.57905300	2.97603600	-1.55599500	H	0.30778900	2.45022300	2.06961800
C	-2.33832600	1.67709600	-3.73768300	C	-3.48712900	2.08837300	1.94485400
H	-3.41098700	1.82068900	-3.93284600	H	-2.98006000	0.03920700	1.45646700
H	-2.01862000	0.78163300	-4.28709800	C	-2.96502400	3.33869900	2.25455300
H	-1.80191700	2.54098200	-4.15482800	H	-1.12097300	4.44794400	2.52492700
C	2.64638400	0.57630200	-0.61058300	H	-4.55948800	1.91543300	1.89309500
C	2.58767700	1.96906800	-0.39590100	H	-3.62265800	4.18072400	2.46118100

Complex **20at**

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G= -2110.092055 a.u.

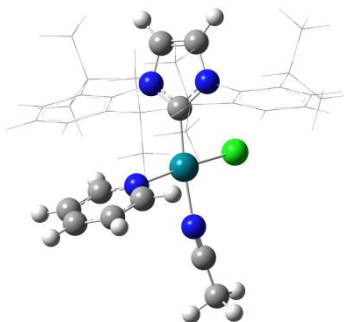


Rh	-0.11576900	1.13535400	0.03635300	C	-4.97070000	-1.36461700	0.55517300
Cl	-0.57399400	1.33259600	-2.29533800	H	-6.02734800	-1.30467300	0.81273100
N	1.21697600	-1.50780700	-0.61489200	C	-4.57960500	-1.34260700	-0.77391800
N	-0.91280400	-1.73137200	-0.43097600	H	-5.33299700	-1.25687200	-1.55639000
C	0.08678000	-0.80776300	-0.29131900	C	-3.23119300	-1.42163600	-1.13203500
C	-0.41566500	-2.95931700	-0.85376200	C	-2.83069300	-1.40763000	-2.59153900
H	-1.06988300	-3.80422900	-1.02498400	H	-1.74945600	-1.21196500	-2.64427900
C	0.92054900	-2.81835500	-0.97232100	C	-3.12645000	-2.75769400	-3.24566400
H	1.69535900	-3.51115200	-1.27420900	H	-4.20317900	-2.98183000	-3.21281500
C	2.55894200	-1.04142500	-0.42208000	H	-2.81849400	-2.75066600	-4.30004300
C	3.14726200	-1.25126800	0.83620100	H	-2.60266400	-3.58547200	-2.74770000
C	4.46531500	-0.83308400	1.01149800	C	-3.51462100	-0.28250400	-3.36218900
H	4.95385800	-0.98265300	1.97447300	H	-4.59722300	-0.44999100	-3.46281100
C	5.16473200	-0.22884100	-0.02632700	H	-3.34440600	0.68384800	-2.87318000
H	6.19408500	0.09212100	0.12854200	H	-3.09633100	-0.21991400	-4.37561400
C	4.55826300	-0.03812900	-1.25956400	C	-1.62285100	-1.69042900	2.35621000
H	5.11614600	0.43318100	-2.06845700	H	-0.70274200	-1.20620000	2.00087600
C	3.24004500	-0.44000500	-1.48661800	C	-1.30598600	-3.16015600	2.63222000
C	2.60857400	-0.27871700	-2.85035200	H	-2.19961400	-3.69119500	2.99288300
H	1.51917500	-0.37699300	-2.74035200	H	-0.52340100	-3.24793200	3.40148400
C	2.85884100	1.09878100	-3.45279200	H	-0.94564900	-3.67590100	1.73156500
H	2.54475100	1.88986700	-2.76032000	C	-2.01117800	-0.98053700	3.64697800
H	2.27172800	1.21243000	-4.37306800	H	-2.28686500	0.06674700	3.45648300
H	3.91720300	1.25430400	-3.71061900	H	-1.16092100	-0.99351400	4.34561100
C	3.10520800	-1.37941700	-3.78843500	H	-2.85179800	-1.47111600	4.15874500
H	2.63564600	-1.28495500	-4.77687400	N	-0.42102200	3.25731000	0.20137500
H	2.87585200	-2.38153900	-3.39967600	C	-1.19375900	3.77392200	1.16830300
H	4.19546600	-1.31810600	-3.92503800	C	0.12386200	4.09939700	-0.69007400
C	2.40220900	-1.94715600	1.95633900	C	-1.44080100	5.13339500	1.29130900
H	1.32341500	-1.83694400	1.76712000	H	-1.63189100	3.05264900	1.85730400
C	2.68262600	-1.33788400	3.32652100	C	-0.06679400	5.47332200	-0.63350500
H	2.63277100	-0.24188700	3.29300100	H	0.70962700	3.63060000	-1.47829300
H	1.94322400	-1.70543700	4.05492500	C	-0.86180800	6.00352200	0.37466300
H	3.67583500	-1.61820300	3.70586400	H	-2.08307300	5.49587100	2.09072900
C	2.72666300	-3.44142900	1.98008000	H	0.40106500	6.11123600	-1.37942900
H	3.80529500	-3.59711400	2.12917500	H	-1.03298500	7.07641300	0.44249900
H	2.44059300	-3.93634500	1.04362300	N	0.26164200	1.10620200	1.96676900
H	2.19531000	-3.94391700	2.80089900	C	0.42934200	1.23908700	3.11300600
C	-2.29468900	-1.53539500	-0.09719000	C	0.63655000	1.43182500	4.53615900
C	-2.66017500	-1.54771800	1.26109000	H	1.31278100	2.27637300	4.71698600
C	-4.01738700	-1.45996300	1.56282700	H	-0.31457800	1.63390000	5.04537500
H	-4.34011900	-1.47118900	2.60298100	H	1.08196600	0.53551000	4.98584000

Complex **20bt**

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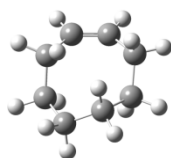


Rh	-0.05597300	-0.92319700	1.00301600	C	4.91005700	1.60899900	1.20398300
Cl	1.36484900	-2.65449800	0.17731100	H	5.77972900	1.89604300	1.79377200
N	-0.42422100	0.10190900	-1.79169100	C	4.97523100	0.51430100	0.35906500
N	1.56756100	0.55217500	-1.11337600	H	5.89996200	-0.05720700	0.28856700
C	0.37071600	0.04412800	-0.67613200	C	3.87456000	0.12048300	-0.40714100
C	1.51539600	0.87443700	-2.46639200	C	4.00859900	-1.05247600	-1.35545400
H	2.37428700	1.28316400	-2.98228200	H	2.99777900	-1.35976700	-1.65781400
C	0.26781300	0.59028300	-2.89305700	C	4.80742600	-0.64757200	-2.59576100
H	-0.20277900	0.68553100	-3.86307500	H	5.83399200	-0.35934400	-2.32426900
C	-1.84726500	-0.05766300	-1.77224200	H	4.87271300	-1.48704300	-3.30128000
C	-2.62872100	1.10252100	-1.62530700	H	4.36022900	0.20376600	-3.12650600
C	-4.01634700	0.95700600	-1.64917600	C	4.65600500	-2.26560800	-0.69344800
H	-4.65005800	1.83893500	-1.55275200	H	5.71396200	-2.08659200	-0.45070000
C	-4.59834600	-0.29601800	-1.79299900	H	4.11573600	-2.54376500	0.21853600
H	-5.68334500	-0.39239000	-1.81171100	H	4.61854200	-3.12323400	-1.37858700
C	-3.80073400	-1.42661200	-1.91693600	C	1.36632000	2.87450000	0.59234500
H	-4.26690100	-2.40534700	-2.03051100	H	0.48901100	2.20907900	0.53865000
C	-2.40647600	-1.33432000	-1.91412500	C	1.33197700	3.82415500	-0.60896200
C	-1.55345600	-2.56821400	-2.09932100	H	2.20488200	4.49346200	-0.58773200
H	-0.51519900	-2.31408000	-1.84727900	H	0.42726200	4.45060800	-0.58515400
C	-1.95506200	-3.69873200	-1.15809100	H	1.34177600	3.28811700	-1.56707400
H	-1.94481800	-3.35490700	-0.11411600	C	1.23225600	3.69221100	1.87365300
H	-1.22807700	-4.51712900	-1.23688600	H	1.37921300	3.08124200	2.77481200
H	-2.95044000	-4.10540600	-1.39344800	H	0.23116000	4.14346000	1.92615100
C	-1.59633900	-3.01554300	-3.55963800	H	1.95747000	4.51801900	1.91053200
H	-0.94535800	-3.88630600	-3.71353800	N	-1.47247100	0.38777300	1.79167600
H	-1.25749000	-2.21507700	-4.23282600	C	-1.15460700	1.30110300	2.72662800
H	-2.61604400	-3.29812600	-3.86222300	C	-2.77799600	0.17268800	1.54195900
C	-2.00474800	2.47715200	-1.48173000	C	-2.10822900	2.02751300	3.42616600
H	-0.93765900	2.34373300	-1.25497000	H	-0.08939700	1.42847100	2.91007200
C	-2.59574300	3.29331200	-0.33604400	C	-3.79078500	0.85186400	2.20506200
H	-2.46166500	2.79276900	0.63164600	H	-2.99635100	-0.57835800	0.78411500
H	-2.09709300	4.27163000	-0.27941900	C	-3.45536200	1.80075200	3.16432600
H	-3.66956900	3.48652200	-0.47252000	H	-1.78693500	2.75695900	4.16667600
C	-2.10607500	3.25428000	-2.79416900	H	-4.82715700	0.63648700	1.95367500
H	-3.15712000	3.45064600	-3.05265400	H	-4.22769900	2.35414900	3.69523500
H	-1.65543800	2.70136100	-3.62845200	N	-0.36464600	-2.14517000	2.63515900
H	-1.59157000	4.22228500	-2.71175700	C	-0.40085200	-2.96655900	3.45175500
C	2.70011600	0.87642300	-0.29009100	C	-0.41821300	-4.01426200	4.45269900
C	2.61034700	2.00573900	0.54910600	H	0.12435500	-3.70062300	5.35184400
C	3.73635200	2.34772800	1.29490900	H	-1.44648800	-4.26740100	4.73433400
H	3.70365700	3.21379700	1.95369700	H	0.06484800	-4.91257300	4.05220600

Cyclooctene

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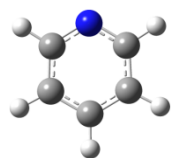


C	-1.93665100	-0.08563800	-0.19684700	H	-2.09416600	2.01861000	-0.06184000
C	-1.36353500	1.24523600	0.21174600	H	1.75003700	-2.14128300	-0.58607300
C	1.09365500	-1.26714700	-0.46986800	H	0.02294900	2.74897500	-0.41173100
C	0.00306100	1.65026300	-0.37984300	H	2.70007700	-0.35861100	0.64874900
C	1.96319100	-0.06143300	-0.11436900	H	1.97341900	1.99316800	0.43754300
C	1.23518900	1.17833700	0.40471700	H	0.94525000	1.02355300	1.45622300
H	-1.28867800	1.29904800	1.31164600	C	-1.38925600	-1.29057800	-0.02623200
H	0.06484300	1.32373800	-1.42959000	H	-1.94629000	-2.15577600	-0.39298700
H	0.63677300	-1.10922200	-1.45759800	C	-0.03039000	-1.57058800	0.54553900
H	2.55151700	0.21165200	-1.00462100	H	0.12696200	-0.97620400	1.45951100
H	-2.91522900	-0.04814300	-0.68056000	H	0.02094700	-2.62021900	0.86226100

Pyridine

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G= -248.032669 a.u.

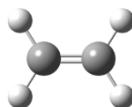


C	-1.13780000	-0.71919000	-0.00021400	H	-0.00001000	2.46803700	0.00016200
C	-1.19473700	0.67048000	-0.00012500	H	-2.05799500	-1.30655300	-0.00036800
C	0.00000400	1.37937400	0.00010600	H	-2.15526600	1.18113300	-0.00025400
C	1.19473500	0.67048300	0.00021700	H	2.15530700	1.18106700	0.00035500
C	1.13780000	-0.71918600	0.00011300	H	2.05797500	-1.30656300	0.00017300
N	-0.00000300	-1.41555500	-0.00009200				

Ethylene

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G= -78.483936 a.u.

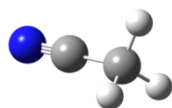


C	0.66326900	0.00000000	0.00000300	H	1.23977500	-0.92365000	0.00002400
C	-0.66326900	0.00000000	-0.00000400	H	-1.23977500	-0.92365000	0.00001100
H	1.23977500	0.92365000	-0.00001000	H	-1.23977500	0.92365000	-0.00002200

Acetonitrile

E= -132.65684412 a.u.

G= -132.634287 a.u.



C	0.00000000	0.00000000	-1.17522000
H	0.00000000	1.02626500	-1.55829600
H	0.88877100	-0.51313200	-1.55829600

H	-0.88877100	-0.51313200	-1.55829600
C	0.00000000	0.00000000	0.27734500
N	0.00000000	0.00000000	1.43744800