

Supporting Information
For

**A potential role of substrate as a base for deprotonation pathway in
Rh-catalysed C-H amination of heteroArenes: DFT insights**

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Details of computational method adopted in the manuscript

Geometry optimizations and frequency calculations were performed using Gaussian 09 quantum chemistry package.¹ All the geometries were optimized at B3LYP/Gen level² where Gen stands for 6-311+G** basis set³ for all atoms except for Rh and Sb, which are treated with SDDAll basis set.⁴ Transition states (first order saddle points) were characterized by one and only one imaginary frequency (negative Eigen value for the Hessian) pertaining to the desired reaction coordinates whereas all the reactants and intermediates were characterized by no imaginary frequency (Hessian is positive definite). In order to account for missing London dispersion effects and basis set superposition error, dispersion (D3) corrections including Becke Johnson damping function (BJ) and geometrical counterpoise corrections (gCP) are also added.⁵ Energies are further refined by single point solvation energy correction (solvent is 1,2 dichloroethane) using SMD method.⁶ The discussions presented in the main text are based on the relative Gibbs energies at 358.15 K and 1 atm with respect to the infinitely separated reactants. The activation energy $\Delta G^\ddagger$ is the Gibbs energy difference between a reactant and the corresponding transition state.

Table S1. Energy parameters of all key stationary points.

Geometries	E _{ele} (a.u)	G _{corr} (298.15 K) (a.u)	SMD-E _{ele} (a.u)	G _{corr} (358.15 K) (a.u)	gCP-D3 corrections (a.u)
a	-2189.91635	0.34253	-2189.99047	0.31602	0.08688
b	-2669.38169	0.49240	-2669.48030	0.45929	0.06984
TS₁	-2669.36061	0.49268	-2669.43751	0.46066	0.06516
c	-2669.39458	0.49550	-2669.47888	0.46301	0.06379
d	-1584.51237	0.32870	-1584.55787	0.30721	0.02605
e	-1980.44419	0.42075	-1980.50616	0.39471	0.01141
TS₂	-1980.42373	0.41975	-1980.47568	0.39410	0.01174
f	-1870.91715	0.41510	-1870.97598	0.39043	0.01762
TS₃	-1870.90405	0.41514	-1870.96484	0.39074	0.01660
g	-1870.98107	0.42000	-1871.03391	0.39590	0.01699
h	-2955.87392	0.58991	-2955.95719	0.55515	0.05155
TS₄	-2955.86569	0.58826	-2955.94155	0.55418	0.04646
i	-2955.86457	0.59411	-2955.95971	0.55998	0.04597
j	-2350.43257	0.57546	-2350.50144	0.54589	-0.00944
TS₅	-2350.39261	0.57454	-2350.46367	0.54587	-0.01119
k	-2350.46182	0.57949	-2350.52841	0.55041	-0.00786
N ₂	-109.55969	-0.01286	-109.55453	-0.01730	0.00081
Phenylazide	-395.94308	0.07115	-395.95270	0.06286	0.00035
2pb	-479.46573	0.13422	-479.48546	0.12489	-0.00252
2pbH ⁺ SbF ₆ ⁻	-1084.88474	0.14607	-1084.92466	0.13110	0.05678
pdt	-765.94613	0.22340	-765.97295	0.21105	-0.00719

Table S2. Coordinates (Å) and energy parameters (a.u) of the optimized geometries at B3LYP level of theory. Imaginary frequencies of the transition states at 298.15 K is also given.

a
SCF Energy = -2189.91635326 a.u

symmetry c1

C	-0.198579000	-1.337172000	1.687432000
C	0.447323000	-0.156870000	2.117531000
C	-1.115217000	-1.975449000	2.528436000
H	-1.647784000	-2.849732000	2.177373000
C	0.151366000	0.368342000	3.387902000
C	-1.399179000	-1.435368000	3.776008000
H	0.689236000	1.239161000	3.742739000
H	-2.128107000	-1.921976000	4.413661000
C	-0.772804000	-0.259525000	4.207913000
H	-0.996967000	0.143405000	5.188634000
C	0.066925000	-1.819944000	0.321536000
N	0.146879000	-0.851783000	-0.622813000
C	0.229651000	-3.162710000	-0.004409000
C	0.415260000	-1.192643000	-1.892792000
C	0.506802000	-3.510511000	-1.316307000
H	0.473482000	-0.389971000	-2.610761000
C	0.604850000	-2.507654000	-2.276868000
C	-1.143024000	2.565509000	-1.320739000
C	-1.420467000	3.037106000	0.033673000
C	-0.182313000	3.179984000	0.710262000
C	0.888953000	2.803680000	-0.203975000
C	0.285067000	2.465993000	-1.467481000
Rh	-0.419449000	1.073338000	0.081671000
C	1.027291000	2.178986000	-2.728894000
H	1.366542000	3.131504000	-3.153982000
H	1.909626000	1.563708000	-2.547204000
H	0.390135000	1.702636000	-3.474459000
C	2.345445000	2.989473000	0.052550000
H	2.563726000	4.064914000	0.034234000
H	2.651982000	2.596790000	1.021062000
H	2.953684000	2.497778000	-0.701893000
C	-2.152561000	2.379044000	-2.403803000
H	-1.897108000	1.543011000	-3.054850000
H	-3.147913000	2.194865000	-2.004124000
H	-2.187885000	3.288912000	-3.016003000
C	-2.777461000	3.337628000	0.577496000
H	-3.517551000	2.613104000	0.238131000
H	-2.779323000	3.353388000	1.667128000
H	-3.092669000	4.327528000	0.226298000

C	0.022604000	3.723512000	2.087427000
H	-0.795722000	3.461106000	2.757811000
H	0.959281000	3.374428000	2.520811000
H	0.073069000	4.817347000	2.034595000
H	0.830248000	-2.733770000	-3.310494000
H	0.657093000	-4.548455000	-1.587142000
H	0.169091000	-3.909852000	0.775100000
H	1.351440000	0.171859000	1.606006000
Sb	4.380272000	-0.552417000	-0.123695000
F	5.526535000	-1.319294000	1.213657000
F	3.139359000	0.253380000	-1.410425000
F	5.478085000	1.025507000	-0.298497000
F	3.099275000	-1.994210000	0.052566000
F	5.281497000	-1.454764000	-1.563059000
F	3.351717000	0.383398000	1.254751000
Sb	-3.929987000	-0.850206000	-0.360381000
F	-2.846711000	-0.722594000	-1.959895000
F	-4.813937000	-0.825316000	1.343374000
F	-2.406112000	0.096524000	0.531767000
F	-5.378972000	-1.709085000	-1.266530000
F	-4.600945000	0.927628000	-0.746449000
F	-3.045868000	-2.501633000	0.092329000

Number of imaginary frequencies= 0

b

SCF Energy = -2669.38168759 a.u

symmetry c1

C	-0.866389000	0.101877000	-1.985951000
C	0.266259000	-0.259514000	-1.217290000
C	-1.264326000	-0.705315000	-3.050676000
H	-2.159864000	-0.466393000	-3.610587000
C	0.977506000	-1.431202000	-1.523386000
C	-0.554419000	-1.868881000	-3.337231000
H	1.873879000	-1.680578000	-0.970306000
H	-0.885864000	-2.504496000	-4.150044000
C	0.555074000	-2.237782000	-2.572834000
H	1.103901000	-3.141165000	-2.810127000
C	-1.665912000	1.261105000	-1.559394000
N	-1.849905000	1.366987000	-0.221912000
C	-2.231231000	2.183991000	-2.439972000
C	-2.592136000	2.376875000	0.262892000
C	-2.993051000	3.224865000	-1.934774000
H	-2.726310000	2.407870000	1.334613000
C	-3.177408000	3.325027000	-0.556652000
C	-1.414672000	-1.547333000	2.692451000
C	-0.044126000	-1.652037000	2.301042000

C	0.535525000	-0.322950000	2.371326000
C	-0.492726000	0.596914000	2.791575000
C	-1.711899000	-0.156876000	2.983215000
Rh	-1.095724000	-0.297558000	0.909861000
C	-3.011590000	0.346421000	3.521162000
H	-3.125390000	0.017847000	4.560638000
H	-3.058968000	1.435432000	3.516483000
H	-3.854479000	-0.042522000	2.948611000
C	-0.275702000	2.043348000	3.098350000
H	0.286405000	2.125282000	4.035844000
H	0.296477000	2.564004000	2.327398000
H	-1.217695000	2.573532000	3.235700000
C	-2.376109000	-2.679673000	2.805670000
H	-3.410220000	-2.341343000	2.798009000
H	-2.251845000	-3.401573000	1.998423000
H	-2.187898000	-3.202136000	3.751817000
C	0.680832000	-2.923265000	1.995573000
H	0.051728000	-3.615082000	1.433266000
H	1.602819000	-2.753380000	1.441747000
H	0.947939000	-3.414937000	2.938729000
C	1.966984000	0.021124000	2.167305000
H	2.467511000	-0.638937000	1.463043000
H	2.097424000	1.054164000	1.847800000
H	2.489059000	-0.093659000	3.126309000
H	-3.771420000	4.117525000	-0.120942000
H	-3.440361000	3.951073000	-2.603013000
H	-2.059520000	2.076199000	-3.502702000
Sb	5.241802000	-1.813002000	-0.086266000
F	4.545933000	-0.894164000	-1.650743000
F	5.760230000	-2.695116000	1.546358000
F	3.366936000	-2.256943000	0.319320000
F	7.039623000	-1.268812000	-0.493123000
F	5.382803000	-3.448841000	-1.091373000
F	4.912310000	-0.175594000	0.916663000
Sb	-4.506641000	-1.743025000	-0.602723000
F	-4.725049000	-0.868411000	1.119029000
F	-4.038257000	-2.551140000	-2.280796000
F	-4.367911000	-3.425750000	0.320782000
F	-4.400185000	0.004848000	-1.415460000
F	-6.393525000	-1.885864000	-0.878589000
F	-2.542934000	-1.535649000	-0.250818000
N	0.726436000	4.942898000	1.193985000
C	0.090354000	5.903408000	1.869648000
H	-0.179443000	5.665217000	2.895791000
C	-0.228393000	7.148461000	1.335831000
H	-0.744771000	7.888826000	1.934628000
H	-0.056222000	8.368915000	-0.435844000
C	0.152063000	7.407905000	0.021231000

C	0.824394000	6.423713000	-0.690821000
H	1.165586000	6.613738000	-1.700468000
C	1.096051000	5.189632000	-0.077579000
H	1.034798000	4.575123000	-2.746865000
C	1.699514000	3.934871000	-2.177056000
C	1.828593000	4.114679000	-0.792552000
C	2.683369000	3.258222000	-0.082537000
H	2.807184000	3.412114000	0.982832000
C	3.385152000	2.247405000	-0.733116000
H	4.042616000	1.590811000	-0.175340000
H	3.779616000	1.270154000	-2.600982000
C	3.239885000	2.071407000	-2.110589000
C	2.399162000	2.920628000	-2.828798000
H	2.281152000	2.789563000	-3.899008000
H	0.737304000	0.487708000	-0.582882000

Number of imaginary frequencies= 0

TS₁

SCF Energy = -2669.36060789 a.u

symmetry c1

C	1.517832000	1.115018000	-1.476738000
C	1.397181000	1.591138000	-0.135175000
C	2.547326000	1.552416000	-2.308920000
H	2.659682000	1.144129000	-3.305652000
C	2.398600000	2.473444000	0.320915000
C	3.496134000	2.447712000	-1.822059000
H	2.352485000	2.853659000	1.334186000
H	4.312290000	2.761526000	-2.462801000
C	3.429105000	2.905050000	-0.505562000
H	4.182206000	3.587407000	-0.128802000
C	0.571937000	0.069344000	-1.888513000
N	0.034953000	-0.638009000	-0.858578000
C	0.229576000	-0.222351000	-3.207403000
C	-0.827667000	-1.631953000	-1.118578000
C	-0.677258000	-1.240326000	-3.469654000
H	-1.226956000	-2.167925000	-0.272523000
C	-1.219521000	-1.956890000	-2.408433000
C	1.000551000	-1.697037000	2.691701000
C	1.736367000	-0.476812000	3.034449000
C	0.808240000	0.594861000	3.111273000
C	-0.495216000	0.079821000	2.721288000
C	-0.363730000	-1.359168000	2.541477000
Rh	0.849531000	-0.155385000	1.048198000
C	-1.490562000	-2.314160000	2.328530000
H	-1.913449000	-2.583589000	3.303958000
H	-2.301213000	-1.888217000	1.741026000

H	-1.155053000	-3.240207000	1.860241000
C	-1.788710000	0.822853000	2.810691000
H	-2.175199000	0.751761000	3.835085000
H	-1.663025000	1.881523000	2.580148000
H	-2.541455000	0.406238000	2.142946000
C	1.586101000	-3.070135000	2.632743000
H	1.102159000	-3.685918000	1.875065000
H	2.650916000	-3.050245000	2.408491000
H	1.450751000	-3.559084000	3.605537000
C	3.201706000	-0.434788000	3.325596000
H	3.763805000	-1.042666000	2.615112000
H	3.593263000	0.581829000	3.294968000
H	3.387261000	-0.839075000	4.327703000
C	1.072265000	1.976381000	3.618204000
H	2.127873000	2.239456000	3.554960000
H	0.493762000	2.724978000	3.076968000
H	0.779777000	2.036100000	4.672734000
H	-1.958728000	-2.732182000	-2.552714000
H	-0.962998000	-1.468869000	-4.489518000
H	0.670758000	0.348023000	-4.013562000
Sb	-5.066035000	-1.264844000	-0.173483000
F	-4.169910000	-2.296358000	-1.546805000
F	-5.804503000	-0.148143000	1.217295000
F	-6.777307000	-2.007668000	-0.619756000
F	-3.301557000	-0.512742000	0.267940000
F	-4.661405000	-2.649485000	1.114920000
F	-5.262567000	0.197542000	-1.436228000
Sb	3.833085000	-2.353807000	-0.793289000
F	2.234953000	-3.402578000	-0.484196000
F	5.316474000	-1.146417000	-1.004982000
F	4.441742000	-2.809062000	0.990687000
F	3.081828000	-1.733350000	-2.460654000
F	4.758635000	-3.821996000	-1.604795000
F	2.852585000	-0.872344000	0.095860000
N	-0.978936000	2.877679000	-0.284370000
C	-2.032990000	2.092488000	-0.566339000
H	-1.985548000	1.067546000	-0.227989000
C	-3.141844000	2.553059000	-1.261718000
H	-3.970893000	1.879833000	-1.444778000
H	-3.976406000	4.270378000	-2.256312000
C	-3.134585000	3.872582000	-1.701328000
C	-2.044490000	4.685502000	-1.405527000
H	-2.029046000	5.727056000	-1.700272000
C	-0.969170000	4.172869000	-0.678525000
H	0.599354000	5.688870000	-2.292242000
C	0.849443000	5.800201000	-1.243221000
C	0.160683000	5.050634000	-0.282235000
C	0.498709000	5.199575000	1.067922000

H	-0.056544000	4.650660000	1.819648000
C	1.509500000	6.077025000	1.450305000
H	1.750660000	6.197725000	2.500387000
H	2.988682000	7.491447000	0.782912000
C	2.201029000	6.808586000	0.485965000
C	1.869707000	6.666947000	-0.860792000
H	2.405687000	7.232033000	-1.614573000
H	0.146322000	2.201698000	0.001158000

Number of Imaginary frequencies= 1 (-1378.8653 cm⁻¹)

c

SCF Energy = -2669.39458211 a.u

symmetry c1

C	0.898834000	0.605648000	0.574647000
C	0.351615000	-0.508496000	1.246966000
C	1.558271000	1.616988000	1.289187000
H	2.060170000	2.419062000	0.763188000
C	0.430923000	-0.548869000	2.640169000
C	1.652430000	1.542717000	2.677810000
H	0.005801000	-1.384002000	3.186536000
H	2.211827000	2.294689000	3.221325000
C	1.074902000	0.466484000	3.353938000
H	1.157540000	0.399206000	4.434201000
C	0.703715000	0.633104000	-0.880201000
N	-0.094201000	-0.363274000	-1.346959000
C	1.235875000	1.579141000	-1.758837000
C	-0.445470000	-0.390648000	-2.640528000
C	0.905045000	1.523206000	-3.104942000
H	-1.132760000	-1.171670000	-2.933050000
C	0.027518000	0.539497000	-3.554243000
C	-0.329118000	-3.830837000	-1.280150000
C	0.932051000	-3.398271000	-0.670104000
C	0.812087000	-3.558667000	0.766547000
C	-0.546792000	-3.891976000	1.042012000
C	-1.229957000	-4.102326000	-0.242737000
Rh	-0.462073000	-1.927991000	0.040542000
C	-2.651209000	-4.549501000	-0.370439000
H	-2.741753000	-5.591969000	-0.043528000
H	-3.326123000	-3.952132000	0.246105000
H	-3.004643000	-4.487656000	-1.399197000
C	-1.146723000	-4.211709000	2.377912000
H	-1.164260000	-5.295614000	2.542061000
H	-0.572367000	-3.768164000	3.192245000
H	-2.174727000	-3.851715000	2.451456000
C	-0.568172000	-3.994465000	-2.750462000
H	-1.616809000	-3.844360000	-3.012155000

H	0.031713000	-3.297658000	-3.337301000
H	-0.287316000	-5.004861000	-3.068837000
C	2.203957000	-3.110410000	-1.402928000
H	2.013326000	-2.691051000	-2.391408000
H	2.836691000	-2.412672000	-0.854675000
H	2.766881000	-4.041311000	-1.543332000
C	1.950846000	-3.452488000	1.730840000
H	2.652542000	-2.669171000	1.441490000
H	1.610421000	-3.252958000	2.746732000
H	2.494295000	-4.404692000	1.744327000
H	-0.278162000	0.477120000	-4.590691000
H	1.332261000	2.239140000	-3.797259000
H	1.939725000	2.311851000	-1.393621000
C	-1.314872000	5.156167000	-2.363269000
C	-2.021060000	4.514533000	-1.352009000
C	-0.026981000	5.635878000	-2.125502000
C	0.560623000	5.468794000	-0.872395000
C	-0.138079000	4.824057000	0.143113000
C	-1.435477000	4.344565000	-0.089632000
C	-2.197435000	3.687946000	0.984385000
N	-1.565026000	2.797496000	1.785160000
C	-2.161527000	2.151146000	2.810215000
C	-3.485519000	2.391475000	3.093571000
C	-4.184099000	3.298950000	2.294311000
C	-3.542473000	3.945944000	1.249347000
H	-1.766630000	5.271818000	-3.341366000
H	0.519344000	6.138122000	-2.915458000
H	1.559043000	5.844588000	-0.682975000
H	0.315726000	4.724947000	1.122938000
H	-1.539724000	1.444674000	3.340928000
H	-3.969004000	1.856302000	3.897874000
H	-5.232303000	3.492605000	2.486355000
H	-4.065983000	4.661585000	0.631146000
H	-3.005315000	4.107258000	-1.548870000
H	-0.596255000	2.538851000	1.571810000
Sb	5.212588000	0.300136000	0.059897000
F	6.724126000	1.438273000	-0.307026000
F	3.646556000	-0.817067000	0.393951000
F	6.342939000	-1.108406000	0.739149000
F	4.001511000	1.686998000	-0.589551000
F	5.003601000	1.050219000	1.833417000
F	5.264926000	-0.444158000	-1.726301000
Sb	-4.113472000	-0.352707000	-0.304326000
F	-3.367981000	-1.020208000	-1.957485000
F	-4.707840000	0.298412000	1.418235000
F	-4.918543000	-2.068914000	0.034766000
F	-3.156283000	1.319357000	-0.538662000
F	-2.489055000	-1.020301000	0.601618000

F -5.668689000 0.356411000 -1.179050000

Number of Imaginary frequencies= 0

d

SCF Energy = -1584.51237336 a.u

symmetry c1

C	1.839460000	2.296580000	-0.467618000
C	1.836753000	1.022122000	-1.077242000
C	2.351913000	3.410797000	-1.146660000
H	2.355398000	4.388523000	-0.677955000
C	2.292321000	0.918894000	-2.391606000
C	2.836996000	3.277894000	-2.441990000
H	2.249350000	-0.029518000	-2.913605000
H	3.226907000	4.141854000	-2.967293000
C	2.789547000	2.033513000	-3.069988000
H	3.133862000	1.929833000	-4.093689000
C	1.196843000	2.375668000	0.845526000
N	0.690006000	1.194990000	1.288204000
C	1.031690000	3.535621000	1.608769000
C	-0.023579000	1.151896000	2.422838000
C	0.327258000	3.481994000	2.802187000
H	-0.468088000	0.198780000	2.670906000
C	-0.223665000	2.271547000	3.215234000
C	0.589715000	-2.730206000	0.583547000
C	1.298886000	-2.559793000	-0.696607000
C	2.576177000	-1.999127000	-0.428195000
C	2.591584000	-1.623246000	0.971567000
C	1.382822000	-2.183577000	1.593993000
Rh	1.047705000	-0.481463000	0.046506000
C	1.100675000	-2.179534000	3.064513000
H	1.613728000	-3.019153000	3.547660000
H	1.457980000	-1.266685000	3.544818000
H	0.034877000	-2.280705000	3.272270000
C	3.774907000	-1.087524000	1.719189000
H	4.402331000	-1.909761000	2.084096000
H	4.391742000	-0.451253000	1.083799000
H	3.467095000	-0.497908000	2.584024000
C	-0.727407000	-3.423439000	0.725506000
H	-1.193441000	-3.217489000	1.688051000
H	-1.433236000	-3.122047000	-0.049638000
H	-0.581620000	-4.507259000	0.639964000
C	0.786474000	-3.073442000	-2.007015000
H	-0.268132000	-2.825629000	-2.141306000
H	1.340257000	-2.656714000	-2.848806000
H	0.878919000	-4.164902000	-2.051382000
C	3.738110000	-1.895872000	-1.365570000

H	3.428424000	-1.946910000	-2.409091000
H	4.299563000	-0.972211000	-1.225108000
H	4.419408000	-2.735422000	-1.184640000
H	-0.814526000	2.192021000	4.118078000
H	0.190709000	4.379583000	3.394219000
H	1.437275000	4.473878000	1.255542000
Sb	-2.803749000	0.099240000	-0.433976000
F	-2.222520000	-0.654630000	1.265662000
F	-3.198669000	0.828498000	-2.164620000
F	-0.888444000	0.013398000	-0.964032000
F	-4.638350000	0.117361000	0.128388000
F	-2.922808000	-1.708412000	-1.116025000
F	-2.435792000	1.849801000	0.288335000

Number of Imaginary frequencies= 0

e

SCF Energy = -1980.44418675 a.u

symmetry c1

C	-0.185546000	-1.930525000	0.171638000
C	-0.714311000	-3.183643000	-0.163637000
C	0.688198000	-1.262802000	-0.711546000
C	-0.370391000	-3.789658000	-1.365212000
C	1.022362000	-1.888165000	-1.912280000
H	-0.793931000	-4.751979000	-1.626888000
H	1.685762000	-1.400515000	-2.617404000
C	0.501352000	-3.142534000	-2.239182000
H	0.765797000	-3.605247000	-3.184497000
C	-0.505919000	-1.228257000	1.413495000
N	0.100524000	-0.019018000	1.547207000
C	-1.353755000	-1.701004000	2.420168000
C	-0.125721000	0.723455000	2.643611000
C	-1.583223000	-0.931964000	3.547666000
H	0.376733000	1.680855000	2.687104000
C	-0.956143000	0.306443000	3.668670000
C	2.540670000	2.465222000	-0.656641000
C	2.200904000	1.642837000	-1.817544000
C	0.774000000	1.635592000	-1.936249000
C	0.240605000	2.344062000	-0.796234000
C	1.354383000	2.904072000	-0.043065000
Rh	1.337750000	0.572187000	-0.079315000
C	3.938753000	2.815269000	-0.252044000
H	4.618009000	1.967396000	-0.357774000
H	4.320890000	3.615556000	-0.896524000
H	3.988264000	3.172626000	0.777444000
C	1.219627000	3.868518000	1.097149000
H	2.056721000	3.806623000	1.795776000

H	1.182580000	4.897994000	0.722386000
H	0.295402000	3.704581000	1.653276000
C	-1.196252000	2.689318000	-0.577452000
H	-1.345568000	3.749728000	-0.815454000
H	-1.856812000	2.105036000	-1.211677000
H	-1.518311000	2.530146000	0.452260000
C	-0.051506000	1.102827000	-3.064895000
H	-0.332082000	1.931416000	-3.725733000
H	0.494529000	0.372938000	-3.661567000
H	-0.966150000	0.633649000	-2.700720000
C	3.188492000	1.162820000	-2.839944000
H	2.762066000	0.384643000	-3.473535000
H	3.489513000	1.987286000	-3.497133000
H	4.093431000	0.761232000	-2.380038000
N	3.078444000	-0.451431000	1.039799000
N	3.030806000	-0.284442000	2.273488000
N	2.888293000	-0.103687000	3.378830000
C	4.346575000	-0.938161000	0.541321000
C	4.331925000	-1.787630000	-0.562475000
C	5.552287000	-0.560377000	1.137372000
C	5.539409000	-2.260409000	-1.070667000
C	6.751639000	-1.045891000	0.622048000
C	6.749778000	-1.894360000	-0.483496000
H	3.386499000	-2.083214000	-0.995762000
H	5.560994000	0.105887000	1.992887000
H	5.529308000	-2.929396000	-1.923354000
H	7.686891000	-0.755854000	1.086511000
H	7.684608000	-2.271007000	-0.881187000
H	-1.415145000	-3.677538000	0.497642000
H	-1.861464000	-2.645270000	2.291364000
H	-2.261204000	-1.283344000	4.316113000
H	-1.120036000	0.947820000	4.524593000
F	-5.742854000	0.085118000	0.851628000
F	-3.089897000	0.741037000	1.174988000
F	-4.410576000	1.659501000	-1.014764000
F	-2.508350000	-0.244272000	-1.260022000
Sb	-4.156290000	-0.093192000	-0.228758000
F	-3.754617000	-1.814479000	0.577065000
F	-5.139360000	-0.941124000	-1.652339000

Number of Imaginary frequencies= 0

TS₂

SCF Energy = -1980.42372507 a.u

symmetry c1

C	-3.279436000	1.531962000	-1.196423000
C	-4.360192000	2.358393000	-1.531436000

C	-3.449665000	0.475335000	-0.272965000
C	-5.604500000	2.160478000	-0.942459000
C	-4.699684000	0.306582000	0.322954000
H	-6.436078000	2.804574000	-1.203301000
H	-4.860192000	-0.480763000	1.051249000
C	-5.770962000	1.141730000	-0.005228000
H	-6.734726000	0.993292000	0.470235000
C	-1.914780000	1.734531000	-1.690030000
N	-0.998805000	0.893827000	-1.139287000
C	-1.504664000	2.714100000	-2.596377000
C	0.307488000	1.040447000	-1.414004000
C	-0.156804000	2.844878000	-2.907674000
H	0.997593000	0.384798000	-0.900686000
C	0.771084000	2.007047000	-2.296856000
C	-0.670016000	-2.682281000	0.522263000
C	-2.087451000	-2.754662000	0.850817000
C	-2.837226000	-2.616136000	-0.361484000
C	-1.910485000	-2.319853000	-1.413288000
C	-0.562256000	-2.431156000	-0.861658000
Rh	-1.782078000	-0.654001000	0.060291000
C	0.452922000	-2.910096000	1.486324000
H	0.202607000	-2.544024000	2.483601000
H	0.662338000	-3.982674000	1.573690000
H	1.365077000	-2.408281000	1.166960000
C	0.695269000	-2.396388000	-1.669556000
H	1.563331000	-2.119000000	-1.076482000
H	0.880195000	-3.393103000	-2.087878000
H	0.622410000	-1.706923000	-2.512032000
C	-2.244439000	-2.195422000	-2.870054000
H	-1.515923000	-1.577513000	-3.396583000
H	-2.244828000	-3.180804000	-3.350630000
H	-3.230091000	-1.751642000	-3.017849000
C	-4.301920000	-2.871026000	-0.533999000
H	-4.449068000	-3.905810000	-0.864823000
H	-4.855025000	-2.747514000	0.397278000
H	-4.748799000	-2.215591000	-1.281564000
C	-2.637210000	-3.152784000	2.185341000
H	-3.657608000	-2.795370000	2.333536000
H	-2.656536000	-4.245173000	2.275216000
H	-2.022086000	-2.775546000	3.003541000
N	-1.226976000	0.268237000	1.788621000
N	-2.436269000	0.319425000	2.891483000
N	-3.038837000	-0.211847000	3.659288000
C	-0.607678000	1.549937000	1.855262000
C	0.784444000	1.534371000	2.004117000
C	-1.291281000	2.766494000	1.735277000
C	1.492605000	2.735305000	1.988488000
C	-0.579746000	3.959853000	1.783095000

C	0.812972000	3.947053000	1.895531000
H	1.310241000	0.592286000	2.082852000
H	-2.368535000	2.767310000	1.617067000
H	2.573289000	2.700314000	2.055426000
H	-1.111829000	4.902505000	1.718886000
H	1.363818000	4.880399000	1.912185000
H	-4.232998000	3.169732000	-2.239485000
H	-2.236729000	3.373648000	-3.043153000
H	0.167460000	3.605561000	-3.608590000
H	1.837148000	2.078542000	-2.466627000
F	3.571500000	1.056109000	-1.390523000
F	6.105302000	0.246993000	-0.622036000
Sb	4.311014000	-0.198026000	-0.099421000
F	2.447018000	-0.614230000	0.362466000
F	4.894146000	-1.472925000	1.223529000
F	4.168116000	-1.598893000	-1.427986000
F	4.255604000	1.199221000	1.239966000

Number of Imaginary frequencies= 1 (-686.2783 cm⁻¹)

f

SCF Energy = -1870.91714673 a.u

symmetry c1

C	-3.290522000	-1.656498000	-1.339418000
C	-4.388129000	-2.119011000	-2.078503000
C	-3.296201000	-0.343445000	-0.820300000
C	-5.471019000	-1.283468000	-2.327579000
C	-4.373521000	0.491137000	-1.103073000
H	-6.313990000	-1.646817000	-2.903537000
H	-4.380772000	1.515855000	-0.749177000
C	-5.457034000	0.027483000	-1.853042000
H	-6.287285000	0.692004000	-2.067219000
C	-2.058430000	-2.427797000	-1.141376000
N	-1.104355000	-1.772830000	-0.434917000
C	-1.778255000	-3.687771000	-1.675591000
C	0.131862000	-2.273074000	-0.317668000
C	-0.510176000	-4.235418000	-1.516623000
H	0.869516000	-1.657399000	0.176807000
C	0.471563000	-3.511682000	-0.846281000
C	-0.909813000	1.401904000	2.096835000
C	-2.299910000	1.692342000	1.859812000
C	-3.056549000	0.492549000	2.162972000
C	-2.145619000	-0.534205000	2.505369000
C	-0.806458000	0.023314000	2.466915000
Rh	-1.651094000	0.120063000	0.328197000
C	0.223702000	2.376978000	2.042388000
H	0.019155000	3.194514000	1.348888000

H	0.380152000	2.818608000	3.033621000
H	1.150867000	1.894317000	1.732869000
C	0.434201000	-0.677511000	2.923892000
H	1.323429000	-0.296948000	2.425529000
H	0.558372000	-0.531235000	4.003802000
H	0.380668000	-1.753476000	2.750811000
C	-2.493410000	-1.922976000	2.950675000
H	-2.568196000	-1.966511000	4.043302000
H	-3.449917000	-2.250774000	2.540994000
H	-1.733303000	-2.644845000	2.648625000
C	-4.548237000	0.409068000	2.246438000
H	-4.870274000	0.687819000	3.256986000
H	-5.039538000	1.085699000	1.547880000
H	-4.913655000	-0.598808000	2.048339000
C	-2.901267000	3.057180000	1.696273000
H	-3.767353000	3.052144000	1.030929000
H	-3.245710000	3.430811000	2.668007000
H	-2.177798000	3.773430000	1.309012000
N	-0.579236000	0.733997000	-1.112402000
C	-0.235029000	1.990391000	-1.440597000
C	1.068812000	2.170926000	-1.998357000
C	-1.098621000	3.121358000	-1.346826000
C	1.498141000	3.434827000	-2.364163000
C	-0.678425000	4.359544000	-1.796456000
C	0.626324000	4.525020000	-2.281158000
H	1.722776000	1.310703000	-2.074508000
H	-2.109513000	2.970485000	-0.992854000
H	2.505514000	3.569046000	-2.739879000
H	-1.355789000	5.206015000	-1.772215000
H	0.955472000	5.504436000	-2.610013000
H	-4.394642000	-3.127978000	-2.475320000
H	-2.537063000	-4.218361000	-2.235205000
H	-0.283273000	-5.207330000	-1.939669000
H	1.491040000	-3.857506000	-0.741328000
F	5.727866000	-1.059903000	-0.510009000
F	3.194059000	-2.117677000	-0.192703000
F	3.540024000	0.059372000	-1.810269000
F	2.228523000	0.259336000	0.527659000
Sb	4.015880000	-0.366688000	0.022631000
F	4.327682000	-0.765275000	1.887775000
F	4.692704000	1.425838000	0.254807000

Number of Imaginary frequencies= 0

TS₃

SCF Energy = -1870.90405389 a.u

symmetry c1

C	-2.583784000	-1.027543000	-2.064477000
C	-3.539807000	-1.182629000	-3.073043000
C	-2.653660000	0.098586000	-1.215787000
C	-4.530133000	-0.221943000	-3.261872000
C	-3.619708000	1.076928000	-1.438551000
H	-5.264842000	-0.352103000	-4.047780000
H	-3.637782000	1.978619000	-0.838902000
C	-4.565635000	0.911664000	-2.449998000
H	-5.323587000	1.670973000	-2.608151000
C	-1.482765000	-1.969444000	-1.832402000
N	-0.835036000	-1.812083000	-0.651641000
C	-1.052130000	-2.926415000	-2.752132000
C	0.255151000	-2.539877000	-0.386386000
C	0.058745000	-3.709399000	-2.459731000
H	0.788164000	-2.325595000	0.528390000
C	0.731838000	-3.508486000	-1.261737000
C	-1.144142000	0.790500000	2.593134000
C	-2.534648000	0.895473000	2.257347000
C	-3.082141000	-0.451710000	2.179550000
C	-2.033811000	-1.364551000	2.445173000
C	-0.819128000	-0.605530000	2.673627000
Rh	-1.516050000	-0.164549000	0.572312000
C	-0.197477000	1.910117000	2.891029000
H	0.804064000	1.690828000	2.519029000
H	-0.524555000	2.849472000	2.443944000
H	-0.134718000	2.062786000	3.975228000
C	0.503255000	-1.157316000	3.106325000
H	1.330836000	-0.624901000	2.639232000
H	0.605184000	-1.057584000	4.193890000
H	0.602989000	-2.217092000	2.870651000
C	-2.146060000	-2.856468000	2.528975000
H	-2.244687000	-3.169091000	3.574596000
H	-3.016222000	-3.228287000	1.986871000
H	-1.262360000	-3.351826000	2.124239000
C	-4.530377000	-0.776770000	1.968689000
H	-5.080899000	-0.686010000	2.912524000
H	-4.995723000	-0.101225000	1.249117000
H	-4.667538000	-1.795566000	1.604704000
C	-3.371317000	2.139956000	2.291584000
H	-4.115795000	2.162336000	1.493323000
H	-3.917425000	2.187344000	3.241065000
H	-2.764008000	3.042495000	2.226211000
N	-0.735319000	0.793871000	-0.909030000
C	-0.430431000	2.114599000	-1.053918000
C	0.662313000	2.364024000	-1.926720000
C	-1.038103000	3.212853000	-0.397259000
C	1.160562000	3.649565000	-2.076042000

C	-0.578345000	4.499886000	-0.614552000
C	0.532351000	4.720311000	-1.439562000
H	1.130177000	1.512225000	-2.403510000
H	-1.883006000	3.032430000	0.251287000
H	2.032066000	3.817943000	-2.697032000
H	-1.066320000	5.339903000	-0.132421000
H	0.904599000	5.728576000	-1.581671000
H	-3.519989000	-2.057777000	-3.712513000
H	1.629908000	-4.054653000	-1.006432000
H	0.409822000	-4.445173000	-3.173829000
H	-1.561588000	-3.031310000	-3.700660000
F	2.313974000	-0.400553000	-1.432280000
F	2.980281000	-1.810082000	0.770861000
F	4.948480000	-1.078445000	-1.020349000
Sb	3.608776000	-0.132932000	-0.007962000
F	4.091153000	1.568567000	-0.783599000
F	2.194636000	0.736679000	1.018886000
F	4.814443000	0.118913000	1.475120000

Number of Imaginary frequencies= 1 (-269.4201 cm⁻¹)

g

SCF Energy = -1870.98107367 a.u

symmetry c1

C	-2.806125000	-1.616321000	-1.292130000
C	-3.965071000	-2.281705000	-1.744951000
C	-2.721492000	-0.187716000	-1.428664000
C	-4.975813000	-1.636900000	-2.430268000
C	-3.705757000	0.413510000	-2.268256000
H	-5.859556000	-2.174955000	-2.749842000
H	-3.599080000	1.453832000	-2.533612000
C	-4.798022000	-0.283280000	-2.742349000
H	-5.527363000	0.235634000	-3.355277000
C	-1.662124000	-2.436835000	-0.886333000
N	-0.710623000	-1.965138000	-0.043426000
C	-1.485919000	-3.719598000	-1.453123000
C	0.394643000	-2.701998000	0.216361000
C	-0.374740000	-4.482651000	-1.158732000
H	1.150239000	-2.233890000	0.829365000
C	0.598313000	-3.961258000	-0.304742000
C	-0.149618000	1.397938000	2.449278000
C	-1.561715000	1.304548000	2.444305000
C	-1.914974000	-0.086167000	2.673316000
C	-0.684828000	-0.801227000	2.991446000
C	0.396522000	0.090830000	2.834101000
Rh	-0.774214000	-0.096557000	0.880258000
C	0.671991000	2.627964000	2.229483000

H	0.129260000	3.373475000	1.648285000
H	0.933473000	3.075283000	3.196352000
H	1.602345000	2.397123000	1.708745000
C	1.835193000	-0.175726000	3.136571000
H	2.498740000	0.438054000	2.530547000
H	2.026427000	0.059436000	4.191370000
H	2.109725000	-1.217900000	2.974694000
C	-0.612505000	-2.222095000	3.457316000
H	-0.803792000	-2.264615000	4.535597000
H	-1.356895000	-2.850471000	2.966300000
H	0.370613000	-2.657942000	3.280942000
C	-3.302976000	-0.619201000	2.842027000
H	-3.642370000	-0.469380000	3.874263000
H	-4.008702000	-0.114204000	2.181735000
H	-3.351212000	-1.687701000	2.629074000
C	-2.530298000	2.436692000	2.348492000
H	-3.480543000	2.127817000	1.913215000
H	-2.736042000	2.809976000	3.359035000
H	-2.139486000	3.263478000	1.758544000
N	-1.725786000	0.542012000	-0.832699000
C	-1.598849000	1.939979000	-1.089454000
C	-2.630640000	2.865312000	-0.854548000
C	-0.374077000	2.416694000	-1.580170000
C	-2.441354000	4.221217000	-1.108918000
C	-0.186813000	3.774859000	-1.825887000
C	-1.218048000	4.683589000	-1.595099000
H	-3.584888000	2.519814000	-0.477598000
H	0.428367000	1.716405000	-1.762258000
H	-3.252634000	4.918049000	-0.926246000
H	0.770456000	4.113902000	-2.204946000
H	-1.073957000	5.739451000	-1.794586000
H	-4.061577000	-3.342971000	-1.549292000
H	1.513992000	-4.491114000	-0.079352000
H	-0.244148000	-5.454746000	-1.620139000
H	-2.206521000	-4.075874000	-2.174208000
F	2.983811000	-1.286594000	-2.148242000
F	5.177339000	0.025048000	-1.013589000
F	3.000992000	1.479550000	-2.018652000
Sb	3.273762000	0.032090000	-0.774102000
F	1.330559000	0.059145000	-0.444168000
F	3.338474000	-1.395605000	0.547542000
F	3.408640000	1.307529000	0.687700000

Number of Imaginary frequencies= 0

h

SCF Energy = -2955.87392299 a.u

symmetry c1

C	-1.357982000	1.502415000	0.658478000
C	-2.588394000	2.124694000	0.922033000
C	-0.270465000	1.669881000	1.564190000
C	-2.775439000	2.910636000	2.052474000
C	-0.496769000	2.455017000	2.714971000
H	-3.742842000	3.358775000	2.243982000
H	0.304275000	2.580217000	3.430344000
C	-1.720925000	3.067185000	2.951570000
H	-1.855359000	3.652809000	3.855119000
C	-1.243838000	0.670107000	-0.558337000
N	-0.511475000	-0.471278000	-0.530912000
C	-1.913582000	1.032019000	-1.735213000
C	-0.454567000	-1.261538000	-1.621513000
C	-1.869233000	0.211560000	-2.850204000
H	0.150936000	-2.154299000	-1.538924000
C	-1.120804000	-0.960158000	-2.795365000
C	1.293196000	-2.469233000	2.793071000
C	0.388474000	-1.530869000	3.347941000
C	-0.882254000	-1.669013000	2.649357000
C	-0.762432000	-2.805580000	1.739606000
C	0.565983000	-3.274181000	1.805365000
Rh	0.558558000	-1.079254000	1.189795000
C	2.695574000	-2.741711000	3.238160000
H	3.106843000	-1.909471000	3.808602000
H	2.704800000	-3.627317000	3.884765000
H	3.354175000	-2.947257000	2.393318000
C	1.114295000	-4.474983000	1.104751000
H	2.197615000	-4.434695000	1.016435000
H	0.851813000	-5.371018000	1.680678000
H	0.700776000	-4.590630000	0.103417000
C	-1.879020000	-3.385560000	0.934430000
H	-1.507915000	-3.968485000	0.090964000
H	-2.463624000	-4.061959000	1.569466000
H	-2.560761000	-2.619459000	0.566076000
C	-2.163078000	-0.983705000	2.994644000
H	-2.825092000	-0.908817000	2.131899000
H	-2.683861000	-1.567922000	3.763894000
H	-1.992704000	0.015819000	3.393976000
C	0.653342000	-0.599709000	4.486122000
H	0.043546000	0.300589000	4.415427000
H	0.396901000	-1.098420000	5.428045000
H	1.701495000	-0.304178000	4.535738000
N	0.948138000	1.024714000	1.294752000
C	2.162533000	1.525264000	1.808536000

C	2.396960000	2.905262000	2.019629000
C	3.261286000	0.663657000	1.990546000
C	3.646541000	3.373595000	2.416903000
C	4.505866000	1.140128000	2.387750000
C	4.713097000	2.499466000	2.615325000
H	1.599023000	3.621034000	1.872237000
H	3.142627000	-0.389022000	1.779833000
H	3.781066000	4.439066000	2.572535000
H	5.324142000	0.437826000	2.502743000
H	5.683311000	2.868741000	2.924993000
H	-3.424834000	1.946322000	0.257696000
H	-1.061207000	-1.640963000	-3.633988000
H	-2.427479000	0.472244000	-3.740297000
H	-2.504559000	1.936690000	-1.750101000
C	1.207213000	7.293255000	-0.346451000
C	1.819737000	6.247865000	-1.027312000
C	-0.028458000	7.097949000	0.271278000
C	-0.647807000	5.851344000	0.211073000
C	-0.036149000	4.798459000	-0.462350000
C	1.203501000	4.988117000	-1.088916000
C	1.848927000	3.897189000	-1.838409000
N	1.806830000	2.628270000	-1.353754000
C	2.344400000	1.564370000	-1.983109000
C	2.987185000	1.727983000	-3.193265000
C	3.069170000	3.012469000	-3.728046000
C	2.500715000	4.089068000	-3.056261000
H	1.696641000	8.258529000	-0.292717000
H	-0.506614000	7.916158000	0.797111000
H	-1.609743000	5.691021000	0.681999000
H	-0.543654000	3.843043000	-0.516216000
H	2.248707000	0.617445000	-1.471998000
H	3.405635000	0.857662000	-3.677865000
H	3.565724000	3.174500000	-4.677691000
H	2.527882000	5.083399000	-3.479794000
H	2.789951000	6.400698000	-1.485434000
H	1.387773000	2.429012000	-0.438582000
F	4.991814000	-1.027167000	-0.985209000
F	3.991741000	-3.270514000	0.229656000
F	2.357224000	-1.198604000	-0.400419000
Sb	3.642390000	-2.328299000	-1.419473000
F	3.157701000	-1.249912000	-2.955312000
F	4.831586000	-3.428616000	-2.436643000
F	2.121543000	-3.470600000	-1.760199000
F	-4.625983000	-1.016150000	-2.452400000
F	-3.739333000	-0.919779000	0.101788000
F	-5.042494000	1.180049000	-0.931246000
F	-7.194898000	-0.441505000	-1.598567000
F	-5.781044000	-2.603863000	-0.524161000

F	-6.230787000	-0.343633000	1.002322000
Sb	-5.491986000	-0.708502000	-0.744767000

Number of Imaginary frequencies= 0

TS4

SCF Energy = -2955.86569499 a.u

symmetry c1

C	-1.372509000	1.609835000	0.362174000
C	-2.624950000	2.184126000	0.616001000
C	-0.270345000	1.936817000	1.195956000
C	-2.819540000	3.052193000	1.684769000
C	-0.496650000	2.781262000	2.291637000
H	-3.803405000	3.465654000	1.869939000
H	0.317275000	3.021709000	2.959284000
C	-1.752349000	3.333658000	2.531804000
H	-1.889222000	3.984140000	3.388945000
C	-1.273621000	0.624605000	-0.741628000
N	-0.513612000	-0.486538000	-0.576222000
C	-2.002670000	0.794185000	-1.924027000
C	-0.482643000	-1.431445000	-1.536583000
C	-1.986059000	-0.185294000	-2.903872000
H	0.146898000	-2.291290000	-1.347263000
C	-1.207324000	-1.321626000	-2.709559000
C	1.397790000	-1.901027000	2.982135000
C	0.487127000	-0.904857000	3.411591000
C	-0.798774000	-1.164237000	2.776603000
C	-0.675883000	-2.413852000	2.036383000
C	0.665016000	-2.851276000	2.143602000
Rh	0.611558000	-0.804466000	1.191767000
C	2.815091000	-2.076993000	3.425555000
H	3.223206000	-1.156370000	3.841419000
H	2.858274000	-2.845947000	4.205951000
H	3.455234000	-2.407462000	2.606757000
C	1.205620000	-4.144219000	1.629327000
H	2.291567000	-4.134855000	1.562516000
H	0.911366000	-4.942179000	2.322809000
H	0.808076000	-4.397289000	0.647295000
C	-1.793410000	-3.137947000	1.359906000
H	-1.428099000	-3.804778000	0.578284000
H	-2.314314000	-3.757401000	2.100343000
H	-2.527599000	-2.456915000	0.932863000
C	-2.088140000	-0.468311000	3.062691000
H	-2.773301000	-0.520956000	2.217485000
H	-2.573292000	-0.962621000	3.914055000
H	-1.937426000	0.577210000	3.327368000
C	0.765946000	0.178472000	4.400320000

H	0.099736000	1.028495000	4.262082000
H	0.600639000	-0.210395000	5.411864000
H	1.796539000	0.528650000	4.339246000
N	1.007461000	1.369565000	0.866329000
C	2.206450000	1.913006000	1.475821000
C	2.394902000	3.291564000	1.669871000
C	3.296573000	1.065653000	1.706017000
C	3.610829000	3.785207000	2.137079000
C	4.512916000	1.563620000	2.166921000
C	4.675000000	2.926347000	2.401019000
H	1.601806000	3.988698000	1.442096000
H	3.207414000	0.012822000	1.483316000
H	3.723742000	4.853746000	2.284070000
H	5.339120000	0.879251000	2.322519000
H	5.620421000	3.314908000	2.760979000
H	-3.470587000	1.898826000	0.003340000
H	-1.167511000	-2.118966000	-3.439628000
H	-2.587616000	-0.071545000	-3.796459000
H	-2.613729000	1.676838000	-2.048214000
C	1.450644000	6.816214000	-0.521112000
C	1.963241000	5.682564000	-1.143806000
C	0.112917000	6.853458000	-0.127344000
C	-0.707608000	5.751193000	-0.356556000
C	-0.194306000	4.610225000	-0.969009000
C	1.146373000	4.563964000	-1.364872000
C	1.692852000	3.395243000	-2.098352000
N	1.583121000	2.138478000	-1.599456000
C	2.050581000	1.093081000	-2.304580000
C	2.658171000	1.229007000	-3.541072000
C	2.793843000	2.509500000	-4.063697000
C	2.307933000	3.591203000	-3.337741000
H	2.094384000	7.670407000	-0.344963000
H	-0.288389000	7.740245000	0.349693000
H	-1.750391000	5.775554000	-0.064469000
H	-0.843578000	3.765221000	-1.155268000
H	1.944237000	0.131237000	-1.831204000
H	3.019712000	0.344619000	-4.046292000
H	3.265234000	2.667418000	-5.026898000
H	2.373742000	4.597164000	-3.730806000
H	3.005402000	5.653951000	-1.441103000
H	1.224714000	1.772129000	-0.429827000
F	4.991120000	-1.139293000	-0.956355000
F	4.067593000	-3.216793000	0.555822000
F	2.378948000	-1.284599000	-0.290757000
Sb	3.670247000	-2.514079000	-1.200239000
F	3.112259000	-1.687695000	-2.855105000
F	4.866258000	-3.722862000	-2.074292000
F	2.158062000	-3.711068000	-1.336209000

F	-4.669785000	-1.355330000	-2.253010000
F	-3.715178000	-0.889441000	0.229106000
F	-5.117687000	1.009998000	-1.023627000
F	-7.236307000	-0.749318000	-1.397198000
F	-5.713096000	-2.704405000	-0.091354000
F	-6.191790000	-0.274452000	1.133918000
Sb	-5.501049000	-0.848723000	-0.576327000

Number of Imaginary frequencies= 1 (-1289.5039 cm⁻¹)

i

SCF Energy = -2955.86456577 a.u

symmetry c1

C	0.236716000	3.999260000	-0.763083000
C	0.224134000	5.126042000	-1.599545000
C	-1.000285000	3.490095000	-0.322021000
C	-0.963990000	5.728308000	-1.994619000
C	-2.194057000	4.094505000	-0.714195000
H	-0.941820000	6.591169000	-2.649040000
H	-3.135873000	3.709210000	-0.348855000
C	-2.175964000	5.207255000	-1.550232000
H	-3.112348000	5.665760000	-1.845358000
C	1.539380000	3.392830000	-0.388119000
N	1.664142000	2.040549000	-0.260389000
C	2.656853000	4.217305000	-0.211830000
C	2.885169000	1.516718000	-0.036587000
C	3.910855000	3.666209000	0.014043000
H	2.952371000	0.441537000	0.034917000
C	4.034411000	2.285663000	0.083606000
C	-1.054332000	-0.965124000	-1.876379000
C	-1.283208000	0.314168000	-2.466262000
C	-0.003927000	0.887462000	-2.810140000
C	1.018164000	-0.089445000	-2.490600000
C	0.378181000	-1.202061000	-1.863988000
Rh	0.023128000	0.630239000	-0.640598000
C	-2.099361000	-1.989433000	-1.591800000
H	-3.030331000	-1.553911000	-1.243612000
H	-2.331539000	-2.514671000	-2.526033000
H	-1.769040000	-2.737581000	-0.874247000
C	1.038849000	-2.466509000	-1.424712000
H	0.463657000	-2.968977000	-0.647204000
H	1.098791000	-3.150231000	-2.280427000
H	2.051303000	-2.297030000	-1.061666000
C	2.454462000	-0.010272000	-2.883903000
H	2.556824000	-0.450373000	-3.883778000
H	2.813106000	1.017136000	-2.946127000
H	3.107494000	-0.574591000	-2.222414000

C	0.202380000	2.120810000	-3.630148000
H	0.183163000	1.853477000	-4.693363000
H	-0.580312000	2.858849000	-3.460306000
H	1.166722000	2.587189000	-3.429103000
C	-2.611698000	0.911272000	-2.788569000
H	-2.612833000	1.994582000	-2.655768000
H	-2.827959000	0.717460000	-3.846877000
H	-3.421329000	0.473169000	-2.206039000
N	-0.995404000	2.329467000	0.543274000
C	-2.138171000	2.206452000	1.453205000
C	-3.306996000	1.552486000	1.083391000
C	-2.025438000	2.795998000	2.714064000
C	-4.370914000	1.483763000	1.984575000
C	-3.085995000	2.718852000	3.612656000
C	-4.260088000	2.063740000	3.246364000
H	-3.412706000	1.083990000	0.113613000
H	-1.120131000	3.328006000	2.989252000
H	-5.273279000	0.957192000	1.700834000
H	-2.992645000	3.172778000	4.592483000
H	-5.087269000	1.997971000	3.943223000
H	1.163012000	5.515882000	-1.972399000
H	4.980127000	1.779350000	0.227221000
H	4.775910000	4.308095000	0.134230000
H	2.530040000	5.290602000	-0.252372000
C	1.959058000	0.042218000	2.660955000
C	1.717193000	1.347349000	3.112713000
C	3.261521000	-0.467424000	2.718911000
H	3.475291000	-1.469973000	2.371687000
C	2.759505000	2.130705000	3.601245000
C	4.305747000	0.323130000	3.192243000
H	2.556227000	3.129291000	3.972327000
H	5.309289000	-0.084226000	3.201605000
C	4.057080000	1.619896000	3.638855000
H	4.868937000	2.227287000	4.022800000
H	0.698774000	1.718718000	3.147433000
C	0.804445000	-0.833436000	2.329650000
C	0.627517000	-1.977303000	3.117723000
N	-0.129714000	-0.470839000	1.408896000
C	-0.546615000	-2.713051000	3.044821000
C	-1.294426000	-1.158621000	1.406991000
C	-1.554502000	-2.264055000	2.200352000
H	1.404986000	-2.240736000	3.822838000
H	-0.684926000	-3.591829000	3.664015000
H	-2.063419000	-0.811674000	0.737520000
H	-2.525721000	-2.736434000	2.124781000
F	6.069807000	-0.048782000	0.005621000
F	3.786384000	-1.438002000	-0.223797000
F	5.480191000	-1.416978000	-2.268557000

Sb	5.687532000	-1.911744000	-0.407330000
F	7.553827000	-2.303093000	-0.609808000
F	5.692578000	-2.272674000	1.493891000
F	5.150370000	-3.721448000	-0.788418000
H	-0.175237000	2.398745000	1.141885000
F	-4.925750000	-0.318529000	-0.899241000
F	-5.182812000	-2.921178000	-1.579348000
Sb	-5.978027000	-1.826016000	-0.195531000
F	-4.399374000	-2.187468000	0.896740000
F	-6.615546000	-0.632358000	1.188339000
F	-6.911124000	-3.317457000	0.573803000
F	-7.439210000	-1.344144000	-1.347566000

Number of Imaginary frequencies= 0

j

SCF Energy = -2350.43256928 a.u

symmetry c1

Rh	-0.836404000	-1.156950000	0.330990000
C	-0.910794000	-2.688400000	1.937555000
C	-1.662057000	-3.188071000	0.817070000
C	-0.771676000	-3.313789000	-0.310677000
C	0.527437000	-2.889148000	0.105565000
C	0.447966000	-2.502648000	1.498138000
C	-1.363047000	-2.594798000	3.362010000
H	-0.960213000	-3.443330000	3.926833000
H	-1.012137000	-1.679927000	3.840873000
H	-2.447029000	-2.613643000	3.450986000
C	-3.089342000	-3.632103000	0.828063000
H	-3.129359000	-4.725738000	0.902467000
H	-3.636683000	-3.221532000	1.675384000
H	-3.607266000	-3.347526000	-0.089193000
C	-1.120946000	-3.925781000	-1.631912000
H	-0.974593000	-5.011716000	-1.588346000
H	-2.159222000	-3.740193000	-1.906658000
H	-0.486346000	-3.545547000	-2.433001000
C	1.781137000	-2.929584000	-0.708773000
H	2.284182000	-3.891653000	-0.555631000
H	1.576300000	-2.834545000	-1.775677000
H	2.483937000	-2.148698000	-0.423477000
C	1.598527000	-2.113992000	2.366183000
H	2.107089000	-3.021923000	2.714885000
H	2.330964000	-1.511763000	1.830348000
H	1.267754000	-1.563780000	3.247788000
C	-4.771837000	-0.844468000	-1.627864000
C	-3.468152000	-0.351595000	-1.605798000
C	-5.192945000	-1.684622000	-2.656994000

C	-4.302826000	-2.025130000	-3.675057000
C	-3.002837000	-1.527131000	-3.659525000
C	-2.565202000	-0.690442000	-2.621232000
C	-1.184961000	-0.135315000	-2.670998000
N	-0.377038000	-0.160724000	-1.578474000
C	0.875889000	0.326521000	-1.691326000
C	1.389513000	0.858324000	-2.866462000
C	0.564611000	0.906316000	-3.981475000
C	-0.727559000	0.407276000	-3.877095000
H	-5.463583000	-0.554523000	-0.845151000
H	-6.208756000	-2.063333000	-2.672214000
H	-4.619436000	-2.677352000	-4.481146000
H	-2.314900000	-1.803766000	-4.450506000
H	1.499917000	0.275973000	-0.811537000
H	2.414414000	1.206646000	-2.868260000
H	0.916854000	1.325362000	-4.917259000
H	-1.404328000	0.445603000	-4.720705000
H	-3.159070000	0.315946000	-0.814104000
C	-2.653277000	3.025076000	-0.234627000
C	-2.934273000	3.523682000	-1.518513000
H	-2.124593000	3.760460000	-2.197396000
C	-4.256519000	3.695057000	-1.907940000
H	-4.491950000	4.078396000	-2.894709000
C	-5.270215000	3.360746000	-1.013849000
H	-6.315716000	3.481948000	-1.271060000
C	-4.900357000	2.856546000	0.230056000
H	-5.657037000	2.577640000	0.958989000
N	-3.633494000	2.689346000	0.616386000
H	2.540322000	2.832529000	1.217674000
C	1.489467000	2.876211000	0.956182000
C	0.950393000	3.995836000	0.332116000
H	1.570512000	4.859467000	0.121912000
C	-0.393024000	3.998297000	-0.029198000
H	-0.810781000	4.876509000	-0.508642000
C	-1.239609000	2.908343000	0.224754000
C	-0.691632000	1.770979000	0.869278000
N	-1.442952000	0.581450000	1.156138000
C	0.666424000	1.784779000	1.216261000
C	-2.229360000	0.617293000	2.321752000
C	-3.389701000	-0.174849000	2.395551000
C	-1.918049000	1.433958000	3.426076000
C	-4.200195000	-0.158439000	3.523197000
C	-2.730333000	1.440447000	4.554575000
C	-3.876071000	0.646881000	4.615839000
H	-3.666210000	-0.767907000	1.532809000
H	-1.038537000	2.063850000	3.394627000
H	-5.100386000	-0.764432000	3.545502000
H	-2.465480000	2.074391000	5.393834000

H	-4.510236000	0.663723000	5.494544000
H	1.086027000	0.906419000	1.689471000
F	4.995265000	-1.417741000	-0.916912000
F	4.264392000	1.103539000	-1.647129000
F	3.117205000	-0.116981000	0.454548000
Sb	4.974951000	0.301990000	-0.024705000
F	5.534457000	-0.527385000	1.625145000
F	6.777733000	0.704092000	-0.552073000
F	4.747422000	1.999491000	0.875017000

Number of Imaginary frequencies= 0

TS₅

SCF Energy = -2350.39260711 a.u

symmetry c1

Rh	1.657212000	-0.627238000	-0.762257000
C	1.748253000	0.408741000	-2.779360000
C	2.623417000	-0.718858000	-2.784502000
C	1.822186000	-1.905999000	-2.540432000
C	0.456034000	-1.493882000	-2.428417000
C	0.404121000	-0.056592000	-2.536608000
C	2.099386000	1.830326000	-3.082012000
H	1.663247000	2.107220000	-4.048482000
H	1.695702000	2.507502000	-2.328579000
H	3.174321000	1.989595000	-3.135328000
C	4.067654000	-0.741796000	-3.180115000
H	4.149261000	-1.047549000	-4.229789000
H	4.538198000	0.236553000	-3.089961000
H	4.640218000	-1.456246000	-2.587588000
C	2.325882000	-3.315845000	-2.591476000
H	2.384518000	-3.655927000	-3.632108000
H	3.322113000	-3.402749000	-2.156055000
H	1.663570000	-3.999514000	-2.060019000
C	-0.725380000	-2.402133000	-2.310564000
H	-1.043922000	-2.690339000	-3.319779000
H	-0.484302000	-3.318891000	-1.770941000
H	-1.578335000	-1.922343000	-1.831764000
C	-0.829982000	0.779473000	-2.637024000
H	-1.150497000	0.822577000	-3.686169000
H	-1.662489000	0.370002000	-2.067335000
H	-0.649432000	1.801498000	-2.308478000
C	4.574359000	-1.689110000	0.381069000
C	3.192564000	-1.582783000	0.599518000
C	5.288507000	-2.799087000	0.826155000
C	4.622606000	-3.831607000	1.486820000
C	3.251953000	-3.748114000	1.717144000
C	2.530710000	-2.629067000	1.288343000

C	1.081029000	-2.487667000	1.510855000
N	0.463326000	-1.539577000	0.758097000
C	-0.843822000	-1.295459000	0.935710000
C	-1.617175000	-2.004251000	1.848613000
C	-1.003197000	-2.990562000	2.608504000
C	0.357329000	-3.226320000	2.445781000
H	5.101997000	-0.880237000	-0.108167000
H	6.358605000	-2.858726000	0.662033000
H	5.170550000	-4.704712000	1.822505000
H	2.749462000	-4.568363000	2.216041000
H	-1.293540000	-0.525041000	0.327115000
H	-2.669649000	-1.773425000	1.938448000
H	-1.574623000	-3.563339000	3.329482000
H	0.860608000	-3.967354000	3.052279000
H	2.796257000	-0.366941000	0.789828000
C	-0.367669000	2.706838000	0.719386000
C	-1.731714000	2.704810000	0.388739000
H	-2.418144000	2.028966000	0.881972000
C	-2.192366000	3.566549000	-0.600170000
H	-3.240910000	3.553721000	-0.874047000
C	-1.281446000	4.412943000	-1.227044000
H	-1.593458000	5.115260000	-1.991345000
C	0.058413000	4.326488000	-0.853376000
H	0.803361000	4.963223000	-1.325084000
N	0.516547000	3.493908000	0.085213000
H	1.250723000	0.100455000	5.153911000
C	0.921085000	0.592425000	4.245436000
C	-0.282759000	1.290122000	4.212645000
H	-0.914282000	1.347940000	5.091554000
C	-0.664470000	1.932755000	3.041729000
H	-1.587952000	2.498795000	3.028168000
C	0.120361000	1.899686000	1.876509000
C	1.325880000	1.159173000	1.901694000
N	2.183303000	0.977843000	0.768741000
C	1.705796000	0.534691000	3.099811000
C	3.249971000	1.886718000	0.623504000
C	4.214555000	1.718777000	-0.385040000
C	3.431334000	2.973618000	1.504741000
C	5.307283000	2.573280000	-0.503078000
C	4.520852000	3.826271000	1.376983000
C	5.475343000	3.638963000	0.377111000
H	4.099483000	0.905521000	-1.085157000
H	2.704490000	3.159346000	2.282280000
H	6.030997000	2.403946000	-1.294602000
H	4.619540000	4.654612000	2.070715000
H	6.322419000	4.308092000	0.284507000
H	2.648764000	0.000282000	3.120113000
F	-4.813239000	-2.006686000	0.684239000

F	-3.718212000	0.355844000	1.284368000
F	-3.227810000	-0.726884000	-1.087963000
Sb	-4.885436000	-0.260998000	-0.152648000
F	-5.899658000	-0.935169000	-1.641350000
F	-6.460061000	0.229200000	0.835100000
F	-4.755209000	1.503353000	-0.939217000

Number of Imaginary frequencies= 1 (-1085.0398 cm⁻¹)

k

SCF Energy = -2350.46181528 a.u

symmetry c1

Rh	-1.073676000	-1.425399000	-0.024133000
C	-1.021973000	-2.766717000	1.820055000
C	-1.484746000	-3.507240000	0.699322000
C	-0.440619000	-3.479061000	-0.296887000
C	0.740040000	-2.873494000	0.319745000
C	0.377484000	-2.400134000	1.589900000
C	-1.729694000	-2.622548000	3.130296000
H	-1.392340000	-3.408946000	3.816512000
H	-1.521796000	-1.663878000	3.604231000
H	-2.810019000	-2.715838000	3.022741000
C	-2.742458000	-4.314525000	0.618970000
H	-2.526876000	-5.344021000	0.928967000
H	-3.520392000	-3.932965000	1.281175000
H	-3.144129000	-4.350060000	-0.393257000
C	-0.441331000	-4.240353000	-1.588776000
H	-0.072186000	-5.261046000	-1.432536000
H	-1.443959000	-4.307457000	-2.012840000
H	0.205975000	-3.769946000	-2.330169000
C	2.100530000	-2.865069000	-0.297665000
H	2.579763000	-3.835291000	-0.119223000
H	2.059480000	-2.728166000	-1.379534000
H	2.748206000	-2.098266000	0.117779000
C	1.281327000	-1.772896000	2.608613000
H	1.695840000	-2.545336000	3.267527000
H	2.116965000	-1.249612000	2.144246000
H	0.743689000	-1.066983000	3.244710000
C	-4.052515000	-1.695109000	-0.858842000
C	-2.750938000	-1.316051000	-1.198347000
C	-5.096058000	-1.628051000	-1.785920000
C	-4.856567000	-1.171001000	-3.081596000
C	-3.575896000	-0.762390000	-3.436208000
C	-2.529214000	-0.823817000	-2.506379000
C	-1.168602000	-0.359506000	-2.794896000
N	-0.307132000	-0.472899000	-1.748418000
C	0.962605000	-0.050397000	-1.873815000

C	1.453193000	0.491185000	-3.054361000
C	0.587100000	0.605115000	-4.137486000
C	-0.729630000	0.183374000	-4.005091000
H	-4.272678000	-2.058928000	0.138144000
H	-6.094557000	-1.939999000	-1.496130000
H	-5.661370000	-1.128365000	-3.806495000
H	-3.398793000	-0.392101000	-4.439797000
H	1.603565000	-0.140824000	-1.008148000
H	2.488813000	0.803766000	-3.087149000
H	0.932938000	1.022263000	-5.076440000
H	-1.417982000	0.273181000	-4.834768000
H	-2.504323000	0.814871000	0.154822000
C	-2.808377000	3.272666000	-0.232542000
C	-3.411186000	4.530681000	-0.069960000
H	-2.847044000	5.358041000	0.339344000
C	-4.745439000	4.695467000	-0.416818000
H	-5.224063000	5.660827000	-0.295912000
C	-5.460277000	3.605790000	-0.908526000
H	-6.501638000	3.692499000	-1.193130000
C	-4.800177000	2.386005000	-1.008244000
H	-5.314293000	1.499816000	-1.367572000
N	-3.516218000	2.219810000	-0.680092000
H	2.444900000	2.680185000	0.823499000
C	1.386468000	2.799526000	0.630662000
C	0.884300000	4.000704000	0.140605000
H	1.551337000	4.834719000	-0.043023000
C	-0.471526000	4.120102000	-0.137518000
H	-0.845055000	5.049346000	-0.550963000
C	-1.367178000	3.058712000	0.069219000
C	-0.838429000	1.837454000	0.549564000
N	-1.715410000	0.693529000	0.801991000
C	0.519410000	1.727167000	0.826418000
C	-2.276689000	0.679082000	2.142624000
C	-3.613209000	0.298712000	2.303153000
C	-1.533972000	1.052013000	3.265618000
C	-4.193751000	0.283379000	3.568049000
C	-2.123234000	1.034086000	4.529495000
C	-3.452172000	0.649408000	4.690390000
H	-4.198935000	0.028258000	1.433178000
H	-0.507682000	1.375784000	3.159012000
H	-5.233903000	-0.004895000	3.673268000
H	-1.534732000	1.331029000	5.390291000
H	-3.906349000	0.643564000	5.674208000
H	0.917172000	0.784156000	1.176072000
F	5.186253000	-1.409831000	-0.355415000
F	4.290111000	0.761552000	-1.737214000
F	3.154671000	0.062102000	0.583973000
Sb	5.000502000	0.473408000	0.050103000

F	5.566518000	0.164279000	1.867121000
F	6.781862000	0.876746000	-0.546126000
F	4.621469000	2.326608000	0.467300000

Number of Imaginary frequencies= 0

N₂

SCF Energy = -109.559693682 a.u

symmetry c1

N	0.000000000	0.000000000	0.547790000
N	0.000000000	0.000000000	-0.547790000

Number of Imaginary frequencies= 0

Phenylazide

SCF Energy = -395.943084998 a.u

symmetry c1

N	1.472372000	-0.877492000	-0.000010000
N	2.415858000	-0.086242000	-0.000158000
N	3.368182000	0.528976000	-0.000301000
C	0.148530000	-0.361407000	0.000028000
C	-0.880192000	-1.308026000	0.000199000
C	-0.153874000	1.004584000	-0.000092000
C	-2.205005000	-0.886535000	0.000247000
C	-1.485320000	1.412992000	-0.000042000
C	-2.515130000	0.473935000	0.000127000
H	-0.625210000	-2.360650000	0.000290000
H	0.639231000	1.744220000	-0.000224000
H	-2.998911000	-1.624626000	0.000379000
H	-1.715228000	2.472437000	-0.000136000
H	-3.548826000	0.798656000	0.000166000

Number of Imaginary frequencies= 0

2pb

SCF Energy = -479.465728675 a.u

symmetry c1

C	-2.810731000	-1.195505000	0.240341000
C	-1.420051000	-1.173132000	0.227899000
C	-3.536039000	-0.026527000	0.010350000
C	-2.856889000	1.165376000	-0.235140000
C	-1.464623000	1.189652000	-0.242102000
C	-0.724766000	0.022342000	-0.004944000
C	0.762870000	0.024683000	-0.001755000
N	1.370316000	-1.149531000	-0.245951000

C	2.702536000	-1.192399000	-0.255170000
C	3.513992000	-0.083868000	-0.024586000
C	2.890937000	1.131351000	0.244740000
C	1.503083000	1.188218000	0.262055000
H	-3.330772000	-2.128124000	0.429468000
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H	-0.956693000	2.121894000	-0.459564000
H	3.144971000	-2.163917000	-0.459497000
H	4.593077000	-0.176068000	-0.048251000
H	3.476681000	2.020982000	0.448387000
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H	-0.851466000	-2.078501000	0.396238000

Number of Imaginary frequencies= 0

2pbH⁺SbF₆⁻

SCF Energy = -1084.88473888 a.u

symmetry c1

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C	-2.458247000	-2.762418000	-0.435956000
C	-2.085604000	-1.422429000	-0.427505000
C	-3.000543000	-0.446679000	-0.000650000
C	-2.620167000	0.974170000	0.003939000
N	-1.345585000	1.303619000	0.323237000
C	-0.859251000	2.559780000	0.297919000
C	-1.691097000	3.609195000	-0.033697000
C	-3.024141000	3.329150000	-0.342252000
C	-3.485401000	2.019698000	-0.330441000
H	-5.637104000	-2.467062000	0.731143000
H	-4.017444000	-4.186829000	-0.027466000
H	-1.746790000	-3.507778000	-0.770090000
H	-1.101200000	-1.138211000	-0.781141000
H	0.194483000	2.654427000	0.531938000
H	-1.300604000	4.617068000	-0.056672000
H	-3.698442000	4.133080000	-0.613734000
H	-4.502670000	1.787717000	-0.613358000
H	-4.992424000	-0.089219000	0.762182000
H	-0.683627000	0.564723000	0.626505000
F	2.077411000	1.713591000	0.135747000
F	0.660791000	-0.230488000	1.220412000
F	0.826383000	-0.125247000	-1.359366000
Sb	2.226938000	-0.225103000	-0.002016000
F	3.623591000	-0.092473000	-1.306884000
F	3.416112000	-0.265069000	1.501045000

F 2.139465000 -2.144084000 -0.085018000

Number of Imaginary frequencies= 0

pdt

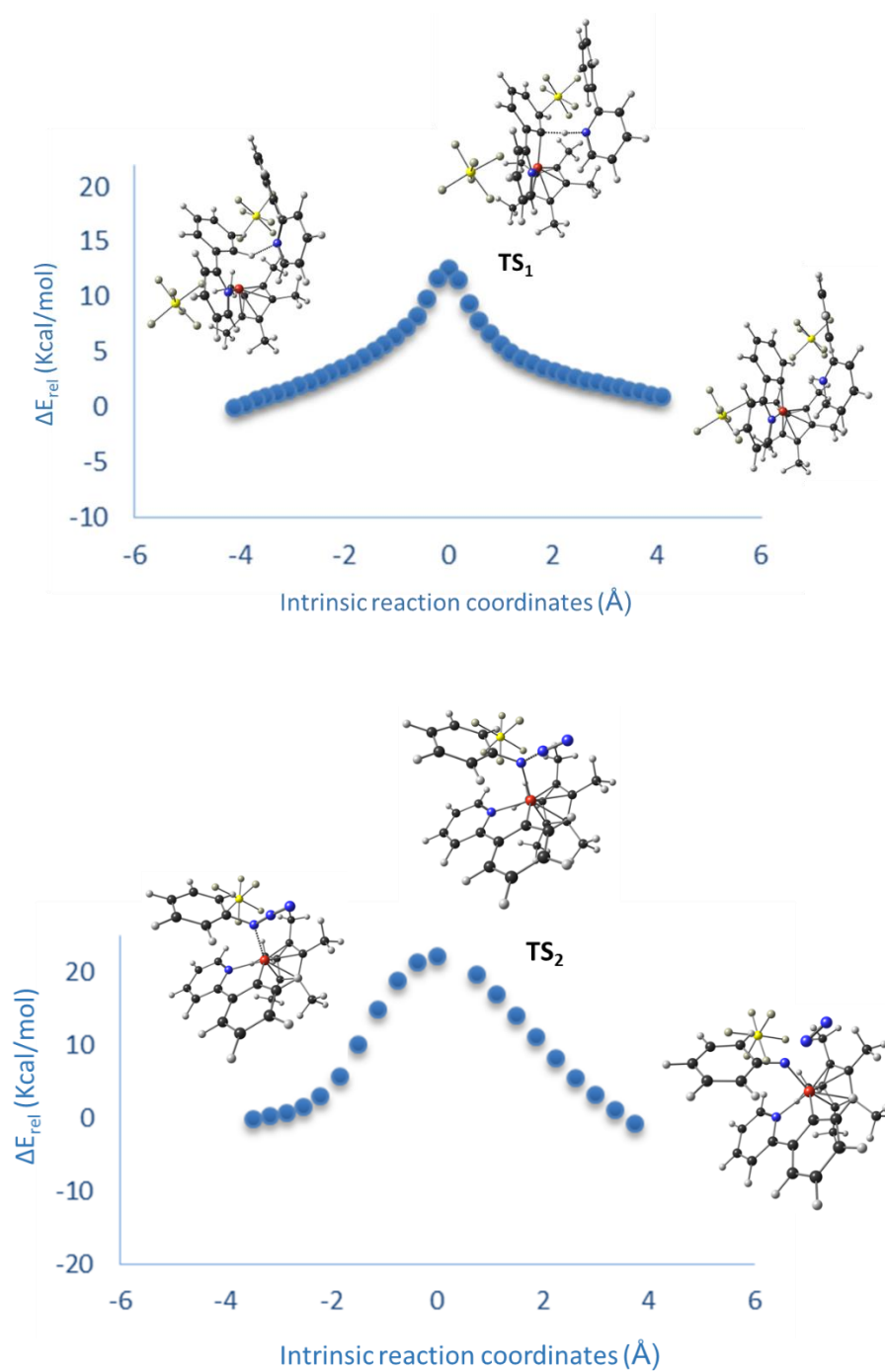
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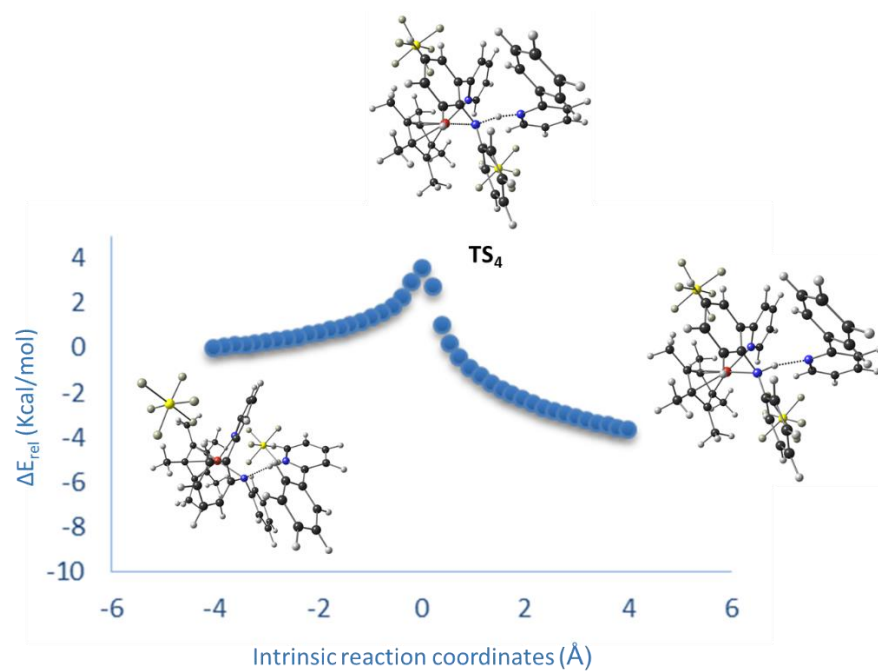
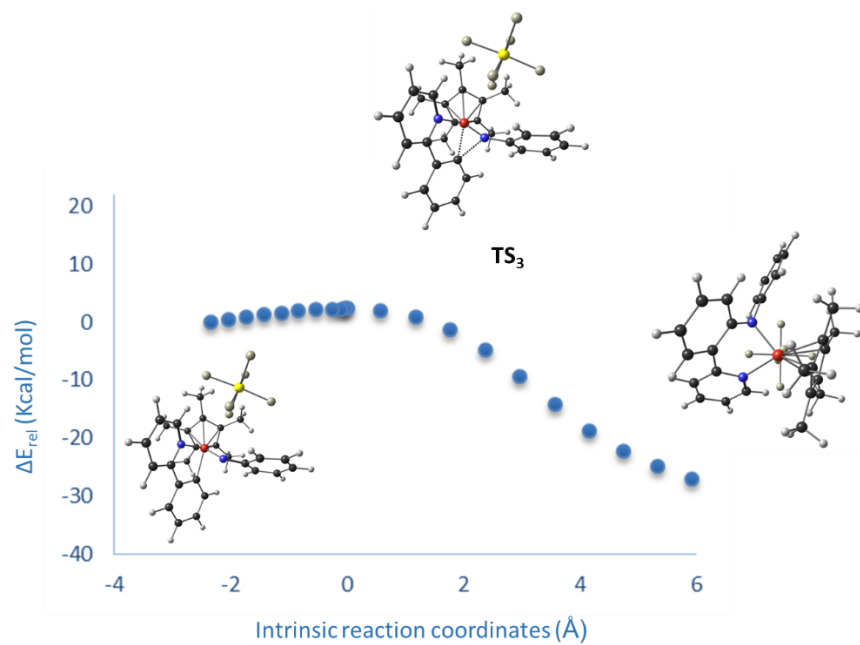
symmetry c1

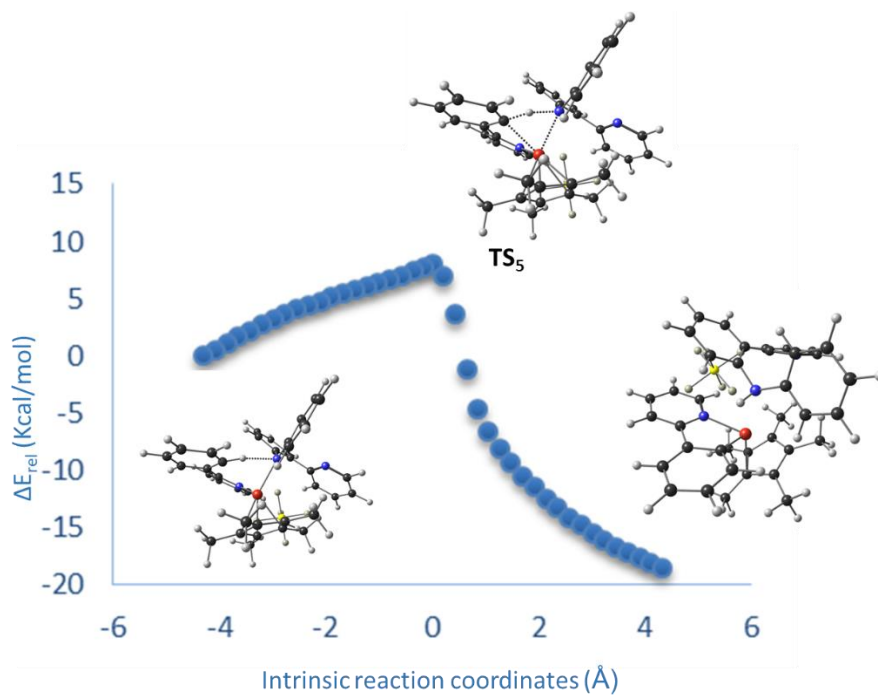
C	1.392511000	0.986473000	-0.125644000
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H	3.160365000	2.202989000	-0.055188000
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C	1.426846000	3.433948000	-0.194954000
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H	1.992365000	4.357776000	-0.187231000
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H	-0.496140000	4.387743000	-0.401673000
C	2.173035000	-0.268218000	0.008743000
N	1.691664000	-1.392326000	-0.560831000
C	3.389549000	-0.296308000	0.718305000
C	2.395053000	-2.525152000	-0.474625000
C	4.114158000	-1.475691000	0.795298000
H	1.953414000	-3.394909000	-0.952838000
C	3.616963000	-2.622825000	0.178300000
N	-0.742414000	-0.173633000	-0.353872000
H	-0.172172000	-0.970644000	-0.626880000
C	-2.099007000	-0.405845000	-0.096759000
C	-2.833232000	0.310716000	0.861539000
C	-2.736488000	-1.452665000	-0.783856000
C	-4.167447000	-0.003791000	1.103903000
C	-4.064921000	-1.768950000	-0.522649000
C	-4.795329000	-1.041907000	0.417175000
H	-2.353667000	1.095282000	1.432523000
H	-2.179283000	-2.010147000	-1.529333000
H	-4.715329000	0.560854000	1.850621000
H	-4.534567000	-2.581557000	-1.066140000
H	-5.833428000	-1.282627000	0.613373000
H	3.746359000	0.591645000	1.222389000
H	5.050133000	-1.504459000	1.342204000
H	4.148809000	-3.565435000	0.215401000

Number of Imaginary frequencies= 0

Figure S1. Intrinsic reaction coordinates of the TSs.







In order to reduce the computational cost, all the transition states obtained at B3LYP/6-311+G** (SDDAll for Rh and Sb) level were re-optimized at B3LP/6-31G* (LANL2DZ for Rh and Sb) and IRC calculations were carried out at B3LYP level.

Figure S2. Comparison of Potential energy Surfaces (PESs) obtained at different levels of DFT.

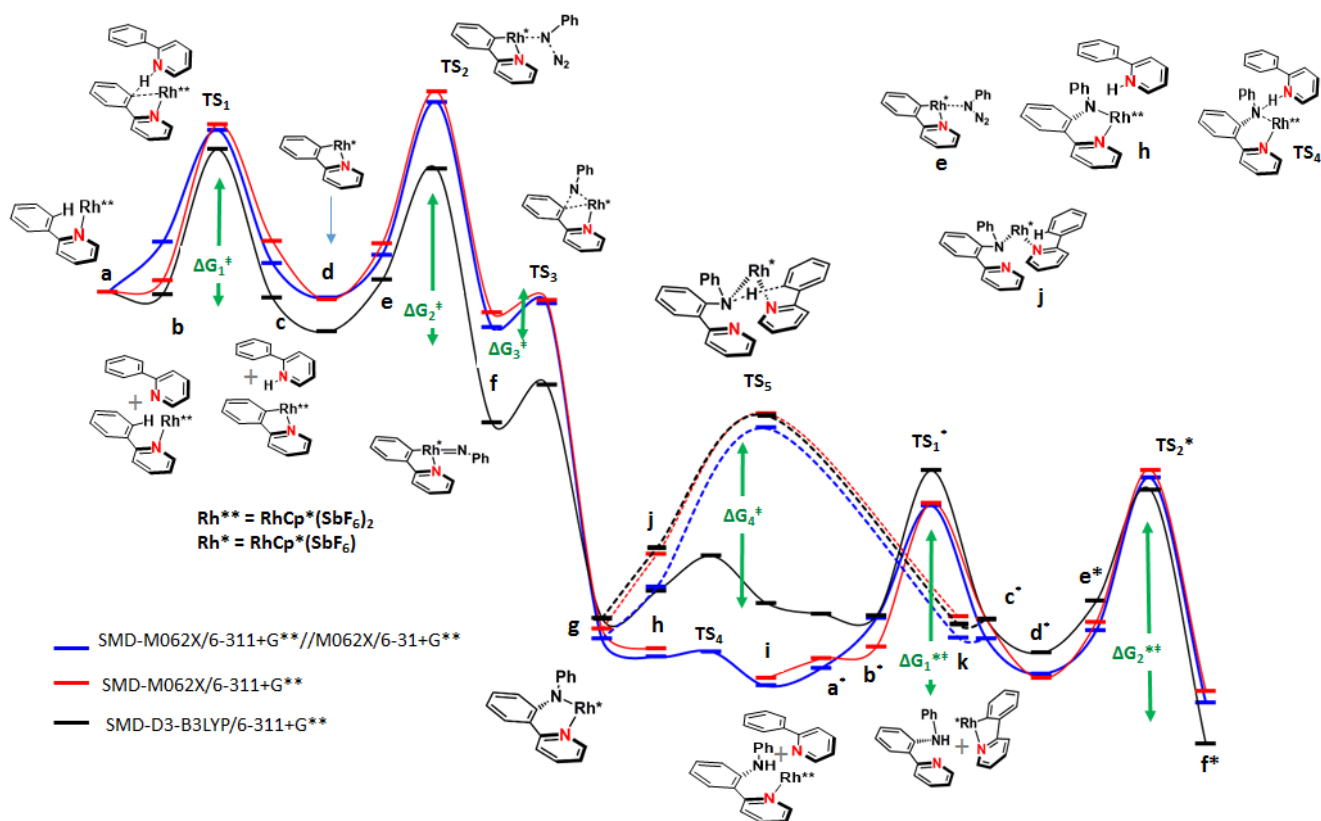


Table S3. A summary of activation barriers ($\Delta G^\ddagger$) obtained at different levels of DFT. $\Delta G^\ddagger$ is the energy difference between TS and the most stable pre-reacting complex before the TS.

	SMD-M062X/6-311+G**// M062X/6-31+G**	SMD-M062X/6-311+G**	SMD-D3-B3LYP/6- 311+G**
$\Delta G_1^\ddagger$	27.8 (w. r to a)	28.7 (w. r to a)	24.8 (w. r to b)
$\Delta G_2^\ddagger$	33.5 (w. r to d)	35.6 (w. r to d)	27.7 (w. r to d)
$\Delta G_3^\ddagger$	4.1 (w. r to f)	2.1 (w. r to f)	6.5 (w. r to f)
$\Delta G_4^\ddagger$	44.1 (w. r to i) i is thermodynamically more stable than g	45.2 (w. r to i) i is thermodynamically more stable than g	34.5 (w. r to g)
$\Delta G_1^{*\ddagger}$	30.8 (w. r to i)	29.9 (w. r to i)	25.2 (w. r to g)
$\Delta G_2^{*\ddagger}$	35.5 (w. r to i)	35.6 (w. r to i)	27.7 (w. r to d*)

$\Delta G^{*\ddagger}$ denotes the activation barriers for the second catalytic cycle. Both in the first and second cycles, the Rh-nitrenoid formation is calculated to be the RDS, rather than C-H activation, consistent with experiments.

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