**SUPPORTING INFORMATION**

# Electronic Structure and Mechanism for the Uptake of Nitric Oxide by the Ru(III) Antitumor complex NAMI-A

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# Tables

**Table S 1:** Energy Values obtained for the **NAMI-$H_2O$** + NO Reaction (Energy values in a.u and bond length in Å). Gibbs free energy difference (ΔG) are given relative to the most stable (triplet) reactant.*

| Parameter | Singlet Surface | | |
|---|---|---|---|
| | Reactant | TS | Product |
| $E_h$ | -2461.19471284 | -2461.18927691 | -2461.25607305 |
| ZPE | 0.19175919 | 0.19127118 | 0.19255212 |
| $G_{el}$ | 0.14342381 | 0.14440313 | 0.14415090 |
| G ($E_h$ + $G_{el}$) | -2461.0512890 | -2461.0448708 | -2461.1119222 |
| $G_{total}$ ($G_{gas}$ + $G_{solv}$) | -2461.0838676 | -2461.0720207 | -2461.1470149 |
| $\Delta G_g$ (kcal/mol) | 15.67 | 19.70 | -22.38 |
| $\Delta G_{solution}$ (kcal/mol) | 14.18 | 21.62 | -25.44 |
| r (Ru-NO) | 3.721 | 2.216 | 1.746 |
| | Triplet Surface | | |
| $E_h$ | -2461.21623210 | -2461.19159159 | -2461.21131986 |
| ZPE | 0.19028267 | 0.18858941 | 0.18978040 |
| $G_{el}$ | 0.13996716 | 0.13731995 | 0.14008567 |
| $G_{gas}$ ($E_h$ + $G_{el}$) | -2461.0762649 | -2461.0542716 | -2461.0712342 |
| $G_{total}$ ($G_{gas}$ + $G_{solv}$) | -2461.1064709 | -2461.0834231 | -2461.1081457 |
| $\Delta G_g$ (kcal/mol) | 0.00 | 13.80 | 3.16 |
| $\Delta G_{solution}$ (kcal/mol) | 0.00 | 14.46 | -1.05 |
| r (Ru-NO) | 4.801 | 3.675 | 1.912 |

* $E_h$ is the total electronic energy in gas phase; ZPE is the Zero Point Energy correction; $G_{el}$ is the thermal correction to the Gibbs free energy; $G_{gas}$ is the Gibbs free energy in gas phase. $G_{total}$ is the total Gibbs free energy of the species including the free energy of solvation. $\Delta G_g$ is the variation of the Gibbs free energy in gas phase and $\Delta G_{solution}$ is the variation of the Gibbs free energy in solution.

**Table S2:** Energy values obtained for the Minimum Energy Crossing Points located between the singlet and triplet potential energy surfaces for the **NAMI-H2O** + NO Reaction (Energy values in a.u and bond length in Å).*

| Parameter | MECP1* | MECP2** | MECP3 |
|---|---|---|---|
| $E_h$ | -2461.16705241 | -2461.22313327 | -2461.21211064 |
| ZPE | 0.18816361 | 0.19031238 | 0.18913759 |
| $G_{el}$ | 0.14034759 | 0.14231518 | 0.14077524 |
| G ($E_h + G_{el}$) | -2461.0267048 | -2461.0808181 | -2461.0713354 |
| $\Delta G_{gas}$ | 31.10 | 15.97 | 3.10 |
| r (Ru-NO) | 3.311 | 1.853 | 1.974 |

* $E_h$ is the total electronic energy in gas phase; ZPE is the Zero Point Energy correction; $G_{el}$ is the thermal correction to the Gibbs free energy; $G_{gas}$ is the Gibbs free energy in gas phase. $\Delta G_g$ is the variation of the Gibbs free energy in gas phase relative to the most stable (triplet) reactant.

**Table S3:** Details of the CASSCF active space for the calculated molecules.

| Molecule | Multiplicity | $n_{elec}$ | $n_{orb}$ | $N^{FOD}$ (a.u.) |
|---|---|---|---|---|
| NAMI-A | 2 | 5 | 5 | 1.15 |
| NAMI-A-$H_2O$ | 2 | 5 | 5 | 1.13 |
| NAMI-A-NO-s | 1 | 8 | 8 | 0.52 |
| NAMI-A-NO-t | 3 | 6 | 6 | 1.56 |

$n_{elec}$ = number of electrons
$n_{orb}$ = number of orbitals
$N^{FOD}$ = amount of static correlation given by the FOD calculation. The larger the number the higher the system is correlated.

**Table S4:** SA-CASSCF(4,4)/NEVPT2 (1 root each state) electronic energies (Hartree) for each stationary point of singlet and triplet DFT reaction paths.*

| Path | Reactants | | TS | | Products | |
|---|---|---|---|---|---|---|
| | CASSCF | SA-CASSCF | CASSCF | SA-CASSCF | CASSCF | SA-CASSCF |
| singlet | -7044.776303 | -7045.425769 | -7045.564376 | -7045.465138 | **-7045.634316** | -7045.582499 |
| triplet | -7045.572162 | **-7045.586165** | **-7045.573647** | **-7045.573606** | -7045.560354 | ** |

* The numbers in bold shows the structure with lower energy in each one of the stationary points (reactants, TS and products).
**The triplet geometry of the products could not be converged with the SA-CASSCF wavefunction.

**Table S5:** SA-CASSCF spin-orbit coupling, SOC, ($T_1$-$S_1$) calculations, at the MECP geometry, with *n* electrons and *m* orbitals and increasing number of singlet (S) and triplet (T) roots.

| $N_{roots}$ (T,S) | Active Space (n,m) | SOC ($cm^{-1}$) |
|---|---|---|

| | | |
|---|---|---|
| 1,1 | (4,4) | 60.80 |
| 2,2 | (4,4) | 56.57 |
| 4,4 | (4,4) | 65.25 |
| 6,6 | (4,4) | 403.9 |
| 8,8 | (4,4) | 510.2 |
| 10,10 | (4,4) | 476.4 |
| 6,10 | (2,4) | 251.7 |
| 10,10 | (6,8) | 442.2 |
| 10,10 | (8,8) | 450.7 |

# Figures

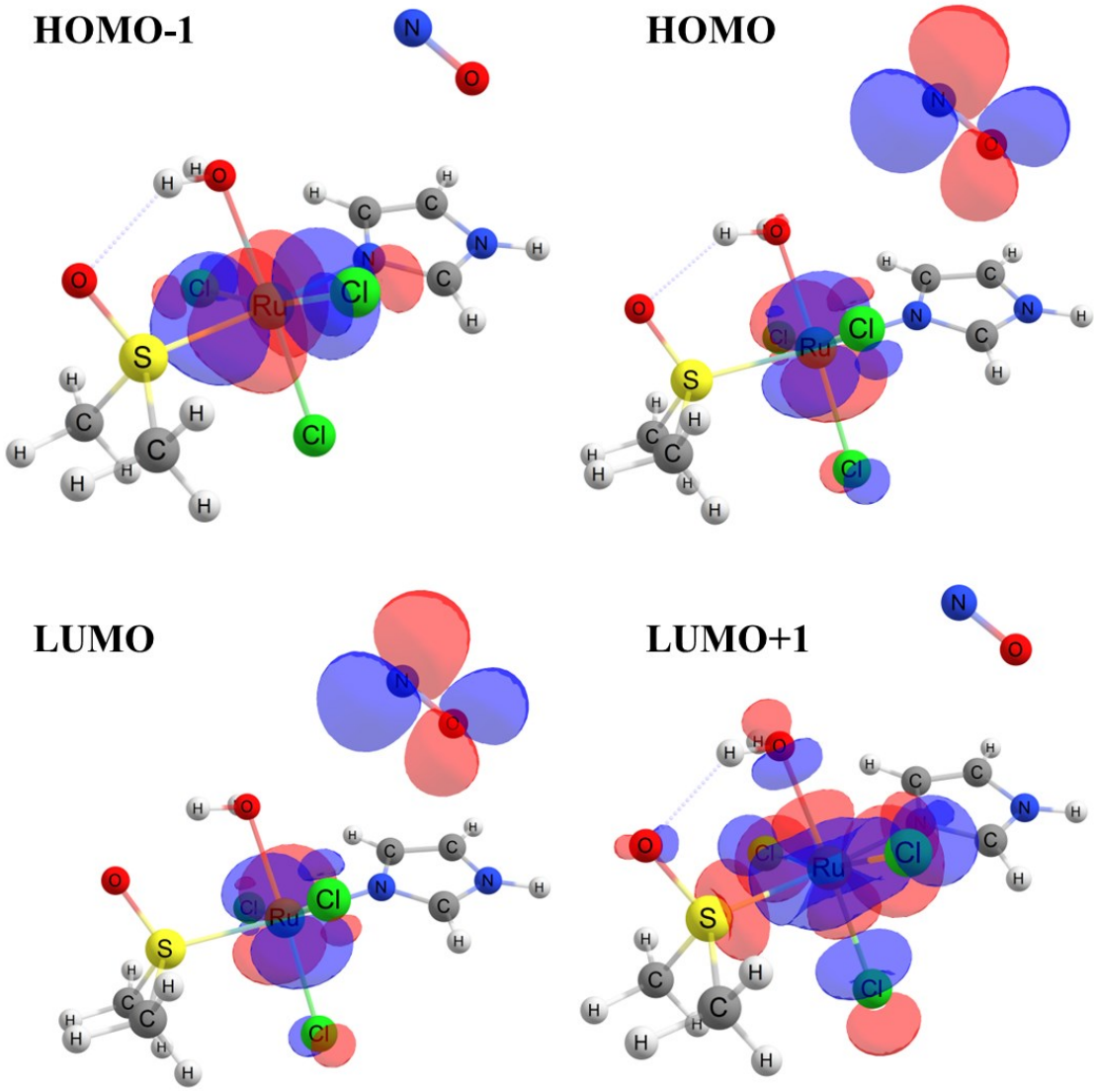


**Figure S1**: SA-CASSCF active orbitals for the reactants at the triplet PES. OBS: Although illustrated in the picture as HOMO and LUMO, both orbitals are SOMO orbitals with occupation of 1.0. Orbital occupations: HOMO-1 (2.0), HOMO (1.0), LUMO (1.0), LUMO+1 (0.0 )

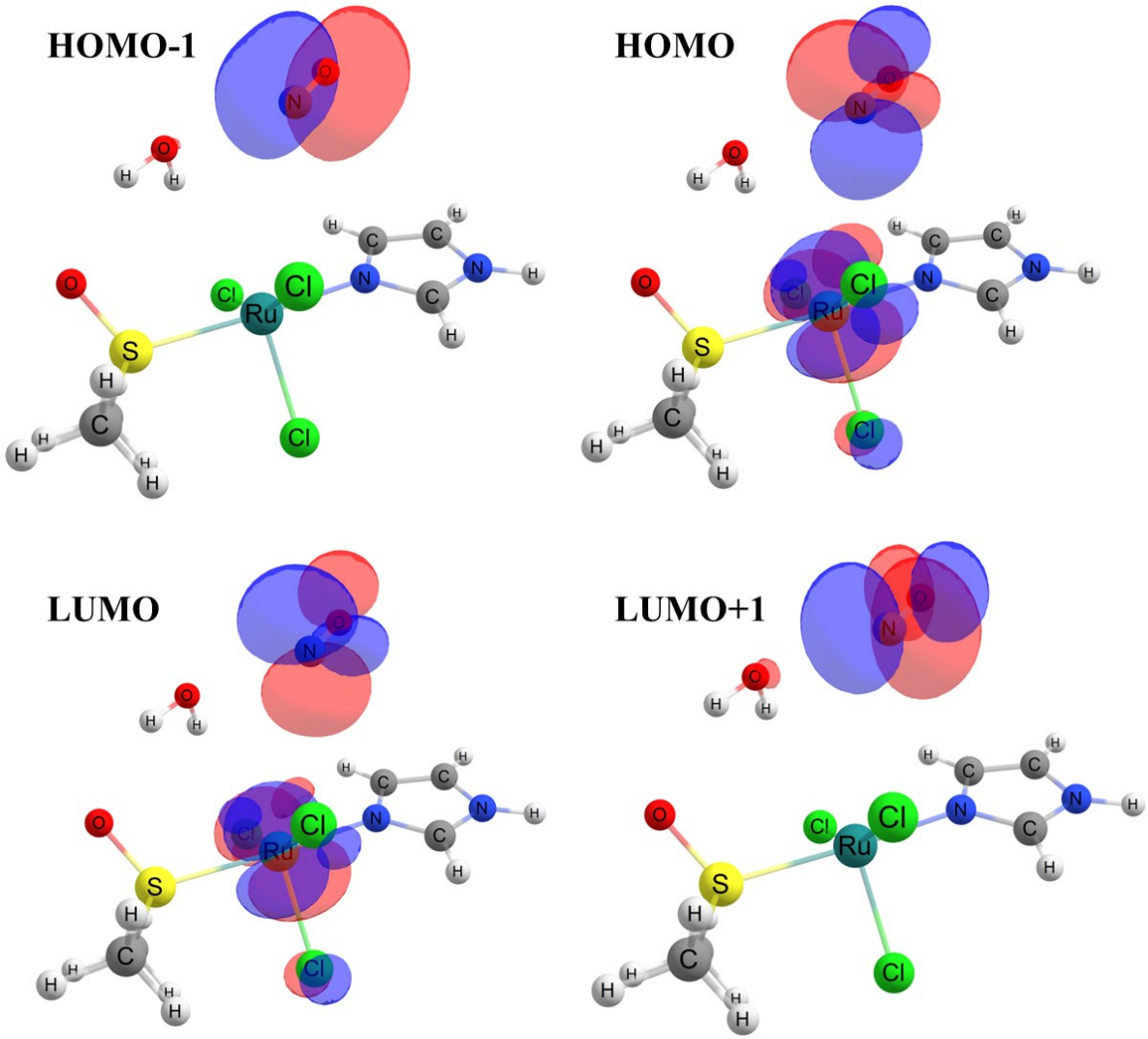


**Figure S2:** SA-CASSCF active orbitals for the transition state at the triplet PES. OBS: Although illustrated in the picture as HOMO and LUMO, both orbitals are SOMO orbitals with occupation of 1.0. Orbital occupations: HOMO-1 (1.9), HOMO (1.0), LUMO (1.0), LUMO+1 (0.1)

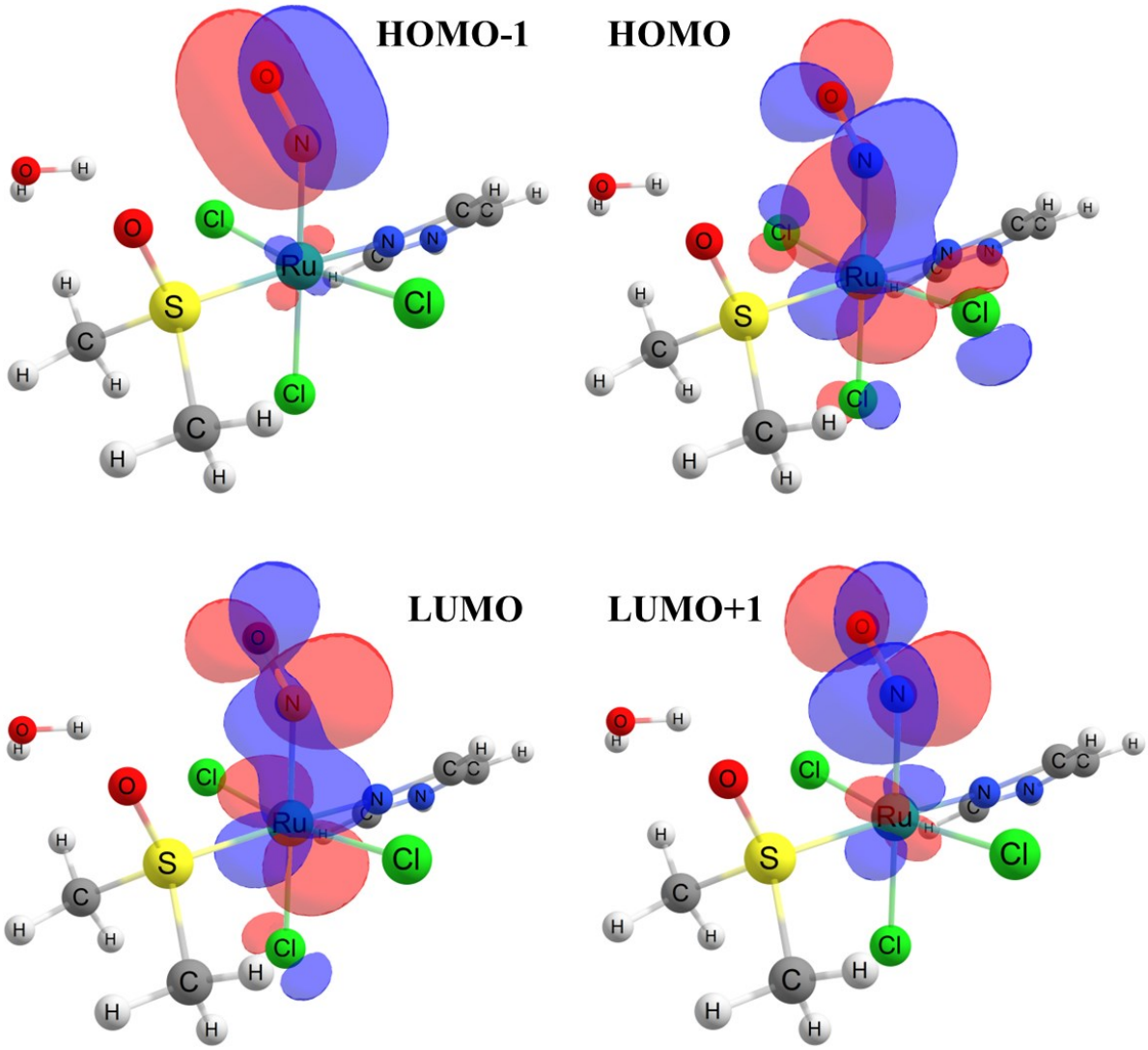


**Figure S3:** SA-CASSCF active orbitals for the MECP3. **OBS:** HOMO and LUMO orbitals at this point are partially SOMO orbitals in which the NO charge transfer partially happened. **Orbital occupations:** HOMO-1 (1.9), HOMO (1.2), LUMO (0.8), LUMO+1 (0.1)

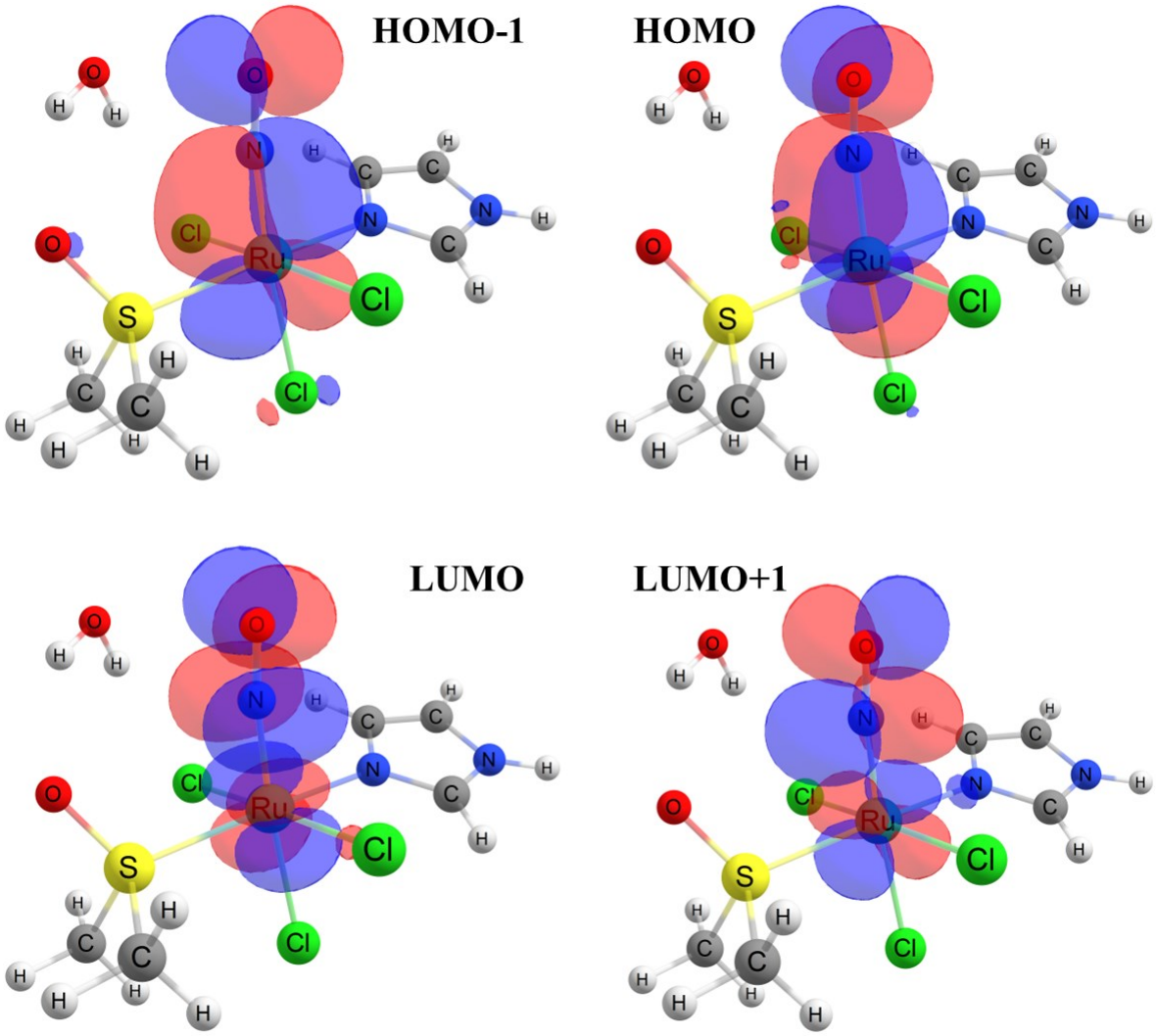


**Figure S4:** CASSCF active orbitals for the products at the singlet PES. **Orbital occupations:** HOMO-1 (1.8), HOMO (1.8), LUMO (0.2), LUMO+1 (0.2)

# ORCA Input Examples

**SA-CASSCF(4,4) – 10 triplet, 10 singlet roots**

```
! old-DKH-TZVP SARC/J RIJCOSX GRIDX6
! DKH NEVPT2 def2-TZVP/C
#--- CASSCF Active Space Parameters
%casscf
      NEl     4
      NOrb    4
      Mult    3,1
      NRoots  10,10
      NEVPT2  SC
      #---- CAS Relativistic ----
      rel
            DoSOC          True
      end
      #---- CAS Convergence ----
      MaxIter 800
      #---- Post Analysis ----
      PrintWF det
      CI TPrintWF 0.1 end
end
#--- Read Pre MO Calculation (CAS 4,4 with 1 root each)
! moread
%moinp "namia-no.mecp3.sacas44.nr1.gbw"
#--- Print Orbitals
%output
      Print[ P_Basis ] 2
      Print[ P_MOs ] 1
end
```

**MECP optimization**

```
! RKS B3LYP def2-TZVP GRID5
! RIJCOSX def2/J GRIDX6
! Freq
! SurfCrossOpt SurfCrossNumFreq
%scf
          MaxIter 350
          LShift  1.0
          ShiftErr 0.05
end
%geom
          MaxIter 250
end
%mecp
          Mult 3
end
```

# XYZ Structures (all gas phase)

### NAMIA-A-$H_2O$ optimized

| | | | |
|---|---|---|---|
| Ru | 1.190622000 | 1.062794000 | -0.047438000 |
| Cl | 3.261206000 | 1.979984000 | 0.307235000 |
| Cl | 1.236639000 | 1.067451000 | -2.443532000 |
| Cl | 0.447299000 | 0.853213000 | 2.179723000 |
| N | 0.364065000 | 3.041512000 | -0.111654000 |
| C | 0.716460000 | 3.959519000 | -0.991331000 |
| H | 1.396398000 | 3.808683000 | -1.810858000 |
| C | -0.515561000 | 3.641439000 | 0.766134000 |
| H | 0.210019000 | 5.979709000 | -1.231518000 |
| C | -0.696000000 | 4.939827000 | 0.397539000 |
| H | -1.287802000 | 5.728264000 | 0.825820000 |
| N | 0.094064000 | 5.123745000 | -0.716566000 |
| H | -0.909929000 | 3.107639000 | 1.611601000 |
| S | 2.130650000 | -1.055271000 | 0.040059000 |
| O | 2.538887000 | -1.628708000 | 1.327144000 |
| C | 3.543826000 | -1.151066000 | -1.069300000 |
| H | 3.247132000 | -0.822942000 | -2.063331000 |
| H | 3.896615000 | -2.181613000 | -1.057578000 |
| H | 1.521248000 | -3.199187000 | -0.769576000 |
| C | 1.015016000 | -2.234928000 | -0.747372000 |
| H | 0.753309000 | -1.886830000 | -1.744775000 |
| H | 0.129426000 | -2.286980000 | -0.118801000 |
| H | 4.291751000 | -0.478713000 | -0.655934000 |
| O | -0.866125000 | 0.270177000 | -0.444254000 |
| H | -1.227394000 | 0.777817000 | -1.184269000 |
| H | -1.359656000 | 0.484679000 | 0.362855000 |

### NAMIA-A-NO singlet reactants optimized

| | | | |
|---|---|---|---|
| N | 2.423879000 | 2.416057000 | 2.532241000 |
| O | 2.505880000 | 3.172627000 | 1.719160000 |
| Ru | 0.491401000 | 0.985177000 | -0.307980000 |
| Cl | 2.733346000 | 1.724171000 | -0.791372000 |
| Cl | -0.175982000 | 0.962873000 | -2.621760000 |
| Cl | 0.721236000 | 1.008880000 | 2.076358000 |
| S | 1.120726000 | -1.173235000 | -0.416973000 |
| O | 0.008215000 | -2.135269000 | -0.165977000 |
| C | 2.452052000 | -1.605106000 | 0.715388000 |
| H | 3.284923000 | -0.926876000 | 0.536526000 |
| H | 2.730478000 | -2.644352000 | 0.545072000 |
| H | 2.205859000 | -2.668367000 | -1.919216000 |

| | | | |
|---|---|---|---|
| C | 1.893919000 | -1.626085000 | -1.975595000 |
| H | 2.732048000 | -0.951879000 | -2.143828000 |
| H | 1.140535000 | -1.475172000 | -2.743981000 |
| H | 2.059203000 | -1.469775000 | 1.719983000 |
| N | -0.208572000 | 2.996264000 | -0.244237000 |
| C | 0.171345000 | 3.927295000 | -1.096211000 |
| H | 0.872608000 | 3.783678000 | -1.898964000 |
| C | -1.110569000 | 3.580275000 | 0.618559000 |
| H | -0.324277000 | 5.953766000 | -1.315187000 |
| C | -1.270031000 | 4.890582000 | 0.277265000 |
| H | -1.877226000 | 5.672574000 | 0.695854000 |
| N | -0.445787000 | 5.093141000 | -0.809713000 |
| H | -1.573010000 | 3.019039000 | 1.410594000 |
| O | -1.569507000 | 0.252719000 | -0.060150000 |
| H | -1.426129000 | -0.709300000 | 0.058030000 |
| H | -1.854133000 | 0.352596000 | -0.987645000 |

**NAMIA-A-NO singlet products optimized**

| | | | |
|---|---|---|---|
| N | 0.014679000 | 1.159926000 | 1.390579000 |
| O | -0.311230000 | 1.172850000 | 2.474967000 |
| Ru | 0.744128000 | 1.275882000 | -0.191944000 |
| Cl | 1.953334000 | 1.545181000 | -2.199566000 |
| Cl | -1.246221000 | 0.699326000 | -1.441921000 |
| Cl | 2.788253000 | 1.880081000 | 0.978332000 |
| S | 1.299134000 | -1.059808000 | -0.202711000 |
| O | 0.464901000 | -1.901682000 | 0.677023000 |
| C | 3.027606000 | -1.327435000 | 0.203590000 |
| H | 3.637331000 | -0.687995000 | -0.431310000 |
| H | 3.241380000 | -2.384953000 | 0.050003000 |
| H | 1.584209000 | -2.768666000 | -1.798595000 |
| C | 1.250412000 | -1.733308000 | -1.863545000 |
| H | 1.890588000 | -1.131578000 | -2.503731000 |
| H | 0.217680000 | -1.663422000 | -2.196179000 |
| H | 3.159999000 | -1.040835000 | 1.243689000 |
| N | 0.237793000 | 3.322008000 | -0.334869000 |
| C | 1.100429000 | 4.320571000 | -0.319675000 |
| H | 2.165834000 | 4.216404000 | -0.214991000 |
| C | -1.024203000 | 3.860291000 | -0.470803000 |
| H | 0.864535000 | 6.394659000 | -0.452065000 |
| C | -0.912409000 | 5.214409000 | -0.530812000 |
| H | -1.651666000 | 5.987061000 | -0.637573000 |
| N | 0.436648000 | 5.484467000 | -0.438201000 |
| H | -1.894951000 | 3.234665000 | -0.543345000 |
| O | -2.373882000 | -0.685363000 | 1.420116000 |
| H | -1.683674000 | -1.361261000 | 1.375857000 |

| | | | |
|---|---|---|---|
| H | -2.410468000 | -0.344093000 | 0.514264000 |

**NAMIA-A-NO singlet TS optimized**

| | | | |
|---|---|---|---|
| N | 0.172039000 | 1.376219000 | 1.982625000 |
| O | -0.322713000 | 2.298860000 | 2.416387000 |
| Ru | 0.640992000 | 1.126085000 | -0.168521000 |
| Cl | 2.240282000 | 1.637442000 | -1.784861000 |
| Cl | -1.049044000 | 0.767053000 | -1.788379000 |
| Cl | 2.465704000 | 1.591865000 | 1.466996000 |
| S | 1.255266000 | -1.120150000 | -0.212451000 |
| O | 0.460269000 | -2.025813000 | 0.660732000 |
| C | 2.997510000 | -1.403756000 | 0.124090000 |
| H | 3.575699000 | -0.738690000 | -0.515379000 |
| H | 3.209674000 | -2.452242000 | -0.082736000 |
| H | 1.541274000 | -2.794257000 | -1.868738000 |
| C | 1.177925000 | -1.767285000 | -1.888650000 |
| H | 1.781583000 | -1.131577000 | -2.533241000 |
| H | 0.136266000 | -1.717991000 | -2.194858000 |
| H | 3.172295000 | -1.159853000 | 1.167846000 |
| N | 0.108040000 | 3.180793000 | -0.259119000 |
| C | 0.988640000 | 4.161886000 | -0.317118000 |
| H | 2.056291000 | 4.042608000 | -0.275985000 |
| C | -1.142433000 | 3.750260000 | -0.367774000 |
| H | 0.799404000 | 6.236254000 | -0.539886000 |
| C | -1.006007000 | 5.098744000 | -0.488614000 |
| H | -1.730817000 | 5.884166000 | -0.601316000 |
| N | 0.350795000 | 5.340205000 | -0.456954000 |
| H | -2.034840000 | 3.152169000 | -0.376071000 |
| O | -1.616947000 | -0.166245000 | 1.082776000 |
| H | -1.096345000 | -0.991447000 | 1.114198000 |
| H | -1.981595000 | -0.128429000 | 0.185381000 |

**NAMIA-A-NO triplet reactants optimized**

| | | | |
|---|---|---|---|
| N | -1.004991000 | 2.857048000 | 3.587140000 |
| O | -0.196318000 | 3.609612000 | 3.285543000 |
| Ru | 0.732540000 | 0.978531000 | -0.476267000 |
| Cl | 2.345395000 | 1.578888000 | -2.015714000 |
| Cl | -0.980858000 | 0.564896000 | -2.083743000 |
| Cl | 2.044193000 | 1.336171000 | 1.447874000 |
| S | 1.336457000 | -1.233932000 | -0.500590000 |
| O | 0.476547000 | -2.060435000 | 0.394070000 |
| C | 3.058827000 | -1.523979000 | -0.079559000 |
| H | 3.671425000 | -0.924928000 | -0.751781000 |
| H | 3.262287000 | -2.588736000 | -0.187384000 |

| | | | |
|---|---|---|---|
| H | 1.666623000 | -2.988958000 | -2.065470000 |
| C | 1.301645000 | -1.965041000 | -2.137663000 |
| H | 1.923556000 | -1.356550000 | -2.792371000 |
| H | 0.268189000 | -1.930597000 | -2.472254000 |
| H | 3.196545000 | -1.187605000 | 0.944697000 |
| N | 0.098387000 | 3.000976000 | -0.386876000 |
| C | 0.900933000 | 4.011890000 | -0.122674000 |
| H | 1.948187000 | 3.931137000 | 0.106468000 |
| C | -1.155096000 | 3.526221000 | -0.615798000 |
| H | 0.596969000 | 6.081872000 | -0.002856000 |
| C | -1.100173000 | 4.879109000 | -0.478352000 |
| H | -1.853061000 | 5.639625000 | -0.577909000 |
| N | 0.210402000 | 5.168713000 | -0.169058000 |
| H | -1.986123000 | 2.903348000 | -0.889487000 |
| O | -0.861674000 | 0.333779000 | 0.922010000 |
| H | -0.599449000 | -0.593744000 | 1.111419000 |
| H | -1.623866000 | 0.262119000 | 0.323836000 |

**NAMIA-A-NO triplet products optimized**

| | | | |
|---|---|---|---|
| N | 0.122448000 | 2.191269000 | 1.455057000 |
| O | -0.464607000 | 1.866625000 | 2.395256000 |
| Ru | 0.902029000 | 1.473487000 | -0.136950000 |
| Cl | 1.832776000 | 0.526704000 | -2.172088000 |
| Cl | -1.260954000 | 0.920101000 | -0.899807000 |
| Cl | 3.056612000 | 2.030821000 | 0.574150000 |
| S | 1.163582000 | -0.734326000 | 0.848442000 |
| O | 0.773870000 | -0.874394000 | 2.259994000 |
| C | 2.864708000 | -1.279237000 | 0.640578000 |
| H | 3.123475000 | -1.202567000 | -0.413965000 |
| H | 2.917870000 | -2.302215000 | 1.012387000 |
| H | 0.659394000 | -2.942577000 | 0.195156000 |
| C | 0.299184000 | -1.967549000 | -0.132639000 |
| H | 0.511161000 | -1.784587000 | -1.184354000 |
| H | -0.762369000 | -1.858800000 | 0.088059000 |
| H | 3.486468000 | -0.612621000 | 1.230184000 |
| N | 0.723838000 | 3.376113000 | -1.057023000 |
| C | 0.676314000 | 3.583788000 | -2.359428000 |
| H | 0.715633000 | 2.812552000 | -3.109684000 |
| C | 0.665646000 | 4.605635000 | -0.438559000 |
| H | 0.537937000 | 5.323219000 | -3.512845000 |
| C | 0.585291000 | 5.571746000 | -1.391810000 |
| H | 0.528781000 | 6.642451000 | -1.316819000 |
| N | 0.590545000 | 4.904315000 | -2.599481000 |
| H | 0.701001000 | 4.704699000 | 0.630935000 |
| O | -2.880225000 | -1.388403000 | 0.828597000 |

| | | | |
|---|---|---|---|
| H | -2.679758000 | -0.529754000 | 0.429696000 |
| H | -2.755302000 | -1.265026000 | 1.776039000 |

**NAMIA-A-NO triplet TS optimized**

| | | | |
|---|---|---|---|
| N | -0.711638000 | 2.051040000 | 2.738619000 |
| O | -1.590985000 | 2.771304000 | 2.875294000 |
| Ru | 0.858845000 | 1.116458000 | -0.449975000 |
| Cl | 2.348896000 | 1.492391000 | -2.124861000 |
| Cl | -1.130535000 | 0.619924000 | -1.605777000 |
| Cl | 2.320423000 | 1.508161000 | 1.311953000 |
| S | 1.364622000 | -1.134282000 | -0.424415000 |
| O | 0.533157000 | -1.955839000 | 0.484181000 |
| C | 3.096365000 | -1.461992000 | -0.062901000 |
| H | 3.707616000 | -0.851753000 | -0.725756000 |
| H | 3.277353000 | -2.525588000 | -0.213323000 |
| H | 1.588214000 | -2.883657000 | -2.013243000 |
| C | 1.265990000 | -1.844628000 | -2.072365000 |
| H | 1.899914000 | -1.262326000 | -2.738284000 |
| H | 0.226604000 | -1.767737000 | -2.381884000 |
| H | 3.264952000 | -1.171589000 | 0.970616000 |
| N | 0.294234000 | 3.161204000 | -0.429449000 |
| C | 1.137468000 | 4.172646000 | -0.352963000 |
| H | 2.205715000 | 4.087784000 | -0.265005000 |
| C | -0.974120000 | 3.695391000 | -0.522672000 |
| H | 0.872793000 | 6.252656000 | -0.351662000 |
| C | -0.884915000 | 5.052311000 | -0.496932000 |
| H | -1.637454000 | 5.818306000 | -0.543879000 |
| N | 0.459676000 | 5.336817000 | -0.393048000 |
| H | -1.841355000 | 3.068616000 | -0.614019000 |
| O | -1.696395000 | -0.231879000 | 1.625002000 |
| H | -1.028168000 | -0.926819000 | 1.514558000 |
| H | -2.078065000 | -0.140050000 | 0.742567000 |

**MECP3 (B3LYP)**

| | | | |
|---|---|---|---|
| N | -0.157477057 | 1.123116161 | 1.824442526 |
| O | -1.189560699 | 0.759800224 | 2.166977125 |
| Ru | 0.913399932 | 1.385538882 | 0.186080292 |
| Cl | 2.210845457 | 1.650820323 | -1.741899061 |
| Cl | -1.071392787 | 0.948964541 | -1.042807750 |
| Cl | 2.672690824 | 1.917655958 | 1.668348092 |
| S | 1.525105126 | -0.905769051 | 0.246061152 |
| O | 1.022408150 | -1.665691063 | 1.400430910 |
| C | 3.313946785 | -1.085037855 | 0.182478937 |

| | | | |
|---|---|---|---|
| H | 3.692636777 | -0.582177631 | -0.704634777 |
| H | 3.525043171 | -2.153731197 | 0.172368398 |
| H | 1.522863940 | -2.751233098 | -1.224328139 |
| C | 1.062062188 | -1.764726167 | -1.264278755 |
| H | 1.411910810 | -1.187027210 | -2.117871506 |
| H | -0.022946059 | -1.853945061 | -1.273304408 |
| H | 3.705159444 | -0.614443938 | 1.080456001 |
| N | 0.430572381 | 3.461875498 | 0.080787925 |
| C | -0.027066950 | 4.070094061 | -0.996065119 |
| H | -0.235104938 | 3.598059302 | -1.939102315 |
| C | 0.562787122 | 4.417371806 | 1.065385555 |
| H | -0.529939354 | 6.063121720 | -1.400355085 |
| C | 0.170320597 | 5.621250808 | 0.566175492 |
| H | 0.125464166 | 6.599171098 | 1.009902301 |
| N | -0.197295318 | 5.381277738 | -0.740065081 |
| H | 0.949264379 | 4.171904027 | 2.037654233 |
| O | -2.478679078 | -2.076125276 | -1.347397156 |
| H | -2.283584931 | -1.173188738 | -1.056257062 |
| H | -2.822481077 | -1.975502863 | -2.241337725 |