

Supplementary Information

The Ru–NO Bonding in Nitrosyl-[poly(1-pyrazolyl)borate]ruthenium Complexes: a Theoretical Insight based on EDA

Giovanni F. Caramori, André G. Kunitz, Daniel F. Coimbra,
Leone C. Garcia and David E. P. Fonseca*

*Departamento de Química, Centro de Ciências Físicas e Matemáticas, Universidade Federal de Santa Catarina,
Campus Universitário Trindade, 88040-900 Florianópolis-SC, Brazil*

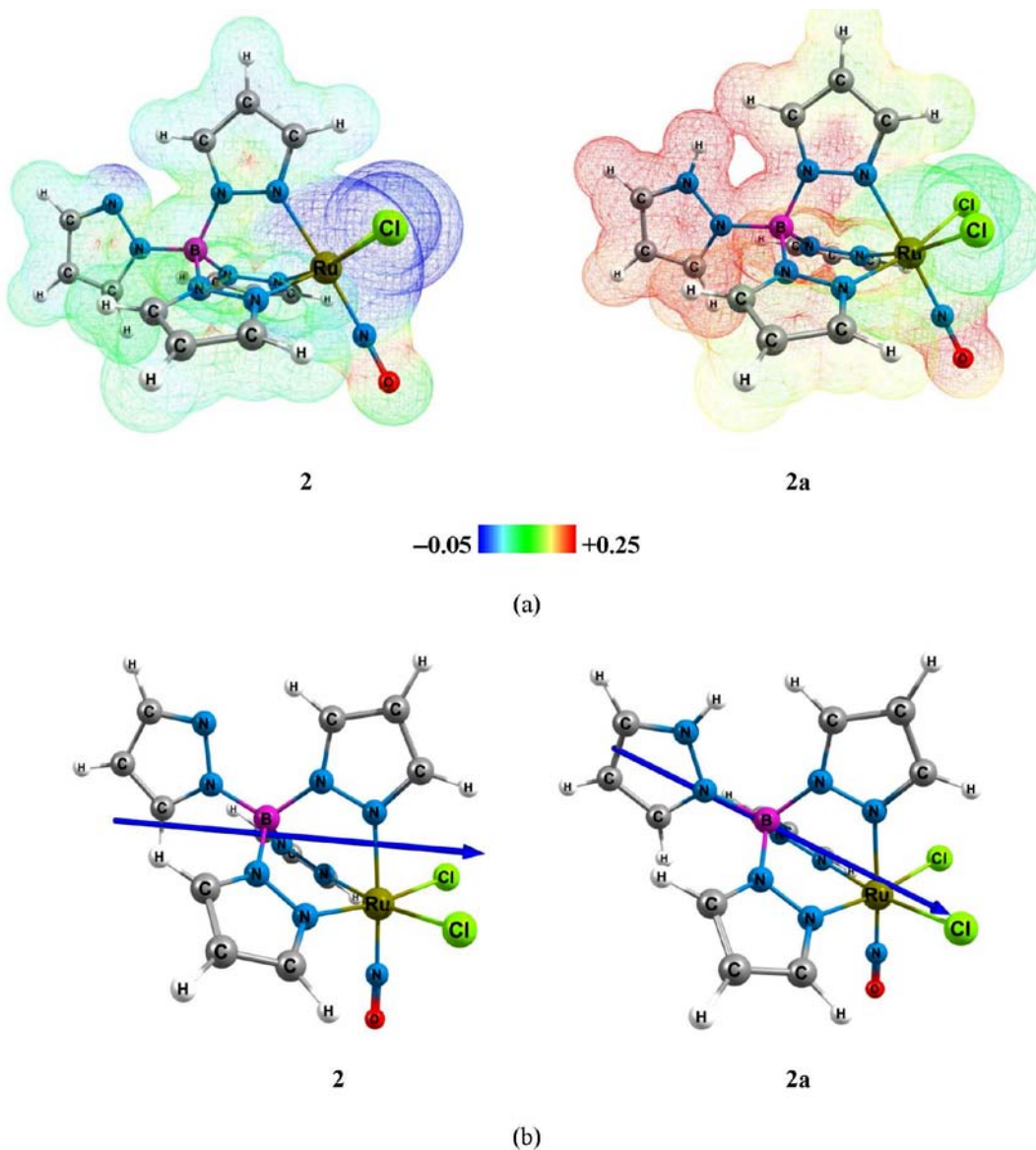


Figure S1. (a) Electrostatic potential surfaces $V(r)$ of complexes **2** and **2a** mapped on electron density isovalue = 0.005 a.u., in which regions of attractive potential appear in blue and those of repulsive potential appear in red. (b) Graphical representation of the dipole moment for complexes **2** ($-6.9764, 0.0000, -3.8752$, Tot = 7.9805 D) and **2a** ($19.136, -0.010, -1.104$, Tot = 19.169 D).

*e-mail: giovanni.caramori@ufsc.br

Table S1. Calculated vibrational frequencies, bond lengths R (Å), bond angles and relative energies of GS, MS1 and MS2 (eV) for complexes [TpRuCl₂(NO)]^a (Tp = BL(pyrazol-1-yl)₃) **1-6**, at BP86/TZVP level of theory (experimental values are given in italics)

| | GS | | | | | | |
|--|------------------------|-----------|-----------|----------|----------|----------|----------|
| | 1 | 2 | 2a | 3 | 4 | 5 | 6 |
| $\nu(\text{NO}^+) / \text{cm}^{-1}$ | 1880/1893 ^a | 1880/1894 | 1937 | 1904 | 1903 | 1904 | 1905 |
| $\nu(\text{BH}) / \text{cm}^{-1}$ | 2542/2522 | – | – | – | – | – | – |
| $R(\text{N–O}) / \text{Å}$ | 1.16 | 1.16 | 1.15 | 1.15 | 1.15 | 1.15 | 1.15 |
| $R(\text{Ru–N}) / \text{Å}$ | 1.75 | 1.75 | 1.71 | 1.76 | 1.76 | 1.76 | 1.76 |
| $R(\text{Ru–O}) / \text{Å}$ | – | – | – | – | – | – | – |
| $R(\text{Ru–Cl}) / \text{Å}$ | 2.38 | 2.38 | 2.36 | 2.37 | 2.37 | 2.36 | 2.37 |
| $R(\text{Ru–N1}) / \text{Å}$ | 2.11 | 2.09 | 2.06 | 2.11 | 2.11 | 2.11 | 2.12 |
| $R(\text{Ru–N2}) / \text{Å}$ | 2.11 | 2.11 | 2.14 | 2.14 | 2.13 | 2.12 | 2.13 |
| $R(\text{Ru–N3}) / \text{Å}$ | 2.11 | 2.09 | 2.05 | 2.11 | 2.10 | 2.11 | 2.09 |
| $\angle \text{Ru–N–O} / \text{degree}$ | 178.6 | 178.2 | 178.9 | 179.9 | 179.7 | 179.7 | 179.7 |
| $\angle \text{Ru–O–N} / \text{degree}$ | – | – | – | – | – | – | – |
| $\Delta E_{\text{rel}} / \text{eV}$ | 0.00 ^b | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MS1 | | | | | | |
| | 1 | 2 | 2a | 3 | 4 | 5 | 6 |
| $\nu(\text{NO}^+) / \text{cm}^{-1}$ | 1791 | 1790 | 1840 | 1808 | 1807 | 1807 | 1806 |
| $\nu(\text{BH}) / \text{cm}^{-1}$ | 2542 | – | – | – | – | – | – |
| $R(\text{N–O}) / \text{Å}$ | 1.16 | 1.16 | 1.15 | 1.15 | 1.15 | 1.15 | 1.15 |
| $R(\text{Ru–N}) / \text{Å}$ | – | – | – | – | – | – | – |
| $R(\text{Ru–O}) / \text{Å}$ | 1.86 | 1.86 | 1.82 | 1.87 | 1.87 | 1.87 | 1.87 |
| $R(\text{Ru–Cl}) / \text{Å}$ | 2.37 | 2.38 | 2.36 | 2.36 | 2.36 | 2.36 | 2.37 |
| $R(\text{Ru–N1}) / \text{Å}$ | 2.09 | 2.08 | 2.07 | 2.10 | 2.10 | 2.11 | 2.11 |
| $R(\text{Ru–N2}) / \text{Å}$ | 2.04 | 2.04 | 2.05 | 2.06 | 2.05 | 2.04 | 2.05 |
| $R(\text{Ru–N3}) / \text{Å}$ | 2.09 | 2.08 | 2.03 | 2.10 | 2.09 | 2.10 | 2.08 |
| $\angle \text{Ru–N–O} / \text{degree}$ | – | – | – | – | – | – | – |
| $\angle \text{Ru–O–N} / \text{degree}$ | 178.7 | 178.5 | 179.6 | 178.6 | 179.2 | 179.1 | 179.2 |
| $\Delta E_{\text{rel}} / \text{eV}$ | 39.51 | 39.47 | 37.06 | 39.52 | 39.50 | 39.22 | 39.54 |
| | MS2 | | | | | | |
| | 1 | 2 | 2a | 3 | 4 | 5 | 6 |
| $\nu(\text{NO}^+) / \text{cm}^{-1}$ | 1536 | 1538 | 1566 | 1564 | 1562 | 1565 | 1561 |
| $\nu(\text{BH}) / \text{cm}^{-1}$ | 2543 | – | – | – | – | – | – |
| $R(\text{N–O}) / \text{Å}$ | 1.20 | 1.20 | 1.20 | 1.19 | 1.19 | 1.19 | 1.20 |
| $R(\text{Ru–N}) / \text{Å}$ | 1.95 | 1.95 | 1.91 | 1.96 | 1.96 | 1.96 | 1.96 |
| $R(\text{Ru–O}) / \text{Å}$ | 2.21 | 2.22 | 2.18 | 2.22 | 2.22 | 2.22 | 2.22 |
| $R(\text{Ru–Cl}) / \text{Å}$ | 2.35 | 2.35 | 2.32 | 2.33 | 2.34 | 2.33 | 2.34 |
| $R(\text{Ru–N1}) / \text{Å}$ | 2.10 | 2.09 | 2.04 | 2.11 | 2.11 | 2.12 | 2.12 |
| $R(\text{Ru–N2}) / \text{Å}$ | 2.04 | 2.05 | 2.02 | 2.06 | 2.05 | 2.05 | 2.06 |
| $R(\text{Ru–N3}) / \text{Å}$ | 2.14 | 2.12 | 2.13 | 2.14 | 2.12 | 2.14 | 2.12 |
| $\angle \text{Ru–N–O} / \text{degree}$ | 86.0 | 86.2 | 85.7 | 86.0 | 85.9 | 86.1 | 85.9 |
| $\angle \text{Ru–O–N} / \text{degree}$ | 61.3 | 61.1 | 61.1 | 61.6 | 61.6 | 61.5 | 61.6 |
| $\Delta E_{\text{rel}} / \text{eV}$ | 31.94 | 31.83 | 30.10 | 32.54 | 32.48 | 32.34 | 33.66 |

^aExperimental values from reference 1. ^bRelative energy values correspond to the ZPE corrected electronic energy differences between each complex in different states.

Table S2. Cartesian coordinates (Å) of optimized structure of **1** in GS

| | | | |
|-------------------|-------------------|-------------------|----|
| -1.43823454511364 | -5.81649533462842 | -2.74425252171036 | H |
| 2.81220139908169 | -6.19539484396843 | -3.10496341841030 | C |
| 0.46879377461672 | -5.09022261461585 | -2.53302461988497 | C |
| 4.60878846286152 | -4.43246946922316 | -2.33789529375629 | C |
| 6.65916572690751 | -4.48626807839201 | -2.37662711761820 | H |
| 0.84420862923379 | -2.79307926180326 | -1.51156347237445 | N |
| -4.69580467545762 | 0.00015873698304 | -4.83505291437803 | O |
| 3.38797823108983 | -2.38456396677023 | -1.39406786930857 | N |
| -4.11593469695822 | -3.21231686209548 | 1.78502005100374 | Cl |
| -3.52354339405850 | -0.00023999520055 | -2.98392079966386 | N |
| -1.68227564900471 | -0.00015873698304 | -0.22810693435537 | Ru |
| 4.40437113349898 | 0.00023243629660 | -0.01792216127568 | B |
| 6.67883021554466 | 0.00038172464969 | 0.04641167027950 | H |
| 0.68827599956022 | 0.00036093766382 | 2.97654519913043 | N |
| 3.38768910301357 | 2.38496647840580 | -1.39395448574925 | N |
| 3.25509458929894 | 0.00013417054519 | 2.68354885377924 | N |
| 0.84385525047393 | 2.79289973783434 | -1.51202645524165 | N |
| 0.18035922780195 | -0.00001700753390 | 5.46542581992220 | C |
| -1.77052585267134 | -0.00004346369774 | 6.09743711789847 | H |
| 4.35348648180451 | 0.00007747876553 | 4.99746919391843 | C |
| 4.60826689848868 | 4.43338031714965 | -2.33699767391171 | C |
| 0.46818150339642 | 5.09031899064126 | -2.53278273495843 | C |
| 6.65864038308268 | 4.48759277631000 | -2.37534777312393 | H |
| 6.39791677816444 | 0.00009826575141 | 5.17052841022649 | H |
| -1.43894697181133 | 5.81627801613973 | -2.74417882239680 | H |
| -4.11657531406835 | 3.21173482649100 | 1.78466100306591 | Cl |
| 2.45564789955662 | -0.00021731848869 | 6.82415959269632 | C |
| 2.81147007512411 | 6.19606947614636 | -3.10409792390753 | C |
| 2.68680674138355 | -0.00048376985308 | 8.86063792209631 | H |
| 3.14734430315616 | 8.03562512945450 | -3.94342539091283 | H |

Table S3. Cartesian coordinates (Å) of optimized structure of **2** in GS

| | | | |
|--------------------|-------------------|-------------------|----|
| -1.79433640012744 | -8.23498366234562 | -3.43790668143407 | H |
| -1.45986434877891 | -6.33344877606407 | -2.74989335378627 | C |
| 2.79285816386260 | -5.84312346353348 | -2.61864054552353 | H |
| 0.87988287644619 | -5.14269652586670 | -2.37687845117468 | C |
| -5.30570617936751 | -4.68072466206876 | -1.94075425944852 | H |
| -3.26044440357261 | -4.56492036376265 | -2.01797602224581 | C |
| -6.49156781870643 | -0.00023243629660 | -4.06207372683174 | H |
| 0.49925426782662 | -2.78643498522742 | -1.50820164984077 | N |
| 5.95121390035421 | 0.00104501847168 | -4.97989852167662 | O |
| -2.04529012168473 | -2.41394164698868 | -1.29988581576378 | N |
| -11.52738900156307 | 0.00008125821751 | -2.75975016454269 | H |
| -7.37536242794898 | -0.00007936849152 | -2.20860969024766 | C |
| 4.82727291248305 | 0.00046109314121 | -3.09879157333160 | N |
| -9.89726978984314 | 0.00007180958757 | -1.51460971066804 | C |
| 5.52553044471494 | -3.20136401026568 | 1.66179290901450 | Cl |
| -5.95535617972117 | -0.00006236095762 | -0.03093670415903 | N |
| -3.07517944710431 | -0.00007747876553 | 0.08635102904811 | B |
| 3.03862836703322 | 0.00000566917797 | -0.30732802724858 | Ru |
| -9.85038379834051 | 0.00022865684462 | 1.15811668237460 | C |
| -2.04524854771298 | 2.41396243397456 | -1.29955700344177 | N |
| 0.49926560618255 | 2.78670710576977 | -1.50766685738600 | N |
| -7.48923731602074 | 0.00019842122880 | 2.05845206319518 | N |
| -11.42904577139143 | 0.00041573971749 | 2.47432028204977 | H |
| -3.26053888987204 | 4.56502996786999 | -2.01719934486450 | C |
| -5.30581011429688 | 4.68069442645294 | -1.93998325124518 | H |
| -1.88920253448009 | -0.00023621574857 | 2.77916520934935 | N |
| 0.87975059562699 | 5.14313305257007 | -2.37593736763237 | C |
| 0.70720916423979 | -0.00023054657061 | 2.92920567339054 | N |
| -1.46007032891166 | 6.33376625003015 | -2.74887101202644 | C |
| 2.79269375770159 | 5.84371683749390 | -2.61752749691626 | H |
| -1.79464064601160 | 8.23537672535124 | -3.43662922666579 | H |
| -2.85273602153671 | -0.00042140889545 | 5.16219849806884 | C |
| -4.88899325299603 | -0.00035715821184 | 5.40326706297988 | H |
| 1.34418099293607 | -0.00053479245477 | 5.38630866195837 | C |
| 5.52562115156239 | 3.20096905753407 | 1.66241651859073 | Cl |
| 3.32812305012758 | -0.00060282259036 | 5.90533135335151 | H |
| -0.84912380653009 | -0.00074077258752 | 6.86717164592237 | C |
| -0.96801402737554 | -0.00102801093779 | 8.91327246005619 | H |

Table S4. Cartesian coordinates (Å) of optimized structure of **2a** in GS

| | | | |
|-------------------|-------------------|-------------------|----|
| -5.89097321529029 | -0.02220617009179 | -4.98704357563944 | O |
| -4.76662593633159 | -0.01347374629857 | -3.11862802703372 | N |
| -3.04704520658635 | -0.00709214163514 | -0.37818708264232 | Ru |
| -5.49350525838650 | 3.16514741169456 | 1.57382616424615 | Cl |
| -5.47364801769851 | -3.19309456933966 | 1.57334050466709 | Cl |
| -0.54490815798470 | 2.74863101682590 | -1.49211819195197 | N |
| 1.99770115211435 | 2.41199522922045 | -1.21793028936510 | N |
| -0.74648900863839 | 0.00173287873153 | 2.94635493673690 | N |
| 1.84371494020900 | 0.02306410569061 | 2.88128789149815 | N |
| -0.53323910000522 | -2.74444905321317 | -1.49551969873142 | N |
| 2.00537532935396 | -2.39012920980660 | -1.21429256683709 | N |
| -0.92503598921729 | 5.11130061829245 | -2.31933818454844 | C |
| 1.40375082527405 | 6.34749888878915 | -2.60243047599350 | C |
| 3.20342759104521 | 4.59854614800343 | -1.85627972830706 | C |
| -0.89604948227848 | -5.11192422786869 | -2.31649225720964 | C |
| 1.44147731491004 | -6.33392687673918 | -2.58841248861022 | C |
| 3.22738553712841 | -4.57082008829900 | -1.84355809295195 | C |
| -1.48561942427725 | 0.00380968759298 | 5.35763207008168 | C |
| 0.63732142800417 | 0.03156220346125 | 6.94097489440632 | C |
| 2.68989077419691 | 0.04582774494903 | 5.31807632568875 | C |
| 2.93874501018089 | 0.01401987710927 | 0.15648442966224 | B |
| -2.84330061967573 | 5.78143146891033 | -2.59834677813218 | H |
| 1.72751379944530 | 8.26334466998221 | -3.25238094277934 | H |
| 5.24270082518230 | 4.75803524198751 | -1.72729459123062 | H |
| -3.49373107686268 | -0.00979256007282 | 5.77761233268742 | H |
| 0.67731747855245 | 0.04636442712978 | 8.98909960507391 | H |
| 4.67037652255530 | 0.09603776446557 | 5.84555365115479 | H |
| -2.80902099024291 | -5.79526615287272 | -2.59960155618860 | H |
| 1.77949071276116 | -8.24920196068369 | -3.23272590277214 | H |
| 5.26769056165527 | -4.71521783053829 | -1.71270212714682 | H |
| 5.88369588050827 | 0.00501533277369 | -0.06620088083190 | N |
| 7.16626802676470 | 0.04724125998848 | -2.27532835600043 | C |
| 9.75716172559792 | 0.01981755644223 | -1.79161519470388 | C |
| 9.98359058327544 | -0.04589766481060 | 0.82889806927433 | C |
| 7.63071165215570 | -0.05163109345995 | 1.80028336781349 | N |
| 6.12548821047293 | 0.09631366445990 | -4.04152673615793 | H |
| 11.27834768270621 | 0.04250371693512 | -3.16356193159015 | H |
| 11.62736684471482 | -0.09099597552804 | 2.05598030160212 | H |
| 7.08446556817109 | -0.12239944200625 | 3.63682679789584 | H |

Table S5. Cartesian coordinates (Å) of optimized structure of **3** in GS

| | | | |
|-------------------|-------------------|-------------------|----|
| 1.86456617676698 | 8.36031217963416 | -3.08771022013458 | H |
| 1.51254990934049 | 6.42454490706950 | -2.51198252100215 | C |
| -2.73975686358353 | 5.93155508089502 | -2.57712893473242 | H |
| -0.83971864028493 | 5.20828324575231 | -2.29668225967137 | C |
| 5.32493603102729 | 4.79981519386900 | -1.63193334866896 | H |
| 3.28734465302003 | 4.63624240202360 | -1.80287985132180 | C |
| 6.14009390263866 | -0.01246085316869 | -4.06960806434821 | H |
| -0.50380472800712 | 2.81062914705919 | -1.55051072499906 | N |
| -6.10972222655022 | 0.00901021351354 | -4.94476851554894 | O |
| 2.04520508401524 | 2.42448442827896 | -1.27198401154242 | N |
| 11.30932596083699 | 0.00274010268344 | -3.07290043756208 | H |
| 7.24832181891478 | -0.00623987521429 | -2.34154624436622 | C |
| -4.90581748347235 | 0.00622664713237 | -3.12672739262077 | N |
| 9.73171845488769 | 0.00146831709313 | -1.76135879190075 | C |
| -5.51218142033162 | 3.18223809353527 | 1.61245027372672 | Cl |
| 5.87661129777709 | -0.00596019576798 | -0.08520963455101 | O |
| 2.85030016473743 | -0.00338638897153 | 0.11090423881772 | B |
| -3.07019434994644 | 0.00213350064111 | -0.36281794117721 | Ru |
| 9.84799329496495 | 0.00770252312945 | 0.95075138046987 | C |
| 2.04158436902113 | -2.42794640629004 | -1.27583905255912 | N |
| -0.50818511284864 | -2.80849753614408 | -1.55588321598459 | N |
| 7.66127985974696 | 0.00449754785282 | 2.08566789688269 | N |
| 11.52505707969316 | 0.01466049421940 | 2.15166468730782 | H |
| 3.27933599428043 | -4.64172638684245 | -1.80870020736662 | C |
| 5.31646816887247 | -4.80991577927796 | -1.63672758350199 | H |
| 1.86584930071323 | -0.00511926770306 | 2.82247017010363 | N |
| -0.84866460311486 | -5.20455859582882 | -2.30512177593637 | C |
| -0.74635672781919 | -0.00275522049135 | 2.93755637253407 | N |
| 1.50115108217738 | -6.42543307828413 | -2.52087368177841 | C |
| -2.75007098802919 | -5.92361823174299 | -2.58713881329392 | H |
| 1.84940490516061 | -8.36122869673862 | -3.09879157333160 | H |
| 2.80203278353715 | -0.01005712171122 | 5.23197096101915 | C |
| 4.81995400372929 | -0.01236825659525 | 5.57016199311320 | H |
| -1.39892068564724 | -0.00589594508437 | 5.38330021818455 | C |
| -5.51722698872113 | -3.17788605458357 | 1.60643338617908 | Cl |
| -3.38802925369152 | -0.00473754305337 | 5.88815941329330 | H |
| 0.77906788468149 | -0.01051254567446 | 6.89684601312102 | C |
| 0.86836877599778 | -0.01365704971946 | 8.94464002174062 | H |

Table S6. Cartesian coordinates (Å) of optimized structure of **4** in GS.

| | | | |
|--------------------|-------------------|-------------------|----|
| -1.90463632725072 | -3.35279674315704 | 8.30479306565956 | H |
| -1.58651178331365 | -2.70955652706075 | 6.38621536807604 | C |
| 2.65744064896486 | -2.56441184416830 | 5.88231554716745 | H |
| 0.74453060055876 | -2.35001800691549 | 5.17446799569420 | C |
| -5.43168471704270 | -1.96887232769147 | 4.79215391400925 | H |
| -3.39364161704541 | -2.03641809249437 | 4.61672660647586 | C |
| 6.02676585024539 | -4.81952904970788 | 0.00000000000000 | O |
| -11.80728985572847 | -2.66156876294582 | 0.00000000000000 | H |
| -6.84530224578873 | -3.97814278670926 | 0.00000000000000 | H |
| 0.36231714489298 | -1.54934846225787 | 2.80136246560366 | N |
| -2.19157200955176 | -1.37403464410844 | 2.42463228421976 | N |
| 4.78972798583032 | -3.02337727486089 | 0.00000000000000 | N |
| -10.13120154188639 | -1.48632212266556 | 0.00000000000000 | C |
| -7.62148462282059 | -2.17521127405838 | 0.00000000000000 | C |
| 5.29761364891936 | 1.72932341428004 | 3.18187205361128 | Cl |
| 2.89531907483800 | -0.30029749634985 | 0.00000000000000 | Ru |
| -3.11008351570307 | -0.00488115277987 | 0.00000000000000 | B |
| -2.19157200955176 | -1.37403464410844 | -2.42463228421976 | N |
| 0.36231714489298 | -1.54934846225787 | -2.80136246560366 | N |
| -9.96774918038852 | 0.99463706535879 | 0.00000000000000 | C |
| -6.09927604049357 | -0.20422194114396 | 0.00000000000000 | N |
| -3.39364161704541 | -2.03641809249437 | -4.61672660647586 | C |
| -5.43168471704270 | -1.96887232769147 | -4.79215391400925 | H |
| 0.74453060055876 | -2.35001800691549 | -5.17446799569420 | C |
| 2.65744064896486 | -2.56441184416830 | -5.88231554716745 | H |
| -11.33417007313555 | 2.40360436017158 | 0.00000000000000 | H |
| -1.58651178331365 | -2.70955652706075 | -6.38621536807604 | C |
| -1.90463632725072 | -3.35279674315704 | -8.30479306565956 | H |
| -2.10017887409215 | 2.72782193438554 | 0.00000000000000 | N |
| 0.49666826473865 | 2.92633119607151 | 0.00000000000000 | N |
| -7.55239393332271 | 1.81692149051555 | 0.00000000000000 | O |
| 5.29761364891936 | 1.72932341428004 | -3.18187205361128 | Cl |
| -3.09558809282823 | 5.10072133883443 | 0.00000000000000 | C |
| 1.08952496179593 | 5.38214639118017 | 0.00000000000000 | C |
| -5.11643424980275 | 5.40903969777431 | 0.00000000000000 | H |
| 3.06366357787237 | 5.94167431034058 | 0.00000000000000 | H |
| -1.12561042472179 | 6.82766185210657 | 0.00000000000000 | C |
| -1.27092427588473 | 8.86631718930910 | 0.00000000000000 | H |

Table S7. Cartesian coordinates (Å) of optimized structure of **5** in GS

| | | | |
|-------------------|-------------------|-------------------|----|
| 0.40581865604732 | 8.81245935801749 | -2.83360065617636 | H |
| 0.32149152353298 | 6.84257119300305 | -2.27292462454296 | C |
| -3.82528917073682 | 5.78116501754594 | -2.30141035409480 | H |
| -1.84222016695204 | 5.31935378045703 | -2.04265584365665 | C |
| 4.32250631394775 | 5.75145474555351 | -1.44023954438752 | H |
| 2.32480327210741 | 5.30125020548644 | -1.59376655287764 | C |
| 7.71622931204285 | 2.20573730674502 | -3.91706938255012 | H |
| -1.18284941611313 | 2.98537021949710 | -1.31149251278564 | N |
| -6.28088226823977 | -0.33686633417606 | -5.00575375265236 | O |
| 1.39884509660770 | 2.94736027096282 | -1.04107839299796 | N |
| 11.40810949716396 | -1.14869072914357 | -3.06377873021521 | H |
| 8.04809732097912 | 1.04703480931396 | -2.25133450512344 | C |
| -5.12558505704012 | -0.29313996452633 | -3.15685340433069 | N |
| 9.90965316424630 | -0.64320792445860 | -1.74396575390187 | C |
| -6.23585009793193 | 2.44713090452609 | 1.77140079580405 | Cl |
| 6.27380713413853 | 1.43968963412484 | 0.56189868434801 | S |
| 2.50724308822279 | 0.53069363909861 | 0.14843986612886 | B |
| -3.35311656605252 | -0.22668775013795 | -0.34996024555092 | Ru |
| 9.65326081129387 | -1.71250559564400 | 0.76793550888277 | C |
| 2.07659532241153 | -1.81664839487459 | -1.49343344124003 | N |
| -0.40556732249084 | -2.56983270269051 | -1.68506299483786 | N |
| 7.78313128121651 | -0.94891267708299 | 2.20015883562674 | N |
| 10.92917923234451 | -3.13139690553854 | 1.56105350628935 | H |
| 3.58405808939076 | -3.67937586825468 | -2.46095991931051 | C |
| 5.62305920298550 | -3.49886546237365 | -2.48287885105204 | H |
| 1.47956663193583 | 0.13706182595163 | 2.82478886389161 | N |
| -0.42937598022095 | -4.85293539140796 | -2.78096989766845 | C |
| -1.10685786493440 | -0.13217121509319 | 2.96788836437675 | N |
| 2.05463292697226 | -5.62020382701676 | -3.32518074676336 | C |
| -2.21685267500984 | -5.81868930650116 | -3.07420245876822 | H |
| 2.65000621748196 | -7.36528451925188 | -4.22082771740627 | H |
| 2.46076149808171 | 0.02832321311682 | 5.21400722577172 | C |
| 4.48276641613517 | 0.13828069921426 | 5.54557665800179 | H |
| -1.71431217368908 | -0.40220549995716 | 5.41031763064326 | C |
| -5.35766041597151 | -3.84139530533748 | 1.34781115656013 | Cl |
| -3.68339531543239 | -0.65644356528260 | 5.93063856379056 | H |
| 0.48167036750289 | -0.30726377656497 | 6.89794583364637 | C |
| 0.60856168818399 | -0.47511490804851 | 8.93676931299819 | H |

Table S8. Cartesian coordinates (Å) of optimized structure of **6** in GS

| | | | |
|--------------------|-------------------|-------------------|----|
| -0.66508906168035 | -7.83852292939374 | -4.69818950965520 | H |
| -0.54364960047630 | -6.00802473274886 | -3.78346197570561 | C |
| 3.62525600566777 | -5.08403943118121 | -3.54555681209946 | H |
| 1.65018243254067 | -4.61586359696276 | -3.24398111076011 | C |
| -4.52839762958139 | -4.97705637378980 | -2.79545086791893 | H |
| -2.52169382285745 | -4.56108988918380 | -2.85948801249390 | C |
| -5.93042502475385 | -0.92812947066060 | -4.20549637046093 | H |
| 1.03300737330074 | -2.43679977254653 | -2.10282660885899 | N |
| 6.52362135092471 | 1.31809332566374 | -4.61775521267733 | O |
| -1.55526527558633 | -2.36242771654002 | -1.89535359257291 | N |
| -10.89903432337470 | -0.19230607550175 | -3.79885379388259 | H |
| -6.95458092152408 | -0.51224046482013 | -2.46770813081573 | C |
| 5.27267187936116 | 0.90025223287708 | -2.88028066754623 | N |
| -9.56326828026577 | -0.08652110438709 | -2.23925537660445 | C |
| 5.96976156093211 | -3.10606701838763 | 1.15744582964866 | Cl |
| -5.64616110319588 | -0.33749183347828 | -0.29775845484242 | N |
| -2.66084946520443 | -0.29474056243865 | -0.13136430209606 | B |
| 3.35690357693363 | 0.25620338035356 | -0.25015436746412 | Ru |
| -10.19840329530116 | 0.49737210074200 | 0.22239429269190 | C |
| -1.85529140161504 | 2.39456628642778 | -1.00038314383391 | N |
| 0.64911520789889 | 3.03014916652246 | -0.98440551060048 | N |
| -7.60643245265444 | 0.50327560473032 | 2.16264588502746 | S |
| -12.05658219822674 | 0.91366550794401 | 1.00596350467818 | H |
| -3.23872767251186 | 4.52211051121739 | -1.51396909355791 | C |
| -5.28668230784049 | 4.48609422360106 | -1.59745907745932 | H |
| -1.63523847942299 | -0.81605549145595 | 2.56379502815700 | N |
| 0.83603934378517 | 5.50601713415688 | -1.48837086531662 | C |
| 0.93161601510952 | -0.52771165148863 | 2.86122845012938 | N |
| -1.58793485847688 | 6.52534100157431 | -1.85872503373629 | C |
| 2.68030230453086 | 6.40610496087295 | -1.50979468884914 | H |
| -2.06721850205620 | 8.46789805961594 | -2.30446604101833 | H |
| -2.60050484521114 | -1.78162988258023 | 4.75925978442811 | C |
| -4.58244946203271 | -2.26862171846696 | 4.95297937496931 | H |
| 1.52990893227158 | -1.23644582460120 | 5.21784147980254 | C |
| 5.49135663993748 | 3.12267582010125 | 2.42888937955834 | Cl |
| 3.48825654067377 | -1.15298040713765 | 5.82477233445839 | H |
| -0.65291733658792 | -2.03282548906406 | 6.49506948096327 | C |
| -0.79037411527116 | -2.71941963249444 | 8.42141457974887 | H |

Reference

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