Electronic Supporting Information of

A Mechanistic Investigation of the Ruthenium Porphyrin-Catalysed Aziridination of Olefins by Aryl Azides

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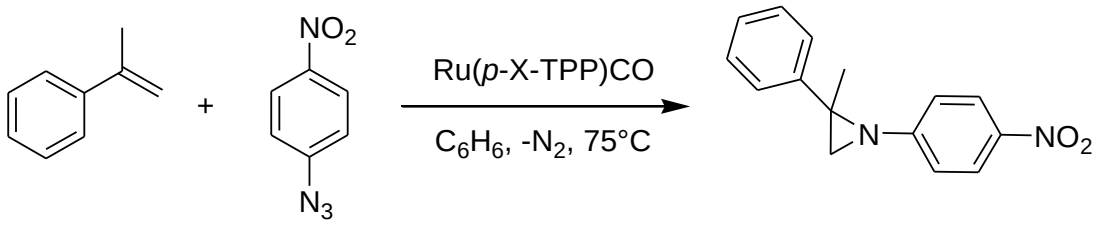
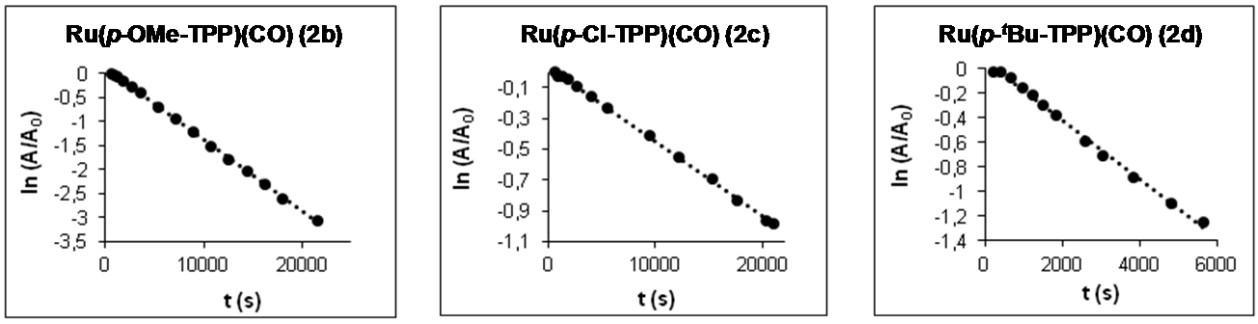
Table of Contents

1. Determination of the kinetic order with respect to 4-nitrophenyl azide concentration using Ru(*p*-X-TPP)CO catalysts 2b-g.

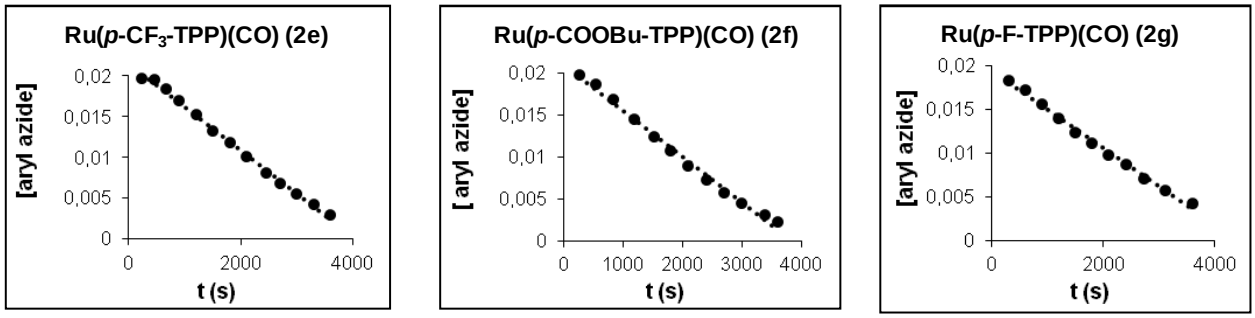


Ru(*p*-X-TPP)CO (1.2×10^{-2}mmol), 4-nitrophenyl azide (100 mg, 6.1×10^{-1} mmol) and α-methylstyrene (4.00×10^{-2} mL, 3.1 mmol) were dissolved in benzene (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. Rate constants with respect to the aryl azide concentration for each catalyst were determined from the specific variation of *A* with respect to time.



$k = 1.50\times10^{-4}$ s^{-1} $k = 4.86\times10^{-5}$ s^{-1} $k = 2.42\times10^{-4}$ s^{-1}

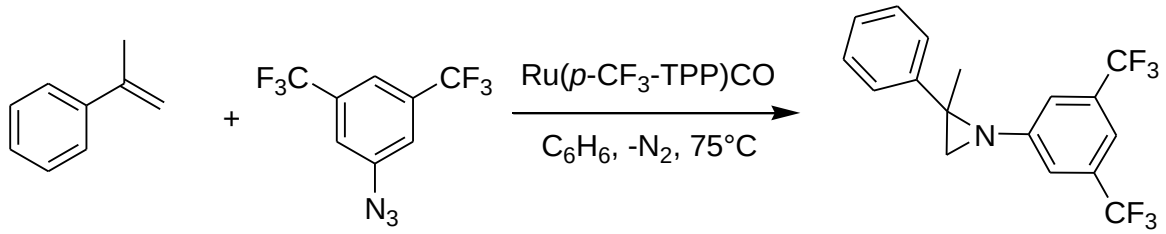
Figure S1. *First order kinetic dependence with respect to 4-nitrophenyl azide concentration using complex **2b**, complex **2c** or complex **2d** as the catalyst.*



$k = 5.30\times10^{-6}$ M s^{-1} $k = 5.46\times10^{-6}$ M s^{-1} $k = 4.42\times10^{-6}$ M s^{-1}

Figure S2. *Zero order kinetic dependence with respect to 4-nitrophenyl azide concentration using complex **2e**, complex **2f** or complex **2g** as the catalyst.*

2. Kinetics of the reaction between α-methylstyrene and 3,5-*bis*(trifluoromethyl)phenyl azide promoted by complex 2e.



2.1. Rate constants and reaction rate at different olefin concentrations.

Complex **2e** (12.5 mg, 1.2×10^{-2} mmol) and 3,5-*bis*(trifluoromethyl)phenyl azide (153 mg, 6.0×10^{-1} mmol) were dissolved in the opportune α-methylstyrene/benzene mixture (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. Rate constants with respect to the aryl azide concentration were determined from the specific variation of *A* with respect to time. The reaction rate was calculated at 90% of azide conversion.

Table S1. *Rate constants with respect to 3,5-bis(trifluoromethyl)phenyl azide and reaction rates at different α-methylstyrene concentrations.*

[olefin] (mol/L)	**[catalyst] (mol/L)**	***k***	***k*/[cat]**	**reaction rate -Δ[Ar'N_3]/Δt (M s^{-1})**
0.10	4.10×10^{-4}	1.70×10^{-5} M s^{-1}	$4{,}15\times10^{-2}$ s^{-1}	1.49×10^{-5}
0.38	4.07×10^{-4}	2.60×10^{-5} M s^{-1}	$6{,}39\times10^{-2}$ s^{-1}	2.26×10^{-5}
0.77	4.07×10^{-4}	3.29×10^{-5} M s^{-1}	$8{,}08\times10^{-2}$ s^{-1}	2.95×10^{-5}
1.50	4.17×10^{-4}	3.40×10^{-3} M s^{-1}	$8{,}16\times10^{-2}$ s^{-1}	2.90×10^{-5}
2.05	$4{,}10\times10^{-4}$	mixed order	mixed order	2.51×10^{-5}
3.08	3.94×10^{-4}	3.04×10^{-3} s^{-1}	7,73 M^{-1} s^{-1}	2.01×10^{-5}
4.36	4.07×10^{-4}	2.76×10^{-3} s^{-1}	6,78 M^{-1} s^{-1}	1.94×10^{-5}

2.2. Kinetic order with respect to the catalyst 2e concentration.

The opportune catalyst amount, 3,5-*bis*(trifluoromethyl)phenyl azide (153 mg, 6.0×10^{-2} mmol) and α-methylstyrene (0.390 mL, 3.0 mmol) were dissolved in benzene (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. Zero order rate constants with respect to the aryl azide concentration were determined from the variation of *A* with respect to time.

Table S2. *Rate constants with respect to 3,5-bis(trifluoromethyl)phenyl azide and reaction rates at different catalyst concentrations.*

molar ratio cat/azide/olefin	**[Ru(*p*-CF_3-TPP)CO] (M)**	***k*** **(M s^{-1})**
0.4:50:250	1.58×10^{-4}	9.31×10^{-6}
0.6:50:250	2.38×10^{-4}	1.08×10^{-5}
0.8:50:250	3.17×10^{-4}	1.66×10^{-5}
1:50:250	4.00×10^{-4}	$1{,}83\times10^{-5}$
1.2:50:250	4.75×10^{-4}	2.10×10^{-5}
3:50:250	1.20×10^{-3}	3.74×10^{-5}

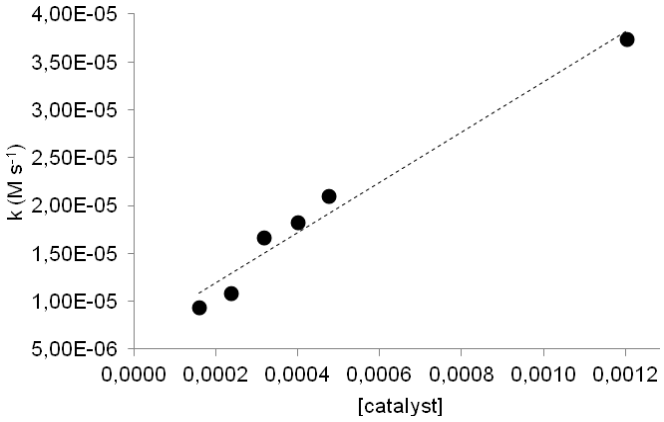
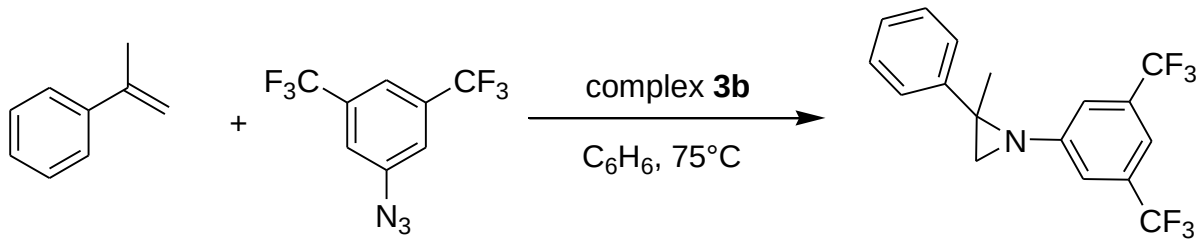


Figure S3. Dependence of the measured rate constants on **2e** concentrations.

3. Reaction between α-methylstyrene and 3,5-bis(trifluoromethyl)phenyl azide promoted by complex 3b.



3.1. Rate constants at different olefin concentrations.

Complex **3b** (16.7 mg, 1.2×10^{-2} mmol) and 3,5-*bis*(trifluoromethyl)phenyl azide (153 mg, 6.0×10^{-2} mmol) were dissolved in the opportune α-methylstyrene/benzene mixture (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. First order rate constants with respect to the aryl azide concentration were determined from the variation of *A* with respect to time.

Table S3. *Rate constants with respect to 3,5-bis(trifluoromethyl)phenyl azide and reaction rates at different α-methylstyrene concentrations.*

molar ratio cat./azide/olefin	**[α-methylstyrene] (M)**	**[catalyst] (M)**	***k*** **(s^{-1})**	***k*/[cat] (M^{-1} s^{-1})**
1:50:250	0.100	3.74×10^{-4}	1.13×10^{-4}	0,302
1:50 :641	0.256	3.98×10^{-4}	1.97×10^{-4}	0,495
1:50:1923	0.769	4.03×10^{-4}	9.93×10^{-5}	0,246
1:50:3200	1.28	4.06×10^{-4}	6.76×10^{-5}	0,167

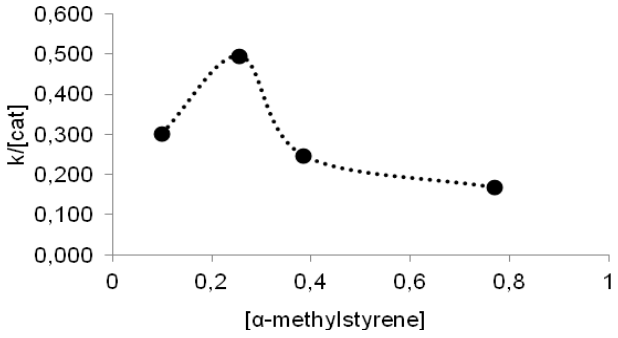


Figure S4. Dependence of the measured rate constants on α-methylstyrene concentrations.

3.2. Kinetic order with respect to the catalyst 3b concentration.

The opportune catalyst amount, 3,5-*bis*(trifluoromethyl)phenyl azide (153 mg, 6.0×10^{-2} mmol) and α-methylstyrene (0.390 mL, 3.0 mmol) were dissolved in benzene (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. First order rate constants with respect to the aryl azide concentration were determined from the variation of *A* with respect to time.

Table S4. *Rate constants with respect to 3,5-bis(trifluoromethyl)phenyl azide and reaction rates at different catalyst concentrations.*

molar ratio catalyst/azide/substrate	**[catalyst]**	***k*** **(s^{-1})**
0.5:50:250	2.00×10^{-4}	4.00×10^{-5}
0.7:50:250	2.80×10^{-4}	6.10×10^{-5}
1:50:250	4.00×10^{-4}	1.14×10^{-4}

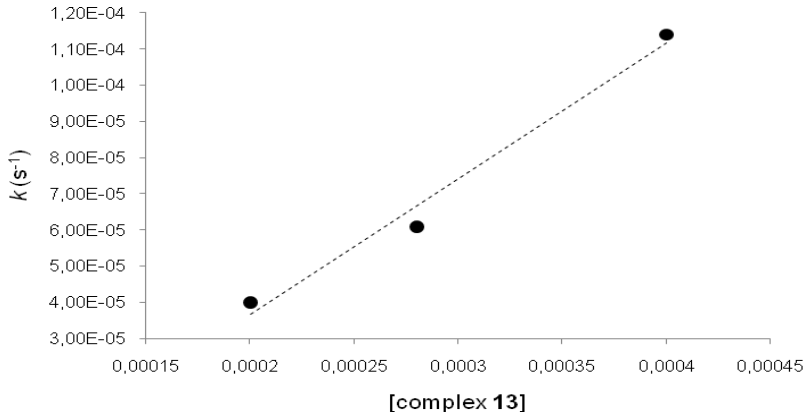


Figure S5. Dependence of the measured rate constants on **3b** concentrations.

4. Kinetics of the uncatalysed reaction between α-methylstyrene and 3,5-bis(trifluoromethyl)phenyl azide.

α-Methylstyrene (15.0 ml, 115 mmol) was dissolved in benzene (15.0 mL) then 3,5-*bis*(trifluoromethyl)phenyl azide (153 mg, 6.0×10^{-1} mmol) was added. The resulting solution was immediately placed in a preheated oil bath at 75 °C. The solution was stirred for one minute and then 0.2 mL samples were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2116 cm^{-1}. A fist-order rate constant (k_1) of 1.34×10^{-5} s^{-1} was obtained. The rate constant of the uncatalysed reaction between α-methylstyrene and 4-nitrophenyl azide (k_2 = 1.15×10^{-5} s^{-1}) was reported in a previous paper.[1] k_2/k_1 = 0.86.

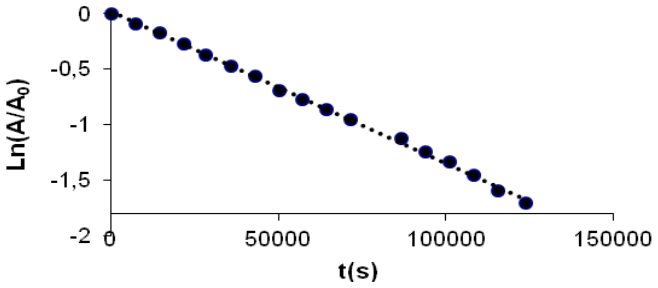
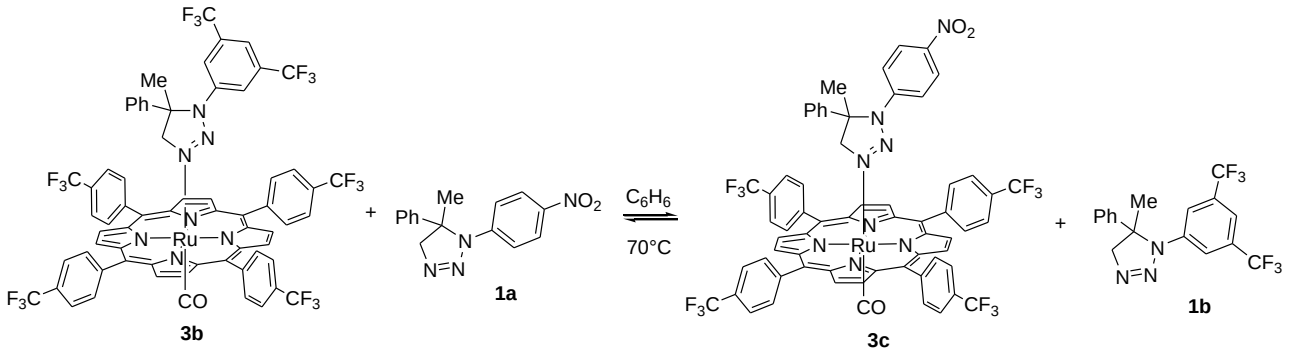


Figure S6. 3,5-*Bis*(trifluoromethyl)phenyl azide consumption in absence of the catalyst.

5. Ligand exchange reaction between complex 3b and triazoline 1a.



Complex **3b** (22.2 mg, 1.6×10^{-2} mmol) and triazoline **1a** (5.0 mg, 1.8×10^{-2} mmol) were dissolved in deuterated benzene (0.75 mL) in a NMR tube. ^{1}H NMR and ^{19}F NMR spectra of the sample were immediately recorded and the appearance of the signals related to the formation of complex **3c** demonstrated that the exchange reaction takes place even at room temperature. The NMR tube was heated at 70°C for 3 hours and ^{1}H NMR analysis showed the presence of both complexes **3c** and **3b** in a 1:2 ratio (Figure S7). The trifluoromethyl groups signals of the free triazoline **1b** and of the axial ligand of complex **3b** were detected in a 1:2 ratio by ^{19} F NMR analysis (Figure S8).

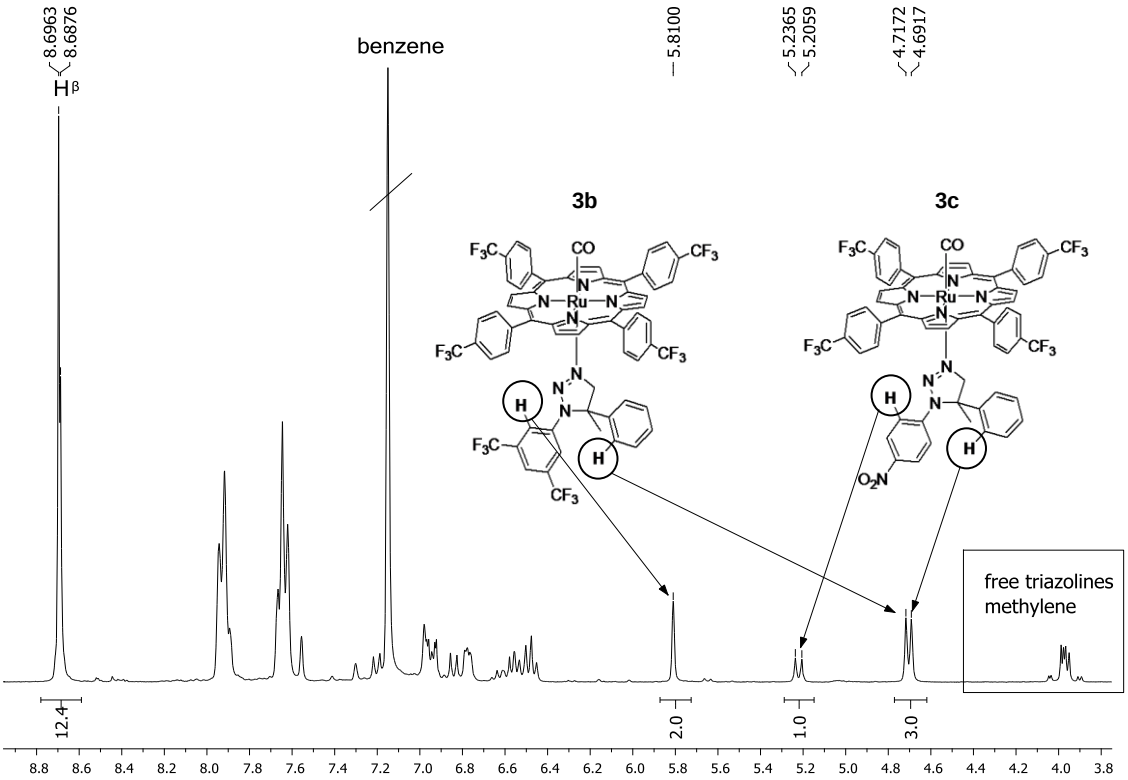


Figure S7. ^{1}H NMR spectrum at the end of the reaction.

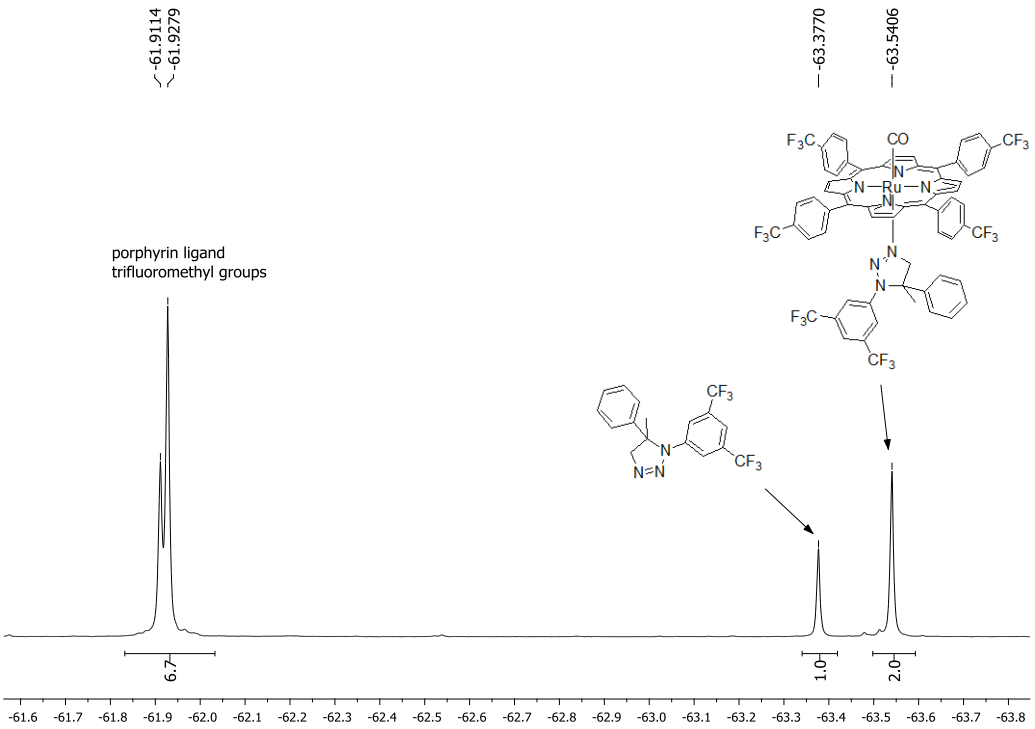


Figure S8. ^{19}F NMR spectrum at the end of the reaction.

6. Synthesis of other ruthenium triazoline porphyrin complexes.

6.1. General procedure for the synthesis of Ru(porphyrin)(1-(*p*-nitrophenyl)-5-methyl,5-phenyl-1,2,3-triazoline)CO (10, 11 and 3c)

In a typical experiment a slight molar excess of **1a** was added to a benzene suspension of the Ru(porphyrin)(CO) complex (**2b**, **2c** or **2e**). The resulting solution was stirred at 75°C (unless otherwise specified), until TLC or infrared monitoring confirmed the consumption of the starting complex. The solution was then concentrated to one fifth of the starting volume and *n*-hexane was added to precipitate the product. The solid was collected by filtration, washed with *n*-hexane and dried *in vacuo.*

6.2 Synthesis of Ru(*p*-MeO-TPP)(1-p-nitrophenyl-5-methyl-5-phenyl-1,2,3-triazoline)CO (10).

Reaction conditions: **2b**: **(**40 mg, 4.6×10^{-2} mmol), **1a** (13.5 mg 4.8×10^{-2} mmol), benzene (10 mL). Stirring time: 60 min. 44.7 mg, 84% yield. Anal. Calcd for $C_{64}H_{50}N_8O_7Ru$ (1144.22): C, 67.18; H, 4.40; N, 9.76. Found: C, 66.80; H, 4.67; N 9.21. ^{1}H NMR (C_6D_6, 300 MHz) δ 9.08 (s, 8H), 8.12 (d, 4H, *J* = 8.2 Hz), 8.02 (d, 4H, *J* = 8.2 Hz), 7.16 (overlapping with the solvent signal, 2H), 7.10 (d, 4H, *J* = 8.2 Hz), 7.05 (d, 4H, *J* = 8.2 Hz), 6.63 (t, 1H, *J* = 7.0 Hz), 6.57 (t, 2H, *J* = 7.0 Hz), 5.30 (d, 2H, *J* = 8.4 Hz), 4.75 (d, 2H, *J* = 7.0 Hz), 3.61 (s, 3H), -0.92 (s, 3H), -0.99 (d, 1H, *J* = 16.9 Hz), -1.14 (d, 1H, *J* = 16.9 Hz). IR (nujol): ν (cm^{-1}) = 1948 (CO).

6.3 Synthesis of Ru(*p*-Cl-TPP)(1-*p*-nitrophenyl-5-methyl-5-phenyl-1,2,3-triazoline)CO (11). Reaction conditions: **2c** (77 mg, 8.8×10^{-2} mmol), **1a** (25.5 mg, 9.0×10^{-2} mmol), benzene (10 mL). Stirring time: 10 h at room temperature. 80.5 mg, 79% yield. Anal. Calcd for $C_{60}H_{38}Cl_4N_8O_3Ru$ (1161.90): C, 62.02; H, 3.30; N, 9.64. Found: C, 62.30; H, 3.52; N 9.39. ^{1}H NMR (C_6D_6, 300 MHz) δ8.80 (s, 8H), 7.78 (m, 8H), 7.38 (m, 8H), 7.16 (overlapping with the solvent signal), 6.60 (t, 1H, *J* = 7.2 Hz), 6.52 (t, 2H, *J* = 7.2 Hz), 5.20 (d, 2H, *J* = 9.2 Hz), 4.67 (d, 2H, *J* = 7.2 Hz), -0.94 (s, 3H), -1.11 (d, 1H, *J* = 16.6 Hz), -1.33 (d, 1H, *J* = 16.6 Hz). IR (nujol): ν (cm^{-1}) = 1963 (CO).

6.4 Synthesis of Ru(*p*-CF_3-TPP)(1-*p*-nitrophenyl-5-methyl-5-phenyl-1,2,3-triazoline)CO (3c). The stoichiometric reaction between **2e** and **1a** was followed by ^{1}H NMR analysis: **2e** (16.9 mg, 1.7×10^{-2} mmol) and **1a** (4.9 mg, 1.7×10^{-2} mmol) were dissolved in C_6D_6 (1.0 mL) at room temperature. After 10 minutes the signals of **2e** and **1a** were no more detectable, and a new pattern attributable to **3c** was monitored. ^{1}H NMR (C_6D_6, 300 MHz) δ8.71 (s, 8H), 7.90-7.96 (m, 8H), 7.63-7.66 (m, 8H), 7.22 (d, 2H, *J* = 9.0 Hz), 6.65 (t, 1H, *J* = 7.5 Hz), 6.55 (t, 2H, *J* = 7.5 Hz), 5.24 (d, 2H, *J* = 9.0 Hz), 4.71 (d, 2H, *J* = 7.5 Hz), -0.80 (s, 3H), -1.07 (d, 1H, *J* = 17.0 Hz), -1.31 (d, 1H, *J* = 17.0 Hz).

7. ATR-IR spectrum of the crude of the Ru(*p*-CF_3-TPP)CO-catalysed reaction between 3,5-*bis*(trifluoromethyl)phenyl azide and α-methylstyrene.

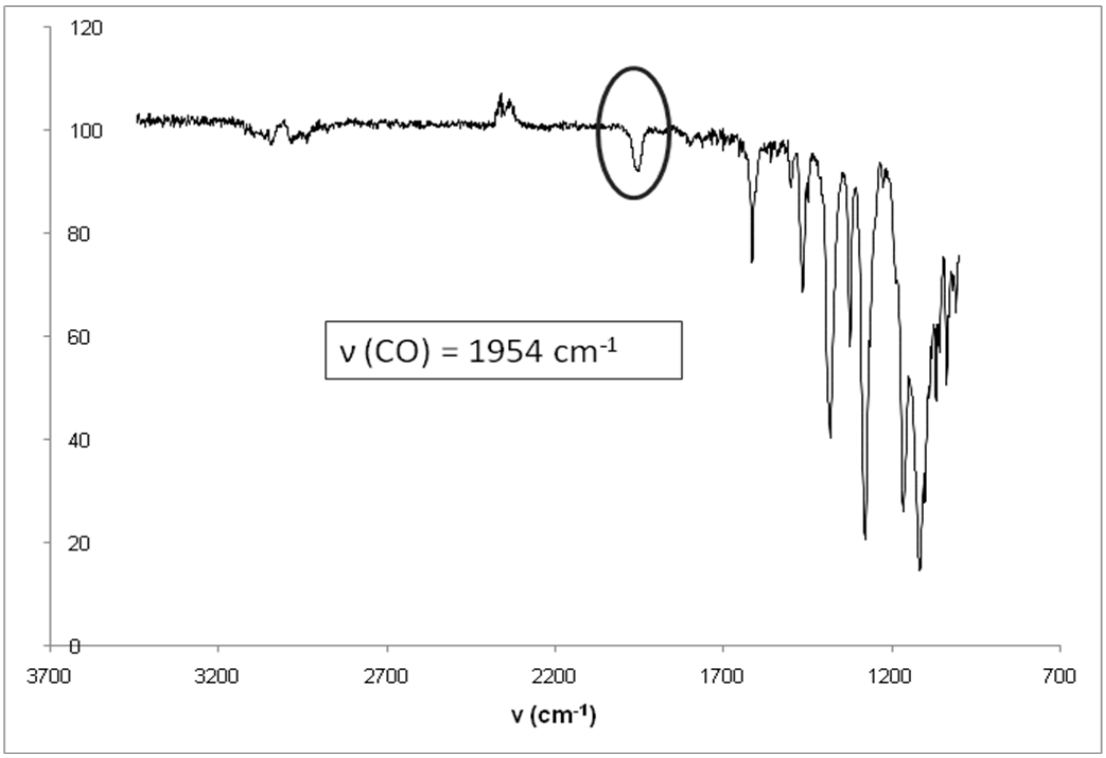


Figure S9. ATR-IR spectrum between 2100-1550 cm^{-1} of the reaction crude at the end of the reaction (a) and of the starting catalyst (Ru(*p*-CF_3-TPP)CO) (**2e**) (b).

8. Variation of the kinetics of the Ru(TPP)CO-catalysed reaction between 4-nitrophenyl azide and α-methylstyrene upon catalyst drying.

The "wet" catalyst Ru(TPP)CO (**2a**) was obtained after the chromatographic purification following a reported procedure.[2] The dried catalyst was obtained after drying "wet" Ru(TPP)CO for 2 hours at 120°C.

The catalyst, 4-nitrophenyl azide (98.5 mg, 0.60 mmol) and α-methylstyrene (400 µL, 3.1 mmol) were dissolved in benzene (30 mL). The resulting solution was immediately placed in a preheated oil bath at 75°C and stirred for one minute to completely dissolve all reagents, then 0.2 mL were withdrawn for IR analysis at regular time intervals. The consumption of the organic azide was then followed by measuring the absorbance (*A*) of the ν(N=N) signal at 2150-2100 cm^{-1}. First order rate constants with respect to the aryl azide concentration for each catalyst were determined from the variation of *A* with respect to time.

Experiment A. Catalyst: "wet" Ru(TPP)CO (7.4 mg, 1.0×10^{-2} mmol); $k_{wet}= 2.67\times10^{-4}$ s^{-1}.

Experiment B. Catalyst: dried Ru(TPP)CO (7.4 mg, 1.0×10^{-2} mmol); $k_{dried}= 6.11\times10^{-4}$ s^{-1}.

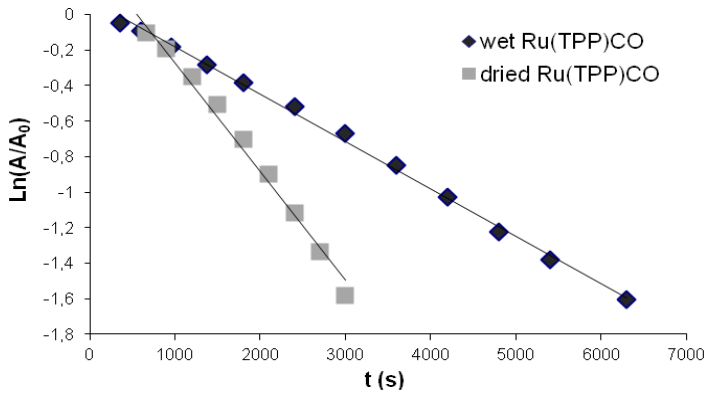


Figure S10. Aryl azide consumption using "wet" (dark grey) and dried (light grey) Ru(TPP)CO.

9. DFT data

Figure S11: Free/energy reaction pathway for the [Ru](CO)-catalysed aziridination of isobutene by CH_3N_3.

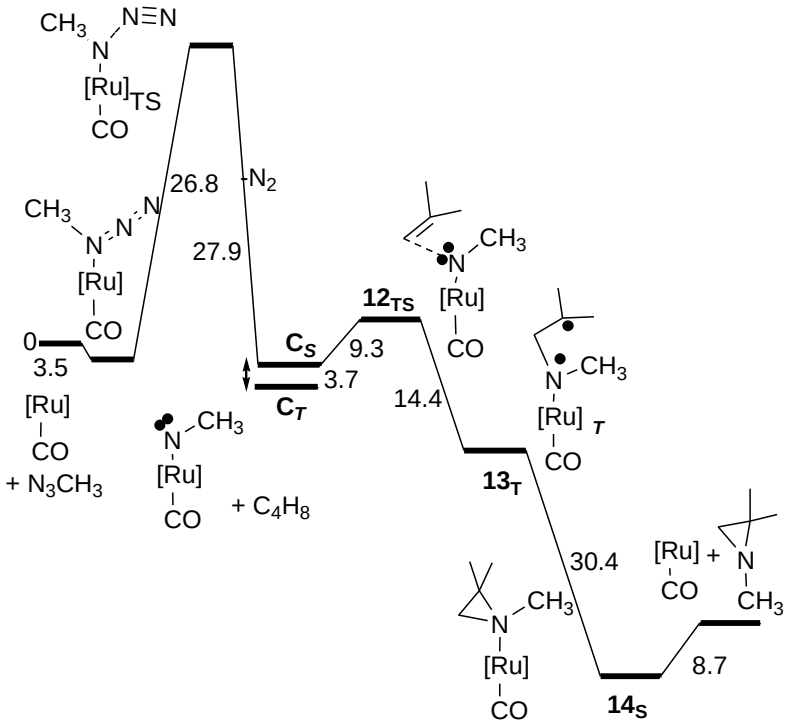


Figure S12: Optimised structure of compound [Ru](Ar'N_3)(CO)

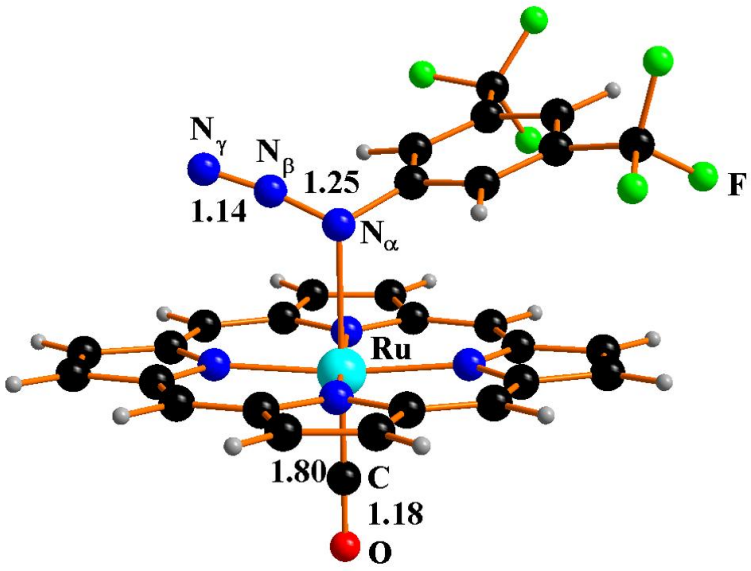


Figure S13: Optimised structure of compound [Ru](Ar'N_3)$(CO)_{TS}$

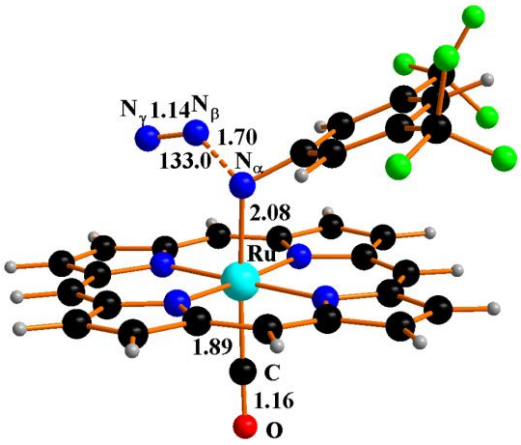


Figure S14: Optimised structure of compound [Ru](NAr')$(CO)_S$

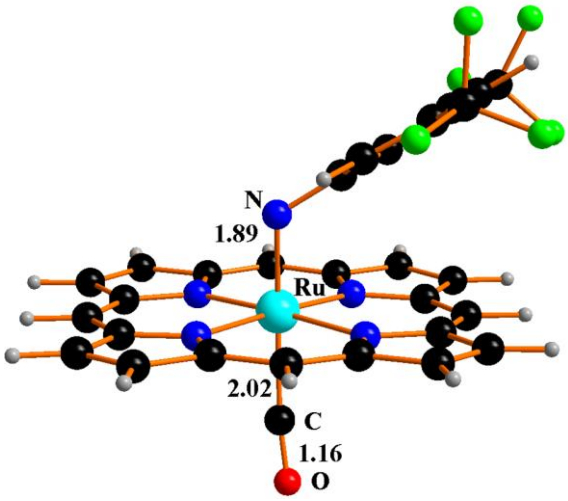


Figure S15: Optimised structure of compound [Ru](NAr')$(CO)_T$

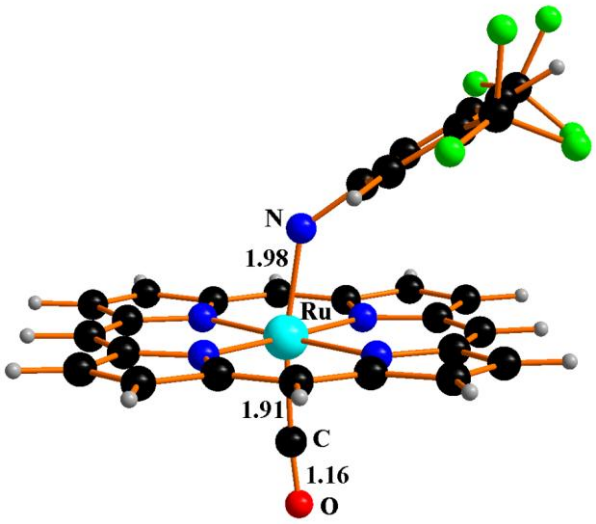
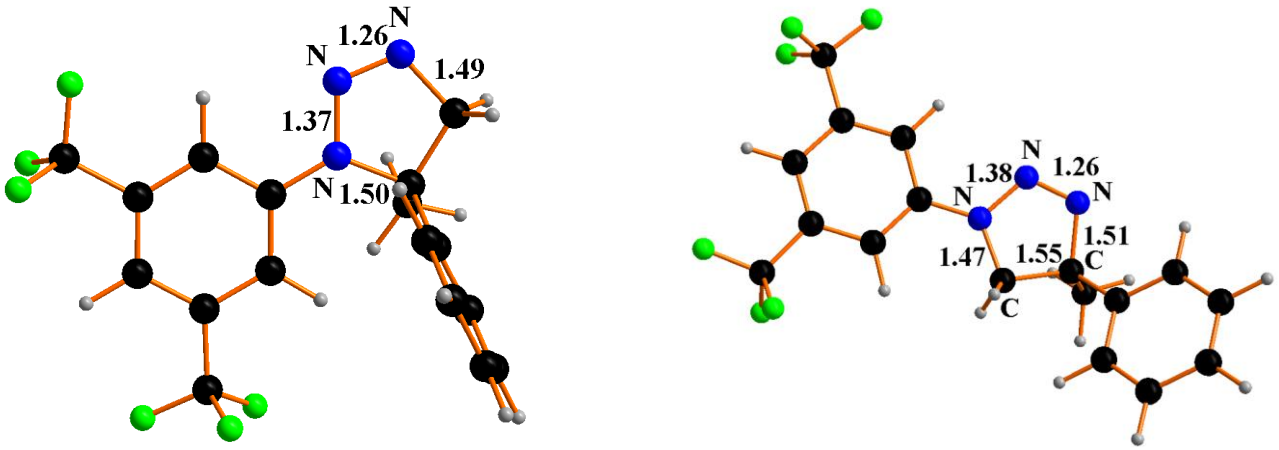
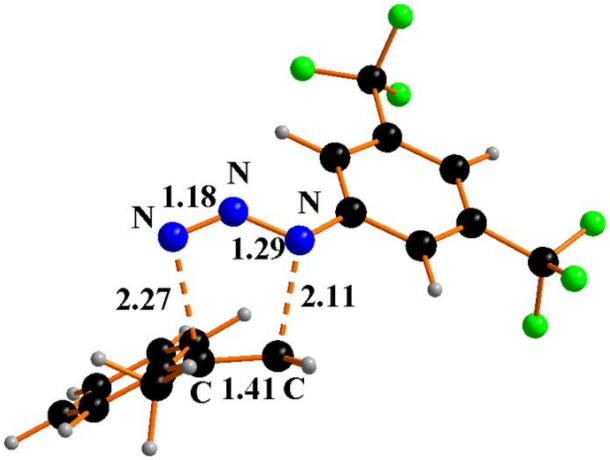


Figure S17: Optimised structure of a) **1b** and b) **1b'** from α-methylstyrene and Ar'N_3.



a **b**

Figure S18: Optimised structure of $\mathbf{8_{TS}}'$ from α-methylstyrene Ar'N_3.



COORDINATES, ENERGIES AND THERMAL PARAMETERS OF ALL THE OPTIMISED STRUCTURES at the B97D level of theory

Compound [Ru](CO)

Cartesian Coordinates

Ru -0.010515 -0.064575 -0.064257
O -0.049065 -0.048000 -3.020049
N 2.053464 -0.114348 0.101813
N 0.040740 1.996300 0.139213
C -2.389855 2.432549 0.183979
C 2.373545 -2.563719 0.096956
C -1.050815 2.844974 0.170752
H 5.145934 1.173157 0.147118
C 4.277739 0.519055 0.124885
C 0.781136 4.186829 0.188943
C 1.172177 2.791701 0.141640
C 2.902441 0.977415 0.109936
H -1.246005 5.087439 0.249812
C 4.244609 -0.854370 0.117994
C 2.490050 2.316492 0.121141
C -0.033599 -0.054904 -1.839163
C -0.592187 4.219796 0.206997
C 2.848918 -1.245752 0.098825
H 1.477220 5.021740 0.213988
H 5.079920 -1.550255 0.133489
C 1.034528 -2.976143 0.112907
N -0.057338 -2.127257 0.118156
C -2.865206 1.114579 0.183580
N -2.070120 -0.016680 0.154734
C -2.918760 -1.108543 0.172005
C -4.293227 -0.650560 0.226049
C -4.260073 0.722861 0.233186
H -5.094639 1.418441 0.276795
H -5.160709 -1.304966 0.262747
C -2.506393 -2.447594 0.158752
C -1.188484 -2.922783 0.141153
C -0.796580 -4.318273 0.163705
H -1.491946 -5.153464 0.197727
C 0.576751 -4.351312 0.146304
H 1.231290 -5.219298 0.163364
H 3.279290 3.069089 0.127066
H 3.126196 -3.352924 0.095436
H -3.295329 -3.200319 0.176290
H -3.142202 3.221625 0.209635

Energy parameters

HF=-1196.2144935
Zero-point vibrational energy 726560.5 (Joules/Mol)
Zero-point correction= 0.276732 (Hartree/Particle)
Thermal correction to Energy= 0.296265
Thermal correction to Enthalpy= 0.297209
Thermal correction to Gibbs Free Energy= 0.230227
Sum of electronic and zero-point Energies= -1195.937761
Sum of electronic and thermal Energies= -1195.918228
Sum of electronic and thermal Enthalpies= -1195.917284
Sum of electronic and thermal Free Energies= -1195.984266

Compound [Ru](CO)(Ar'N_3)

Cartesian Coordinates

Ru -0.007244 -0.178093 0.135471
O 0.241440 0.295264 -2.791296
N 2.044284 -0.342627 0.393639
N 0.104817 1.837041 0.620363
C -2.303771 2.376008 0.529127
C 2.267613 -2.778222 0.063956
C -0.955141 2.715861 0.714237
H 5.160724 0.773905 0.880036
C 4.275410 0.174562 0.683938
C 0.914271 3.941380 1.120379
C 1.258940 2.559535 0.849903
C 2.923207 0.694096 0.636762
H -1.078261 4.916636 1.182723
C 4.195319 -1.177762 0.461136
C 2.556529 2.029954 0.844925
C 0.146023 0.105389 -1.633452
C -0.454003 4.038337 1.037241
C 2.793124 -1.495903 0.278114
H 1.634097 4.722017 1.352733
H 5.001138 -1.906736 0.441462
C 0.916271 -3.125220 -0.078717
N -0.139472 -2.237753 -0.048209
C -2.825679 1.104142 0.255642
N -2.076709 -0.050124 0.127285
C -2.958112 -1.089524 -0.092807
C -4.314066 -0.574158 -0.101693
C -4.231962 0.780510 0.112553
H -5.041239 1.503215 0.182066
H -5.204413 -1.181605 -0.244749
C -2.592514 -2.434069 -0.254217
C -1.296165 -2.968240 -0.225277
C -0.960058 -4.373686 -0.363938
H -1.685799 -5.170601 -0.506890
C 0.406895 -4.470868 -0.272648
H 1.025849 -5.363192 -0.326247
H 3.366460 2.730223 1.049776
H 2.987703 -3.595631 0.013024
H -3.406388 -3.142991 -0.410001
H -3.026329 3.187124 0.624665
N -0.207640 -0.495850 2.542910
N -1.330286 -0.189893 3.002696
N -2.422668 0.001052 3.285041
C 0.945033 -0.054466 3.275966
C 2.015379 -0.956007 3.358888
C 1.043376 1.248737 3.781443
C 3.203018 -0.537373 3.970669
H 1.917287 -1.951090 2.933960
C 2.240448 1.643393 4.396652
H 0.219347 1.948788 3.663968
C 3.326319 0.760996 4.491903
H 4.254829 1.079237 4.961787
C 4.370860 -1.488092 4.131705
C 2.413891 3.065963 4.884035
F 4.193714 -2.669256 3.477657
F 4.576297 -1.792063 5.455498
F 5.540670 -0.942470 3.678559
F 3.063338 3.118916 6.086541
F 1.228818 3.722019 5.036195
F 3.166980 3.803464 4.003309

Energy parameters

HF=-2265.5900791

Zero-point vibrational energy 1016100.2 (Joules/Mol)

Zero-point correction= 0.387012 (Hartree/Particle)

Thermal correction to Energy= 0.422830

Thermal correction to Enthalpy= 0.423774

Thermal correction to Gibbs Free Energy= 0.319134

Sum of electronic and zero-point Energies= -2265.203067

Sum of electronic and thermal Energies= -2265.167249

Sum of electronic and thermal Enthalpies= -2265.166305

Sum of electronic and thermal Free Energies= -2265.270945

Compound [Ru](CO)(Ar'N_3)$_{TS}$

Cartesian Coordinates

Ru -0.084105 0.481508 0.401698
O -0.534745 -0.271042 -2.523696
N 1.859311 1.125510 0.095864
N -0.760740 2.397521 0.168735
C -3.189610 1.982228 0.481897
C 3.013196 -1.055763 0.270334
C -2.097799 2.803633 0.180135
H 4.285411 3.354361 -0.483267
C 3.705250 2.454180 -0.296413
C -0.873464 4.643030 -0.352136
C 0.001486 3.509189 -0.160526
C 2.261550 2.420200 -0.146105
H -3.082100 4.786593 -0.192125
C 4.153387 1.163399 -0.162944
C 1.397952 3.518643 -0.272587
C -0.367449 0.030316 -1.410599
C -2.162664 4.208722 -0.143912
C 2.989372 0.330742 0.073972
H -0.535579 5.644598 -0.606490
H 5.174324 0.793830 -0.211347
C 1.920741 -1.897641 0.533521
N 0.616461 -1.480871 0.638878
C -3.160157 0.613095 0.798413
N -2.028411 -0.158791 0.816973
C -2.401039 -1.447749 1.127450
C -3.839596 -1.484567 1.343491
C -4.309798 -0.211584 1.136636
H -5.333005 0.149929 1.201773
H -4.400858 -2.376259 1.611635
C -1.540578 -2.554214 1.177699
C -0.153613 -2.577453 0.944612
C 0.700778 -3.745994 1.031046
H 0.355711 -4.747154 1.275696
C 1.984469 -3.325355 0.777164
H 2.897956 -3.914214 0.769765
H 1.860412 4.479034 -0.501557
H 3.993403 -1.531348 0.233789
H -2.001678 -3.511792 1.422141
H -4.169281 2.460783 0.475539
N 0.078251 0.603717 2.469876
N 0.035237 2.204196 3.046354
N -0.564997 3.120802 2.744337
C 1.154110 -0.027560 3.119539
C 0.887245 -1.302829 3.664611
C 2.464260 0.493777 3.176104
C 1.936138 -2.066984 4.190769
H -0.127316 -1.690937 3.626862
C 3.485797 -0.257465 3.769252
H 2.667741 1.470214 2.744794
C 3.240166 -1.550476 4.260747
H 4.046281 -2.140627 4.692462
C 1.683891 -3.447696 4.754826
C 4.905643 0.262854 3.788550
F 1.848376 -3.471484 6.118622
F 2.562642 -4.371215 4.249548
F 0.427284 -3.911746 4.500961
F 5.677003 -0.357329 2.832472
F 5.523105 0.029229 4.988519
F 4.988242 1.602301 3.549442

Energy parameters

HF=-2265.5541417
Zero-point vibrational energy 1006246.2 (Joules/Mol)
Zero-point correction= 0.383259 (Hartree/Particle)
Thermal correction to Energy= 0.419010
Thermal correction to Enthalpy= 0.419954
Thermal correction to Gibbs Free Energy= 0.315732
Sum of electronic and zero-point Energies= -2265.170883
Sum of electronic and thermal Energies= -2265.135132
Sum of electronic and thermal Enthalpies= -2265.134188
Sum of electronic and thermal Free Energies= -2265.238410

Compound [Ru](CO)(NAr')$_S$

Cartesian Coordinates

Ru -0.052590 0.452877 0.474762	C -1.550655 -2.595670 1.085878
O -0.518869 -0.326829 -2.565423	C -0.164330 -2.622470 0.848926
N 1.868301 1.081517 0.040925	C 0.682144 -3.798570 0.901165
N -0.717156 2.398667 0.288980	H 0.332279 -4.801151 1.134450
C -3.139870 1.997262 0.657609	C 1.966194 -3.387653 0.625306
C 3.001610 -1.122583 0.098502	H 2.871522 -3.987713 0.582862
C -2.033831 2.817500 0.397494	H 1.927814 4.476052 -0.264708
H 4.309027 3.295979 -0.516355	H 3.975003 -1.605779 0.013671
C 3.718445 2.397340 -0.356718	H -2.015685 -3.556412 1.309337
C -0.794773 4.688347 0.034197	H -4.105454 2.499007 0.725889
C 0.058117 3.516093 0.066962	N 0.066340 0.436282 2.360776
C 2.286249 2.383932 -0.134239	C 1.110741 -0.135434 3.033235
H -2.994605 4.849209 0.278725	C 0.865466 -1.326705 3.777167
C 4.146531 1.091880 -0.320788	C 2.420588 0.419227 3.033042
C 1.449324 3.508891 -0.109854	C 1.923771 -1.977123 4.413089
C -0.403939 0.023300 -1.469259	H -0.138558 -1.743695 3.778240
C -2.084009 4.256988 0.236086	C 3.436348 -0.198592 3.769716
C 2.982536 0.266884 -0.073295	H 2.610197 1.330117 2.473419
H -0.440737 5.704114 -0.123727	C 3.215340 -1.415882 4.436517
H 5.157049 0.708985 -0.436650	H 4.025517 -1.913398 4.965448
C 1.912803 -1.957474 0.400522	C 1.708276 -3.293631 5.127342
N 0.614806 -1.530688 0.541924	C 4.837098 0.374003 3.741745
C -3.139911 0.606152 0.861308	F 1.923186 -3.179848 6.478117
N -2.027232 -0.188538 0.805075	F 2.579908 -4.255156 4.680801
C -2.407705 -1.482687 1.067579	F 0.450154 -3.794123 4.966304
C -3.842986 -1.508546 1.303642	F 5.610045 -0.243304 2.785157
C -4.296221 -0.217485 1.174164	F 5.490594 0.203465 4.931883
H -5.312047 0.155193 1.279477	F 4.859644 1.708500 3.459917
H -4.414606 -2.402827 1.539686	

Energy parameters

HF=-2156.1216913
Zero-point vibrational energy 985661.9 (Joules/Mol)
Zero-point correction= 0.375419 (Hartree/Particle)
Thermal correction to Energy= 0.409593

Thermal correction to Enthalpy= 0.410537
Thermal correction to Gibbs Free Energy= 0.306487
Sum of electronic and zero-point Energies= -2155.746273
Sum of electronic and thermal Energies= -2155.712098
Sum of electronic and thermal Enthalpies= -2155.711154
Sum of electronic and thermal Free Energies= -2155.815205

Compound [Ru](CO)(NAr')$_T$

Cartesian Coordinates

Ru -0.153354 0.415224 0.365732	C -1.670561 -2.623078 1.000132
O -0.367259 -0.100436 -2.656729	C -0.279508 -2.659843 0.801142
N 1.817177 1.037982 0.034367	C 0.564171 -3.837285 0.894948
N -0.795400 2.377382 0.252806	H 0.205156 -4.838945 1.117652
C -3.205754 2.002474 0.639361	C 1.855816 -3.424734 0.671337
C 2.920330 -1.166141 0.202582	H 2.764304 -4.021732 0.673672
C -2.094590 2.820097 0.384156	H 1.876619 4.423676 -0.308186
H 4.280282 3.245248 -0.422900	H 3.892517 -1.659192 0.179133
C 3.681862 2.349165 -0.278463	H -2.153384 -3.577213 1.213540
C -0.829257 4.669858 0.007375	H -4.169636 2.505407 0.722140
C 0.001706 3.480466 0.020538	N 0.320164 0.491140 2.283440
C 2.236850 2.334927 -0.138152	C 1.269359 -0.075047 3.046382
H -3.020608 4.872171 0.293112	C 1.029305 -1.343860 3.661558
C 4.108153 1.046028 -0.181040	C 2.553811 0.536828 3.182279
C 1.393810 3.458393 -0.152842	C 2.060209 -1.979325 4.350505
C -0.331236 0.126508 -1.516717	H 0.055424 -1.810042 3.538045
C -2.122651 4.262466 0.230450	C 3.558265 -0.123019 3.892662
C 2.927363 0.226239 0.018182	H 2.736761 1.489867 2.692692
H -0.457671 5.679633 -0.148678	C 3.331959 -1.383638 4.476181
H 5.124377 0.662866 -0.226214	H 4.128310 -1.893265 5.014545
C 1.810563 -1.993062 0.437649	C 1.851509 -3.343405 4.974084
N 0.504476 -1.568637 0.515765	C 4.951099 0.467649 3.956960
C -3.209999 0.609192 0.807468	F 2.025963 -3.306197 6.334110
N -2.098524 -0.199346 0.738174	F 2.756557 -4.256336 4.495426
C -2.507439 -1.497533 0.967974	F 0.609955 -3.855335 4.744909
C -3.941601 -1.507725 1.193791	F 5.777838 -0.112287 3.023987
C -4.375566 -0.208140 1.093078	F 5.540940 0.265530 5.174617
H -5.386362 0.176455 1.204517	F 4.970740 1.809682 3.718602
H -4.526143 -2.399955 1.404166	

Energy parameters

HF=-2156.1308337
Zero-point vibrational energy 985975.4 (Joules/Mol)
Zero-point correction= 0.375538 (Hartree/Particle)
Thermal correction to Energy= 0.409573
Thermal correction to Enthalpy= 0.410517
Thermal correction to Gibbs Free Energy= 0.307026
Sum of electronic and zero-point Energies= -2155.755295
Sum of electronic and thermal Energies= -2155.721261
Sum of electronic and thermal Enthalpies= -2155.720317
Sum of electronic and thermal Free Energies= -2155.823807

Compound [Ru](CO)(Ar'N)•••H_2C=C(Me)Ph, 5_{TS}

Cartesian Coordinates

Ru	-2.0883	0.2286	0.4580	C	0.5081	-2.4526	-1.9800
N	-2.4970	-1.8133	0.5272	C	-0.4519	-1.4818	-2.2427
N	-3.2116	0.3801	-1.2788	C	-3.5760	0.6050	1.5693
C	-2.8405	2.7803	-1.7355	O	-4.4573	0.8550	2.2925
C	-1.1527	-2.3711	2.5244	H	-1.4955	-1.7161	-2.0527
C	-3.4058	1.5268	-2.0181	H	-0.2660	-0.6447	-2.9140
H	-3.9610	-4.6762	-0.3907	C	0.0639	-3.7031	-1.2509
C	-3.3839	-3.8995	0.1049	H	0.3178	-4.6130	-1.8207
C	-4.6255	-0.0981	-3.0376	H	0.5569	-3.7927	-0.2687
C	-3.9463	-0.6267	-1.8684	H	-1.0193	-3.6707	-1.0895
C	-3.3327	-2.5094	-0.3165	C	0.9009	0.2296	-0.2603
H	-4.6040	1.9551	-3.8792	C	1.7411	-0.6829	0.4350
C	-2.5772	-4.0126	1.2116	C	1.4104	1.4964	-0.6358
C	-4.0050	-1.9564	-1.4191	C	3.0586	-0.3309	0.7269
C	-4.2896	1.2311	-3.1314	H	1.3331	-1.6437	0.7330
C	-2.0260	-2.6959	1.4737	C	2.7433	1.8138	-0.3449
H	-5.2689	-0.6796	-3.6935	H	0.7629	2.1992	-1.1572
H	-2.3563	-4.9023	1.7964	C	3.5795	0.9164	0.3339
C	-0.6191	-1.1097	2.8357	H	4.6134	1.1767	0.5483
N	-0.8814	0.0534	2.1509	C	3.9582	-1.2685	1.5025
C	-2.0090	3.1170	-0.6553	C	3.2390	3.1782	-0.7417
N	-1.6088	2.2504	0.3352	F	4.5453	3.3821	-0.4000
C	-0.7800	2.9422	1.1893	F	2.4872	4.1584	-0.1324
C	-0.6633	4.3142	0.7301	F	3.1099	3.3695	-2.0946
C	-1.4123	4.4200	-0.4162	F	5.1678	-1.4462	0.8867
H	-1.5556	5.2914	-1.0505	F	4.2475	-0.7702	2.7501
H	-0.0640	5.0782	1.2178	F	3.4242	-2.5099	1.6904
C	-0.1179	2.3942	2.2990	C	1.9311	-2.2409	-2.2457
C	-0.1505	1.0607	2.7363	C	2.8900	-3.2179	-1.8561
C	0.6001	0.5153	3.8533	C	2.4233	-1.0431	-2.8408
H	1.2653	1.0919	4.4913	C	4.2619	-3.0020	-2.0328
C	0.3136	-0.8267	3.9121	H	2.5559	-4.1475	-1.3974
H	0.6980	-1.5687	4.6076	C	3.7929	-0.8280	-3.0125
H	-4.6291	-2.6372	-1.9989	H	1.7310	-0.2635	-3.1527
H	-0.8572	-3.1934	3.1772	C	4.7246	-1.8036	-2.6055
H	0.5200	3.0738	2.8648	H	4.9726	-3.7646	-1.7110
H	-3.0755	3.5842	-2.4342	H	4.1372	0.1061	-3.4587
N	-0.3801	-0.1335	-0.5597	H	5.7943	-1.6285	-2.7280

Energy parameters

HF=-2504.87146062

Zero-point vibrational energy 151253.2 (Joules/Mol)

Zero-point correction= 0.521257 (Hartree/Particle)

Thermal correction to Energy= 0.5423995

Thermal correction to Enthalpy= 0.5620939

Thermal correction to Gibbs Free Energy= 0.4512661

Sum of electronic and zero-point Energies= -2504.331416

Sum of electronic and thermal Energies= -2504.283688

Sum of electronic and thermal Enthalpies= -2504.274234

Sum of electronic and thermal Free Energies= -2504.431532

Compound [Ru](CO)(Ar'$NCH_2C(Me)Ph)_T$, 6_T

Cartesian Coordinates

Ru -2.002730 0.298416 0.484631	C 0.284220 -2.250386 -2.023898
N -2.805105 -1.606817 0.248321	C -0.533988 -0.975598 -1.993345
N -3.020248 0.922908 -1.215434	C -3.454258 0.793891 1.600292
C -2.150886 3.232716 -1.318322	O -4.346102 1.097487 2.287719
C -1.658291 -2.708504 2.137102	H -1.595847 -1.199119 -2.128138
C -2.936718 2.169852 -1.793269	H -0.229632 -0.276441 -2.792982
H -4.791329 -3.944030 -1.082059	C -0.389723 -3.472247 -1.458116
C -4.084095 -3.382622 -0.476414	H -0.094411 -4.389424 -1.990650
C -4.401169 0.980190 -3.061600	H -0.133319 -3.618775 -0.391309
C -3.906073 0.174099 -1.960490	H -1.481596 -3.376299 -1.505368
C -3.738716 -1.989447 -0.690213	C 0.902832 0.102382 -0.333621
H -3.919490 3.076132 -3.609155	C 1.659466 -0.778257 0.456473
C -3.349509 -3.817586 0.600978	C 1.438876 1.334695 -0.739094
C -4.247601 -1.163685 -1.705754	C 2.964640 -0.426182 0.820270
C -3.798567 2.211330 -2.961163	H 1.220890 -1.719632 0.772665
C -2.552552 -2.693276 1.054591	C 2.745438 1.672598 -0.361874
H -5.111267 0.635360 -3.809335	H 0.831463 2.012390 -1.333059
H -3.335361 -4.806636 1.052450	C 3.518762 0.798470 0.416903
C -0.898234 -1.636761 2.631127	H 4.535358 1.064215 0.700785
N -0.908501 -0.356302 2.126603	C 3.803473 -1.346547 1.677080
C -1.330426 3.243997 -0.179278	C 3.350933 2.996608 -0.767773
N -1.142514 2.180235 0.673238	F 2.582108 3.688867 -1.656269
C -0.248350 2.575014 1.644731	F 4.583417 2.833525 -1.349418
C 0.139537 3.951874 1.402882	F 3.546237 3.818331 0.315473
C -0.526115 4.364793 0.274854	F 5.040103 -1.566254 1.127008
H -0.477141 5.331037 -0.221238	F 4.028614 -0.809245 2.922109
H 0.845135 4.510306 2.012483	F 3.231919 -2.568537 1.872347
C 0.251401 1.754360 2.666086	C 1.675355 -2.250537 -2.375726
C -0.039129 0.398846 2.881976	C 2.495346 -3.402684 -2.129222
C 0.553301 -0.440203 3.906526	C 2.334867 -1.105562 -2.934900
H 1.287525 -0.102274 4.633284	C 3.867008 -3.394417 -2.395384
C 0.024214 -1.698211 3.751121	H 2.049027 -4.295427 -1.693770
H 0.236106 -2.594739 4.328622	C 3.705135 -1.106436 -3.199322
H -4.971862 -1.617303 -2.383040	H 1.768025 -0.202174 -3.149913
H -1.550106 -3.658946 2.660910	C 4.489132 -2.247546 -2.929189
H 0.968628 2.211565 3.348158	H 4.460353 -4.283827 -2.175760
H -2.190124 4.157791 -1.894603	H 4.170093 -0.210341 -3.614148
N -0.413995 -0.248122 -0.707622	H 5.561588 -2.241233 -3.127482

Energy parameters

HF=-2504.897573

Zero-point vibrational energy 1410567.2 (Joules/Mol)

Zero-point correction= 0.537257 (Hartree/Particle)

Thermal correction to Energy= 0.579995

Thermal correction to Enthalpy= 0.580939

Thermal correction to Gibbs Free Energy= 0.459661
Sum of electronic and zero-point Energies= -2504.360316
Sum of electronic and thermal Energies= -2504.317578
Sum of electronic and thermal Enthalpies= -2504.316634
Sum of electronic and thermal Free Energies= -2504.437912

Compound [Ru](4b)(CO), 7

Cartesian Coordinates

Ru 1.866067 0.325834 -0.608376
N 2.513066 -1.636795 -0.767234
N 3.278850 0.655445 0.874548
C 2.644546 2.967277 1.467867
C 0.863952 -2.427319 -2.426714
C 3.457107 1.828426 1.580606
H 4.590162 -4.213985 -0.281277
C 3.789455 -3.552321 -0.602984
C 5.161633 0.456321 2.195654
C 4.316090 -0.191851 1.210574
C 3.644363 -2.169508 -0.186745
H 4.984940 2.471577 3.108530
C 2.740383 -3.830419 -1.445982
C 4.491014 -1.489372 0.702325
C 4.625211 1.699770 2.432276
C 1.959897 -2.611549 -1.568448
H 6.044519 0.006423 2.643461
H 2.515938 -4.762098 -1.959877
C 0.162212 -1.235483 -2.662908
N 0.390152 -0.042258 -2.013114
C 1.573709 3.163924 0.580929
N 1.118827 2.236432 -0.331544
C 0.123375 2.836746 -1.072987
C -0.080286 4.190018 -0.592312
C 0.808720 4.389558 0.436389
H 0.950531 5.281880 1.041448
H -0.821089 4.879747 -0.987686
C -0.603712 2.214081 -2.098465
C -0.493429 0.884400 -2.525945
C -1.319152 0.248444 -3.535002
H -2.112461 0.746028 -4.086981
C -0.918246 -1.061816 -3.615781
H -1.317308 -1.851138 -4.247406
H 5.355131 -2.043085 1.071062
H 0.551405 -3.295911 -3.007606
H -1.366688 2.819986 -2.586710
H 2.899768 3.809440 2.112297
N 0.213842 -0.225849 1.089647
C 0.277225 -1.255745 2.235622
C 0.493384 0.202185 2.479446
C 3.023210 0.867482 -1.888585
O 3.773438 1.225605 -2.720759
H 1.512947 0.547085 2.642255
H -0.280809 0.792724 2.970844
C 1.490197 -2.165589 2.222240
H 1.552240 -2.680813 3.192360
H 1.428136 -2.918410 1.426742
H 2.397101 -1.580034 2.072806
C -1.100885 0.057831 0.593077
C -1.751226 -0.930376 -0.162951
C -1.720087 1.291869 0.819410
C -3.030703 -0.686614 -0.667296
H -1.249230 -1.873125 -0.351178
C -3.003457 1.526819 0.298975
H -1.201807 2.066898 1.377667
C -3.672000 0.543576 -0.441470
H -4.669983 0.727109 -0.833886
C -3.786512 -1.773684 -1.395331
C -3.657367 2.876963 0.477368
F -3.141549 3.582936 1.526325
F -5.006579 2.775529 0.688539
F -3.503643 3.665912 -0.639568
F -4.774649 -2.306212 -0.598957
F -4.415569 -1.306460 -2.518826
F -2.994777 -2.815151 -1.780853
C -1.022586 -1.917449 2.623526
C -1.957366 -1.306232 3.482080
C -1.338045 -3.179029 2.072895
C -3.181146 -1.931954 3.774142
H -1.737002 -0.338994 3.931799
C -2.560698 -3.804410 2.357853
H -0.631055 -3.666468 1.401766
C -3.490418 -3.180207 3.208153
H -3.891173 -1.441189 4.441387
H -2.790205 -4.772247 1.909786
H -4.444640 -3.661430 3.426786

Energy parameters

HF=-2504.9423569

Zero-point vibrational energy 1421023.4 (Joules/Mol)
Zero-point correction= 0.541239 (Hartree/Particle)
Thermal correction to Energy= 0.582907
Thermal correction to Enthalpy= 0.583851
Thermal correction to Gibbs Free Energy= 0.467071
Sum of electronic and zero-point Energies= -2504.401118
Sum of electronic and thermal Energies= -2504.359450
Sum of electronic and thermal Enthalpies= -2504.358506
Sum of electronic and thermal Free Energies= -2504.475286

Compound of the 1,3-cycloaddition between Ar'N_3 and α-methtylstirene, 8_{TS}

Cartesian Coordinates

N -2.875680 -0.246517 1.147513	C -1.439333 -0.381335 4.405147
C -1.957525 -1.640342 2.289956	C -1.582759 -0.255134 5.810670
C -2.246611 -1.355453 3.644077	C -0.564651 0.527320 3.750293
H -2.436836 -2.514457 1.845307	C -0.879897 0.723992 6.527454
N -3.572847 0.394981 1.874280	H -2.249810 -0.924051 6.351560
N -3.963130 0.257810 3.097625	C 0.142399 1.499469 4.467720
H -0.980068 -1.388870 1.880076	H -0.454292 0.492131 2.667146
C -3.211216 -2.261037 4.386310	C -0.013005 1.606573 5.861830
H -2.643217 -3.006683 4.969372	H -1.019149 0.801806 7.606552
H -3.848914 -1.707947 5.088357	H 0.799143 2.189006 3.935458
H -3.855533 -2.796080 3.676965	H 0.524855 2.375289 6.417747
C -3.947299 1.355415 3.954035	C -2.255151 4.744140 4.500014
C -3.175473 2.520337 3.722089	C -5.118034 1.935362 7.533101
C -4.606391 1.192832 5.190743	F -5.337351 3.088506 8.229036
C -3.070994 3.488604 4.723474	F -4.316834 1.145105 8.325296
H -2.656270 2.642863 2.774604	F -6.319301 1.289413 7.435593
C -4.481368 2.176134 6.182306	F -1.533045 4.715652 3.343512
H -5.198861 0.296919 5.365606	F -1.365861 4.959646 5.520667
C -3.712824 3.328557 5.965398	F -3.054305 5.858582 4.444061
H -3.613863 4.084862 6.740351	

Energy parameters

HF=-1418.0567833
Zero-point vibrational energy 702878.8 (Joules/Mol)
Zero-point correction= 0.267712 (Hartree/Particle)
Thermal correction to Energy= 0.290832
Thermal correction to Enthalpy= 0.291776
Thermal correction to Gibbs Free Energy= 0.213024
Sum of electronic and zero-point Energies= -1417.789071
Sum of electronic and thermal Energies= -1417.765952
Sum of electronic and thermal Enthalpies= -1417.765007
Sum of electronic and thermal Free Energies= -1417.843759

Triazoline from the 1,3-cycloaddition between Ar'N_3 and α-methtylstirene, 1b

Cartesian Coordinates

N 0.063668 -0.035560 2.362697	C -2.416328 -1.173431 4.704526
C -0.890498 -1.140456 2.648820	C -3.615604 -1.879334 4.916722
C -2.105742 -0.480678 3.376048	C -1.466620 -1.113650 5.746314
H -1.179647 -1.627600 1.707501	C -3.862485 -2.510887 6.149435
N -0.312931 1.024711 2.924315	H -4.367339 -1.935736 4.130633
N -1.495756 0.874701 3.604396	C -1.712011 -1.740629 6.976123
H -0.371684 -1.879544 3.277688	H -0.539728 -0.558125 5.594998
C -3.301661 -0.341108 2.412193	C -2.914597 -2.442161 7.182949
H -3.647798 -1.337763 2.104646	H -4.798637 -3.050745 6.298851
H -4.140970 0.197601 2.869882	H -0.970242 -1.676287 7.773430
H -2.974964 0.204242 1.516322	H -3.110018 -2.926150 8.140718
C -2.074814 1.968244 4.258741	C -5.151941 2.697341 6.372269
C -3.296619 1.821977 4.947069	C -1.366497 5.674627 4.905581
C -1.434800 3.233571 4.251109	F -2.130922 6.587175 4.221806
C -3.865751 2.922780 5.606243	F -0.134242 5.676293 4.324657
H -3.801966 0.863068 4.983370	F -1.212749 6.175328 6.172758
C -2.022365 4.309046 4.922393	F -5.789202 3.858294 6.696214
H -0.493962 3.359125 3.724757	F -4.922927 2.027465 7.549074
C -3.243574 4.176080 5.609792	F -6.043620 1.934143 5.664070
H -3.688056 5.022533 6.126890	

Energy parameters

HF=-1418.1001112
Zero-point vibrational energy 713258.6 (Joules/Mol)
Zero-point correction= 0.271666 (Hartree/Particle)
Thermal correction to Energy= 0.294217
Thermal correction to Enthalpy= 0.295161
Thermal correction to Gibbs Free Energy= 0.216688
Sum of electronic and zero-point Energies= -1417.828445
Sum of electronic and thermal Energies= -1417.805894
Sum of electronic and thermal Enthalpies= -1417.804950
Sum of electronic and thermal Free Energies= -1417.883424

Compound [Ru](1b)(CO), 9

Cartesian Coordinates

Ru 2.752922 -0.487329 0.168936	C 1.365051 -3.123169 -0.682347
N 1.622663 -2.223813 0.327020	H 4.159214 -0.256296 -4.943172
N 3.028161 -0.861405 -1.852744	C 0.190129 -3.851406 1.119759
C 4.261624 1.196027 -2.438739	C 1.841767 -3.020698 -1.997693
C 0.865075 -1.954417 2.662513	C 3.701386 -0.682570 -4.053660
C 3.696186 -0.051835 -2.744639	C 0.914099 -2.631953 1.434461
H 0.102380 -4.990439 -0.781470	H 2.819377 -2.615786 -4.694055
C 0.472173 -4.157264 -0.188866	H -0.456456 -4.383983 1.812832
C 3.026577 -1.872339 -3.927984	C 1.496954 -0.745959 2.994139
C 2.603044 -1.975537 -2.542259	N 2.278764 0.000516 2.139479

C 4.259262 1.849022 -1.196566
N 3.689032 1.356739 -0.042573
C 3.909127 2.281848 0.956109
C 4.641101 3.410694 0.409745
C 4.854885 3.144411 -0.921300
H 5.366584 3.758555 -1.658576
H 4.940819 4.287111 0.979566
C 3.459379 2.164419 2.280731
C 2.690235 1.122627 2.825687
C 2.154714 1.081382 4.174381
H 2.323184 1.844812 4.930308
C 1.413068 -0.071448 4.276864
H 0.854834 -0.440836 5.133954
H 1.559777 -3.823121 -2.680460
H 0.260080 -2.414966 3.444680
H 3.707049 2.987250 2.952412
H 4.755973 1.717909 -3.259076
N 0.848681 0.513290 -0.252806
C 0.571064 1.923622 0.101069
C -0.959158 1.952773 0.370902
N -0.216191 -0.125742 -0.484641
N -1.311800 0.631700 -0.285807
O 5.304208 -1.867239 0.970867
C 4.310433 -1.327972 0.651801
H 1.163791 2.207828 0.976156
H 0.870312 2.549501 -0.752081
C -2.561360 -0.017772 -0.229139
C -2.641183 -1.428122 -0.282961
C -3.740682 0.742729 -0.115612
C -3.896120 -2.047283 -0.238027
H -1.735396 -2.026126 -0.349311
C -4.982051 0.092919 -0.053180
H -3.698879 1.827054 -0.082444
C -5.082119 -1.303591 -0.115725
H -6.048827 -1.796645 -0.071586
C -1.640815 3.121688 -0.336808
C -2.256160 4.166808 0.376480
C -1.644337 3.161573 -1.747484
C -2.866665 5.233379 -0.308684
H -2.272411 4.154456 1.465399
C -2.256083 4.221254 -2.431332
H -1.180749 2.348534 -2.308464
C -2.870763 5.263633 -1.712315
H -3.341523 6.034967 0.258657
H -2.257836 4.231436 -3.522135
H -3.350227 6.087449 -2.242478
C -3.939056 -3.562442 -0.249169
C -6.214168 0.958492 0.106620
F -3.538306 -4.080176 0.958040
F -3.105704 -4.093217 -1.194490
F -5.187628 -4.055415 -0.493726
F -6.268127 1.946384 -0.841459
F -6.220375 1.595313 1.323795
F -7.377881 0.255497 0.020205
C -1.235488 1.827616 1.880840
H -0.849408 2.714834 2.400387
H -2.308509 1.728888 2.090184
H -0.705093 0.946719 2.268164

Energy parameters

HF=-2614.3578265
Zero-point vibrational energy 1445630.0 (Joules/Mol)
Zero-point correction= 0.550611 (Hartree/Particle)
Thermal correction to Energy= 0.594241
Thermal correction to Enthalpy= 0.595185
Thermal correction to Gibbs Free Energy= 0.471096
Sum of electronic and zero-point Energies= -2613.807215
Sum of electronic and thermal Energies= -2613.763586
Sum of electronic and thermal Enthalpies= -2613.762642
Sum of electronic and thermal Free Energies= -2613.886730

Inverted compound from the 1,3-cycloaddition between Ar'N_3 and α-methtylstirene, 8'$_{TS}$

Cartesian Coordinates

N -3.155416 0.171907 0.849432
C -2.419879 -1.720613 1.857624
C -2.979940 -1.488930 3.130104
N -3.519314 0.790242 1.792358
N -3.723919 0.480690 3.029634
C -3.498663 1.426874 4.040138

C -2.985678 2.724871 3.807996
C -3.769590 1.008060 5.359547
C -2.756901 3.578518 4.893876
H -2.774628 3.050172 2.791538
C -3.520555 1.879044 6.429712
H -4.170917 0.012365 5.537163
C -3.015983 3.170181 6.214445
H -2.828775 3.840779 7.049093
C -2.270201 4.993832 4.654833
C -3.748798 1.374678 7.839886
F -2.704627 0.585675 8.257089
F -4.876858 0.606775 7.937732
F -3.869044 2.382566 8.750184
F -3.308069 5.890688 4.708420
F -1.674748 5.152119 3.437619
F -1.364412 5.390895 5.599418
C -3.136029 -2.674302 0.911944
H -4.215686 -2.674391 1.114287
H -2.975564 -2.397626 -0.139002
H -2.760121 -3.701801 1.052498
C -0.974770 -1.437007 1.640494
C -0.307990 -0.437187 2.393587
C -0.228113 -2.141989 0.667301
C 1.052447 -0.168720 2.195877
H -0.863294 0.146934 3.128286
C 1.137115 -1.874611 0.469903
H -0.711139 -2.911155 0.065713
C 1.785367 -0.889092 1.232946
H 1.539827 0.608942 2.786284
H 1.691923 -2.438005 -0.282157
H 2.844446 -0.678891 1.077047
H -3.944926 -1.936829 3.366696
H -2.338678 -1.248157 3.977957

Energy parameters

HF=-1418.0470151
Zero-point vibrational energy 702473.7 (Joules/Mol)
Zero-point correction= 0.267558 (Hartree/Particle)
Thermal correction to Energy= 0.290835
Thermal correction to Enthalpy= 0.291779
Thermal correction to Gibbs Free Energy= 0.211095
Sum of electronic and zero-point Energies= -1417.779457
Sum of electronic and thermal Energies= -1417.756180
Sum of electronic and thermal Enthalpies= -1417.755236
Sum of electronic and thermal Free Energies= -1417.835920

Inverted triazoline from the 1,3-cycloaddition between Ar'N_3 and α-methtylstirene, 1b'

Cartesian Coordinates

N -1.922415 0.323319 1.066750
C -1.702386 -0.968671 1.823985
C -1.945295 -0.556229 3.302320
N -2.430612 1.196623 1.812090
N -2.578877 0.755984 3.107214
C -3.031570 1.603628 4.117401
C -3.556997 2.885111 3.813339
C -2.980135 1.174244 5.459170
C -4.012541 3.701562 4.850024
H -3.599272 3.219199 2.781080
C -3.449345 2.018965 6.480128
H -2.577839 0.196220 5.712335
C -3.969880 3.285424 6.196042
H -4.332037 3.933466 6.989843
C -4.578129 5.076760 4.558201
C -3.401067 1.496896 7.900595
F -3.740278 2.433408 8.829183
F -2.151718 1.037220 8.230386
F -4.256246 0.435857 8.071228
F -4.587519 5.388778 3.232523
F -3.862208 6.057528 5.195991
F -5.869611 5.190681 5.006052
C -2.798237 -1.944757 1.326314
H -3.796932 -1.531120 1.533088
H -2.689904 -2.107235 0.245612
H -2.689017 -2.908184 1.845634
C -0.318583 -1.547211 1.549275
C 0.285170 -2.400290 2.495498
C 0.338959 -1.311575 0.324968
C 1.530657 -2.995383 2.232473

H -0.217345 -2.608145 3.442048
C 1.585987 -1.904386 0.062796
H -0.122362 -0.657699 -0.414057
C 2.186926 -2.747124 1.014284
H 1.984436 -3.650784 2.977536
H 2.087647 -1.704848 -0.885482
H 3.155356 -3.205709 0.809117
H -2.625012 -1.239142 3.828791
H -1.013866 -0.444883 3.879726

Energy parameters

HF=-1418.0973128
Zero-point vibrational energy 712271.7 (Joules/Mol)
Zero-point correction= 0.271290 (Hartree/Particle)
Thermal correction to Energy= 0.294063
Thermal correction to Enthalpy= 0.295008
Thermal correction to Gibbs Free Energy= 0.215232
Sum of electronic and zero-point Energies= -1417.826023
Sum of electronic and thermal Energies= -1417.803249
Sum of electronic and thermal Enthalpies= -1417.802305
Sum of electronic and thermal Free Energies= -1417.882081

Compound [Ru](NCH$_3$)(CO) in the triplet state, C$_T$

Cartesian Coordinates

Ru -0.005362 -0.197768 0.245429
N 2.074996 -0.364190 0.369436
N 0.141684 1.860294 0.587468
C -2.263843 2.399737 0.527724
C 2.254721 -2.798915 0.020898
C -0.908589 2.743064 0.666641
H 5.204044 0.733605 0.772245
C 4.308451 0.137526 0.614052
C 0.980866 3.965959 0.987816
C 1.307092 2.566187 0.776685
C 2.956348 0.668648 0.591134
H -0.999352 4.967730 1.029479
C 4.212584 -1.217524 0.403354
C 2.599563 2.015365 0.774778
C -0.387833 4.075366 0.919550
C 2.801231 -1.525002 0.249934
H 1.712343 4.750838 1.164654
H 5.013727 -1.951104 0.355160
C 0.898712 -3.132408 -0.120921
N -0.154491 -2.245338 -0.055142
C -2.801360 1.123837 0.295943
N -2.073157 -0.039401 0.163755
C -2.962237 -1.069282 -0.045733
C -4.314227 -0.538662 -0.043269
C -4.214817 0.815301 0.167767
H -5.014927 1.548461 0.235606
H -5.212272 -1.135644 -0.182823
C -2.610771 -2.415962 -0.227817
C -1.317293 -2.960788 -0.232406
C -0.989353 -4.363442 -0.417032
H -1.720463 -5.152800 -0.574179
C 0.378780 -4.469436 -0.347827
H 0.991766 -5.363115 -0.436910
H 3.421132 2.713370 0.939756
H 2.964691 -3.623549 -0.052349
H -3.432785 -3.115745 -0.382209
H -2.980555 3.217409 0.612380
N 0.035956 -0.350149 2.207423
C 0.757157 0.215176 3.284008
H 0.434832 -0.217127 4.250376
H 1.843917 0.032830 3.156006
H 0.601293 1.312992 3.315111
C 0.195754 0.167880 -1.622078
O 0.392348 0.456474 -2.733772

Energy parameters

HF=-1290.7457827
Zero-point vibrational energy 827951.3 (Joules/Mol)
Zero-point correction= 0.315350 (Hartree/Particle)

Thermal correction to Energy= 0.338719
Thermal correction to Enthalpy= 0.339663
Thermal correction to Gibbs Free Energy= 0.263095
Sum of electronic and zero-point Energies= -1290.430433
Sum of electronic and thermal Energies= -1290.407064
Sum of electronic and thermal Enthalpies= -1290.406120
Sum of electronic and thermal Free Energies= -1290.482688

Compound 12, imaginary frequency at -267.1 cm^{-1}

Cartesian Coordinates

Ru -0.156125 -0.057842 0.072790	C -2.001454 -2.396521 -0.789050
N 1.772140 -0.729439 0.465528	C -1.997917 -3.831565 -1.018449
N 0.410893 1.859312 0.636196	H -2.862704 -4.409130 -1.336466
C -1.784061 2.965400 0.389723	C -0.724868 -4.277171 -0.754989
C 1.423724 -3.123506 -0.032135	H -0.339138 -5.292081 -0.816324
C -0.413496 2.960958 0.695243	H 3.749457 1.911834 1.319700
H 5.027169 -0.428966 1.173740	H 1.927213 -4.090237 -0.075483
C 4.035361 -0.787256 0.908268	H -4.043964 -2.015874 -1.242016
C 1.659015 3.690212 1.278652	H -2.298459 3.921939 0.491278
C 1.680624 2.269001 0.978208	N -0.763156 -0.483847 1.962094
C 2.853736 0.051119 0.809006	C -1.992498 -1.055592 2.414751
H -0.039933 5.117472 1.242555	H -2.139978 -2.043790 1.936631
C 3.642033 -2.071012 0.615316	H -2.839933 -0.417518 2.095949
C 2.808486 1.435235 1.042453	H -2.018940 -1.176525 3.508844
C 0.364163 4.116863 1.108118	C 0.756199 -1.098089 4.293779
C 2.218844 -2.025003 0.331061	C 0.502248 0.074287 3.613030
H 2.526582 4.270957 1.583004	C 0.262788 0.265949 -1.744241
H 4.247877 -2.973732 0.592591	O 0.465512 0.441919 -2.882636
C 0.059738 -3.117064 -0.367113	H 1.237723 0.469374 2.917812
N -0.743591 -2.000497 -0.396335	H -0.247966 0.772262 3.991541
C -2.565826 1.882241 -0.044577	C -0.142870 -1.591331 5.397084
N -2.105666 0.600746 -0.239065	H 0.444627 -1.824802 6.302664
C -3.167207 -0.169108 -0.657650	H -0.915967 -0.855203 5.660360
C -4.355034 0.664140 -0.739989	H -0.639776 -2.534134 5.101207
C -3.984228 1.930950 -0.357709	C 1.864763 -2.021639 3.863668
H -4.602004 2.823310 -0.289800	H 2.470255 -2.339769 4.730169
H -5.337455 0.311857 -1.045552	H 1.441400 -2.942020 3.420771
C -3.112885 -1.547356 -0.920762	H 2.518629 -1.557818 3.115055

Energy parameters

HF=-1447.8797099
Zero-point vibrational energy 1108562.5 (Joules/Mol)
Zero-point correction= 0.422229 (Hartree/Particle)
Thermal correction to Energy= 0.451538
Thermal correction to Enthalpy= 0.452482
Thermal correction to Gibbs Free Energy= 0.363119
Sum of electronic and zero-point Energies= -1447.457481
Sum of electronic and thermal Energies= -1447.428172
Sum of electronic and thermal Enthalpies= -1447.427228
Sum of electronic and thermal Free Energies= -1447.516591

Compound 13, [Ru]($CH_3NCH_2C(CH_3)_2$)$(CO)_T$

Cartesian Coordinates

Ru -0.326700 -0.133100 -0.249800	C -2.155100 -2.373700 -1.370900
N 1.578500 -0.856200 0.172300	C -2.153000 -3.786600 -1.709000
N 0.240100 1.734600 0.462800	H -3.002500 -4.324500 -2.123400
C -1.932000 2.881200 0.209600	C -0.903700 -4.270700 -1.403400
C 1.215800 -3.206900 -0.489100	H -0.525500 -5.283600 -1.520200
C -0.574800 2.838700 0.568900	H 3.546000 1.690900 1.293500
H 4.793400 -0.663300 1.071800	H 1.707400 -4.176800 -0.575900
C 3.811900 -0.984700 0.731400	H -4.156500 -1.921700 -1.933200
C 1.480900 3.499300 1.280500	H -2.439500 3.836200 0.351800
C 1.500000 2.102300 0.882600	N -0.908500 -0.649300 1.676600
C 2.651500 -0.118700 0.621700	C -2.120500 -1.392200 1.966900
H -0.200900 4.947200 1.279000	H -2.773800 -1.407100 1.090600
C 3.414700 -2.239600 0.335400	H -2.652100 -0.954100 2.830700
C 2.613500 1.248600 0.941100	H -1.860500 -2.433500 2.236800
C 0.197900 3.953100 1.090800	C 0.192200 -1.474900 3.777600
C 2.010300 -2.148200 -0.021000	C -0.121100 -0.306100 2.881100
H 2.341700 4.046600 1.657300	C 0.198700 0.314300 -2.004700
H 4.006600 -3.150600 0.287700	O 0.520600 0.587500 -3.095400
C -0.131300 -3.155500 -0.882800	H 0.801400 0.168100 2.529300
N -0.921700 -2.028300 -0.865600	H -0.710900 0.444400 3.444000
C -2.704100 1.842400 -0.335600	C -0.677300 -1.805000 4.954700
N -2.253500 0.566900 -0.589600	H -1.405200 -2.610200 4.719300
C -3.296700 -0.144000 -1.141800	H -0.073500 -2.177500 5.801400
C -4.462500 0.717800 -1.237400	H -1.255700 -0.931500 5.293700
C -4.097700 1.943600 -0.735000	C 1.201300 -2.472900 3.296500
H -4.704100 2.841400 -0.640500	H 1.600500 -3.074100 4.129700
H -5.427600 0.410600 -1.633300	H 0.756000 -3.180300 2.566100
C -3.243900 -1.497600 -1.512800	H 2.035600 -1.983800 2.771000

Energy parameters

HF=-1447.9058799

Zero-point vibrational energy 1115248.5 (Joules/Mol)

Zero-point correction= 0.424776 (Hartree/Particle)

Thermal correction to Energy= 0.453880

Thermal correction to Enthalpy= 0.454824

Thermal correction to Gibbs Free Energy= 0.366275

Sum of electronic and zero-point Energies= -1447.481104

Sum of electronic and thermal Energies= -1447.452000

Sum of electronic and thermal Enthalpies= -1447.451055

Sum of electronic and thermal Free Energies= -1447.539605

Compound 14, [Ru](1,2,2-trimethylaziridine)$(CO)_S$

Cartesian Coordinates

Ru -0.241331 -0.297483 -0.164508	C -1.697281 2.753925 0.513955
N 1.630792 -1.122247 0.162917	C 1.121179 -3.443134 -0.503125
N 0.429069 1.502490 0.620039	C -0.324729 2.644860 0.789976

H 4.912478 -1.076739 0.809074
C 3.892405 -1.354635 0.554414
C 1.817764 3.225064 1.279945
C 1.744341 1.831137 0.881270
C 2.773568 -0.430976 0.501181
H 0.199305 4.732806 1.463394
C 3.401445 -2.598885 0.238765
C 2.827004 0.939693 0.801567
C 0.538011 3.724811 1.235575
C 1.983516 -2.437907 -0.035594
H 2.733926 3.741058 1.557369
H 3.941422 -3.540601 0.174009
C -0.210656 -3.292925 -0.922025
N -0.927248 -2.117714 -0.876559
C -2.532058 1.776147 -0.050817
N -2.141501 0.499504 -0.391040
C -3.210772 -0.111382 -1.012590
C -4.336308 0.806453 -1.037529
C -3.920190 1.969050 -0.434560
H -4.485207 2.883894 -0.271782
H -5.311619 0.577657 -1.460694
C -3.209812 -1.425018 -1.510446
C -2.166670 -2.362081 -1.425874
C -2.243059 -3.754946 -1.829394
H -3.112288 -4.218988 -2.289554
C -1.039054 -4.333838 -1.505912
H -0.724126 -5.363987 -1.655349
H 3.809602 1.346968 1.042662
H 1.551161 -4.440308 -0.606171
H -4.134813 -1.768658 -1.975030
H -2.153786 3.725089 0.709475
N -1.056019 -1.000539 1.958999
C -2.171894 -1.963325 1.783729
H -1.767303 -2.921777 1.437414
H -2.849307 -1.562244 1.027377
H -2.742443 -2.115540 2.709945
C -0.338264 -1.060053 3.283175
C -1.311110 0.037590 2.991182
C 0.243877 0.225740 -1.837388
O 0.550237 0.561946 -2.922288
H -0.935867 1.030688 2.743306
H -2.297362 0.005693 3.464511
C -0.679488 -2.166860 4.280901
H -0.298778 -3.136680 3.922783
H -0.176050 -1.938099 5.231869
H -1.751636 -2.261081 4.488698
C 1.145504 -0.750331 3.256666
H 1.480948 -0.533036 4.283021
H 1.720038 -1.605948 2.873690
H 1.349840 0.119402 2.634580

Energy parameters

HF=-1447.964319
Zero-point vibrational energy 1130358.7 (Joules/Mol)
Zero-point correction= 0.430531 (Hartree/Particle)
Thermal correction to Energy= 0.458035
Thermal correction to Enthalpy= 0.458979
Thermal correction to Gibbs Free Energy= 0.376265
Sum of electronic and zero-point Energies= -1447.533788
Sum of electronic and thermal Energies= -1447.506284
Sum of electronic and thermal Enthalpies= -1447.505340
Sum of electronic and thermal Free Energies= -1447.588054

Compound 15, [Ru](4,5-dihydro-1,5,5-trimethyl-1*H*-1,2,3-triazole)$(CO)_5$

Cartesian Coordinates
Ru -0.237293 0.001162 -0.333708
N 1.347427 -0.912268 0.656746
N 0.560055 1.866289 0.102950
C -1.213165 3.268067 -0.886491
C 0.650842 -3.265996 0.388586
C 0.013656 3.085069 -0.230729
H 4.242859 -1.022476 2.329347
C 3.319479 -1.256769 1.804646
C 1.959197 3.543006 0.850202
C 1.742757 2.108464 0.764869
C 2.415832 -0.268743 1.241949
H 0.697794 5.208970 0.102232
C 2.777941 -2.492463 1.541456
C 2.594419 1.122925 1.288341
C 0.891297 4.146702 0.232116
C 1.537722 -2.267097 0.820405
H 2.817237 4.011524 1.326650
H 3.168441 -3.471669 1.808938
C -0.588546 -3.082548 -0.245229
N -1.134019 -1.861877 -0.580028

C -2.114677 2.270854 -1.288075
N -1.920605 0.917152 -1.131593
C -3.045032 0.279366 -1.605125
C -3.990742 1.270885 -2.089656
C -3.413466 2.502347 -1.896884
H -3.820363 3.483357 -2.131038
H -4.964771 1.040190 -2.515009
C -3.249525 -1.109340 -1.606050
C -2.372071 -2.098827 -1.135336
C -2.624040 -3.528953 -1.151148
H -3.530311 -3.992895 -1.533685
C -1.519736 -4.137667 -0.604050
H -1.341881 -5.199087 -0.447113
H 3.495220 1.478784 1.790219
H 0.943647 -4.296679 0.593065
H -4.196836 -1.459036 -2.018784
H -1.511800 4.299259 -1.079613
C 0.607294 -0.086469 -1.966586
O 1.146110 -0.140916 -3.009789
N -1.243843 0.055632 1.589839
C -1.109633 -1.028323 2.597277
C -2.309650 -0.784442 3.532819
H -1.118627 -2.002957 2.099451
N -2.017186 0.969879 2.012924
N -2.510102 0.672475 3.228023
C -3.696868 1.408873 3.656916
H -4.611348 1.035283 3.166779
H -3.796129 1.301715 4.744619
H -3.556713 2.467588 3.408210
H -0.139911 -0.892679 3.103059
C -1.997497 -1.002248 5.016154
H -2.862150 -0.731617 5.640441
H -1.771620 -2.064128 5.191877
H -1.131328 -0.398354 5.321523
C -3.541200 -1.596624 3.077123
H -3.330303 -2.667961 3.208357
H -4.429029 -1.341503 3.673166
H -3.752210 -1.409305 2.014045

Energy parameters

HF=-1557.3944623
Zero-point vibrational energy 1153042.2 (Joules/Mol)
Zero-point correction= 0.439171 (Hartree/Particle)
Thermal correction to Energy= 0.468921
Thermal correction to Enthalpy= 0.469865
Thermal correction to Gibbs Free Energy= 0.379989
Sum of electronic and zero-point Energies= -1556.955292
Sum of electronic and thermal Energies= -1556.925541
Sum of electronic and thermal Enthalpies= -1556.924597
Sum of electronic and thermal Free Energies= -1557.014473

Compound isobutene

Cartesian Coordinates
C -2.613246 0.138610 0.112929
H -2.089652 -0.818782 0.170590
H -3.703533 0.123168 0.184384
C -1.938886 1.296416 -0.041022
C -2.640020 2.635554 -0.123473
H -2.287513 3.307500 0.678383
H -2.406167 3.137427 -1.078559
H -3.731512 2.531412 -0.039803
C -0.429133 1.345511 -0.143109
H -0.120462 1.807672 -1.097005
H -0.006819 1.973222 0.660895
H 0.018144 0.343087 -0.077373

Energy parameters

HF=-157.1260698
Zero-point vibrational energy 274883.0 (Joules/Mol)
Zero-point correction= 0.104697 (Hartree/Particle)
Thermal correction to Energy= 0.110131
Thermal correction to Enthalpy= 0.111076
Thermal correction to Gibbs Free Energy= 0.077289
Sum of electronic and zero-point Energies= -157.021372

Sum of electronic and thermal Energies= -157.015938
Sum of electronic and thermal Enthalpies= -157.014994
Sum of electronic and thermal Free Energies= -157.048781

Compound methylazide CH_3N_3

Cartesian Coordinates

N -0.002226 -0.606884 2.428170
N -1.078385 -1.069532 2.817261
N -2.082670 -1.585694 3.058781
C 0.628220 0.414995 3.304530
H 0.856195 -0.003348 4.298133
H 1.560071 0.711944 2.812096
H -0.024105 1.296019 3.416329

Energy parameters

HF=-203.9794983
Zero-point vibrational energy 128579.6 (Joules/Mol)
Zero-point correction= 0.048973 (Hartree/Particle)
Thermal correction to Energy= 0.053491
Thermal correction to Enthalpy= 0.054436
Thermal correction to Gibbs Free Energy= 0.022352
Sum of electronic and zero-point Energies= -203.930525
Sum of electronic and thermal Energies= -203.926007
Sum of electronic and thermal Enthalpies= -203.925063
Sum of electronic and thermal Free Energies= -203.957146

Compound 1,2,2-trimethylaziridine

Cartesian Coordinates

N -1.068929 -0.982158 2.025669
C -2.154092 -1.930303 1.739481
H -1.720464 -2.888104 1.413048
H -2.759891 -1.522047 0.915876
H -2.827504 -2.122582 2.597130
C -0.343489 -1.070218 3.314386
C -1.331546 0.030604 3.065804
H -0.991917 1.048183 2.844527
H -2.291584 -0.032229 3.595278
C -0.674698 -2.157797 4.333436
H -0.211713 -3.114209 4.038933
H -0.267131 -1.874199 5.316304
H -1.755543 -2.311759 4.447636
C 1.147935 -0.775930 3.201659
H 1.547338 -0.437352 4.171756
H 1.695042 -1.685633 2.903168
H 1.331188 0.003732 2.448909

Energy parameters

HF=-251.7088539
Zero-point vibrational energy 391783.9 (Joules/Mol)
Zero-point correction= 0.149223 (Hartree/Particle)
Thermal correction to Energy= 0.156621
Thermal correction to Enthalpy= 0.157565
Thermal correction to Gibbs Free Energy= 0.118915
Sum of electronic and zero-point Energies= -251.559631
Sum of electronic and thermal Energies= -251.552233
Sum of electronic and thermal Enthalpies= -251.551289
Sum of electronic and thermal Free Energies= -251.589939

Compound (4,5-dihydro-1,5,5-trimethyl-1*H*-1,2,3-triazole)$_{TS}$

Cartesian Coordinates

N -1.301405 0.549337 1.237725	H -0.233968 -1.305354 2.384025
C -1.310860 -1.362821 2.222653	C -1.618824 -0.955845 4.693797
C -2.183067 -1.225238 3.310991	H -2.332893 -0.401259 5.320623
H -1.646436 -1.894160 1.330388	H -1.413762 -1.914933 5.202342
N -2.078439 1.149858 1.915627	H -0.678213 -0.388963 4.639809
N -2.881674 0.849781 2.854618	C -3.561256 -1.859481 3.269618
C -3.249234 1.870282 3.838326	H -3.502066 -2.887794 3.668974
H -3.930984 1.384120 4.548366	H -4.279697 -1.303253 3.889712
H -2.371636 2.253293 4.387895	H -3.946421 -1.909179 2.241597
H -3.782063 2.712807 3.368714	

Energy parameters

HF=-361.0810712
Zero-point vibrational energy 407887.8 (Joules/Mol)
Zero-point correction= 0.155356 (Hartree/Particle)
Thermal correction to Energy= 0.165264
Thermal correction to Enthalpy= 0.166208
Thermal correction to Gibbs Free Energy= 0.120764
Sum of electronic and zero-point Energies= -360.925715
Sum of electronic and thermal Energies= -360.915807
Sum of electronic and thermal Enthalpies= -360.914863
Sum of electronic and thermal Free Energies= -360.960307

Compound (4,5-dihydro-1,5,5-trimethyl-1*H*-1,2,3-triazole)

Cartesian Coordinates

N -1.742508 0.026220 1.179913	H -0.310654 -0.974711 2.363515
C -1.390372 -1.058866 2.149101	C -1.496130 -0.952665 4.727477
C -2.247237 -0.763269 3.403015	H -2.118195 -0.632353 5.577528
H -1.584570 -2.042830 1.701448	H -1.252378 -2.016281 4.869225
N -2.349213 0.947707 1.799311	H -0.564112 -0.369584 4.728558
N -2.497198 0.686366 3.133169	C -3.568363 -1.563227 3.389496
C -3.532580 1.438268 3.836526	H -3.341991 -2.636275 3.477368
H -4.547506 1.065863 3.612719	H -4.214080 -1.277278 4.232701
H -3.349762 1.358363 4.916720	H -4.113639 -1.394636 2.448886
H -3.459812 2.491286 3.537626	

Energy parameters

HF=-361.1375379
Zero-point vibrational energy 420638.8 (Joules/Mol)
Zero-point correction= 0.160213 (Hartree/Particle)
Thermal correction to Energy= 0.168959
Thermal correction to Enthalpy= 0.169904
Thermal correction to Gibbs Free Energy= 0.127579
Sum of electronic and zero-point Energies= -360.977325
Sum of electronic and thermal Energies= -360.968578
Sum of electronic and thermal Enthalpies= -360.967634
Sum of electronic and thermal Free Energies= -361.009959

Compound α-methylstyrene

Cartesian Coordinates

C 1.031773 -1.777992 -0.308123	C -1.889205 -1.765815 -0.959148
C 0.078549 -1.566885 0.630792	C -3.634468 -2.311882 1.164838
H 0.794480 -2.165190 -1.299996	H -1.912230 -2.098647 2.443563
H 2.082068 -1.578451 -0.088134	C -3.246797 -2.007128 -1.211655
C 0.465704 -1.092092 2.020675	H -1.225915 -1.521462 -1.789317
H 0.268855 -1.871703 2.775140	C -4.128760 -2.285739 -0.150060
H 1.534837 -0.842808 2.063081	H -4.306824 -2.520585 1.998868
H -0.120614 -0.206673 2.315066	H -3.620360 -1.964224 -2.236293
C -1.368121 -1.805684 0.358957	H -5.186449 -2.468675 -0.345831
C -2.273422 -2.069166 1.415877	

Energy parameters

HF=-348.7226592
Zero-point vibrational energy 413526.8 (Joules/Mol)
Zero-point correction= 0.157504 (Hartree/Particle)
Thermal correction to Energy= 0.165679
Thermal correction to Enthalpy= 0.166623
Thermal correction to Gibbs Free Energy= 0.124607
Sum of electronic and zero-point Energies= -348.565155
Sum of electronic and thermal Energies= -348.556980
Sum of electronic and thermal Enthalpies= -348.556036
Sum of electronic and thermal Free Energies= -348.598052

Compound 3,5-*bis*(trifluoromethyl)phenyl azide, Ar'N_3

Cartesian Coordinates

N 1.674006 0.897695 -1.315378	C -1.608330 3.861647 2.669368
N 0.744872 0.939713 -0.639580	H -1.964029 4.628835 3.352405
N -0.296923 0.825578 0.025237	C 0.362856 5.328820 2.161307
C -0.681498 1.877723 0.893243	C -3.593003 2.402471 3.279686
C -1.871069 1.673551 1.614940	F -4.060610 3.507696 3.924297
C 0.050604 3.074587 1.052709	F -4.601221 1.948665 2.472852
C -2.324007 2.668957 2.494134	F -3.393750 1.436667 4.233013
H -2.429853 0.749078 1.480597	F -0.447338 6.430722 2.156913
C -0.423448 4.052036 1.936164	F 1.326099 5.534339 1.218415
H 0.969961 3.240861 0.494016	F 0.993383 5.313060 3.379163

Energy parameters

HF=-1069.3441665
Zero-point vibrational energy 285332.7 (Joules/Mol)
Zero-point correction= 0.108678 (Hartree/Particle)
Thermal correction to Energy= 0.123323
Thermal correction to Enthalpy= 0.124267
Thermal correction to Gibbs Free Energy= 0.064453
Sum of electronic and zero-point Energies= -1069.235489
Sum of electronic and thermal Energies= -1069.220844
Sum of electronic and thermal Enthalpies= -1069.219900

Sum of electronic and thermal Free Energies= -1069.279714

Compound Ar'N=NAr'

Cartesian Coordinates

N 0.264491 -1.275521 1.440278	C 2.920950 0.290788 -2.601885
C 1.405460 -0.706872 2.111759	H 3.618575 0.705269 -3.325870
C 1.142608 0.163788 3.183033	C 1.900852 1.670664 5.034971
C 2.726845 -1.096521 1.819370	C 5.193385 -0.966032 2.194031
C 2.215199 0.712024 3.902694	C 2.843726 2.542402 -1.472387
H 0.112606 0.423073 3.424810	C 2.957735 -1.889075 -3.876514
C 3.781421 -0.561639 2.570073	F 1.090461 2.691143 4.615428
H 2.927098 -1.802407 1.016220	F 3.014400 2.237128 5.576351
C 3.540624 0.357232 3.605048	F 1.234986 1.037277 6.051337
H 4.366206 0.777363 4.172939	F 6.132757 -0.488334 3.054846
N 0.192923 -1.384198 0.190375	F 5.518665 -0.503771 0.943670
C 1.153765 -0.791192 -0.703922	F 5.332633 -2.326574 2.152705
C 1.551866 0.556739 -0.598289	F 2.718393 3.054222 -0.213205
C 1.585249 -1.580795 -1.783136	F 4.139923 2.729655 -1.857769
C 2.433894 1.084243 -1.548420	F 2.069729 3.318250 -2.295792
H 1.185408 1.175169 0.217227	F 2.097069 -1.777880 -4.938320
C 2.493993 -1.042244 -2.706681	F 3.022665 -3.215086 -3.559165
H 1.236786 -2.608563 -1.871061	F 4.191453 -1.520122 -4.327046

Energy parameters

HF=-1919.8738328
Zero-point vibrational energy 527231.4 (Joules/Mol)
Zero-point correction= 0.200812 (Hartree/Particle)
Thermal correction to Energy= 0.227051
Thermal correction to Enthalpy= 0.227995
Thermal correction to Gibbs Free Energy= 0.137873
Sum of electronic and zero-point Energies= -1919.673021
Sum of electronic and thermal Energies= -1919.646782
Sum of electronic and thermal Enthalpies= -1919.645838
Sum of electronic and thermal Free Energies= -1919.735960

Compound N_2

Cartesian Coordinates
N 0.000000 0.000000 0.013717
N 0.000000 0.000000 1.126283

Energy parameters

HF=-109.4582665

Zero-point vibrational energy 14213.7 (Joules/Mol)

Zero-point correction= 0.005414 (Hartree/Particle)

Thermal correction to Energy= 0.007774

Thermal correction to Enthalpy= 0.008718

Thermal correction to Gibbs Free Energy= -0.013048

Sum of electronic and zero-point Energies= -109.452853

Sum of electronic and thermal Energies= -109.450492

Sum of electronic and thermal Enthalpies= -109.449548

Sum of electronic and thermal Free Energies= -109.471315

References

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[2] E. Gallo, A. Caselli, F. Ragaini, S. Fantauzzi, N. Masciocchi, A. Sironi, S. Cenini, *Inorg. Chem.* 2005, *44*, 2039-2049.