Supporting Information

Chemoselective Reduction of Imines Catalyzed by Ruthenium(II) Half-Sandwich Complexes: A Mechanistic Study

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1. Complexes studied in this work

Figure S1. Ruthenium half sandwich complexes studied in this work.

2. Reduction of N-benzylideneaniline catalyzed by Ru(thione) complexes

Table S1: Reduction of N-benzylideneaniline by **1a-2e**

Entry ^a	Catalyst	Isolated yield
1	1a	95
2	1b	96
3	1c	95
4	1d	94
5	1e	95
6	1f	93
7	2a	94
8	2b	95
9	2c	96
10	2d	92
11	2e	97
12	1g	94

3. Reduction of 1-(4-methoxyphenyl)-N-phenylethan-1-imine catalyzed by Ru(thione) complexes

Table S2. Reduction of N,1-diphenylethan-1-imine catalyzed by complexes **1a-2e**

Entry ^{a, b}	Catalyst	Isolated yield
1	1a	93
2	1b	91
3 ^c	1b	92
4 ^d	1b	91
5 ^e	1b	93
6	1c	92
7	1d	93
7	1e	91
8	1f	93
9	1g	92
10	2a	92
11	2b	89
12	2c	90
13	2d	91
14	2e	90

^a Ketimine (0.25 mmol), PhSiH₃ (0.5 mmol), and catalyst (0.005 mmol), ethanol (5 mL), room temperature. ^b Conversion (by ¹H NMR spectroscopy) was 100 % in all cases in 2 h (unless mentioned otherwise). ^c 0.5 mmol of Ph₂SiH₂ used. ^d Reaction done at 0 °C, 6 h. ^e 0.0125 mmol of catalyst used, 30 min. ^f ee was zero in all cases (determined by optical activity measurements).

4. Catalyst recyclability

The catalyst recyclability was tested with complex (**1c**) using N-Benzylideneaniline as substrate. 0.0025 mmol of the catalyst was taken in a 10 mL R.B flask. Then ethanol (10 mL) was added to this flask. To this solution was added 0.25 mmol of the N-Benzylideneaniline, followed by the addition of phenylsilane (0.5 mmol). The resulting solution was stirred at room temperature. After 15 minutes, 0.5 mL of the reaction mixture was withdrawn and after removal of the solvent ¹H NMR spectrum was recorded in CDCl₃. It showed complete

conversion of the imine. Also, after 15 minutes, 0.25 mmol of the imine and 0.5 mmol of phenylsilane were freshly added to the reaction mixture. After 75 minutes (1h after the second addition of imine and silane), an aliquot was taken from the reaction mixture and after removal of the solvent, ^1H NMR spectrum was recorded in CDCl_3 . The ^1H NMR spectrum showed only 75% conversion. To maintain the substrate: catalyst ratio of 100: 1, more substrate (75 %) and phenylsilane (150 %) was added to the reaction mixture. Similarly, after 2 h, the conversion was 50% and so 50% of imine and 100 % of silane was added to the reaction mixture. In the fourth cycle conversion further decreased to 20%. This result suggests deactivation of the catalyst over time.

Table S3. Recyclability test

Entry	Cycle no.	Time (min)	Conversion
1	1	15	100
2	2	75	70
3	3	135	50
4	4	195	20

^a Aldimine (0.25 mmol, PhSiH_3 (0.5 mmol), and complex **1c** (0.0025 mmol), ethanol (5 mL).

5. Reduction of various imines by 1c

Table S4. Reduction of various imines by **1c**

Entry ^a	Substrate	Time (min)	Conversion ^b
1		15	100 [95]
2 ^c		15	100 [94]
3 ^d		30	100 [92]
4		15	99 [93]
5		30	98 [91]
6		15	100[91]
7		15	100[92]
8 ^e		120	100[90]
9 ^e		120	100[92]
10 ^e		120	100[91]

11		120	0
12		110	0
13		12 h	0

^a Aldimine (0.25 mmol), PhSiH₃ (0.5 mmol), and complex **1c** (0.0025 mmol), ethanol (5 mL), room temperature. ^b Conversion by ¹H NMR spectroscopy. Values inside the square brackets are the isolated yields. ^c 0.5 mmol of Ph₂SiH₂ used. ^d Reaction done at 0 °C. ^e Catalyst (0.005 mmol), ethanol (5 mL); ee was zero by optical activity measurements.

6. ^1H NMR of 1c in CDCl_3 and CD_3OD .

Figure S2: ^1H NMR of **1c** in CDCl_3 .

Figure S3: ^1H NMR of **1c** in CD_3OD .

Figure S4: ^1H NMR of **1c** in CD_3OD (0-6.5 ppm region).

Figure S5: ^1H NMR of **1c** in CD_3OD (aromatic peaks of cymene).

Figure S6: ^1H NMR of **1c** stacked with free ligand (**L1c**) and $[(\eta^6\text{-cymene})\text{RuCl}_2]_2$; all spectra are in CD_3OD .

Figure S7: ^1H NMR of **1c** in CD_3OD . Peaks corresponding to dinuclear complex (**W**) are marked with #.

7. ESI-MS data

Table S2: Different species detected under ESI-MS conditions.

S. No.	Name of species	Observed peak $[M]^+$	Theoretical formula (Calculated m/z)	Found m/z (Abundance in %)
1	V	$[(\eta^6\text{-cym})\text{Ru}(\text{L-H})]^+$	$[\text{C}_{17}\text{H}_{26}\text{NS}_2\text{Ru}]^+$ (410.0553)	410.0575 (100)
2	T-Cl⁻	$[(\eta^6\text{-cym})\text{Ru}(\text{L-H})]_2[\text{Cl}]^+$	$[\text{C}_{34}\text{H}_{52}\text{N}_2\text{S}_4\text{Ru}_2\text{Cl}]^+$ (855.0792)	855.0871 (20)
3	X	$[(\eta^6\text{-cym})\text{Ru}(\text{L})(\text{L-H})]^+$	$[\text{C}_{24}\text{H}_{38}\text{N}_2\text{S}_4\text{Ru}]^+$ (585.1038)	585.1084 (43)
4	Y	$[(\eta^6\text{-cym})\text{Ru}(\text{OH})(\text{CH}_3\text{CN})]^+$	$[\text{C}_{12}\text{H}_{18}\text{NORu}]^+$ (294.0431)	294.0440 (1)
5	P- Cl⁻		$[\text{C}_{20}\text{H}_{28}\text{Cl}_3\text{Ru}_2]^+$ (576.9408)	576.9561 (1)
6	Z	$[(\eta^6\text{-cym})\text{Ru}(\text{L-H})]_2 [\text{L-H}]^+$	$[\text{C}_{41}\text{H}_{64}\text{N}_3\text{S}_6\text{Ru}_2]^+$ (994.1525)	994.1526 (0.5)

Figure S8: Different species detected under ESI-MS conditions.

Figure S9: HR ESI-MS of **1c**. The subsequent figures show the isotopic distribution of species **V**, **[T-Cl]**, **X**, **Y**, and **Z**.

Figure S10: Comparison of isotopic distribution of $[\mathbf{T-Cl}]^+$ observed in the HR ESI-MS of **1c** (red) with theoretical isotopic distribution obtained from Molecular Weight Calculator software (blue).

Figure S11: Comparison of isotopic distribution of **V** observed in the HR ESI-MS of **1c** (red) with theoretical isotopic distribution obtained from Molecular Weight Calculator software (blue).

Figure S12: Comparison of isotopic distribution of **X** observed in the HR ESI-MS of **1c** (red) with theoretical isotopic distribution obtained from Molecular Weight Calculator software (blue).

Figure S13: Comparison of isotopic distribution of **Y** observed in the HR ESI-MS of **1c** (red) with theoretical isotopic distribution obtained from Molecular Weight Calculator software (blue).

Figure S14: Comparison of isotopic distribution of **Z** observed in the HR ESI-MS of **1c** (red) with theoretical isotopic distribution obtained from Molecular Weight Calculator software (blue).

8. Mechanistic studies

Figure S15: ^1H NMR spectrum recorded 30 minutes after the addition of Ph_2SiH_2 (0.026 mmol) to $[(\eta^6\text{-cymene})\text{RuCl}_2]_2$ (0.008 mmol).

Figure S16: Expansion of spectrum in Figure S14.

The amount of **A** present in the mixture was calculated to be 0.0062 mmols using trimethoxybenzene as internal standard. Hence 0.0062 mmols (2.6 mg) of imine (N-(4-methoxyphenyl)-1-phenylmethanimine) was added.

Figure S17: ^1H NMR spectrum recorded immediately after the imine (2.6 mg) was added to the mixture obtained by reacting $[(\eta^6\text{-cymene})\text{RuCl}_2]_2$ (0.008 mmols) and Ph_2SiH_2 (0.026 mmols) for 30 minutes. Inside box is shown the expansion.

9. ^1H NMR of amines

10. Reductive elimination of Ru(II) dihydride intermediate:

The reductive elimination of the dihydride species (Intermediate **X**) to furnish a 16e species **Y** was examined by DFT calculations using a slightly truncated model (**X'**, **Y'**) and found to be thermodynamically accessible ($\Delta G = 9.47$ kcal/mol) when $L = \text{CH}_2\text{NH}$.

$$\Delta G_{(\text{X}' \rightarrow \text{Y} + \text{H}_2)} = 9.47 \text{ kcal/mol}$$

11. Optimized geometry coordinates:

A'

Ru	0.96102300	-0.61231400	0.14022200
C	3.17719700	-1.10234600	0.99600800
C	3.32127800	-0.44258600	-0.26408700
C	2.73913200	-0.96994600	-1.43818200
C	1.86451500	-2.08834000	-1.33475700
C	1.65958800	-2.72113400	-0.07087700
C	2.34444500	-2.23314200	1.09103800
H	3.91033900	0.46034800	-0.32161600
H	2.88969500	-0.48227400	-2.38883600
H	1.01740200	-3.58350900	0.00336700
H	2.20045600	-2.72524300	2.04056000
H	-0.25766400	-0.99164100	1.11494800

H	3.66653900	-0.70642100	1.87210300
H	1.38189000	-2.48299800	-2.21511500
Si	-1.04832500	0.09514500	-0.93124600
H	-1.16147800	0.22561300	-2.43219300
C	-0.00041500	1.54873900	-0.29232500
C	0.29917900	1.62635800	1.10090400
C	0.72230500	2.41842800	-1.17035300
C	1.28673700	2.53553600	1.57257200
H	-0.34747800	1.15708300	1.82570700
C	1.65484600	3.31457500	-0.69083500
H	0.51307800	2.37740700	-2.23239100
C	1.95263600	3.36604400	0.69481600
H	1.48521600	2.59105800	2.63550000
H	2.15972700	3.98878500	-1.37142600
H	2.68676800	4.07261600	1.06018100
C	-2.83387200	-0.10572100	-0.29806000
C	-3.14268800	-0.51876900	1.01007700
C	-3.90424700	0.16641700	-1.17134300
C	-4.46788200	-0.63472000	1.43760300
H	-2.33985700	-0.76320800	1.69376700
C	-5.23152300	0.04683800	-0.75076700
H	-3.69949100	0.47597100	-2.18920300
C	-5.51646300	-0.35123500	0.55784700
H	-4.68140700	-0.95147700	2.45059700
H	-6.03744100	0.26262500	-1.44065000
H	-6.54336400	-0.44492700	0.88671100

Absolute energies (a.u):

Sum of electronic and zero-point Energies = -1079.804672
Sum of electronic and thermal Energies = -1079.786169
Sum of electronic and thermal Enthalpies = -1079.785225
Sum of electronic and thermal Free Energies = -1079.853788

S1

Ru	1.57852300	-0.72698200	-0.06106700
C	3.72707800	-1.08949300	0.94849300
C	3.18719700	0.10276800	1.50191600
C	2.83901700	1.17912700	0.64341700
C	3.05026000	1.07671400	-0.75665700
C	3.51033700	-0.14119900	-1.30402100
C	3.88297800	-1.22183900	-0.44597100
H	3.05368600	0.19356700	2.56801100
H	2.44104400	2.09124500	1.06074400
H	3.63039200	-0.24216400	-2.37123100
H	4.26617100	-2.13756500	-0.86684800
H	0.91940400	-1.96997200	0.69727100
H	0.96647700	-1.68352800	-1.19528100
H	3.99145200	-1.90889700	1.59915100
H	2.81760300	1.90865200	-1.40307900
Si	-0.58631200	-0.11817700	-0.02990600
C	-1.25782500	1.68155300	0.01692200

C	-2.34716700	2.06272500	0.82681400
C	-0.60591200	2.69073500	-0.71924700
C	-2.76204000	3.39526600	0.90179400
H	-2.87329400	1.31498200	1.40641900
C	-1.03021000	4.02057900	-0.66407300
H	0.23827100	2.42761600	-1.34447500
C	-2.10819000	4.37664300	0.15154800
H	-3.59500200	3.66511100	1.53832500
H	-0.52232600	4.77545400	-1.25088500
H	-2.43464000	5.40718000	0.20237600
C	-2.11983800	-1.25244700	-0.05127100
C	-3.36864900	-0.82037600	-0.54364000
C	-2.01388700	-2.58732000	0.38821100
C	-4.46501100	-1.68502700	-0.59406600
H	-3.48356600	0.19519300	-0.89797000
C	-3.11065000	-3.45016600	0.35172400
H	-1.06153100	-2.94789800	0.75287900
C	-4.33973300	-3.00065000	-0.14051800
H	-5.41140000	-1.33324300	-0.98442300
H	-3.00635900	-4.46950000	0.70041400
H	-5.18957000	-3.67010500	-0.17402900

Absolute energies (a.u):

Sum of electronic and zero-point Energies = -1079.816218
Sum of electronic and thermal Energies = -1079.797413
Sum of electronic and thermal Enthalpies = -1079.796468
Sum of electronic and thermal Free Energies = -1079.866036

S2

Ru	1.78533000	-0.09676200	0.37167800
C	3.95287400	0.74356000	0.00442400
C	3.08625900	1.43374000	-0.90095700
C	2.30059600	0.69293800	-1.80975100
C	2.39785600	-0.73388600	-1.85519500
C	3.24418300	-1.40631200	-0.95020900
C	4.04575900	-0.66281900	-0.02478700
H	3.02455900	2.51012700	-0.87753700
H	1.63773000	1.20571200	-2.49002000
H	3.30985500	-2.48319500	-0.96866600
H	4.70332000	-1.17944000	0.65624200
H	1.55704500	0.80431600	1.69286500
H	1.44083300	-1.25260200	1.44885500
Si	-0.53263900	-0.00584400	0.44431000
C	-1.54295800	1.57611700	-0.04753400
C	-1.39156900	2.76888700	0.68643200
C	-2.34603000	1.62483100	-1.20287500

C	-2.03236800	3.94971400	0.30221900
H	-0.74701500	2.78094500	1.55755900
C	-2.97957800	2.80689900	-1.60163000
H	-2.47958500	0.73211600	-1.80090100
C	-2.83029800	3.97197000	-0.84574500
H	-1.90124400	4.85087600	0.88836400
H	-3.58845200	2.81589100	-2.49710900
H	-3.32268300	4.88661900	-1.14990400
C	-1.68099300	-1.50490700	-0.02492400
C	-1.08157900	-2.74140000	-0.32719900
C	-3.08826200	-1.44147600	-0.04366000
C	-1.85080000	-3.86714200	-0.63736200
H	-0.00131500	-2.81225100	-0.30667100
C	-3.86446500	-2.56428300	-0.34868300
H	-3.58862000	-0.50328200	0.16623000
C	-3.24563900	-3.78114200	-0.64836700
H	-1.36459000	-4.80694200	-0.86753500
H	-4.94478600	-2.48856600	-0.35786800
H	-3.84373100	-4.65090200	-0.88839200
N	-1.20081400	-0.01743900	2.33140200
H	-2.21366600	0.02447600	2.43558200
C	-0.48806000	-0.13478200	3.38875300
H	-0.93577700	-0.18639000	4.37665200

H	0.58695000	-0.18373700	3.26447100
H	4.54143000	1.30634700	0.71239900
H	1.80829800	-1.29172300	-2.56629400

Absolute energies (a.u):

Sum of electronic and zero-point Energies =	-1174.423067
Sum of electronic and thermal Energies =	-1174.401031
Sum of electronic and thermal Enthalpies =	-1174.400087
Sum of electronic and thermal Free Energies =	-1174.477234

S3

Ru	-1.71968100	-0.52816200	0.31567000
C	-3.47403700	-1.54537400	-0.92007100
C	-2.46596900	-1.09372700	-1.82264200
C	-2.08274300	0.27537300	-1.81625600
C	-2.74669300	1.21558800	-0.97054700
C	-3.69515800	0.74004000	-0.04417300
C	-4.08533300	-0.63884600	-0.03175200
H	-1.99097200	-1.78690200	-2.49846300
H	-1.32149600	0.61931400	-2.49934100
H	-4.15865800	1.42514100	0.64943800
H	-4.83247200	-0.98030200	0.66719100
H	-1.03805600	-1.92252200	0.74101600
H	-1.60770100	-0.14322100	1.99014000
Si	0.61591500	-0.02721900	0.48541200

C	2.01094900	-1.27061600	0.03548000
C	3.31254800	-1.16014400	0.56113800
C	1.74498500	-2.34590900	-0.82990000
C	4.30915100	-2.08251000	0.23150600
H	3.54907400	-0.35185200	1.24228300
C	2.74006400	-3.26722900	-1.17272900
H	0.74308700	-2.47118600	-1.22058600
C	4.02539200	-3.13720400	-0.64189000
H	5.30102900	-1.98075900	0.65387600
H	2.51031300	-4.08676100	-1.84209100
H	4.79629700	-3.85206600	-0.89971000
C	1.26563500	1.72908300	-0.00889000
C	0.53327700	2.86838600	0.38283100
C	2.42308200	1.93471100	-0.78124800
C	0.95054600	4.15763200	0.04177200
H	-0.38407800	2.73943300	0.94636300
C	2.83886900	3.22261700	-1.13827200
H	3.00623700	1.08361000	-1.10694800
C	2.10765500	4.33761600	-0.72275900
H	0.37347000	5.01632100	0.36205700
H	3.73225900	3.35283500	-1.73603700
H	2.43109800	5.33402900	-0.99497100
N	0.75000600	0.18923300	2.39832100

H	1.02734000	1.10205800	2.74101900
C	-0.22836700	-0.43276100	3.04875800
H	-0.60734400	-0.04057700	3.98753100
H	-0.40628300	-1.47360200	2.85147300
H	-3.75735400	-2.58663500	-0.90967900
H	-2.47577600	2.25885400	-1.00019600

Absolute energies (a.u):

Sum of electronic and zero-point Energies =	-1174.402016
Sum of electronic and thermal Energies =	-1174.381052
Sum of electronic and thermal Enthalpies =	-1174.380107
Sum of electronic and thermal Free Energies =	-1174.454108

Z1

Ru	1.42117900	-0.58656700	0.02136700
C	3.76108400	-0.50408500	0.66132800
C	3.56701300	0.40864200	-0.42239200
C	3.04622400	-0.02530300	-1.66053200
C	2.56601300	-1.36079400	-1.77953400
C	2.70095800	-2.26863000	-0.68523000
C	3.33059800	-1.83674800	0.52943700
H	3.85142800	1.44265500	-0.29737200
H	2.94178100	0.66580700	-2.48239600
H	2.36205600	-3.28691100	-0.78477300
H	3.44808000	-2.53143700	1.34672400

H	0.47208100	-1.54519300	0.88803600
H	4.19734600	-0.15810800	1.58542500
H	2.13155400	-1.70047200	-2.70657300
Si	-0.80375300	-0.32117900	-0.80477400
H	-1.07924500	0.11584900	-2.22159900
C	-2.37022500	-1.20368100	-0.16742200
C	-3.63522100	-0.76588400	-0.60936400
C	-2.31916200	-2.29333800	0.71860100
C	-4.80433400	-1.39227300	-0.16896600
H	-3.71268300	0.08360300	-1.27675900
C	-3.48758500	-2.92337200	1.15773600
H	-1.35792600	-2.65216000	1.06319800
C	-4.73363100	-2.47357200	0.71412000
H	-5.76618800	-1.03460300	-0.51375800
H	-3.42432400	-3.76195200	1.83978400
H	-5.63962600	-2.96054100	1.05174800
C	-0.18275900	1.19758800	0.16218000
C	0.17391700	2.43280600	-0.47058400
C	0.20102300	1.02603700	1.52731400
C	0.83710600	3.42997300	0.21552600
H	-0.09929500	2.58328000	-1.50810500
C	0.91247200	2.05372100	2.20734300
H	-0.21370700	0.21944500	2.11190000

C	1.22417700	3.23535500	1.56618300
H	1.06415300	4.36802800	-0.27581600
H	1.17867300	1.90915900	3.24685400
H	1.74659100	4.02300500	2.09376600
N	-3.43970400	2.73332700	-0.98609400
H	-2.65531700	2.48693600	-0.36846400
C	-3.86832700	3.92767900	-0.82936500
H	-3.46632300	4.65255400	-0.11692400
H	-4.69657100	4.26848500	-1.44382000

Sum of electronic and zero-point Energies = -1174.387976

Sum of electronic and thermal Energies = -1174.364523

Sum of electronic and thermal Enthalpies = -1174.363578

Sum of electronic and thermal Free Energies = -1174.446379

Z2

Ru	-1.32991200	-0.36089500	-0.36139900
C	-3.38240000	0.38980800	-1.26757800
C	-3.45440300	0.63182700	0.13065700
C	-3.31413500	-0.42304900	1.05893700
C	-3.03692400	-1.73222200	0.57460200
C	-3.02492200	-2.00838800	-0.81803300
C	-3.14433500	-0.93425300	-1.73240700
H	-0.35178700	-0.36293400	-1.63410600
H	-3.48920500	1.20308100	-1.96709100

H	-2.90531900	-2.54205100	1.27679700
Si	0.68503500	-1.11770700	0.41555100
H	0.94330500	-2.76731000	0.69282100
C	2.50277200	-0.83803800	-0.15110800
C	3.27078200	-1.86428800	-0.72916200
C	3.07659800	0.44404200	-0.04618000
C	4.57179600	-1.62436100	-1.18031900
H	2.85001600	-2.85592600	-0.83585800
C	4.37785200	0.68477800	-0.49662900
H	2.50401400	1.26190700	0.37036600
C	5.12887400	-0.34850300	-1.06263800
H	5.14440100	-2.42825100	-1.62487200
H	4.79830400	1.67811700	-0.40956800
H	6.13524400	-0.16028600	-1.41332100
C	-0.38231000	1.47098500	0.02909000
C	-0.27851000	1.96906200	1.34981900
C	0.03955900	2.33572800	-1.00709500
C	0.19690700	3.25961900	1.61737700
H	-0.56388900	1.33519300	2.17985800
C	0.51231700	3.62618100	-0.74275200
H	-0.00570000	1.99284900	-2.03150100
C	0.59419000	4.09732000	0.57161900
H	0.25771600	3.60600000	2.64281900

H	0.81843900	4.26244800	-1.56520000
H	0.96162800	5.09510100	0.77587000
N	1.18307000	-1.14583400	2.38050400
H	2.11903600	-0.77384400	2.52602000
C	1.11842900	-2.49977900	2.35688400
H	0.14423800	-2.95412600	2.47594500
H	1.97088400	-3.13099600	2.59347500
H	-3.08305900	-1.12435400	-2.79284800
H	-3.60181500	1.64023000	0.48633800
H	-3.37016700	-0.23189700	2.11896700
H	-2.86494800	-3.01363600	-1.17511000

Sum of electronic and zero-point Energies = -1174.354106
Sum of electronic and thermal Energies = -1174.332520
Sum of electronic and thermal Enthalpies = -1174.331576
Sum of electronic and thermal Free Energies = -1174.408052

C'

Ru	-1.14783600	-0.57751700	-0.37458600
C	-3.49804000	-0.75440200	-1.05339700
C	-3.46542300	-0.43139800	0.34096300
C	-2.77934700	-1.24655900	1.26256400
C	-1.98126600	-2.32491100	0.77378600
C	-1.96827900	-2.62492100	-0.62304000

C	-2.76658200	-1.85257000	-1.53234900
H	-3.99759200	0.44011600	0.69159200
H	-2.80546800	-1.01936800	2.31733800
H	-1.39264400	-3.46028400	-0.98721900
H	-2.77419900	-2.10051500	-2.58259600
H	0.02456500	-0.86856100	-1.43268600
C	-0.04263200	1.50744600	0.26288200
C	-0.41983200	1.78460700	-1.08289800
C	-0.64259100	2.29819500	1.28913700
C	-1.36615300	2.80367100	-1.36965100
H	0.12534900	1.34276800	-1.90316800
C	-1.53171100	3.31302600	0.99260000
H	-0.37150300	2.09767600	2.31896900
C	-1.91123200	3.55947800	-0.34919900
H	-1.63431500	3.00131600	-2.39995500
H	-1.93999400	3.92804000	1.78513600
H	-2.61514600	4.35126600	-0.57176500
C	2.66149800	-0.14774200	-0.14712500
C	3.39878400	-1.34621600	-0.19145400
C	3.23964100	0.99980000	-0.71863900
C	4.66127400	-1.39882600	-0.78670400
H	2.98126200	-2.24870700	0.23877300
C	4.50300400	0.95276400	-1.31738300

H	2.69876200	1.93727200	-0.69449500
C	5.21669500	-0.24717000	-1.35300700
H	5.20856100	-2.33267800	-0.81091700
H	4.92759900	1.84952300	-1.75063000
H	6.19435100	-0.28589500	-1.81583400
Si	0.93164200	-0.09711200	0.65130600
C	2.34746200	-0.25458300	3.19286400
H	2.25080600	0.56877400	3.91024600
H	2.58527500	-1.16457800	3.75293800
H	3.19950700	-0.03363800	2.55167100
N	1.14503100	-0.42276500	2.37127300
H	0.33312600	-0.73354800	2.88252200
H	-4.05802000	-0.13166500	-1.73391200
H	-1.42535100	-2.94577200	1.45886800

Sum of electronic and zero-point Energies = -1174.441927

Sum of electronic and thermal Energies = -1174.419972

Sum of electronic and thermal Enthalpies = -1174.419028

Sum of electronic and thermal Free Energies = -1174.495514

X

Ru	-0.33376200	-0.33827600	-0.00010400
C	1.32804400	0.98692300	1.23789800
C	1.11242100	1.64559400	-0.00038100
C	1.32853200	0.98620500	-1.23815400

C	1.63325500	-0.39908300	-1.22861700
C	1.83018300	-1.09312100	0.00059700
C	1.63282300	-0.39832300	1.22933400
H	0.83757400	2.69186300	-0.00074500
H	1.21097000	1.51498900	-2.17126600
H	2.09778900	-2.13695500	0.00096400
H	1.76358400	-0.92412400	2.16249200
H	-1.00825300	-1.42722600	-0.94503600
H	1.21008000	1.51627600	2.17063800
H	1.76433400	-0.92546100	-2.16140400
N	-2.17175400	0.54955400	-0.00014400
H	-2.12802400	1.57017200	-0.00050500
C	-3.37884900	0.07921100	0.00019300
H	-4.24707600	0.73036000	0.00008300
H	-3.52322900	-0.98967600	0.00058800
H	-1.00839100	-1.42738300	0.94454800

Sum of electronic and zero-point Energies = -421.789653

Sum of electronic and thermal Energies = -421.779734

Sum of electronic and thermal Enthalpies = -421.778789

Sum of electronic and thermal Free Energies = -421.826220

Y

Ru	0.43198200	0.05275700	-0.15410600
C	-1.66909500	1.08374200	-0.61820600

C	-1.39627900	1.23955400	0.74947500
C	-1.02484000	0.08544500	1.51691200
C	-1.09728300	-1.22624900	0.94497000
C	-1.42759500	-1.38110600	-0.42418000
C	-1.61312800	-0.22011400	-1.21459100
H	-1.40517600	2.21682900	1.20688400
H	-0.76870000	0.19522600	2.55919300
H	-1.43900900	-2.35830200	-0.87969000
H	-1.77507300	-0.31947500	-2.27650100
H	-1.86437200	1.94449100	-1.23884100
H	-0.86612400	-2.08748200	1.55143800
N	2.21055700	0.74020200	-0.11843400
H	2.72069300	1.48880600	0.33870500
C	2.44505400	-0.64470400	0.05778600
H	2.72892100	-1.00945900	1.04426200
H	2.88672800	-1.19277800	-0.76875000

Sum of electronic and zero-point Energies = -420.595142

Sum of electronic and thermal Energies = -420.586264

Sum of electronic and thermal Enthalpies = -420.585320

Sum of electronic and thermal Free Energies = -420.630121