Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

$[Ru^{II}(tpy)(bpy)Cl]^{+}$-Catalyzed Reduction of Carbon Dioxide. Mechanistic Insights by Carbon-13 Kinetic Isotope Effect

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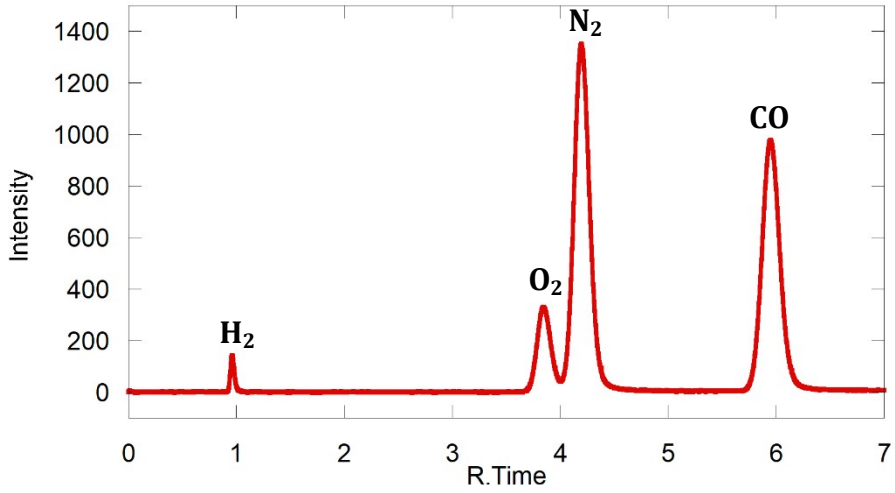
Procedure for Detection of CO by Gas Chromatography

One equivalent each of $[Ru(tpy)(bpy)Cl]PF_6$ and $Ru(bpy)_3Cl_2$ (concentration in runs ranged from 0.35 mM to 1.0 mM) was dissolved in 20 mL of a 5:1 mixture of acetonitrile and triethanolamine, in a 100 mL round bottom flask, which was sealed with a rubber septum and silicone grease. This solution was saturated with CO_2, and each reaction mixture was irradiated for 5 to 24 hours (150W, 21V Halogen lightbulb). After irradiation, a gas-tight syringe was used to extract a 50 µL portion of the headspace gas, which was then injected into the gas chromatograph. A typical GC spectrum is shown in Figure S1. Carbon monoxide was observed as the main gaseous product, but H_2 was also observed to form. This is consistent with observations of $[Ru(tpy)(bpy)Cl]PF_6$ being used to reduce CO_2 under electrocatalytic conditions, in which H_2 was produced, as long as there was a source of protons. In the electrochemical case, the proton source was dihydrogen phosphate, and in our photochemical case, the protons were most likely the result of the decomposition of triethanolamine molecules after donating an electron to the catalytic system.

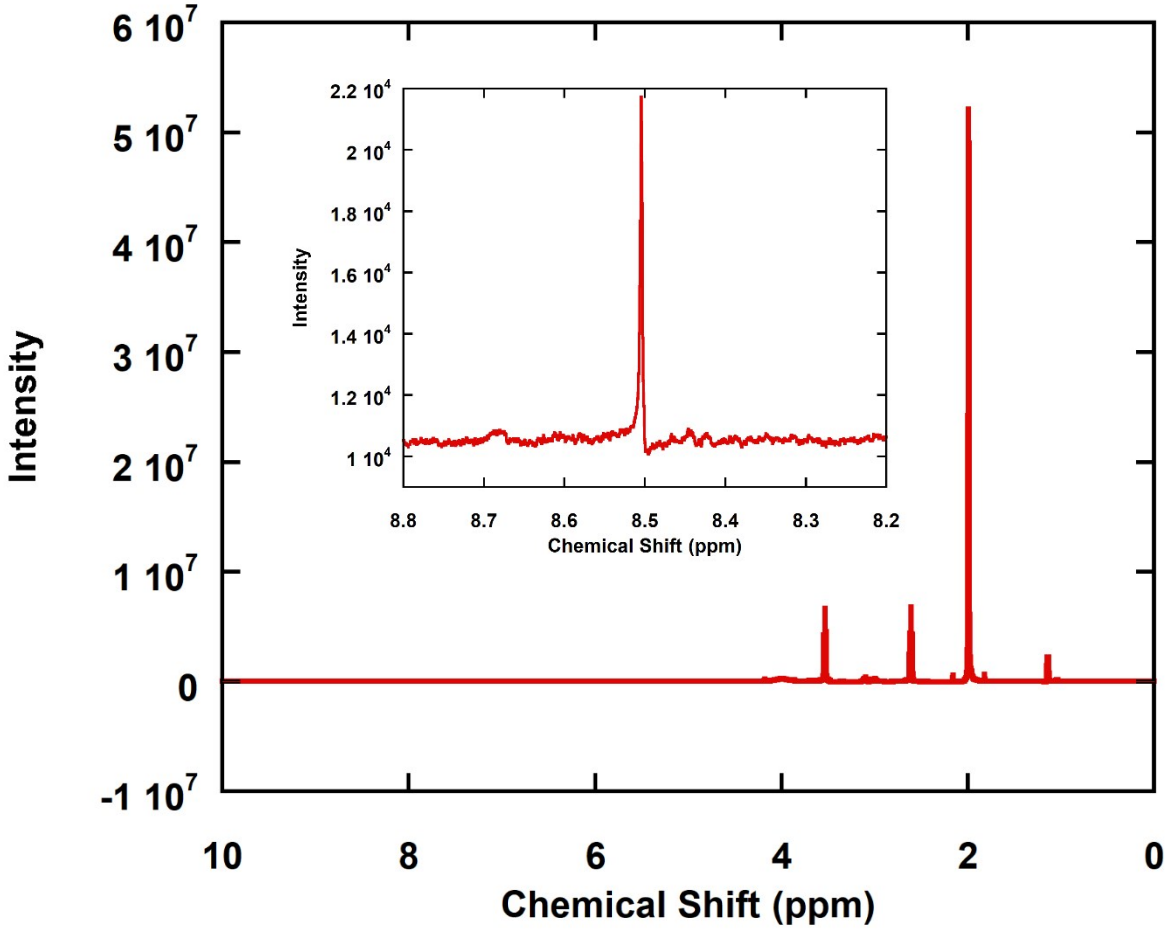
Figure S1. Typical gas chromatogram of the headspace over the 5:1 ACN/TEOA solution containing 1 equivalent each of $[Ru(tpy)(bpy)Cl]PF_6$ and $Ru(bpy)_3Cl_2$, and saturated with 100% CO_2. From earliest to latest, the peaks correspond to H_2, O_2, N_2, and CO.



Use of Verkade's Base and ^{1}H NMR to Detect the Production of Formate from CO_2

Due to the possibility that [Ru(tpy)(bpy)Cl]PF_6 may also be producing formate under photocatalytic conditions (as explained in the main body of the paper), we used a method recently described by Kubiak, involving Verkade's base (2,8,9-triisopropyl-2,5,8,9-tetraza-1-phosphabicyclo[3,3,3]undecane), to detect the presence of formate in solution. For each reaction mixture described above, after determining the species found in the headspace using GC, a 0.8 mL aliquot of the reaction mixture was transferred to a vial containing 0.1 mmol of Verkade's base. To this solution, 1.2 mL of CD_3CN was added, as well as a known amount of ferrocene, usually ranging from 8 to 15 mg. A 700 μL portion of this solution was transferred to an NMR tube, and ^{1}H NMR was performed. When formate is present, the Verkade's base produces a ^{1}H NMR peak at 8.5ppm, as is shown in Figure S2. The most prominent peaks belong to TEOA, due to the high amounts of this compound in the solution. The Verkade's base formate peak is extremely weak by comparison, and easy to miss if one is not expecting to find it. This is demonstrated in Figure S2, where the larger spectrum has the resolution automatically assigned by the NMR software, and the inset is the portion of the spectrum in which the relevant peak is found. As can been seen by comparing the differences in intensity of the two spectra, the Verkade's base formate has an intensity much smaller than the bulk of the reaction mixture.

Figure S2. Typical ^{1}H NMR spectrum used to determine formation of formate. Peaks in the range of 0 to 4 are from the high amounts of acetonitrile and TEOA present in the solution. The inset shows the formate peak, present at 8.50 ppm with an intensity much smaller than those of the solvents. The formate peak would only be visible when the reaction mixture was exposed to a quantity of Verkade's Base prescribed by P. L. Cheung *et al*. in *Inorg. Chem*., **2016**, *55*, 3192-3198.



Procedure for Calibration of Verkade's Base Formate Measurements

The Verkade's base measurements were calibrated by using ferrocene as an intensity standard. Known quantities of ferrocene were dissolved in reaction mixtures containing the same amounts of $[Ru(tpy)(bpy)Cl]PF_6$, $Ru(bpy)_3Cl_2$, and TEOA as described previously, except these mixtures contained no CO_2, and were not irradiated. The intensity of the ferrocene peak at 4.7 ppm was correlated with the amount of protons, based on the facts that the amount of ferrocene was known, and that there are ten protons for each ferrocene. Based on these values, a calibration curve was obtained, whereby the amount of formate produced could be determined based on the height of the characteristic 8.5 ppm peak. The calibration curve is presented in Figure S3, along with its respective linear equation.

Figure S3. Calibration curve using the peak height of the ^1H NMR of ferrocene to calibrate for the concentration of protons in a solution.

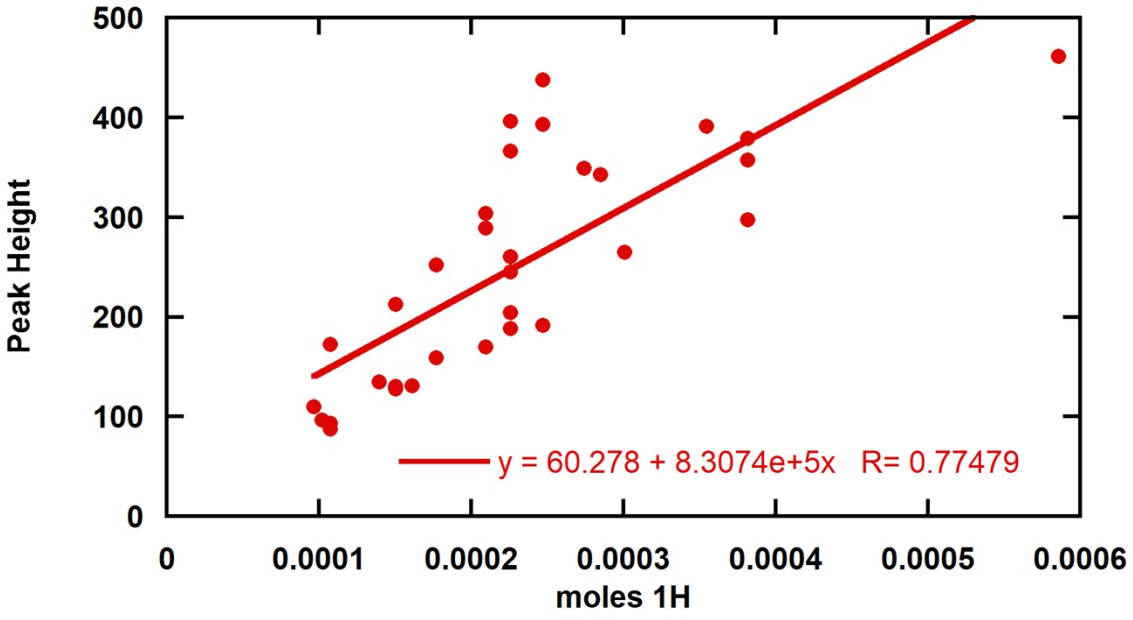


Figure S4. Product quantification and ^{13}C KIE determination in the photochemical reduction of CO_2 in solutions containing 1% H_2O. (A) CO (red circles) and formic acid (blue triangles) are formed during the photocatalytic reduction of CO_2 catalyzed by **1**. Data points are shown with error bars representing standard deviations from two measurements each. (B) Isotope fractionation of CO_2 during its reduction catalysed by **1**. Data points are shown with error bars representing standard errors. The slope of the plot indicates a ^{13}C KIE value of 1.037 ± 0.006. This value was corrected for partition of CO_2 due to CO_2 hydration leading to a ^{13}C KIE_{exp} = 1.044 ± 0.006 (O'Leary, Marion H. *Phytochemistry* **1981**, 20, 553-567).

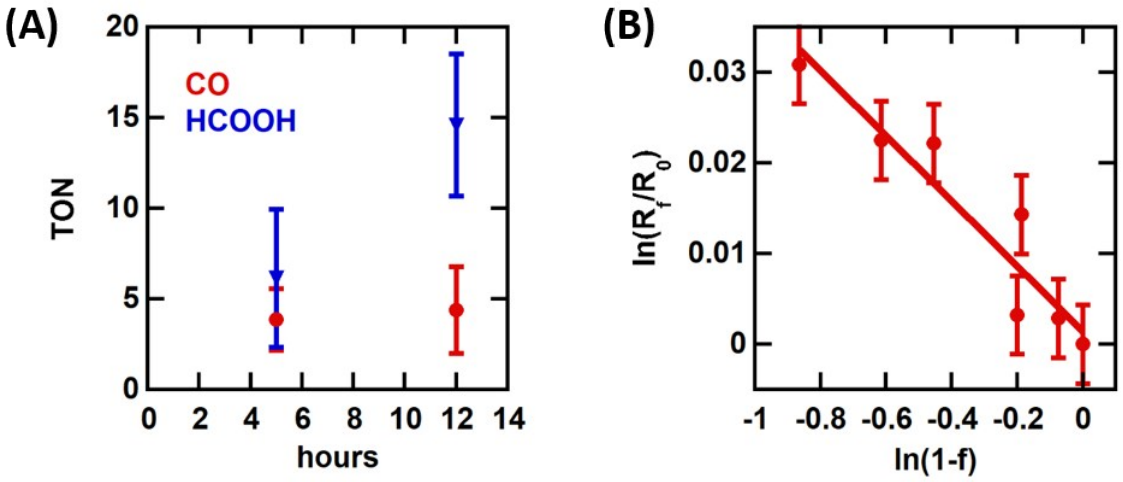


Table S1. Formic acid to carbon monoxide ratios obtained during the experiments. Values were determined from three independent experiments.

Water content	5 hours	12 hours
0%	3.9 ± 2.6	5.4 ± 4.6
1%	1.6 ± 1.2	3.3 ± 2.0

Table S2. Formic acid mole fractions. Values were determined from three independent experiments.

Water content	5 hours	12 hours
0%	0.80 ± 0.11	0.84 ± 0.11
1%	0.62 ± 0.18	0.77 ± 0.11

Computational Methods

Density functional theory calculations. All geometries were fully optimized at the M06 level of density functional theory[1] with the SMD continuum solvation model[2] for acetonitrile as solvent using the Stuttgart [8s7p6d2f | 6s5p3d2f] ECP28MWB contracted pseudopotential basis set[3] on Ru and the 6-31G(d) basis set on all other atoms.[4] Non-analytical integrals were evaluated using the integral=grid=ultrafine option as implemented in the Gaussian 09 software package.[5] The nature of all stationary points was verified by analytic computation of vibrational frequencies, which were also used for the computation of zero-point vibrational energies, molecular partition functions, and for determining the reactants and products associated with each transition-state structure (by following the normal modes associated with imaginary frequencies). Partition functions were used in the computation of 298 K thermal contributions to the free energy employing the usual ideal-gas, rigid-rotator, harmonic oscillator approximation.[6] Free-energy contributions were added to single-point, SMD-solvated M06 electronic energies computed at the optimized geometries obtained with the initial basis with the SDD basis set on Ru and the larger 6-311+G(2df,p) basis set on all other atoms to arrive at final, composite free energies. The quenching studies with TEOA have shown that the oxidized $TEOA^{\bullet+}$ rapidly deprotonates from its α-carbon to produce an α-amino radical[7] and TEOA itself could be the proton acceptor to generate $TEOAH^+$, which is employed as the proton donor species in the current work for modeling of the CO_2 reduction mechanism. The optimized structures and distinct pathways for mechanim of CO_2 reduction by $[Ru(tpy)(bpy)Cl]^+$ are presented in Table S1 and Scheme S1 respectively.

Standard reduction potentials were calculated for various possible redox couples to assess the energetic accessibility of different intermediates at various oxidation states. For a redox reaction of the form

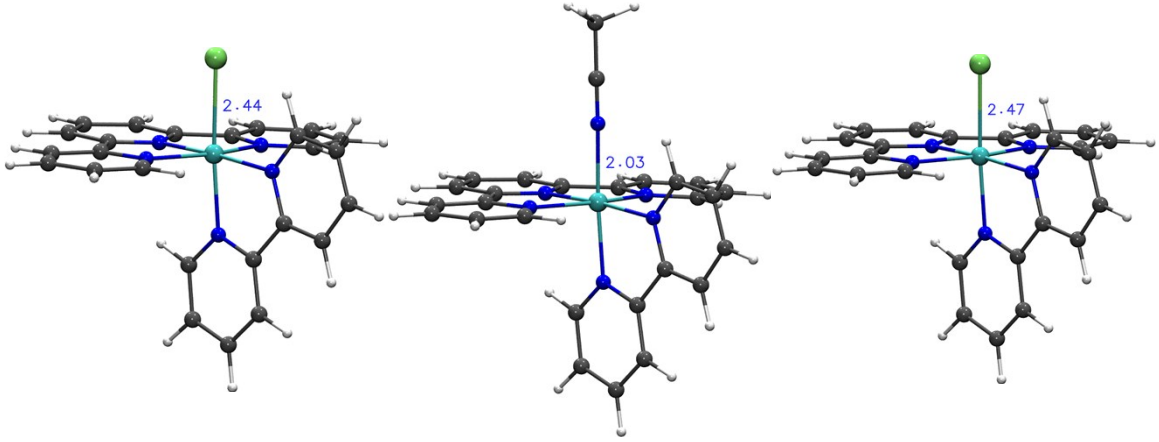
$$O_{(\mathrm{soln})} + n\,e^-_{(\mathrm{g})} \rightarrow R_{(\mathrm{soln})} \qquad (1)$$

where O and R denote the oxidized and reduced states of the redox couple, respectively, and n is the number of electrons involved in redox reaction, the reduction potential $E^{\mathrm{o}}_{O|R}$ relative to SCE was computed as

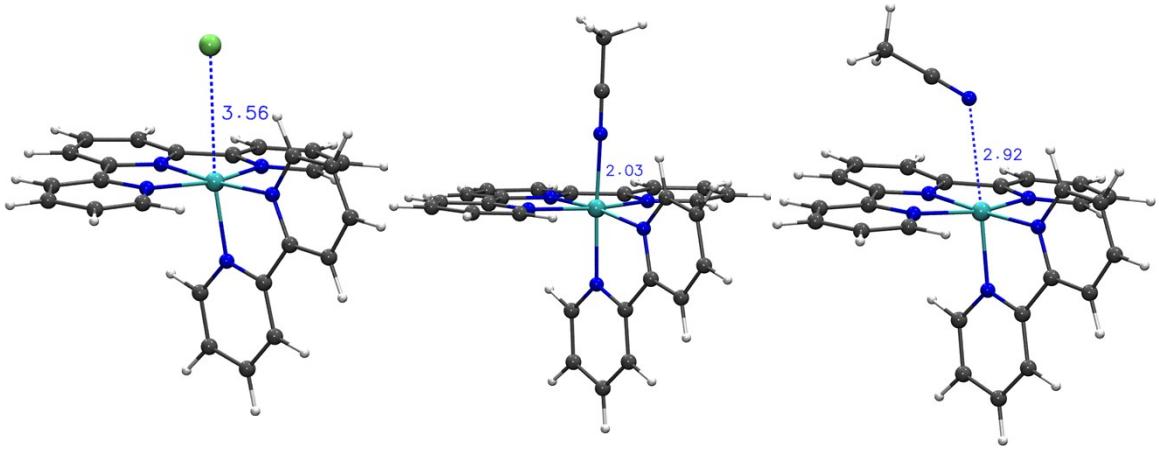
$$E^{o}_{O|R} = -\frac{\Delta G^{o}_{O|R}}{nF} - \Delta E^{o}_{ref} \qquad (2)$$

where $\Delta G^{o}_{O|R}$ is the free energy change associated with eq. 1 (using Boltzmann statistics for the electron) and ΔE^{o}_{ref} is taken as 0.141 V,[12] which is required for the conversion of calculated $E^{o}_{O|R}$ versus normal hydrogen electrode (NHE) in aqueous solution (E_{NHE} = -4.281 V) to $E^{o}_{O|R}$ versus the saturated calomel electrode (SCE) in acetonitrile (E_{SCE} = -4.422 V).[13]

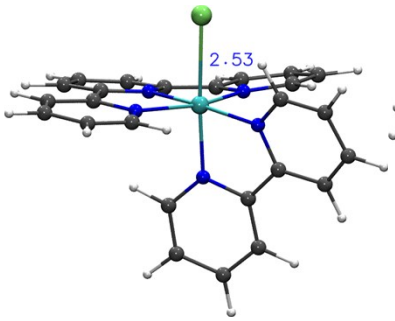
Table S3. Optimized structures at M06 level of theory for mechanistic investigation of photocatalytic CO_2 reduction by $[Ru(tpy)(bpy)Cl]^+$ (see computational methods for details) Color code: Ru, cyan; Cl, green; N, blue; O, red; C, gray; and H, white.



[Ru–Cl]$^+$ **[Ru–NCCH$_3$]$^{2+}$** **[Ru–Cl]^0**



[Ru–Cl]^{0} TS



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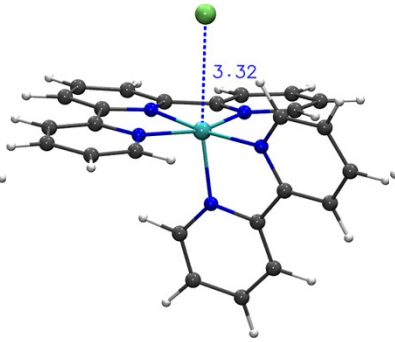
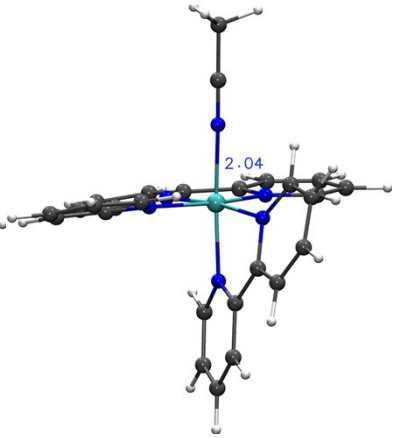


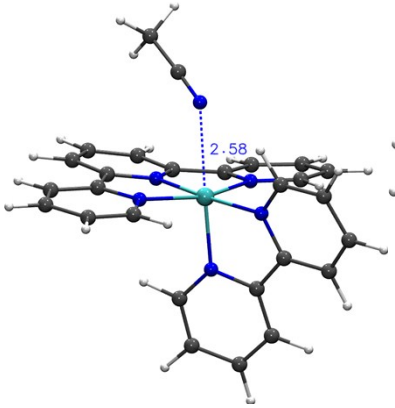
[Ru–NCCH$_3$]$^{+}$ TS



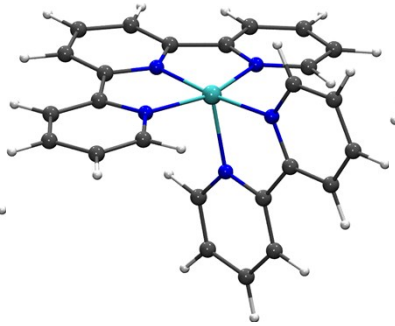
[Ru–Cl]$^{-}$

[Ru–Cl]$^{-}$ TS

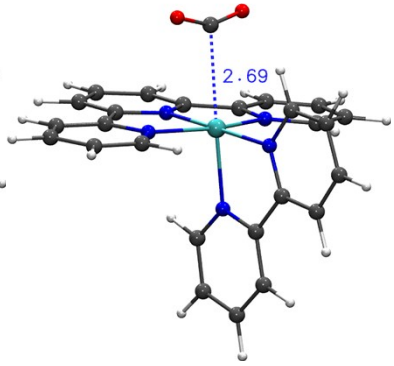
[Ru–NCCH$_3$]^{0}



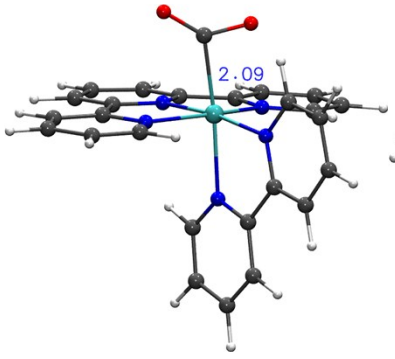
[Ru–NCCH$_3$]^{0} TS



[Ru]$^{+}$



[Ru]$^{+}$ CO_2 binding TS



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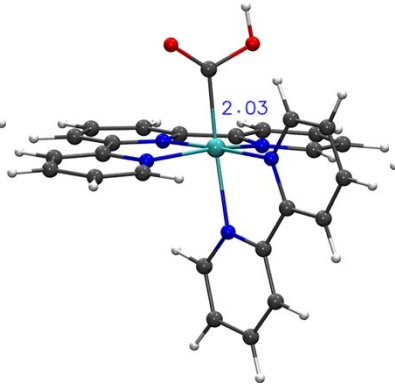
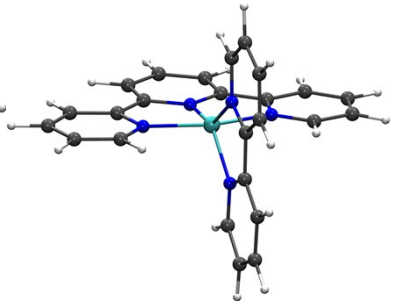
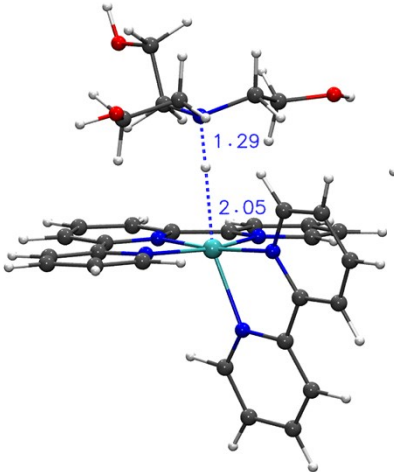


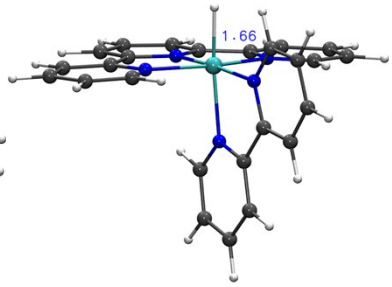
[Ru–CO_2H]$^{2+}$



[Ru]^{0}



[Ru]^{0} TEOAH^{+} PT TS



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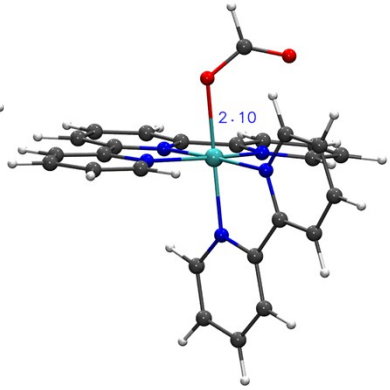

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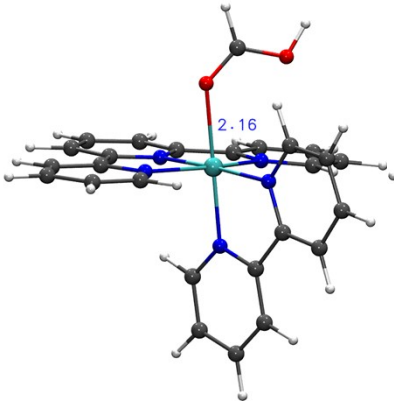

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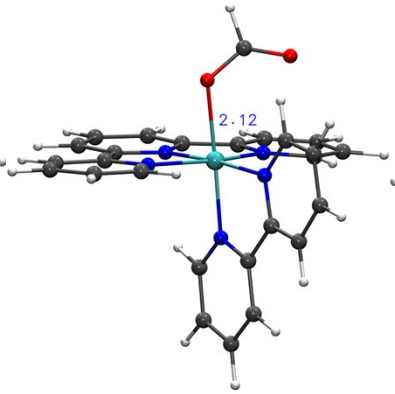

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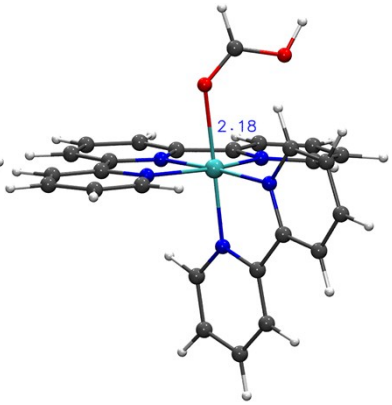

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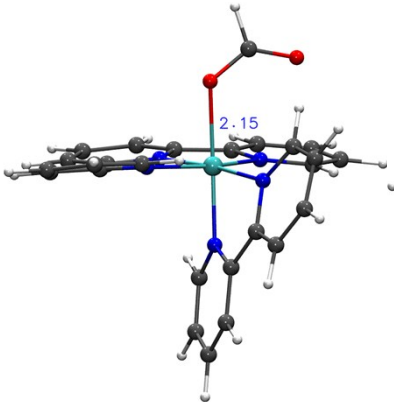

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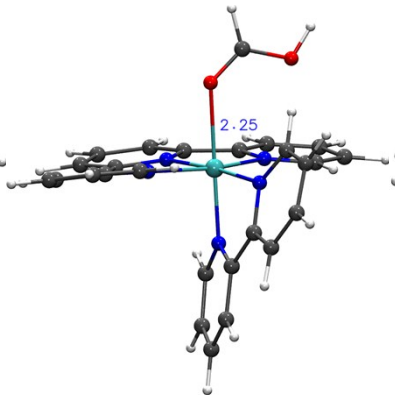

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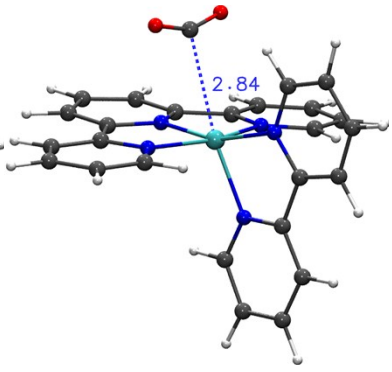
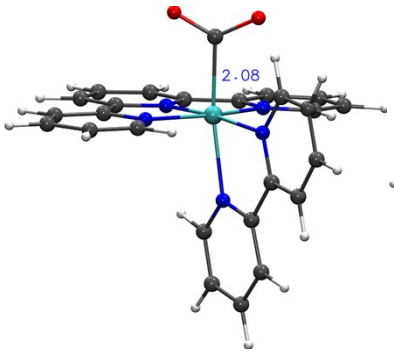


[Ru]^{0} CO_2 binding TS



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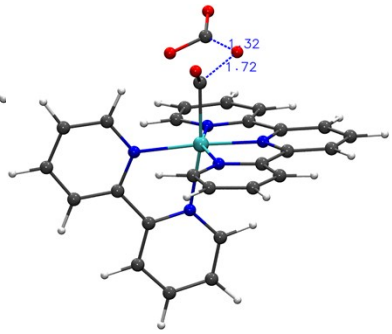

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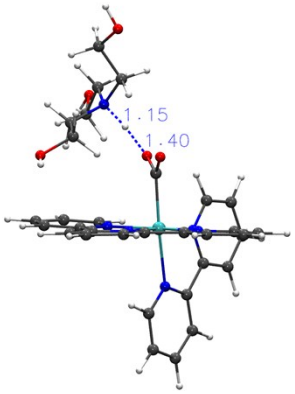

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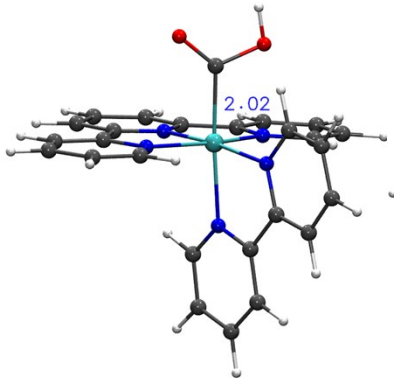

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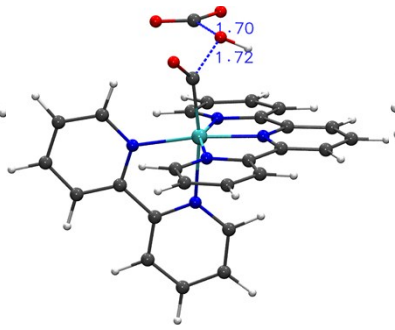
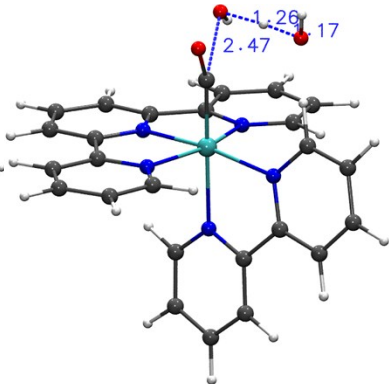
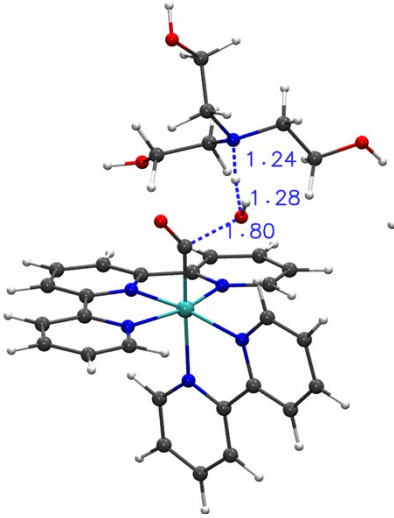


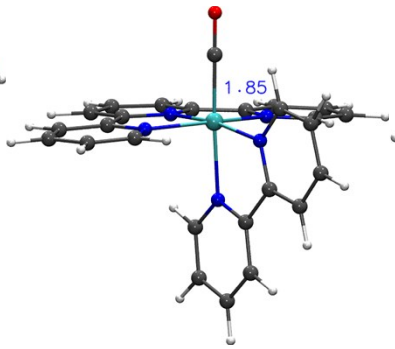
[Ru–CO_2H]$^+$ CO_2 attack TS



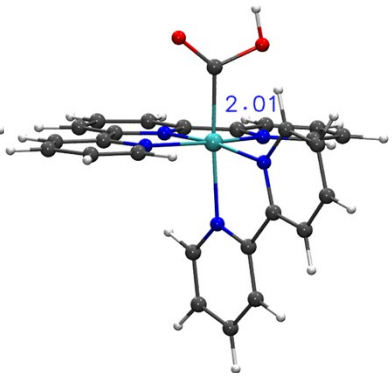
[Ru–CO_2H]$^+$ H_2O C–O bond cleavage TS



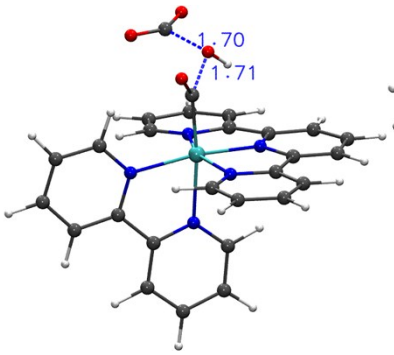
[Ru–CO_2H]$^+$ $TEOAH^+$ C–O bond cleavage TS



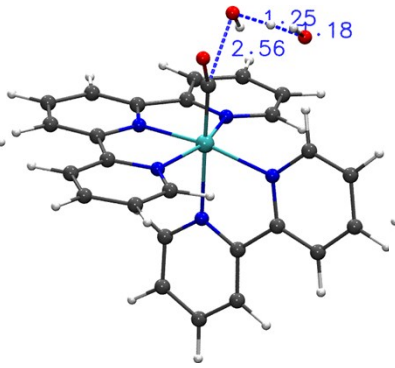
[Ru–CO]$^{2+}$



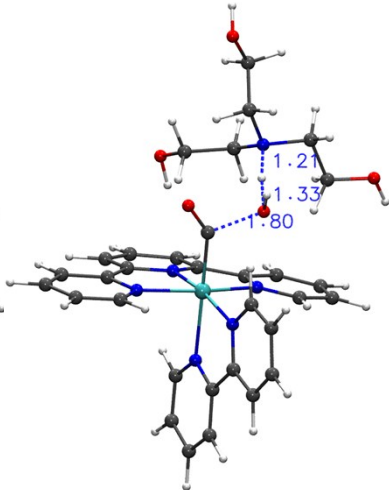
[Ru–CO_2H]^0



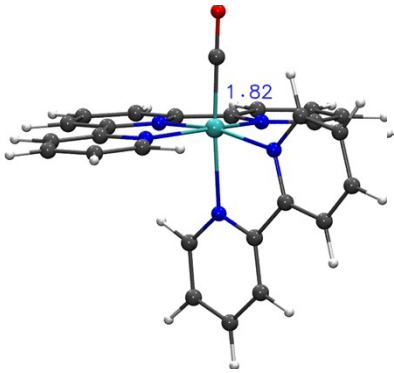
[Ru–CO_2H]^0 CO_2 attack TS



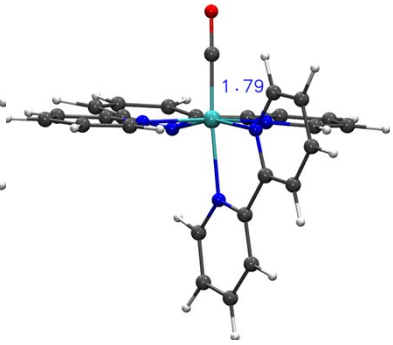
[Ru–CO_2H]^0 H_2O C–O bond cleavage TS



[Ru–CO_2H]^0 $TEOAH^+$ C–O bond cleavage TS

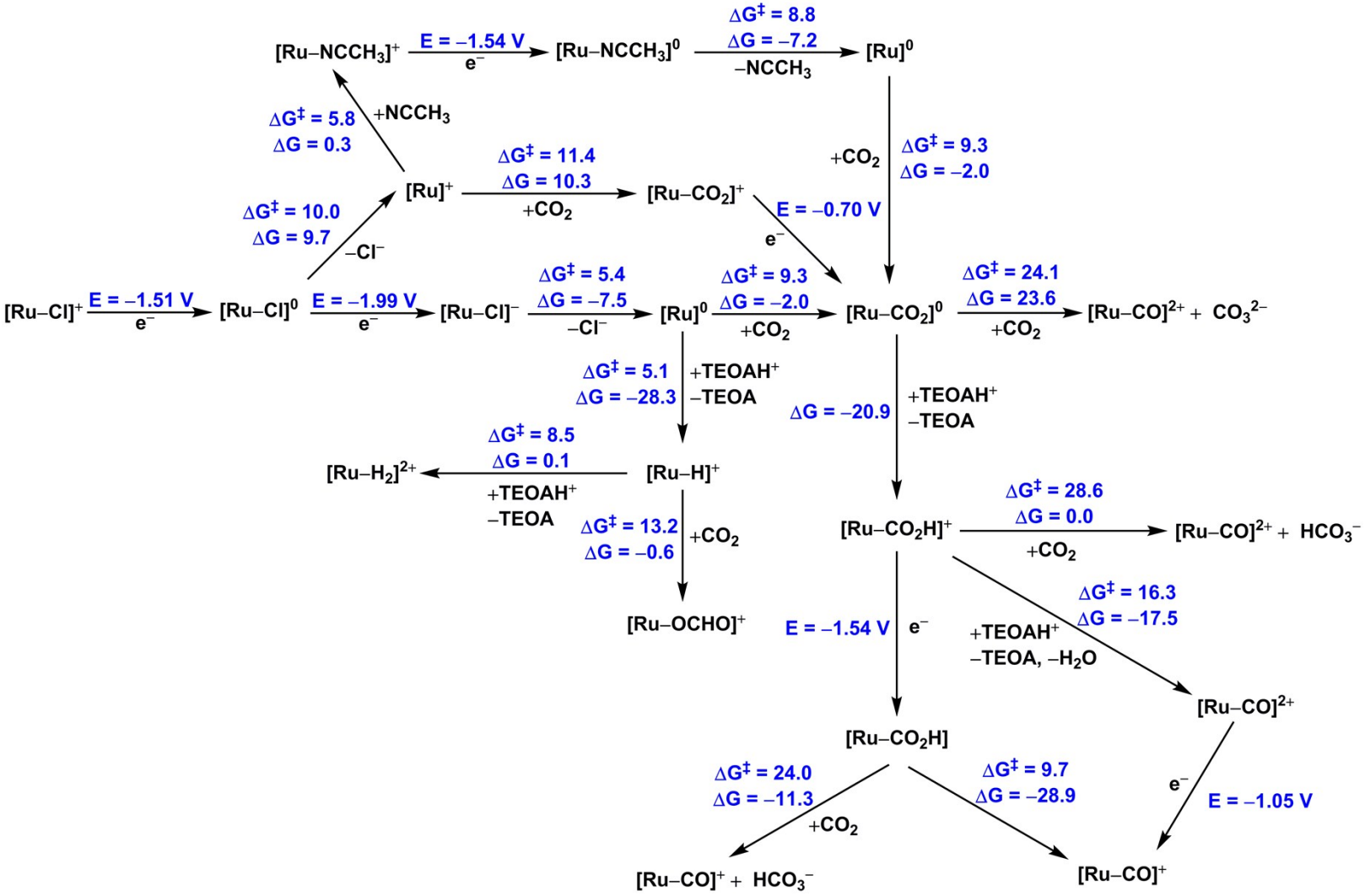


[Ru–CO]$^+$



[Ru–CO]^0

Scheme S1. Proposed reaction pathways for CO_2 reduction by $[Ru(tpy)(bpy)Cl]^+$. Computed free energy changes (ΔG) and activation free energies ($\Delta G^‡$) are reported in units of kcal/mol and computed reduction potentials (E) are repored in units of volts vs SCE.



Calculation of C-13 kinetic isotope effects (^{13}C-KIEs). The ^{13}C equilibrium and kinetic isotope effects were calculated by employing the Transition State Theory as formulated by Bigeleisen and Wolfsberg.[8] For each step of the catalytic mechanism, the vibrational frequencies of reactants and products were analyzed following the Bigeleisen and Goeppert-Mayer approach.[9] The Redlich-Teller product rule[10] was employed to isotope exchange equations (Eqn. S1) for the initial (A) and final (B) states using the full set of vibrational frequencies obtained for both light (^{12}C) and heavy (^{13}C) isotopologues via DFT calculations.

$$A(^{12}C) + B(^{13}C) \longrightarrow A(^{13}C) + B(^{12}C) \quad \text{(S1)}$$

^{13}C-EIEs for the exchange reactions were obtained using the $3N-6$ vibrational frequencies as

$$^{13}\text{C-EIE} = \text{ZPE} \times \text{EXC} \times \text{MMI} \quad \text{(S2)}$$

with

$$ZPE = \frac{\prod_{j}^{3N-6} \frac{exp(h\upsilon^{B(^{13}C)}_{j}/2kT)}{exp(h\upsilon^{B(^{12}C)}_{j}/2kT)}}{\prod_{i}^{3N-6} \frac{exp(h\upsilon^{A(^{13}C)}_{i}/2kT)}{exp(h\upsilon^{A(^{12}C)}_{i}/2kT)}} \quad \text{(S3)}$$

$$EXC = \frac{\prod_{j}^{3N-6} \frac{1-exp(-h\upsilon^{B(^{13}C)}_{j}/kT)}{1-exp(-h\upsilon^{B(^{12}C)}_{j}/kT)}}{\prod_{i}^{3N-6} \frac{1-exp(-h\upsilon^{A(^{13}C)}_{i}/kT)}{1-exp(-h\upsilon^{A(^{12}C)}_{i}/kT)}} \quad \text{(S4)}$$

$$MMI = VP = \frac{\prod_{j}^{3N-6} (\upsilon^{B(^{12}C)}_{j}/\upsilon^{B(^{13}C)}_{j})}{\prod_{i}^{3N-6} (\upsilon^{A(^{12}C)}_{i}/\upsilon^{A(^{13}C)}_{i})} \quad \text{(S5)}$$

where υ is the associated vibrational frequency, h is the Planck's constant, k is the Boltzmann constant and T is the temperature in Kelvin units.

The ^{13}C-KIEs associated with located transition state structures were calculated in a similar way,

$$^{13}\text{C-KIE} = \upsilon_{RC}^{13} \times \text{ZPE} \times \text{EXC} \times \text{VP} \tag{S6}$$

$$^{13}\text{C-KIE} = \upsilon_{RC}^{13} \times {}^{13}\text{K}_{\text{TS}} \tag{S7}$$

where υ_{RC}^{13} [10,11] is the ratio of the imaginary frequencies of the TSs associated with light (e.g. ^{12}C) and heavy (e.g. ^{13}C) isotopologues and $^{13}\text{K}_{\text{TS}}$ is the product of ZPE × EXC × VP with $3N-6$ vibrational frequencies for the reactant and $3N-7$ vibrational frequencies for the TS (S8-S10).

$$ZPE = \frac{\prod_{j}^{3N-7} \frac{exp(h\upsilon_{j}^{B(^{13}C)}/2kT)}{exp(h\upsilon_{j}^{B(^{12}C)}/2kT)}}{\prod_{i}^{3N-6} \frac{exp(h\upsilon_{i}^{A(^{13}C)}/2kT)}{exp(h\upsilon_{i}^{A(^{12}C)}/2kT)}} \tag{S8}$$

$$EXC = \frac{\prod_{j}^{3N-7} \frac{1-exp(-h\upsilon_{j}^{B(^{13}C)}/kT)}{1-exp(-h\upsilon_{j}^{B(^{12}C)}/kT)}}{\prod_{i}^{3N-6} \frac{1-exp(-h\upsilon_{i}^{A(^{13}C)}/kT)}{1-exp(-h\upsilon_{i}^{A(^{12}C)}/kT)}} \tag{S9}$$

$$MMI = VP = \frac{\prod_{j}^{3N-7} (\upsilon_{j}^{B(^{12}C)}/\upsilon_{j}^{B(^{13}C)})}{\prod_{i}^{3N-6} (\upsilon_{i}^{A(^{12}C)}/\upsilon_{i}^{A(^{13}C)})} \tag{S10}$$

The calculated ^{13}C-EIEs and ^{13}C-KIEs along with the reduced partition functions are tabulated in the following section.

Mechanistic Scenarios for First Irreversible Step in CO and HCO_2^- Formation

The following estimated ^{13}C-KIEs for different mechanistic scenarios are based on the assumption of equilibrium conditions at all steps before the first irreversible step.

i) CO_2 Binding to $[Ru]^+$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/ EIE	KIE
$[Ru]^+$ CO_2 binding TS (KIE_1)	1.032	0.9706	0.984	0.999	1.044	1.075

^{13}C–KIE = KIE_1 = 1.075

ii) CO_2 binding to $[Ru]^0$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/ EIE	KIE
$[Ru]^0$ CO_2 binding TS (KIE_2)	1.030	1.053	0.986	0.999	1.037	1.068

^{13}C–KIE = KIE_2 = 1.068

iii) Protonation of $[Ru–CO_2]^0$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/EIE	KIE
$[Ru–CO_2]^0$ (EIE_1)	-	1.021	0.984	1.030	1.034	-

$[Ru–CO_2]^0$ $TEOAH^+$ proton transfer TS (KIE_3)	1.001	0.998	1.000	1.002	1.000	1.001

$^{13}C–KIE = EIE_1 \times KIE_3 = (1.034 \times 1.001) = 1.035$

iv) CO_2 Attack to $[Ru–CO_2H]^+$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/EIE	KIE
$[Ru–CO_2]^0$ (EIE_1)	-	1.021	0.984	1.030	1.034	-
$[Ru–CO_2H]^+$ (EIE_2)	-	1.002	1.001	1.000	1.003	-
$[Ru–^{\square\square}CO_2H]^+$ CO_2 attack TS (KIE_{4a})	1.010	1.040	0.997	0.991	1.028	1.038
$[Ru–CO_2H]^+$ $^{\square\square}CO_2$ attack TS (KIE_{4b})	1.010	1.012	0.985	1.018	1.015	1.026

$^{13}C–KIE = ((EIE_1 \times EIE_2 \times KIE_{4a}) + KIE_{4b})/2 = (1.034 \times 1.003 \times 1.038) + 1.026)/2 = 1.051$

v) C–OH Bond Cleavage in $[Ru–CO_2H]^+$ Assisted by $TEOAH^+$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/EIE	KIE
$[Ru–CO_2]^0$ EIE_1	-	1.021	0.984	1.030	1.034	-
$[Ru–CO_2H]^+$ EIE_2	-	1.002	1.001	1.000	1.003	-
$[Ru–CO_2H]^+$ $TEOAH^+$ C–O bond cleavage TS (KIE_5)	1.005	1.033	0.995	0.997	1.025	1.030

$^{13}C–KIE = EIE_1 \times EIE_2 \times KIE_5 = 1.034 \times 1.003 \times 1.030 = 1.068$

vi) CO_2 Attack to $[Ru–CO_2H]^0$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/EIE	KIE
$[Ru–CO_2]^0$ EIE_1	-	1.021	0.984	1.030	1.034	-
$[Ru–CO_2H]^+$ EIE_2	-	1.002	1.001	1.000	1.003	-
$[Ru–CO_2H]^0$ EIE_3	-	1.003	1.000	1.000	1.003	-
$[Ru–^{\square\square}CO_2H]^+$ CO_2 attack TS (KIE_{6a})	1.010	1.037	0.998	0.991	1.026	1.036
$[Ru–CO_2H]^+$ $^{\square\square}CO_2$ attack TS (KIE_{6b})	1.010	1.014	0.985	1.018	1.016	1.027

$^{13}C–KIE = ((EIE_1 \times EIE_2 \times EIE_3 \times KIE_{6a}) + KIE_{6b})/2 = ((1.034 \times 1.003 \times 1.003 \times 1.036) + 1.027)/2 = 1.052$

vii) C–OH Bond Cleavage in $[Ru–CO_2H]^0$ Assisted by $TEOAH^+$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/EIE	KIE
$[Ru–CO_2]^0$ EIE_1	-	1.021	0.984	1.030	1.034	-
$[Ru–CO_2H]^+$ EIE_2	-	1.002	1.001	1.000	1.003	-
$[Ru–CO_2H]^0$ EIE_3	-	1.003	1.000	1.000	1.003	-
$[Ru–CO_2H]^0$ $TEOAH^+$ C–O bond cleavage TS (KIE_7)	1.003	1.034	0.993	0.999	1.026	1.029

$^{13}C–KIE = EIE_1 \times EIE_2 \times EIE_3 \times KIE_7 = 1.034 \times 1.003 \times 1.003 \times 1.029 = 1.070$

viii) Electrophilic Attack of CO_2 Binding to $[Ru–H]^+$ as the First Irreversible Step

	$^{13}\nu_{RC}$	ZPE	EXC	VP/ MMI	$^{13}K_{TS}$/ EIE	KIE
$[Ru–H]^+$ CO_2 attack TS (KIE_8)	1.029	1.039	0.989	0.999	1.026	1.055

^{13}C–KIE = KIE_8 = 1.055

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Cartesian Coordinates of Geometry Optimized Structures at M06 Level of Theory

H_2O

O	0.00000	0.00000	0.12363
H	0.00000	0.75829	-0.47609
H	0.00000	-0.75829	-0.47609

CO

C	-0.01997	-0.01155	2.26085
O	-0.11989	-0.01100	3.39372

CO_2

C	-3.57497	-0.41512	0.00000
O	-2.41031	-0.41512	0.00000
O	-4.73963	-0.41512	0.00000

HCO_2H

C	-1.39691	1.78311	0.00000
H	-2.50096	1.70464	0.00000
O	-0.79665	2.82429	-0.00000
O	-0.76841	0.60373	0.00001
H	-1.42467	-0.11760	0.00001

HCO_2^-

H	0.20585	-0.08179	2.08908
C	0.01946	0.66518	2.94133
O	1.04074	1.24846	3.35532
O	-1.17096	0.75923	3.29933

CH_3CN

C	0.00002	0.00007	-1.17678
H	-0.00004	1.02839	-1.55451
H	-0.89072	-0.51424	-1.55425
H	0.89074	-0.51429	-1.55422
C	0.00001	0.00042	0.27027
N	0.00000	-0.00036	1.43163

TEOA

O	-2.59138	1.31942	0.29942
H	-2.66274	0.49548	-0.21785
C	-1.37077	1.94118	-0.03596
H	-1.53474	2.71638	-0.80812
H	-1.00411	2.46018	0.86394
C	-0.28353	1.01893	-0.55195
H	-0.65754	0.46907	-1.43962
H	0.52730	1.66680	-0.91547
N	0.29311	0.11419	0.44046
C	-0.62298	-0.88324	0.99129
H	-0.06783	-1.44882	1.75319
H	-1.44205	-0.36662	1.50846
C	-1.22580	-1.88524	0.02054
H	-1.60104	-2.75305	0.58815
H	-0.45596	-2.25734	-0.67675
C	1.53325	-0.47264	-0.05233
H	1.71569	-1.42403	0.46811
H	1.48898	-0.71059	-1.13470
C	2.71853	0.43655	0.20204
H	2.54544	1.43093	-0.24748
H	2.82434	0.59054	1.29045
O	-2.29320	-1.27274	-0.69424
H	-2.61330	-1.88850	-1.37102
O	3.85670	-0.18488	-0.35402
H	4.61659	0.39267	-0.19557

$TEOAH^+$

O	2.67604	-1.15345	0.26753
H	2.73978	-0.39599	-0.34419
C	1.52019	-1.88630	-0.04763
H	1.71704	-2.63019	-0.83947
H	1.23652	-2.45210	0.85229
C	0.33623	-1.08040	-0.53607
H	0.58876	-0.45400	-1.39757
H	-0.45699	-1.77592	-0.82818
N	-0.26610	-0.16078	0.49974
C	0.67086	0.89350	1.04947
H	0.11262	1.39709	1.84516
H	1.51905	0.35946	1.48565
C	1.13965	1.91234	0.04370
H	1.62915	2.71149	0.62115
H	0.29179	2.37048	-0.48802
C	-1.54872	0.44428	0.01314
H	-1.80866	1.25242	0.70617
H	-1.36341	0.87264	-0.97838
C	-2.68802	-0.55458	-0.02158
H	-2.54710	-1.29570	-0.82357
H	-2.72947	-1.10512	0.93647
O	2.04780	1.31430	-0.86624
H	2.37579	1.99881	-1.47118
O	-3.84204	0.21859	-0.23468
H	-4.57529	-0.38595	-0.42508
H	-0.50244	-0.75047	1.31147

$[Ru–Cl]^+$

Ru	0.17120	-0.00959	0.37722
C	0.67147	-3.05695	0.38880
C	-1.54785	-2.34484	0.36627
C	-1.99454	-3.66157	0.36470
C	-1.06872	-4.69662	0.37435
C	0.28696	-4.39042	0.38687
H	1.72186	-2.76868	0.40420
H	-3.06081	-3.87464	0.35685
H	-1.40458	-5.73089	0.37321
H	1.04568	-5.16863	0.39709
C	-2.44615	-1.18209	0.35605
C	-3.83731	-1.20019	0.35659
C	-4.52314	0.01074	0.34511
H	-4.38082	-2.14147	0.36938
C	-2.43532	1.18459	0.34127
C	-3.82626	1.21533	0.34057
H	-5.61046	0.01574	0.34493

H	-4.36106	2.16166	0.34067
C	-1.52722	2.33969	0.33940
C	-1.96343	3.65992	0.32879
C	0.69754	3.03431	0.35332
C	-1.02954	4.68770	0.32913
H	-3.02800	3.88144	0.32147
C	0.32364	4.37072	0.34179
H	1.74578	2.73851	0.36963
H	-1.35715	5.72457	0.32109
H	1.08862	5.14285	0.34526
N	-0.21354	-2.05109	0.37650
N	-1.78966	-0.00175	0.33617
N	-0.19529	2.03520	0.35004
C	1.80285	-0.04133	-2.04989
C	2.13129	-0.07062	-3.40339
C	1.12206	-0.08886	-4.35400
C	-0.20261	-0.07772	-3.93006
C	-0.46911	-0.05065	-2.57168
H	3.17320	-0.08053	-3.71276
H	1.36770	-0.11170	-5.41303
H	-1.02721	-0.09061	-4.63790
H	-1.49195	-0.04250	-2.19955
C	2.79062	-0.01922	-0.96783
C	4.16792	-0.00645	-1.17572
C	3.09752	0.00657	1.33680
C	5.02172	0.01153	-0.08302
H	4.57003	-0.00985	-2.18515
C	4.47605	0.01712	1.19655
H	2.61709	0.01232	2.31422
H	6.09912	0.02126	-0.23029
H	5.10550	0.03049	2.08259
N	0.50403	-0.03329	-1.64346
N	2.26307	-0.01056	0.28419
Cl	0.04016	0.00816	2.81562

$[Ru–NCCH_3]^{2+}$

Ru	0.19368	-0.00518	0.42840
C	0.69521	-3.06039	0.41571
C	-1.52559	-2.34944	0.40426
C	-1.97169	-3.66508	0.39024
C	-1.04423	-4.69988	0.38818
C	0.31048	-4.39438	0.39963
H	1.74531	-2.77229	0.42966
H	-3.03747	-3.87955	0.37973
H	-1.38002	-5.73401	0.37696
H	1.06936	-5.17230	0.39764
C	-2.42965	-1.18787	0.39712
C	-3.82064	-1.21271	0.38214
C	-4.50906	-0.00342	0.36209
H	-4.36186	-2.15507	0.38563
C	-2.42854	1.17947	0.37611
C	-3.81947	1.20538	0.35884
H	-5.59629	-0.00303	0.34896
H	-4.35975	2.14817	0.34340
C	-1.52321	2.33998	0.36160
C	-1.96789	3.65571	0.32697
C	0.69849	3.04817	0.34661
C	-1.03923	4.68907	0.29933
H	-3.03349	3.87124	0.31887
C	0.31518	4.38211	0.30681
H	1.74825	2.75875	0.35925
H	-1.37390	5.72325	0.27097
H	1.07488	5.15889	0.28431
N	-0.19108	-2.05706	0.41930
N	-1.78428	-0.00447	0.38928
N	-0.18898	2.04630	0.37585
C	1.79305	-0.02750	-2.02108
C	2.11283	-0.02698	-3.37614
C	1.09535	-0.02690	-4.31893
C	-0.22585	-0.02684	-3.88722
C	-0.48222	-0.02433	-2.52593
H	3.15190	-0.02495	-3.69462
H	1.33381	-0.02666	-5.37983
H	-1.05492	-0.02742	-4.58963
H	-1.50270	-0.02252	-2.14750
C	2.79079	-0.03036	-0.94609
C	4.16531	-0.05102	-1.16635
C	3.12100	-0.01235	1.35593
C	5.02968	-0.05004	-0.08154
H	4.55762	-0.06967	-2.17912
C	4.49812	-0.02928	1.20324
H	2.66168	0.00141	2.34208
H	6.10536	-0.06586	-0.23947
H	5.13600	-0.02755	2.08305
N	0.49774	-0.02380	-1.60746
N	2.27775	-0.01321	0.31114
N	0.07333	0.01951	2.45309
C	-0.04326	0.03711	3.60562
C	-0.17206	0.05929	5.04307
H	0.27989	-0.84149	5.47328
H	0.33434	0.94180	5.44994
H	-1.23062	0.09501	5.32357

$[Ru–Cl]^{0}$

Ru	0.16333	-0.00966	0.39721
C	0.67289	-3.05302	0.40871
C	-1.54780	-2.34428	0.37191
C	-1.99111	-3.66341	0.36580
C	-1.06436	-4.69672	0.38075
C	0.29164	-4.38680	0.40308
H	1.72208	-2.75972	0.43047
H	-3.05722	-3.87817	0.35010
H	-1.39791	-5.73186	0.37587
H	1.05180	-5.16382	0.41653
C	-2.44732	-1.18408	0.35511
C	-3.83852	-1.20110	0.33310
C	-4.52549	0.00968	0.30936
H	-4.38201	-2.14286	0.33617
C	-2.43650	1.18508	0.33592
C	-3.82755	1.21425	0.31245
H	-5.61276	0.01450	0.29129
H	-4.36230	2.16090	0.29924

C	-1.52737	2.33761	0.33839
C	-1.96007	3.66025	0.31980
C	0.69886	3.02903	0.37067
C	-1.02527	4.68626	0.32560
H	-3.02445	3.88337	0.30208
C	0.32824	4.36559	0.35218
H	1.74575	2.72802	0.39665
H	-1.35049	5.72395	0.31100
H	1.09464	5.13656	0.35933
N	-0.21289	-2.04626	0.39122
N	-1.78676	-0.00247	0.34565
N	-0.19481	2.02891	0.36136
C	1.81293	-0.03477	-2.02662
C	2.11412	-0.05756	-3.41655
C	1.11169	-0.07753	-4.34985
C	-0.23985	-0.07496	-3.92376
C	-0.48895	-0.05275	-2.56592
H	3.15577	-0.06167	-3.73334
H	1.35411	-0.09580	-5.41134
H	-1.06589	-0.08971	-4.62983
H	-1.51345	-0.05030	-2.19023
C	2.77376	-0.01699	-0.98555
C	4.18188	-0.00647	-1.18133
C	3.12234	0.00164	1.34282
C	5.03193	0.00631	-0.10542
H	4.57997	-0.00740	-2.19442
C	4.49836	0.00955	1.20436
H	2.65090	0.00563	2.32708
H	6.10975	0.01449	-0.26200
H	5.13639	0.01910	2.08441
N	0.47506	-0.03251	-1.62962
N	2.26687	-0.01051	0.30914
Cl	0.04704	0.00957	2.85992

[Ru–Cl]^{0} TS

Ru	0.14625	-0.01961	0.25474
C	0.62760	-3.07051	0.24487
C	-1.59651	-2.34960	0.40522
C	-2.03496	-3.67798	0.39089
C	-1.11776	-4.70774	0.30419
C	0.24552	-4.39664	0.22580
H	1.67765	-2.78286	0.19169
H	-3.10060	-3.89175	0.44304
H	-1.45230	-5.74269	0.29331
H	1.00227	-5.17418	0.15642
C	-2.47693	-1.19776	0.48052
C	-3.86068	-1.20056	0.60104
C	-4.54693	0.01389	0.65196
H	-4.40646	-2.14015	0.65928
C	-2.46299	1.19648	0.44725
C	-3.84688	1.21831	0.57048
H	-5.62956	0.02132	0.75351
H	-4.38207	2.16510	0.60786
C	-1.56929	2.33481	0.33929
C	-1.99361	3.66651	0.27649
C	0.66329	3.02788	0.16841
C	-1.06573	4.68366	0.16258
H	-3.05748	3.89212	0.31043
C	0.29490	4.35623	0.10381
H	1.71076	2.72891	0.13064
H	-1.38984	5.72088	0.11464
H	1.05997	5.12339	0.01359
N	-0.25226	-2.05126	0.34039
N	-1.80303	-0.00510	0.42262
N	-0.22710	2.02035	0.29299
C	1.89330	-0.00950	-2.09803
C	2.26357	0.00199	-3.44124
C	1.28371	-0.01410	-4.42164
C	-0.05483	-0.04236	-4.03681
C	-0.36520	-0.05024	-2.68827
H	3.31621	0.02232	-3.71380
H	1.55954	-0.00549	-5.47343
H	-0.85675	-0.05761	-4.77053
H	-1.39699	-0.07133	-2.33983
C	2.83026	-0.00458	-0.97685
C	4.21810	0.01389	-1.09932
C	2.98775	-0.02990	1.34730
C	4.99812	0.01101	0.04697
H	4.68155	0.03012	-2.08278
C	4.37176	-0.01294	1.29172
H	2.43483	-0.04995	2.29018
H	6.08302	0.02615	-0.02859
H	4.94690	-0.01811	2.21420
N	0.58111	-0.03238	-1.73036
N	2.22532	-0.02288	0.23886
Cl	0.12926	-0.14427	3.81710

[Ru–NCCH$_3$]$^{+}$

Ru	0.19622	-0.00197	0.44167
C	0.70635	-3.05163	0.60071
C	-1.51659	-2.33670	0.40013
C	-1.95445	-3.66627	0.43520
C	-1.03244	-4.69157	0.55200
C	0.32748	-4.38556	0.63834
H	1.75404	-2.75717	0.66434
H	-3.01833	-3.88559	0.38134
H	-1.36854	-5.72598	0.58014
H	1.08329	-5.16117	0.72783
C	-2.41366	-1.19577	0.30073
C	-3.81625	-1.22447	0.12604
C	-4.48951	-0.01044	0.02877
H	-4.35202	-2.16691	0.04983
C	-2.41604	1.18473	0.27491
C	-3.81883	1.20658	0.10023
H	-5.56881	-0.01310	-0.11625
H	-4.35673	2.14608	0.00470
C	-1.52117	2.32891	0.34782
C	-1.96134	3.65829	0.34907
C	0.70011	3.05209	0.53685
C	-1.04136	4.68755	0.44432
H	-3.02540	3.87413	0.28560
C	0.31889	4.38593	0.54253

H	1.74814	2.76093	0.60952
H	-1.37911	5.72180	0.44623
H	1.07316	5.16472	0.61601
N	-0.17278	-2.05018	0.47761
N	-1.78264	-0.00418	0.36029
N	-0.17682	2.04644	0.43463
C	1.74034	-0.02476	-2.03300
C	2.02429	-0.01837	-3.40807
C	0.99573	-0.01201	-4.32604
C	-0.32812	-0.01141	-3.86478
C	-0.55348	-0.01290	-2.50212
H	3.05764	-0.01489	-3.74614
H	1.21235	-0.00658	-5.39203
H	-1.17154	-0.00758	-4.54994
H	-1.56813	-0.00920	-2.10583
C	2.75144	-0.03602	-0.99769
C	4.13178	-0.06889	-1.24644
C	3.15470	-0.02063	1.30393
C	5.02091	-0.07445	-0.19073
H	4.49883	-0.09356	-2.26939
C	4.52435	-0.04816	1.11816
H	2.72229	-0.00307	2.30329
H	6.09224	-0.10014	-0.37778
H	5.18694	-0.05088	1.97961
N	0.43956	-0.01812	-1.59232
N	2.27578	-0.01520	0.28600
N	0.12099	0.02126	2.46840
C	0.03392	0.03779	3.62433
C	-0.06138	0.05924	5.06532
H	0.41722	-0.83210	5.48645
H	0.43802	0.95105	5.46060
H	-1.11307	0.07583	5.37205

$[Ru–NCCH_3]^+$ TS

Ru	0.41475	0.07606	0.35507
C	0.85829	-2.98161	0.40623
C	-1.33302	-2.22167	0.75395
C	-1.78730	-3.54440	0.81701
C	-0.89508	-4.58930	0.67662
C	0.45986	-4.30138	0.46284
H	1.90145	-2.71172	0.24207
H	-2.84724	-3.74067	0.96615
H	-1.24265	-5.61891	0.72439
H	1.19638	-5.09218	0.34437
C	-2.18699	-1.05557	0.87945
C	-3.54558	-1.03218	1.17745
C	-4.20144	0.19343	1.28840
H	-4.09017	-1.96069	1.33853
C	-2.14248	1.33592	0.79925
C	-3.49751	1.38585	1.09851
H	-5.26164	0.22215	1.52850
H	-4.00668	2.34274	1.19462
C	-1.24600	2.45999	0.58617
C	-1.65184	3.79810	0.56090
C	0.96697	3.11210	0.17338
C	-0.72285	4.79846	0.34514
H	-2.70160	4.04361	0.70728
C	0.61729	4.44690	0.14325
H	1.99788	2.79344	0.01950
H	-1.03205	5.84109	0.32697
H	1.38147	5.19980	-0.03261
N	0.00485	-1.94606	0.55614
N	-1.51284	0.12410	0.70170
N	0.07733	2.12207	0.39867
C	1.83822	-0.06936	-2.19019
C	2.03019	-0.16098	-3.56697
C	0.93160	-0.20596	-4.41103
C	-0.34563	-0.15961	-3.85740
C	-0.47880	-0.07182	-2.48290
H	3.03878	-0.19682	-3.97143
H	1.06917	-0.27686	-5.48729
H	-1.23650	-0.19164	-4.47925
H	-1.45668	-0.03560	-2.00564
C	2.91490	-0.01175	-1.20398
C	4.27359	-0.01279	-1.51276
C	3.38489	0.10526	1.07148
C	5.20156	0.04633	-0.48448
H	4.60053	-0.05762	-2.54885
C	4.74902	0.10555	0.83207
H	2.97833	0.15215	2.08159
H	6.26615	0.04652	-0.70667
H	5.44255	0.15233	1.66773
N	0.58462	-0.02683	-1.65740
N	2.47789	0.04832	0.08112
N	0.15515	0.12890	3.25893
C	-0.79722	-0.22368	3.82659
C	-1.99769	-0.66330	4.50478
H	-2.13354	-1.74218	4.36449
H	-1.92918	-0.45089	5.57770
H	-2.87001	-0.13897	4.09520

$[Ru–Cl]^-$

Ru	0.20964	-0.18218	0.39470
C	0.50439	-3.27950	0.54238
C	-1.66874	-2.42682	0.52724
C	-2.18840	-3.71743	0.63354
C	-1.33078	-4.80418	0.69498
C	0.04669	-4.58186	0.64443
H	1.57079	-3.05420	0.50877
H	-3.26626	-3.86220	0.67144
H	-1.72832	-5.81335	0.77959
H	0.75785	-5.40296	0.69227
C	-2.48770	-1.21564	0.41508
C	-3.86254	-1.16308	0.27903
C	-4.46290	0.09891	0.04945
H	-4.46778	-2.06615	0.31574
C	-2.29140	1.16697	0.11205
C	-3.69157	1.24035	-0.04251
H	-5.54300	0.16583	-0.06813
H	-4.16619	2.20271	-0.23283
C	-1.34443	2.22394	0.12829
C	-1.65949	3.60523	0.02219

C	0.90461	2.80815	0.58942
C	-0.69814	4.56037	0.21633
H	-2.68740	3.89393	-0.19766
C	0.62781	4.15383	0.53619
H	1.91441	2.44974	0.80310
H	-0.94825	5.61756	0.14108
H	1.41962	4.87881	0.70993
N	-0.31455	-2.21570	0.48818
N	-1.73766	-0.08670	0.34222
N	-0.00834	1.83728	0.35978
C	1.69076	0.26852	-2.01176
C	1.90323	0.52104	-3.39142
C	0.93490	0.21921	-4.31357
C	-0.28608	-0.35562	-3.87290
C	-0.47809	-0.53169	-2.52217
H	2.85754	0.93594	-3.71350
H	1.10658	0.40511	-5.37249
H	-1.07721	-0.61867	-4.57082
H	-1.42013	-0.92105	-2.13338
C	2.68564	0.33353	-1.00131
C	4.02935	0.74275	-1.19856
C	3.21041	-0.27142	1.21330
C	4.94485	0.61801	-0.18380
H	4.33029	1.14936	-2.16314
C	4.53800	0.06718	1.05553
H	2.82426	-0.64722	2.16272
H	5.97650	0.93267	-0.33487
H	5.23627	-0.06075	1.87922
N	0.44295	-0.19988	-1.58893
N	2.27903	-0.10853	0.25392
Cl	0.17993	-0.21307	2.92065

[Ru–Cl]$^-$ TS

Ru	0.15807	-0.17126	0.24362
C	0.50144	-3.25648	0.42975
C	-1.68784	-2.42355	0.55349
C	-2.18196	-3.73418	0.62619
C	-1.31443	-4.80706	0.60823
C	0.06534	-4.56207	0.50229
H	1.56312	-3.01825	0.35030
H	-3.25648	-3.89622	0.69296
H	-1.69497	-5.82468	0.66794
H	0.78736	-5.37526	0.48775
C	-2.51011	-1.23228	0.53229
C	-3.89161	-1.17188	0.56703
C	-4.53379	0.07257	0.43409
H	-4.48025	-2.08066	0.68250
C	-2.38872	1.16227	0.23251
C	-3.78272	1.22862	0.25023
H	-5.62016	0.12692	0.45958
H	-4.28225	2.18928	0.12709
C	-1.45344	2.23421	0.13503
C	-1.78857	3.59983	0.00598
C	0.82584	2.83076	0.29945
C	-0.81596	4.56720	0.03576
H	-2.83716	3.87270	-0.11080
C	0.53466	4.16759	0.20026
H	1.85575	2.48888	0.41695
H	-1.07600	5.61966	-0.06000
H	1.33940	4.89822	0.24566
N	-0.32780	-2.18978	0.46647
N	-1.77193	-0.07190	0.40847
N	-0.11125	1.84396	0.25967
C	1.81757	0.23882	-2.06230
C	2.07511	0.62214	-3.38860
C	1.12082	0.41628	-4.36238
C	-0.10242	-0.18008	-4.00083
C	-0.33701	-0.47755	-2.67730
H	3.03223	1.07664	-3.63993
H	1.31289	0.70465	-5.39362
H	-0.87008	-0.39066	-4.74170
H	-1.28747	-0.89499	-2.34291
C	2.77311	0.24647	-0.98399
C	4.13838	0.55136	-1.11152
C	3.07656	-0.28732	1.27340
C	4.96813	0.42419	-0.01640
H	4.53565	0.87185	-2.07270
C	4.43137	-0.02736	1.19980
H	2.58465	-0.58528	2.20232
H	6.02743	0.65955	-0.10007
H	5.05452	-0.15025	2.08251
N	0.57694	-0.25233	-1.70230
N	2.24321	-0.12027	0.22684
Cl	0.29061	-0.23172	3.56379

[Ru–NCCH$_3$]^0

Ru	0.19724	0.14429	0.44838
C	0.85301	-2.86201	0.69823
C	-1.37891	-2.25490	0.16431
C	-1.70483	-3.63596	0.06621
C	-0.75979	-4.59753	0.29857
C	0.56231	-4.20489	0.65420
H	1.86091	-2.51213	0.93451
H	-2.72899	-3.91745	-0.17834
H	-1.02015	-5.65252	0.22767
H	1.34007	-4.93737	0.85600
C	-2.31395	-1.19101	0.11429
C	-3.70871	-1.25188	-0.09379
C	-4.47138	-0.10310	-0.04195
H	-4.18533	-2.21026	-0.29831
C	-2.50303	1.20161	0.38314
C	-3.87080	1.15974	0.19549
H	-5.54623	-0.16223	-0.20298
H	-4.46925	2.06779	0.18905
C	-1.67671	2.40884	0.49370
C	-2.18832	3.70485	0.56267
C	0.50467	3.24874	0.53550
C	-1.32415	4.78657	0.61824
H	-3.26550	3.85789	0.57464
C	0.05312	4.55508	0.59947
H	1.56957	3.01589	0.52610
H	-1.71635	5.79975	0.67305

H	0.76835	5.37273	0.64218
N	-0.04191	-1.88649	0.42695
N	-1.76593	0.06323	0.36169
N	-0.32195	2.18969	0.48982
C	1.67431	-0.30269	-1.97981
C	1.91681	-0.51109	-3.35833
C	0.94290	-0.23316	-4.28510
C	-0.30331	0.27354	-3.84818
C	-0.50976	0.42642	-2.49530
H	2.89261	-0.86993	-3.68093
H	1.13556	-0.38555	-5.34554
H	-1.10081	0.50876	-4.54831
H	-1.46781	0.77486	-2.10758
C	2.66681	-0.37986	-0.95693
C	4.00619	-0.79023	-1.15440
C	3.18647	0.20774	1.26073
C	4.92008	-0.68093	-0.13450
H	4.30935	-1.19008	-2.12042
C	4.51154	-0.13922	1.10517
H	2.81211	0.59579	2.20930
H	5.95007	-0.99974	-0.28461
H	5.20818	-0.01508	1.93047
N	0.41910	0.12373	-1.56414
N	2.25891	0.05817	0.29459
N	0.15636	0.16229	2.49048
C	0.11931	0.15494	3.65020
C	0.08564	0.14448	5.09534
H	0.60587	-0.74093	5.47809
H	0.57642	1.04147	5.48994
H	-0.95154	0.12508	5.44806

[Ru–NCCH$_3$]^0 TS

Ru	0.40303	-0.19668	0.35859
C	0.73836	-3.29675	0.46917
C	-1.42055	-2.44944	0.81466
C	-1.91752	-3.75508	0.92350
C	-1.06344	-4.83467	0.81253
C	0.29977	-4.60059	0.57347
H	1.78800	-3.06526	0.28424
H	-2.98202	-3.91088	1.08973
H	-1.44554	-5.84959	0.89987
H	1.00909	-5.41939	0.47933
C	-2.23742	-1.24958	0.86988
C	-3.60082	-1.18236	1.09368
C	-4.24203	0.07067	1.05518
H	-4.17463	-2.08463	1.29713
C	-2.13261	1.14412	0.57787
C	-3.51238	1.22308	0.78668
H	-5.31355	0.13488	1.23255
H	-4.01166	2.19119	0.76326
C	-1.20380	2.21501	0.41548
C	-1.54543	3.58396	0.33657
C	1.08287	2.80596	0.36957
C	-0.57160	4.54851	0.29046
H	-2.59938	3.86034	0.31805
C	0.78834	4.14529	0.32534
H	2.11818	2.46064	0.37695
H	-0.83653	5.60252	0.23331
H	1.59584	4.87380	0.30677
N	-0.07487	-2.22728	0.59896
N	-1.52441	-0.10110	0.62453
N	0.14398	1.82261	0.39742
C	1.77216	0.24471	-2.09596
C	1.87464	0.62676	-3.44634
C	0.82671	0.40036	-4.31015
C	-0.34427	-0.21485	-3.81911
C	-0.43054	-0.51271	-2.47875
H	2.79210	1.09356	-3.80140
H	0.90339	0.68613	-5.35709
H	-1.18365	-0.43848	-4.47314
H	-1.33184	-0.94538	-2.04452
C	2.83925	0.26356	-1.13688
C	4.17478	0.61987	-1.40595
C	3.42292	-0.32425	1.05545
C	5.12754	0.48740	-0.41961
H	4.44934	0.98496	-2.39411
C	4.75165	-0.02261	0.83725
H	3.07016	-0.68659	2.02229
H	6.16242	0.76078	-0.61654
H	5.47790	-0.15889	1.63471
N	0.58000	-0.27079	-1.60832
N	2.46607	-0.14576	0.12383
N	0.31928	-0.14270	2.94016
C	-0.59588	-0.00145	3.64623
C	-1.77259	0.17249	4.46885
H	-1.96966	-0.73873	5.04482
H	-1.63292	1.00850	5.16308
H	-2.64274	0.38300	3.83178

[Ru]$^+$

Ru	0.04494	-0.00187	0.19039
C	0.51912	-3.05500	0.25252
C	-1.66070	-2.33196	-0.20367
C	-2.06963	-3.65453	-0.39465
C	-1.15886	-4.68534	-0.25309
C	0.16613	-4.37787	0.07358
H	1.53911	-2.77041	0.50950
H	-3.10301	-3.86335	-0.66399
H	-1.46917	-5.71726	-0.40120
H	0.91674	-5.15559	0.19018
C	-2.53234	-1.17830	-0.34698
C	-3.89456	-1.18029	-0.61640
C	-4.56963	0.03410	-0.74301
H	-4.43149	-2.12005	-0.72726
C	-2.51245	1.21304	-0.34836
C	-3.87442	1.23714	-0.61814
H	-5.63722	0.04284	-0.94889
H	-4.39560	2.18559	-0.73027
C	-1.62341	2.35308	-0.20524
C	-2.01406	3.68194	-0.39073
C	0.56730	3.04441	0.24928
C	-1.08894	4.69959	-0.24721

H	-3.04509	3.90633	-0.65654
C	0.23227	4.37251	0.07611
H	1.58396	2.74528	0.50319
H	-1.38526	5.73623	-0.39081
H	0.99372	5.13933	0.19454
N	-0.35851	-2.03640	0.13301
N	-1.87028	0.01195	-0.18615
N	-0.32440	2.03809	0.12718
C	2.43038	-0.04365	-1.53532
C	3.18891	-0.08700	-2.70344
C	2.54874	-0.12582	-3.93226
C	1.15627	-0.12183	-3.96878
C	0.45473	-0.07977	-2.77619
H	4.27495	-0.09325	-2.64890
H	3.12847	-0.15982	-4.85158
H	0.61233	-0.15181	-4.90926
H	-0.63460	-0.07723	-2.75287
C	2.98552	-0.00184	-0.18425
C	4.34607	0.03243	0.11511
C	2.44174	0.04426	2.07584
C	4.74768	0.07094	1.44147
H	5.08498	0.03139	-0.68246
C	3.77707	0.07598	2.44111
H	1.64393	0.04938	2.81811
H	5.80521	0.09786	1.69359
H	4.04645	0.10551	3.49371
N	1.07015	-0.04074	-1.58009
N	2.04211	0.00671	0.79277

$[Ru]^+$ CO_2 attack TS

Ru	0.03049	-0.00304	-0.26920
C	0.52522	-3.05238	-0.26611
C	-1.69411	-2.34008	-0.20204
C	-2.13851	-3.65942	-0.20123
C	-1.21432	-4.69342	-0.23393
C	0.14245	-4.38441	-0.26950
H	1.57588	-2.76516	-0.28832
H	-3.20463	-3.87286	-0.17673
H	-1.54896	-5.72815	-0.23317
H	0.90180	-5.16180	-0.29631
C	-2.58956	-1.18110	-0.17602
C	-3.97946	-1.19711	-0.13843
C	-4.66948	0.01208	-0.13408
H	-4.52115	-2.13957	-0.11456
C	-2.58339	1.19220	-0.21486
C	-3.97298	1.21696	-0.17896
H	-5.75630	0.01548	-0.10266
H	-4.50986	2.16245	-0.18740
C	-1.68059	2.34443	-0.27514
C	-2.11666	3.66615	-0.30579
C	0.54284	3.04019	-0.36137
C	-1.18572	4.69293	-0.36510
H	-3.18133	3.88700	-0.28362
C	0.16886	4.37447	-0.39657
H	1.59140	2.74480	-0.37893
H	-1.51369	5.72958	-0.38772
H	0.93305	5.14609	-0.44382
N	-0.35836	-2.04201	-0.22864
N	-1.92623	0.00382	-0.19752
N	-0.34731	2.03771	-0.29569
C	1.71418	-0.01304	-2.71447
C	2.07001	0.00120	-4.06225
C	1.07552	0.01714	-5.02924
C	-0.25799	0.01816	-4.63083
C	-0.54681	0.00369	-3.27596
H	3.11725	0.00154	-4.35416
H	1.33929	0.02909	-6.08423
H	-1.06821	0.03022	-5.35538
H	-1.57554	0.00408	-2.91504
C	2.67565	-0.02807	-1.60673
C	4.05841	-0.04900	-1.77740
C	2.92365	-0.03507	0.70611
C	4.88332	-0.06266	-0.66312
H	4.48566	-0.05509	-2.77687
C	4.30459	-0.05583	0.60332
H	2.42430	-0.03008	1.67467
H	5.96415	-0.07908	-0.78158
H	4.91105	-0.06647	1.50519
N	0.41100	-0.01178	-2.33661
N	2.11535	-0.02091	-0.36866
C	-0.47265	0.10905	2.36881
O	-0.50247	-1.04379	2.67596
O	-0.55417	1.27603	2.60137

$[Ru–CO_2]^+$

Ru	0.17338	0.08776	0.50907
C	0.72826	-2.96691	0.44008
C	-1.49902	-2.28261	0.43587
C	-1.92888	-3.60439	0.40875
C	-0.98918	-4.62714	0.40519
C	0.36227	-4.30558	0.42216
H	1.77501	-2.66632	0.45685
H	-2.99149	-3.83345	0.39423
H	-1.31240	-5.66537	0.38951
H	1.13075	-5.07402	0.42338
C	-2.42041	-1.13498	0.43253
C	-3.80852	-1.19206	0.36778
C	-4.52890	-0.00191	0.32745
H	-4.32525	-2.14787	0.34391
C	-2.47819	1.22985	0.40046
C	-3.86790	1.22170	0.33420
H	-5.61471	-0.02960	0.27866
H	-4.42756	2.15217	0.28568
C	-1.60245	2.40842	0.37622
C	-2.06793	3.71747	0.31609
C	0.60770	3.14816	0.35814
C	-1.15371	4.76186	0.27593
H	-3.13652	3.91749	0.30127
C	0.20654	4.47484	0.29570
H	1.66093	2.87105	0.38379
H	-1.50229	5.79093	0.22957
H	0.95416	5.26311	0.26663

N	-0.17069	-1.97619	0.44637
N	-1.80008	0.06389	0.46281
N	-0.26675	2.13536	0.39874
C	1.80709	-0.05425	-2.04779
C	2.15404	-0.11024	-3.39780
C	1.15195	-0.07985	-4.35748
C	-0.17652	0.00471	-3.95549
C	-0.44983	0.05747	-2.59704
H	3.19442	-0.17469	-3.70442
H	1.40959	-0.12199	-5.41340
H	-0.98925	0.03170	-4.67652
H	-1.47478	0.12540	-2.22911
C	2.79036	-0.07842	-0.95061
C	4.16151	-0.19710	-1.16997
C	3.13572	-0.00808	1.34800
C	5.03083	-0.22187	-0.08973
H	4.55172	-0.27159	-2.18099
C	4.50805	-0.12454	1.19415
H	2.67393	0.08305	2.32863
H	6.10212	-0.31616	-0.25162
H	5.14797	-0.13789	2.07257
N	0.51322	0.03049	-1.66968
N	2.28590	0.01335	0.30726
C	-0.06542	-0.15626	2.56757
O	-0.72857	-0.99497	3.16130
O	0.63980	0.82115	2.90678

$[Ru–CO_2]^{2+}$ CO_2 attack TS

Ru	0.00449	-0.01591	0.54783
C	0.41649	-3.07964	0.55942
C	-1.78178	-2.30338	0.43116
C	-2.26615	-3.60318	0.41550
C	-1.36907	-4.66464	0.48493
C	-0.00873	-4.40238	0.55611
H	1.47162	-2.82037	0.61575
H	-3.33528	-3.78977	0.35423
H	-1.73665	-5.68804	0.48025
H	0.72396	-5.20301	0.60896
C	-2.64795	-1.11212	0.36270
C	-4.03427	-1.09256	0.24841
C	-4.67780	0.13752	0.14809
H	-4.60735	-2.01559	0.23488
C	-2.56813	1.25485	0.26610
C	-3.95182	1.32464	0.14525
H	-5.76091	0.17052	0.05935
H	-4.45638	2.28192	0.04736
C	-1.62113	2.38292	0.24698
C	-2.01095	3.70926	0.11456
C	0.62633	3.00970	0.33644
C	-1.04057	4.70450	0.09120
H	-3.06487	3.96313	0.03095
C	0.29778	4.35234	0.20279
H	1.65995	2.68142	0.43829
H	-1.33231	5.74699	-0.01127
H	1.08599	5.10016	0.19192
N	-0.44090	-2.05684	0.50337
N	-1.97383	0.05326	0.38829
N	-0.30224	2.04782	0.35482
C	1.71465	0.00491	-1.88627
C	2.09989	0.07328	-3.22280
C	1.12676	0.09230	-4.21207
C	-0.21384	0.03997	-3.84984
C	-0.53244	-0.02416	-2.50271
H	3.15102	0.10850	-3.49438
H	1.41644	0.14561	-5.25889
H	-1.00674	0.04778	-4.59265
H	-1.56944	-0.06701	-2.17230
C	2.66353	-0.04948	-0.76474
C	4.04474	-0.04373	-0.93478
C	2.91063	-0.27493	1.53923
C	4.87026	-0.14693	0.17585
H	4.47677	0.03699	-1.92817
C	4.29309	-0.27979	1.43178
H	2.41329	-0.42767	2.49553
H	5.95095	-0.13893	0.05566
H	4.89770	-0.39034	2.32796
N	0.40480	-0.04234	-1.54506
N	2.10618	-0.13731	0.47136
C	0.00810	0.37403	2.44291
O	-1.00339	-1.02008	3.08826
O	0.30540	1.10685	3.30583
C	-0.21040	-1.97942	3.60949
O	1.02248	-1.94298	3.46469
O	-0.90740	-2.82982	4.21903

$[Ru–CO_2H]^{2+}$

Ru	0.18466	-0.01326	0.45522
C	0.63488	-3.02390	0.16584
C	-1.58737	-2.34468	0.43349
C	-2.01815	-3.66299	0.44031
C	-1.08003	-4.68135	0.31250
C	0.26399	-4.36078	0.17147
H	1.67395	-2.71916	0.05451
H	-3.07534	-3.89353	0.54305
H	-1.40198	-5.71981	0.31826
H	1.02468	-5.12882	0.06464
C	-2.47936	-1.18308	0.52298
C	-3.86786	-1.20435	0.59293
C	-4.55230	0.00586	0.62252
H	-4.40842	-2.14656	0.61258
C	-2.47210	1.17751	0.49201
C	-3.86026	1.21064	0.56157
H	-5.63786	0.01004	0.67867
H	-4.39425	2.15679	0.55821
C	-1.57023	2.32892	0.37985
C	-1.98897	3.65153	0.36315
C	0.65919	2.98431	0.11234
C	-1.04204	4.65912	0.22095
H	-3.04429	3.89253	0.46067
C	0.29968	4.32378	0.09100
H	1.69693	2.66917	0.01811
H	-1.35453	5.70037	0.20872

H	1.06789	5.08299	-0.02467
N	-0.26537	-2.04251	0.30457
N	-1.82915	-0.00546	0.49117
N	-0.24995	2.01247	0.26232
C	1.87495	-0.02160	-2.04481
C	2.25995	-0.00934	-3.38354
C	1.28009	-0.01163	-4.36745
C	-0.05992	-0.02656	-3.99921
C	-0.37195	-0.03798	-2.64773
H	3.30963	0.00239	-3.66287
H	1.56507	-0.00186	-5.41686
H	-0.85452	-0.02972	-4.74033
H	-1.40667	-0.05101	-2.30437
C	2.82549	-0.02263	-0.92148
C	4.20540	-0.03228	-1.09312
C	3.08979	-0.03164	1.39830
C	5.03553	-0.04296	0.01916
H	4.63430	-0.03349	-2.09084
C	4.46998	-0.04429	1.28777
H	2.60658	-0.02467	2.37172
H	6.11528	-0.05149	-0.10834
H	5.08040	-0.05418	2.18621
N	0.56958	-0.03550	-1.69883
N	2.27965	-0.01952	0.32549
C	-0.01126	0.00545	2.47788
O	-0.45342	-0.88708	3.17671
O	0.43298	1.16142	3.04176
H	0.31260	1.07708	4.01305

[Ru]^0

Ru	-0.04339	0.00436	-0.44978
C	0.44221	-3.03531	-0.49887
C	-1.77308	-2.33026	-0.14590
C	-2.18154	-3.67321	-0.05911
C	-1.26499	-4.69084	-0.19606
C	0.08541	-4.36104	-0.42318
H	1.47689	-2.73808	-0.67291
H	-3.23260	-3.89592	0.11914
H	-1.57878	-5.73063	-0.12934
H	0.84511	-5.13098	-0.53773
C	-2.63350	-1.19459	-0.02309
C	-4.00336	-1.18218	0.18490
C	-4.69661	0.02852	0.27901
H	-4.54147	-2.12567	0.27316
C	-2.62440	1.23033	-0.04589
C	-3.99430	1.23200	0.16268
H	-5.77199	0.03403	0.44121
H	-4.52563	2.18080	0.23378
C	-1.75562	2.35692	-0.19109
C	-2.15442	3.70428	-0.13163
C	0.46477	3.03906	-0.55668
C	-1.23055	4.71248	-0.28754
H	-3.20405	3.93805	0.04052
C	0.11760	4.36850	-0.50692
H	1.49735	2.73130	-0.72468
H	-1.53699	5.75557	-0.24172
H	0.88298	5.13051	-0.63575
N	-0.44020	-2.01072	-0.36743
N	-1.92755	0.01417	-0.14436
N	-0.42494	2.02338	-0.40579
C	2.74908	-0.03109	-1.64012
C	3.75573	-0.05314	-2.60624
C	3.40998	-0.05991	-3.94720
C	2.05860	-0.04407	-4.29118
C	1.11074	-0.02295	-3.28307
H	4.80127	-0.06425	-2.30682
H	4.18050	-0.07691	-4.71480
H	1.73761	-0.04801	-5.32983
H	0.04488	-0.01057	-3.50619
C	2.98200	-0.02164	-0.20053
C	4.24183	-0.03294	0.39931
C	1.94503	0.00994	1.87474
C	4.33637	-0.02201	1.78083
H	5.14005	-0.05014	-0.21354
C	3.16216	-0.00005	2.53294
H	1.00391	0.02676	2.42233
H	5.30941	-0.03046	2.26672
H	3.18449	0.00924	3.61992
N	1.43179	-0.01729	-1.97507
N	1.83756	-0.00045	0.53204

[Ru]^0 proton transfer TS with TEOAH$^+$

Ru	-0.16039	-0.39576	0.26568
C	0.94158	-3.22393	0.80346
C	-1.38263	-3.00682	0.59490
C	-1.53320	-4.38849	0.77651
C	-0.42590	-5.18547	0.98232
C	0.84251	-4.58431	0.99461
H	1.90931	-2.72280	0.80696
H	-2.53126	-4.82252	0.75750
H	-0.53539	-6.25779	1.12863
H	1.74488	-5.17057	1.15233
C	-2.47370	-2.07700	0.43480
C	-3.83534	-2.35888	0.43954
C	-4.76038	-1.32887	0.28403
H	-4.17554	-3.38607	0.55951
C	-2.94902	0.24548	0.08686
C	-4.31037	-0.02126	0.09172
H	-5.82600	-1.54482	0.29270
H	-5.02338	0.78714	-0.06066
C	-2.30661	1.52744	-0.10639
C	-2.98309	2.72661	-0.36025
C	-0.25599	2.65494	-0.17022
C	-2.27197	3.90084	-0.51678
H	-4.06870	2.72264	-0.43670
C	-0.87490	3.86207	-0.42408
H	0.82777	2.58222	-0.07538
H	-2.79054	4.83689	-0.71246
H	-0.27398	4.76046	-0.54390
N	-0.13194	-2.41664	0.61343
N	-2.03795	-0.76962	0.31136
N	-0.93376	1.49774	0.00461

C	1.91900	0.11941	-1.91823
C	2.42421	0.41683	-3.18547
C	1.59902	0.28274	-4.29106
C	0.28395	-0.14173	-4.10819
C	-0.15372	-0.40708	-2.82153
H	3.44944	0.75820	-3.30654
H	1.97532	0.51040	-5.28592
H	-0.39611	-0.26283	-4.94770
H	-1.17644	-0.73243	-2.62428
C	2.68670	0.20583	-0.67498
C	4.06063	0.44785	-0.64618
C	2.63156	0.03740	1.62831
C	4.72566	0.48710	0.56762
H	4.60761	0.59321	-1.57450
C	3.99249	0.26944	1.73055
H	2.03397	-0.14000	2.51790
H	5.79629	0.67460	0.60566
H	4.46206	0.27812	2.71091
N	0.64094	-0.28359	-1.74672
N	1.96070	0.00941	0.46048
H	-0.54575	-0.09668	2.25928
C	-0.14585	-0.92468	4.27728
H	0.90972	-0.88002	3.97629
H	-0.19323	-0.66856	5.34591
C	-0.63672	-2.33823	4.04245
H	-0.80686	-2.50256	2.96722
H	-1.59241	-2.51824	4.56351
C	-0.29608	1.44174	3.81551
H	0.71643	1.46304	3.38562
H	-0.19854	1.54324	4.90609
C	-1.07177	2.61049	3.24307
H	-1.98678	2.80152	3.82906
H	-1.37806	2.39109	2.20902
C	-2.33147	0.01524	3.57762
H	-2.75741	0.78650	2.92411
H	-2.63230	-0.95231	3.15362
C	-2.90184	0.16776	4.97366
H	-2.55672	-0.65006	5.62875
H	-2.56540	1.11518	5.43017
N	-0.85867	0.10828	3.49147
O	0.37940	-3.17739	4.54444
H	0.08097	-4.09357	4.43832
O	-0.19282	3.71128	3.30115
H	-0.67422	4.48557	2.97162
O	-4.30076	0.13967	4.80884
H	-4.70492	0.17991	5.68872

[Ru–H]$^+$

Ru	0.19321	0.00233	0.43241
C	0.67554	-3.05073	0.41956
C	-1.54058	-2.32885	0.42735
C	-1.99130	-3.64520	0.39945
C	-1.07152	-4.68381	0.37992
C	0.28627	-4.38074	0.38706
H	1.72736	-2.76827	0.43384
H	-3.05867	-3.85309	0.39008
H	-1.41098	-5.71669	0.35762
H	1.04274	-5.16120	0.37030
C	-2.43091	-1.16521	0.43067
C	-3.82135	-1.17823	0.40015
C	-4.50770	0.03218	0.37946
H	-4.36528	-2.11955	0.38919
C	-2.41520	1.20253	0.41218
C	-3.80530	1.23348	0.38006
H	-5.59469	0.03925	0.35589
H	-4.33640	2.18176	0.35290
C	-1.51050	2.35477	0.39305
C	-1.94541	3.67613	0.35133
C	0.71401	3.04962	0.37199
C	-1.01328	4.70325	0.31737
H	-3.01024	3.89679	0.34240
C	0.34074	4.38376	0.32456
H	1.76242	2.75495	0.38741
H	-1.34023	5.73987	0.28416
H	1.10659	5.15470	0.29688
N	-0.20410	-2.03640	0.44361
N	-1.76224	0.01456	0.44746
N	-0.17766	2.04618	0.41026
C	1.81845	-0.04840	-2.08193
C	2.15658	-0.08471	-3.43470
C	1.14890	-0.09798	-4.38787
C	-0.17879	-0.07463	-3.97245
C	-0.44585	-0.04049	-2.61293
H	3.19801	-0.10344	-3.74519
H	1.39932	-0.12622	-5.44593
H	-0.99849	-0.08312	-4.68622
H	-1.47033	-0.02161	-2.23937
C	2.80250	-0.02949	-0.99133
C	4.17976	-0.03099	-1.20680
C	3.13275	0.00907	1.30924
C	5.04523	-0.01296	-0.12440
H	4.57420	-0.04577	-2.21909
C	4.50930	0.00702	1.15932
H	2.67291	0.02513	2.29446
H	6.12123	-0.01427	-0.28159
H	5.14433	0.02138	2.04138
N	0.52282	-0.02821	-1.68606
N	2.28100	-0.00837	0.26575
H	0.21524	0.01783	2.09641

[Ru–H]$^+$ CO_2 attack TS

Ru	0.19944	0.01359	0.41042
C	0.68627	-3.03917	0.36305
C	-1.53095	-2.32157	0.40613
C	-1.98034	-3.63756	0.38578
C	-1.05801	-4.67466	0.35088
C	0.29848	-4.37073	0.33555
H	1.73750	-2.75422	0.36070
H	-3.04713	-3.84789	0.39393
H	-1.39641	-5.70796	0.33409
H	1.05548	-5.15013	0.30561
C	-2.42505	-1.15746	0.42063

C	-3.81588	-1.17489	0.41330
C	-4.50260	0.03543	0.39601
H	-4.35918	-2.11643	0.41744
C	-2.41318	1.20802	0.39325
C	-3.80372	1.23847	0.38122
H	-5.58988	0.04081	0.38907
H	-4.33747	2.18525	0.36005
C	-1.50939	2.36405	0.37467
C	-1.94669	3.68384	0.34492
C	0.71520	3.06258	0.38300
C	-1.01472	4.71279	0.33228
H	-3.01156	3.90365	0.33176
C	0.33938	4.39710	0.34980
H	1.76358	2.76806	0.40710
H	-1.34351	5.74907	0.30874
H	1.10340	5.17021	0.34113
N	-0.19554	-2.02946	0.40245
N	-1.76322	0.02214	0.41899
N	-0.17618	2.05995	0.39690
C	1.81728	-0.07090	-2.07279
C	2.14865	-0.13979	-3.42502
C	1.13788	-0.15302	-4.37492
C	-0.18725	-0.09669	-3.95564
C	-0.45120	-0.03266	-2.59680
H	3.18937	-0.18331	-3.73558
H	1.38388	-0.20646	-5.43297
H	-1.00979	-0.10304	-4.66603
H	-1.47360	0.01164	-2.22206
C	2.80445	-0.04180	-0.98673
C	4.18176	-0.05841	-1.19638
C	3.12026	0.05475	1.31650
C	5.03972	-0.02155	-0.10766
H	4.58133	-0.09852	-2.20611
C	4.49805	0.03853	1.17246
H	2.64873	0.11911	2.29548
H	6.11663	-0.03569	-0.25804
H	5.13018	0.07435	2.05595
N	0.52160	-0.02066	-1.67291
N	2.28025	0.01023	0.26672
H	0.20812	-0.07108	2.11298
C	-0.07028	1.00325	3.26311
O	1.01520	1.42632	3.51856
O	-1.24205	0.93159	3.46650

[Ru–H]$^+$ CO_2 attack TS with TEOAH$^+$

Ru	-0.02113	-0.01120	0.55202
C	0.79834	-2.97492	0.81117
C	-1.47882	-2.52370	0.58479
C	-1.77896	-3.87788	0.67253
C	-0.74860	-4.79617	0.83320
C	0.56121	-4.33975	0.90248
H	1.80649	-2.56686	0.86832
H	-2.81086	-4.21558	0.61860
H	-0.97137	-5.85815	0.90483
H	1.39605	-5.02358	1.02957
C	-2.49415	-1.47375	0.39613
C	-3.85827	-1.65746	0.19141
C	-4.65158	-0.54173	-0.05774
H	-4.29802	-2.65104	0.20461
C	-2.72657	0.87013	0.12461
C	-4.09244	0.73165	-0.10578
H	-5.71730	-0.66814	-0.23235
H	-4.71407	1.59499	-0.32624
C	-1.95047	2.12266	0.10700
C	-2.51937	3.37341	-0.10497
C	0.16755	3.07577	0.31235
C	-1.70462	4.49991	-0.11348
H	-3.59046	3.47148	-0.25673
C	-0.33942	4.35050	0.09399
H	1.22859	2.90813	0.49079
H	-2.13686	5.48382	-0.28062
H	0.33371	5.20415	0.09573
N	-0.18785	-2.08389	0.65459
N	-1.98093	-0.22602	0.37327
N	-0.60896	1.98691	0.32174
C	1.63550	0.05724	-1.93440
C	1.99670	0.05470	-3.28058
C	1.01844	-0.11989	-4.24876
C	-0.30306	-0.29142	-3.85452
C	-0.59537	-0.27517	-2.49977
H	3.03289	0.18901	-3.57730
H	1.28905	-0.12336	-5.30206
H	-1.10063	-0.43467	-4.57837
H	-1.61896	-0.40461	-2.14874
C	2.59857	0.21462	-0.83400
C	3.96892	0.35410	-1.04370
C	2.91182	0.30479	1.46523
C	4.82262	0.47059	0.04272
H	4.37207	0.36622	-2.05223
C	4.28304	0.44051	1.32255
H	2.45320	0.29023	2.44934
H	5.89368	0.57868	-0.11090
H	4.90805	0.52090	2.20791
N	0.34447	-0.10317	-1.56037
N	2.07288	0.19839	0.42048
C	-0.16855	-0.01826	2.49840
O	-0.48697	-0.69981	3.41221
O	0.46636	1.52058	3.17885
H	0.93764	1.19539	3.97048
H	-0.48988	2.17294	3.71455
C	-0.58433	4.04787	4.80584
H	-1.23818	4.67366	5.42976
H	0.27922	3.74126	5.41249
C	-0.07418	4.84599	3.62330
H	-0.90724	5.31323	3.07191
H	0.45459	4.17267	2.92371
C	-2.53394	3.11272	3.65236
H	-2.23573	3.57586	2.70094
H	-3.13589	3.84911	4.20628
C	-3.37326	1.89347	3.33118
H	-3.79755	1.44394	4.24317
H	-2.74609	1.11982	2.84309

C	-1.49734	1.91589	5.57896
H	-1.90429	0.96428	5.21507
H	-0.50138	1.70147	5.99027
C	-2.39018	2.46072	6.67491
H	-1.93576	3.35121	7.13945
H	-3.36892	2.76613	6.26496
N	-1.29844	2.80981	4.41117
O	0.78405	5.81904	4.16925
H	1.03965	6.42297	3.45584
O	-4.39300	2.35711	2.47815
H	-5.02481	1.63261	2.35162
O	-2.52245	1.40805	7.60157
H	-3.03847	1.73674	8.35303

[Ru–□□HO]$^{+}$

Ru	0.15517	-0.01523	0.37313
C	0.66752	-3.06400	0.37152
C	-1.55291	-2.35683	0.40562
C	-1.99594	-3.67473	0.42423
C	-1.06797	-4.70786	0.41421
C	0.28662	-4.39831	0.38553
H	1.71758	-2.77520	0.35514
H	-3.06140	-3.89076	0.44519
H	-1.40128	-5.74287	0.42794
H	1.04745	-5.17450	0.37686
C	-2.45635	-1.19770	0.40338
C	-3.84652	-1.22477	0.44854
C	-4.54065	-0.01830	0.44402
H	-4.38335	-2.16902	0.49111
C	-2.46164	1.16832	0.36143
C	-3.85245	1.19041	0.40475
H	-5.62746	-0.02041	0.47807
H	-4.39383	2.13306	0.41125
C	-1.55961	2.32681	0.31238
C	-2.00224	3.64510	0.26558
C	0.65976	3.02386	0.20349
C	-1.07280	4.67205	0.17617
H	-3.06717	3.86347	0.29080
C	0.28089	4.35599	0.13380
H	1.70782	2.73001	0.19770
H	-1.40318	5.70737	0.13486
H	1.04191	5.12821	0.05635
N	-0.21940	-2.05940	0.38156
N	-1.80877	-0.01374	0.34479
N	-0.22840	2.02581	0.29834
C	1.82436	0.04179	-2.02772
C	2.17555	0.10182	-3.37443
C	1.18188	0.12727	-4.34135
C	-0.14957	0.08976	-3.93999
C	-0.43796	0.03294	-2.58682
H	3.22255	0.12844	-3.66502
H	1.44444	0.17456	-5.39553
H	-0.96222	0.10506	-4.66154
H	-1.46619	0.00310	-2.23002
C	2.79252	-0.00762	-0.92875
C	4.17372	-0.02843	-1.10801
C	3.04808	-0.14117	1.37878
C	5.00252	-0.10619	0.00132
H	4.59799	0.01244	-2.10777
C	4.42874	-0.17049	1.26726
H	2.55358	-0.18647	2.34563
H	6.08281	-0.12291	-0.12234
H	5.03831	-0.24199	2.16427
N	0.51947	0.01049	-1.64265
N	2.23834	-0.05160	0.31121
H	0.04752	0.51431	4.33251
C	0.33515	0.75610	3.28080
O	0.97895	1.77483	3.04943
O	-0.07665	-0.13989	2.45663

[Ru–□□HOH]$^{2+}$

Ru	0.18835	-0.01463	0.37887
C	0.68175	-3.06693	0.38986
C	-1.53651	-2.34886	0.40247
C	-1.98663	-3.66309	0.41572
C	-1.06267	-4.70107	0.41488
C	0.29295	-4.39968	0.40027
H	1.73301	-2.78298	0.38234
H	-3.05308	-3.87424	0.42558
H	-1.40177	-5.73414	0.42466
H	1.04947	-5.17992	0.39834
C	-2.43731	-1.18470	0.39415
C	-3.82809	-1.20566	0.41847
C	-4.51393	0.00531	0.40054
H	-4.37146	-2.14626	0.45145
C	-2.43054	1.18184	0.34521
C	-3.82141	1.21187	0.36573
H	-5.60112	0.00864	0.41682
H	-4.35960	2.15604	0.35540
C	-1.52092	2.33804	0.29951
C	-1.96002	3.65521	0.24044
C	0.70270	3.03246	0.22104
C	-1.02693	4.68160	0.16343
H	-3.02460	3.87584	0.24729
C	0.32595	4.36612	0.14596
H	1.75111	2.73740	0.22684
H	-1.35638	5.71668	0.11320
H	1.08882	5.13733	0.08000
N	-0.20086	-2.05977	0.39222
N	-1.78841	-0.00351	0.34975
N	-0.18860	2.03648	0.30432
C	1.81065	0.03694	-2.03003
C	2.13429	0.09236	-3.38287
C	1.12173	0.09878	-4.33050
C	-0.20060	0.04759	-3.90424
C	-0.46447	-0.00082	-2.54572
H	3.17512	0.12924	-3.69347
H	1.36388	0.14130	-5.38965
H	-1.02700	0.04643	-4.60988
H	-1.48550	-0.03947	-2.17214
C	2.79994	-0.00042	-0.95050
C	4.17691	-0.01104	-1.15612

C	3.10167	-0.12054	1.35094
C	5.02788	-0.07370	-0.06260
H	4.58102	0.02539	-2.16409
C	4.48031	-0.13487	1.21452
H	2.63512	-0.17688	2.33199
H	6.10543	-0.08155	-0.20763
H	5.10689	-0.19525	2.10028
N	0.51239	-0.00313	-1.62160
N	2.27043	-0.04521	0.29956
H	-0.03003	0.45190	4.45589
C	0.23814	0.66006	3.41155
O	0.90461	1.76574	3.17171
O	-0.06652	-0.11593	2.51729
H	1.06160	2.25566	4.00518

[Ru–□□HO]^{0}

Ru	0.17299	0.07067	0.38225
C	0.76372	-2.97358	0.43754
C	-1.49879	-2.30251	0.33823
C	-1.88552	-3.66603	0.32479
C	-0.94094	-4.65993	0.37051
C	0.43085	-4.31415	0.43083
H	1.80852	-2.65865	0.48359
H	-2.94523	-3.91460	0.27972
H	-1.24535	-5.70531	0.36079
H	1.21101	-5.07006	0.47052
C	-2.40591	-1.20473	0.31654
C	-3.81862	-1.24022	0.30683
C	-4.53688	-0.06305	0.32476
H	-4.33816	-2.19716	0.29587
C	-2.49478	1.19113	0.35623
C	-3.88048	1.18879	0.35689
H	-5.62496	-0.09654	0.32138
H	-4.44825	2.11542	0.38229
C	-1.62121	2.37384	0.35738
C	-2.09229	3.68472	0.33629
C	0.58246	3.13436	0.29806
C	-1.19114	4.73792	0.28977
H	-3.16351	3.87321	0.34905
C	0.17328	4.45668	0.26016
H	1.63803	2.86687	0.29679
H	-1.54762	5.76548	0.27078
H	0.91606	5.24942	0.21567
N	-0.13679	-1.97788	0.39082
N	-1.80058	0.03518	0.31400
N	-0.27950	2.10580	0.35346
C	1.80013	-0.07299	-2.02940
C	2.12677	-0.10882	-3.38496
C	1.12681	0.00534	-4.33691
C	-0.19110	0.15743	-3.91051
C	-0.45727	0.18336	-2.55345
H	3.16361	-0.22071	-3.69208
H	1.37094	-0.02036	-5.39634
H	-1.01003	0.25204	-4.61917
H	-1.47244	0.29445	-2.17599
C	2.78063	-0.15062	-0.94774
C	4.14544	-0.35512	-1.15006
C	3.10079	-0.02095	1.35152
C	4.99814	-0.39796	-0.05869
H	4.53664	-0.48335	-2.15622
C	4.46455	-0.22051	1.21569
H	2.64064	0.14730	2.32229
H	6.06386	-0.56334	-0.19997
H	5.09502	-0.23617	2.10135
N	0.50730	0.06675	-1.61877
N	2.25919	0.00185	0.30117
H	-0.04179	0.59607	4.36564
C	0.34219	0.79432	3.33332
O	1.13785	1.71824	3.16331
O	-0.13297	-0.02833	2.47783

[Ru–□□HOH]$^{+}$

Ru	0.19859	0.00521	0.38447
C	0.71149	-3.04998	0.42878
C	-1.53727	-2.32864	0.38894
C	-1.95553	-3.67993	0.38661
C	-1.03244	-4.69560	0.40709
C	0.34650	-4.38034	0.42701
H	1.76263	-2.75695	0.44595
H	-3.02126	-3.90368	0.36667
H	-1.36008	-5.73366	0.40553
H	1.10989	-5.15394	0.44274
C	-2.42021	-1.20754	0.36656
C	-3.82907	-1.20825	0.35788
C	-4.51817	-0.01186	0.34135
H	-4.37301	-2.15137	0.36888
C	-2.44618	1.19403	0.34016
C	-3.82811	1.22232	0.33513
H	-5.60634	-0.01673	0.33654
H	-4.37369	2.16258	0.32785
C	-1.54537	2.35334	0.31172
C	-1.98508	3.67422	0.25045
C	0.67810	3.06458	0.25145
C	-1.06036	4.70467	0.18361
H	-3.05174	3.88734	0.24776
C	0.29889	4.39365	0.17554
H	1.72838	2.77421	0.26477
H	-1.39388	5.73874	0.13290
H	1.05902	5.16860	0.11671
N	-0.17021	-2.03356	0.41600
N	-1.78220	0.01476	0.34303
N	-0.20773	2.05655	0.32821
C	1.80414	0.00558	-2.02878
C	2.11371	0.03769	-3.38675
C	1.09323	0.07196	-4.32406
C	-0.22607	0.07264	-3.88103
C	-0.47711	0.04274	-2.52035
H	3.15219	0.03669	-3.70779
H	1.32469	0.09706	-5.38623
H	-1.05982	0.09598	-4.57794
H	-1.49262	0.04260	-2.12970
C	2.80197	-0.04099	-0.95996

C	4.17733	-0.09564	-1.17855
C	3.12518	-0.10245	1.33973
C	5.03839	-0.15138	-0.09355
H	4.57129	-0.09848	-2.19156
C	4.50086	-0.15755	1.19076
H	2.66644	-0.11552	2.32649
H	6.11389	-0.19447	-0.24828
H	5.13510	-0.20744	2.07205
N	0.50880	0.01091	-1.60290
N	2.28028	-0.03955	0.29602
H	-0.03150	0.47442	4.48197
C	0.23850	0.68032	3.43682
O	0.91911	1.78455	3.20765
O	-0.07235	-0.08662	2.54112
H	1.07595	2.26217	4.04715

[Ru–□□HO]$^{-}$

Ru	0.18701	0.17572	0.37346
C	0.88366	-2.81750	0.59036
C	-1.37161	-2.23829	0.14853
C	-1.68601	-3.62280	0.06226
C	-0.72335	-4.57492	0.25800
C	0.60739	-4.16388	0.55906
H	1.89649	-2.45797	0.78684
H	-2.71575	-3.91431	-0.14580
H	-0.97372	-5.63309	0.19694
H	1.40157	-4.88627	0.73298
C	-2.31858	-1.18453	0.13017
C	-3.72452	-1.26383	0.02976
C	-4.49655	-0.12559	0.14480
H	-4.20270	-2.23079	-0.12586
C	-2.51462	1.20148	0.41783
C	-3.89396	1.14140	0.34675
H	-5.58052	-0.19883	0.07519
H	-4.50289	2.04018	0.41423
C	-1.69674	2.41660	0.48473
C	-2.21896	3.70993	0.54206
C	0.47149	3.27464	0.38294
C	-1.36514	4.80046	0.51654
H	-3.29615	3.85373	0.59902
C	0.01101	4.57818	0.42261
H	1.53644	3.05139	0.32860
H	-1.76366	5.81192	0.55952
H	0.71923	5.40278	0.39184
N	-0.03032	-1.84788	0.35924
N	-1.76213	0.07781	0.30844
N	-0.34301	2.20589	0.42435
C	1.71188	-0.31377	-1.99868
C	1.95706	-0.56837	-3.37082
C	1.01433	-0.25511	-4.31726
C	-0.20873	0.33271	-3.90687
C	-0.42904	0.51686	-2.56081
H	2.91469	-0.99194	-3.67051
H	1.21070	-0.44167	-5.37173
H	-0.98099	0.60098	-4.62375
H	-1.37380	0.91928	-2.19307

C	2.67863	-0.40404	-0.95900
C	4.00572	-0.87625	-1.11538
C	3.16925	0.21186	1.26101
C	4.89747	-0.78259	-0.07554
H	4.31305	-1.31252	-2.06480
C	4.48309	-0.19258	1.14164
H	2.77915	0.65567	2.17882
H	5.91619	-1.14963	-0.19231
H	5.16712	-0.07646	1.97911
N	0.46570	0.17611	-1.60615
N	2.25698	0.07226	0.27761
H	0.08087	0.63620	4.41710
C	0.43281	0.88297	3.38102
O	1.19545	1.84173	3.23867
O	-0.03569	0.07964	2.50994

[Ru–□□HOH]^{0}

Ru	0.20745	0.16236	0.37740
C	0.88756	-2.83678	0.56614
C	-1.36808	-2.24361	0.14619
C	-1.68828	-3.62183	0.03527
C	-0.72717	-4.58139	0.20648
C	0.60529	-4.17917	0.50377
H	1.90262	-2.48592	0.76423
H	-2.71950	-3.90512	-0.17548
H	-0.98034	-5.63720	0.12582
H	1.39795	-4.90741	0.65879
C	-2.31067	-1.18160	0.13755
C	-3.71002	-1.25308	0.01931
C	-4.47764	-0.10746	0.12520
H	-4.19169	-2.21589	-0.14912
C	-2.48983	1.21021	0.41680
C	-3.86682	1.15330	0.32356
H	-5.56074	-0.17215	0.04145
H	-4.47116	2.05657	0.37250
C	-1.66962	2.41956	0.47279
C	-2.18379	3.71885	0.49355
C	0.50843	3.26833	0.39521
C	-1.32435	4.80312	0.46637
H	-3.26101	3.87059	0.52268
C	0.05489	4.57348	0.40592
H	1.57360	3.03829	0.36327
H	-1.71864	5.81695	0.48197
H	0.76740	5.39432	0.37747
N	-0.03040	-1.85885	0.37096
N	-1.74523	0.07065	0.34635
N	-0.31223	2.20270	0.44311
C	1.70655	-0.31371	-1.99001
C	1.91921	-0.60269	-3.35740
C	0.95520	-0.30635	-4.28906
C	-0.25390	0.29380	-3.86301
C	-0.44998	0.50335	-2.51786
H	2.86597	-1.04283	-3.66663
H	1.12467	-0.51869	-5.34294
H	-1.03667	0.55992	-4.56892
H	-1.38560	0.91502	-2.13962

C	2.69594	-0.38666	-0.96657
C	4.02705	-0.82742	-1.15057
C	3.20301	0.20698	1.24857
C	4.93210	-0.73042	-0.12140
H	4.32965	-1.23763	-2.11260
C	4.52211	-0.16979	1.10842
H	2.83252	0.61462	2.18983
H	5.95700	-1.07120	-0.25776
H	5.21245	-0.05466	1.94033
N	0.47244	0.18493	-1.57917
N	2.28044	0.06631	0.27613
H	0.09913	0.61884	4.56859
C	0.33986	0.83188	3.51612
O	1.02288	1.94012	3.28933
O	0.00110	0.08488	2.61933
H	1.20600	2.39756	4.13399

$[Ru]^0$ CO_2 attack TS

Ru	-0.10826	0.00455	-0.56251
C	0.37147	-3.03131	-0.69088
C	-1.80599	-2.32482	-0.17839
C	-2.22823	-3.66290	-0.12908
C	-1.33069	-4.68326	-0.35942
C	0.00487	-4.35850	-0.65067
H	1.39764	-2.73535	-0.91126
H	-3.27180	-3.88355	0.08886
H	-1.65375	-5.72160	-0.32110
H	0.74812	-5.12963	-0.83929
C	-2.65280	-1.18576	0.05086
C	-3.99236	-1.17689	0.40920
C	-4.66111	0.03560	0.59854
H	-4.52334	-2.11886	0.54207
C	-2.64159	1.22885	0.03016
C	-3.98131	1.23836	0.38792
H	-5.71080	0.04290	0.88284
H	-4.50391	2.18724	0.50358
C	-1.78463	2.35608	-0.21867
C	-2.19487	3.69855	-0.19151
C	0.39768	3.03421	-0.74866
C	-1.28909	4.70673	-0.44239
H	-3.23579	3.93218	0.02552
C	0.04267	4.36500	-0.73173
H	1.42055	2.72532	-0.96686
H	-1.60291	5.74840	-0.42168
H	0.79197	5.12602	-0.93676
N	-0.48823	-2.01186	-0.45718
N	-1.96060	0.01738	-0.07738
N	-0.47016	2.02655	-0.49423
C	1.92640	-0.03131	-2.79910
C	2.42384	-0.04915	-4.10273
C	1.53828	-0.05955	-5.16821
C	0.16862	-0.05198	-4.90701
C	-0.25911	-0.03340	-3.59127
H	3.49629	-0.05514	-4.28106
H	1.90921	-0.07364	-6.19052
H	-0.56328	-0.06007	-5.71098
H	-1.31874	-0.02627	-3.33480
C	2.74848	-0.02095	-1.59157
C	4.14356	-0.02901	-1.59587
C	2.71217	0.00885	0.72435
C	4.82822	-0.01727	-0.39188
H	4.68849	-0.04428	-2.53686
C	4.09482	0.00247	0.79270
H	2.10821	0.02414	1.62948
H	5.91578	-0.02323	-0.37587
H	4.58384	0.01269	1.76354
N	0.59309	-0.02247	-2.55024
N	2.02938	-0.00299	-0.43649
C	-0.52943	0.02781	2.24345
O	-0.56135	-1.12820	2.51956
O	-0.54458	1.18847	2.50097

$[Ru–CO_2]^0$

Ru	0.11494	0.05356	0.43339
C	0.70717	-2.97449	0.44900
C	-1.52947	-2.31959	0.48828
C	-1.93710	-3.65278	0.49914
C	-0.98783	-4.66257	0.49117
C	0.36191	-4.31519	0.46510
H	1.75101	-2.66130	0.43323
H	-2.99786	-3.89397	0.51446
H	-1.29432	-5.70611	0.50383
H	1.14307	-5.07155	0.46151
C	-2.45177	-1.18850	0.47701
C	-3.84227	-1.24782	0.48143
C	-4.57508	-0.06593	0.44824
H	-4.35081	-2.20883	0.51382
C	-2.52426	1.17950	0.40318
C	-3.91370	1.15986	0.40782
H	-5.66203	-0.09823	0.45448
H	-4.47792	2.08953	0.38692
C	-1.66133	2.36070	0.36815
C	-2.13191	3.67104	0.32038
C	0.54287	3.11431	0.33300
C	-1.22745	4.72186	0.27642
H	-3.20251	3.86361	0.31837
C	0.13607	4.43801	0.27877
H	1.59839	2.84439	0.34347
H	-1.58161	5.74963	0.23931
H	0.88065	5.22947	0.24184
N	-0.20191	-1.98279	0.46067
N	-1.81952	0.01513	0.43203
N	-0.32140	2.08794	0.38017
C	1.86459	-0.02830	-2.12152
C	2.26284	-0.00250	-3.46043
C	1.29890	0.10728	-4.45164
C	-0.04272	0.19207	-4.08915
C	-0.36135	0.16082	-2.74007
H	3.31400	-0.05827	-3.73134
H	1.59326	0.13027	-5.49872
H	-0.82909	0.28095	-4.83467
H	-1.39773	0.22376	-2.40303

C	2.80274	-0.11927	-0.99188
C	4.17225	-0.31511	-1.17215
C	3.08495	-0.04076	1.31107
C	5.00946	-0.38376	-0.06980
H	4.58163	-0.42023	-2.17337
C	4.45226	-0.23530	1.19585
H	2.59007	0.12408	2.26872
H	6.07759	-0.54474	-0.19879
H	5.06613	-0.26716	2.09298
N	0.56326	0.05079	-1.77880
N	2.25635	0.00131	0.24850
C	0.06170	0.13189	2.50609
O	-0.77360	-0.58608	3.11068
O	0.88853	0.92448	3.03848

$[Ru–CO_2]^0$ CO_2 attack TS

Ru	0.00512	-0.02619	0.48300
C	0.40044	-3.08678	0.45836
C	-1.79307	-2.30401	0.40861
C	-2.27995	-3.60727	0.37146
C	-1.38800	-4.67072	0.37930
C	-0.02249	-4.40628	0.41518
H	1.45797	-2.83042	0.50386
H	-3.35191	-3.78720	0.33755
H	-1.75558	-5.69407	0.35277
H	0.71188	-5.20785	0.41848
C	-2.64773	-1.11276	0.38952
C	-4.03765	-1.08397	0.35382
C	-4.68730	0.14700	0.34232
H	-4.61085	-2.00789	0.34185
C	-2.56082	1.25214	0.38242
C	-3.94970	1.32691	0.35471
H	-5.77380	0.18664	0.32122
H	-4.45108	2.29163	0.34375
C	-1.62009	2.37699	0.37555
C	-2.01075	3.71254	0.33503
C	0.62477	2.99510	0.38325
C	-1.04341	4.70751	0.31656
H	-3.06760	3.96941	0.31829
C	0.29902	4.34216	0.33829
H	1.66232	2.66351	0.41422
H	-1.33450	5.75499	0.28576
H	1.09055	5.08728	0.32568
N	-0.45151	-2.05116	0.45943
N	-1.94578	0.04547	0.40302
N	-0.30047	2.02475	0.40229
C	1.78808	-0.11706	-1.95958
C	2.21238	-0.15298	-3.28887
C	1.26792	-0.16920	-4.30434
C	-0.08373	-0.15004	-3.97412
C	-0.43426	-0.11293	-2.63344
H	3.27093	-0.16915	-3.53386
H	1.58520	-0.19726	-5.34438
H	-0.85691	-0.16319	-4.73818
H	-1.48008	-0.09775	-2.32399
C	2.70495	-0.09950	-0.81012
C	4.09221	-0.10751	-0.95070
C	2.90970	-0.04194	1.50350
C	4.89873	-0.07909	0.17601
H	4.54269	-0.13478	-1.93927
C	4.29274	-0.04319	1.42702
H	2.39768	-0.02743	2.46155
H	5.98184	-0.08413	0.07727
H	4.87860	-0.01864	2.34249
N	0.47250	-0.09439	-1.64716
N	2.11426	-0.07057	0.41672
C	-0.07407	0.08927	2.52760
O	-1.40324	-0.82503	3.13756
O	0.14524	1.07988	3.20616
C	-0.53791	-1.75976	3.46514
O	0.66244	-1.29183	3.16316
O	-0.78537	-2.86040	3.94579

$[Ru–CO_2]^0$ proton transfer TS with $TEOAH^+$

Ru	-0.07605	0.01178	0.23329
C	0.91601	-2.90769	0.31899
C	-1.38206	-2.56610	0.14501
C	-1.60490	-3.94060	0.13448
C	-0.52880	-4.81138	0.22323
C	0.75650	-4.28436	0.31518
H	1.90332	-2.45292	0.39455
H	-2.61997	-4.32344	0.05695
H	-0.69132	-5.88674	0.21922
H	1.63027	-4.92703	0.38745
C	-2.44973	-1.57012	0.03808
C	-3.81345	-1.81942	-0.08553
C	-4.68962	-0.74516	-0.20428
H	-4.18966	-2.83987	-0.09501
C	-2.83310	0.76552	-0.05256
C	-4.20144	0.55939	-0.19295
H	-5.75690	-0.92469	-0.30975
H	-4.88131	1.40244	-0.29091
C	-2.14090	2.05515	0.03796
C	-2.79047	3.28688	0.03969
C	-0.07454	3.10060	0.29314
C	-2.04512	4.45096	0.16914
H	-3.87311	3.33147	-0.04509
C	-0.66218	4.35711	0.29648
H	1.00197	2.97595	0.40187
H	-2.53929	5.41993	0.17353
H	-0.04045	5.24277	0.40243
N	-0.11736	-2.05329	0.23926
N	-1.99125	-0.29415	0.04668
N	-0.78362	1.96985	0.16696
C	1.84650	0.19553	-2.12681
C	2.34350	0.25827	-3.42994
C	1.46200	0.17327	-4.49752
C	0.10082	0.02909	-4.24525
C	-0.32166	-0.02447	-2.92600
H	3.40792	0.37700	-3.61387
H	1.83526	0.22159	-5.51811
H	-0.62372	-0.04041	-5.05271

H	-1.37755	-0.13606	-2.67473
C	2.68893	0.28661	-0.92426
C	4.08036	0.36075	-0.98384
C	2.75161	0.41205	1.39494
C	4.81574	0.45607	0.18716
H	4.58943	0.33982	-1.94392
C	4.13484	0.48951	1.39937
H	2.16943	0.46604	2.31298
H	5.90160	0.50834	0.15196
H	4.66320	0.57497	2.34581
N	0.52413	0.05545	-1.89083
N	2.02622	0.29733	0.26516
C	-0.37736	0.07976	2.25563
O	-1.07797	-0.76065	2.86276
O	0.13954	1.10542	2.87059
H	-0.73877	1.48171	3.88691
C	-0.70619	3.06616	5.26935
H	-1.33965	3.57113	6.01101
H	0.15069	2.61842	5.79015
C	-0.18712	4.06627	4.25423
H	-1.01215	4.67396	3.84698
H	0.28619	3.53001	3.41247
C	-2.64088	2.44795	3.88972
H	-2.25162	2.99089	3.01577
H	-3.19464	3.16380	4.51424
C	-3.57472	1.36677	3.38351
H	-4.06289	0.83879	4.22013
H	-3.01052	0.61867	2.79954
C	-1.75046	0.87212	5.63056
H	-2.17497	0.02870	5.07494
H	-0.77866	0.53852	6.01781
C	-2.65888	1.27373	6.77333
H	-2.15725	2.00130	7.43256
H	-3.57676	1.75663	6.39297
N	-1.46393	1.94888	4.64997
O	0.73296	4.86798	4.95904
H	1.00545	5.58961	4.37274
O	-4.52949	2.04969	2.59893
H	-5.15695	1.38914	2.26809
O	-2.94775	0.07641	7.45728
H	-3.45033	0.30341	8.25393

[Ru–CO_2H]$^+$

Ru	0.16600	0.00630	0.45438
C	0.69438	-3.03573	0.48751
C	-1.52911	-2.34315	0.44084
C	-1.96400	-3.66439	0.43673
C	-1.03060	-4.69166	0.46349
C	0.32234	-4.37218	0.49004
H	1.74235	-2.73942	0.51087
H	-3.02827	-3.88669	0.41477
H	-1.35722	-5.72893	0.46380
H	1.08825	-5.14314	0.51428
C	-2.43788	-1.19095	0.41149
C	-3.82866	-1.22613	0.36308
C	-4.52973	-0.02600	0.31170
H	-4.35997	-2.17455	0.36365
C	-2.45770	1.17533	0.35739
C	-3.84704	1.18758	0.30450
H	-5.61635	-0.03538	0.27359
H	-4.39291	2.12665	0.26020
C	-1.56421	2.34207	0.34685
C	-2.01582	3.65606	0.28998
C	0.65049	3.06255	0.38209
C	-1.09392	4.69457	0.27696
H	-3.08256	3.86435	0.25572
C	0.26235	4.39360	0.32213
H	1.70106	2.77814	0.42798
H	-1.43302	5.72689	0.23218
H	1.01844	5.17449	0.31366
N	-0.19790	-2.03555	0.46254
N	-1.79481	-0.00234	0.41134
N	-0.23004	2.05313	0.39461
C	1.80306	-0.00694	-2.07212
C	2.14834	0.02925	-3.42328
C	1.14521	0.06901	-4.38067
C	-0.18424	0.07066	-3.97183
C	-0.45643	0.03389	-2.61315
H	3.19038	0.03024	-3.73088
H	1.40129	0.09843	-5.43738
H	-1.00048	0.09939	-4.68898
H	-1.48288	0.03178	-2.24451
C	2.78504	-0.04953	-0.97812
C	4.15908	-0.12116	-1.20175
C	3.12917	-0.06503	1.31865
C	5.03103	-0.16754	-0.12517
H	4.54815	-0.14456	-2.21593
C	4.50347	-0.13861	1.16050
H	2.67811	-0.02264	2.30647
H	6.10440	-0.22590	-0.28987
H	5.14220	-0.17189	2.03943
N	0.50759	-0.00348	-1.68339
N	2.27099	-0.02198	0.28229
C	0.04597	0.02616	2.47163
O	-0.60568	-0.71312	3.20309
O	0.77795	1.02105	3.09138
H	0.61988	0.90972	4.05247

[Ru–CO_2H]$^+$ CO_2 attack TS

Ru	0.00047	0.05258	0.56770
C	0.43084	-3.01369	0.58439
C	-1.76434	-2.25556	0.38148
C	-2.22873	-3.55965	0.25961
C	-1.32360	-4.61259	0.30339
C	0.02767	-4.33616	0.46487
H	1.47934	-2.74922	0.71413
H	-3.29073	-3.75035	0.12568
H	-1.67373	-5.63777	0.20875
H	0.77009	-5.12901	0.50125
C	-2.64042	-1.07362	0.31543
C	-4.02288	-1.06512	0.15095
C	-4.67677	0.15882	0.05824

H	-4.58291	-1.99461	0.09155
C	-2.58041	1.29462	0.27244
C	-3.95970	1.35129	0.10695
H	-5.75633	0.18464	-0.06782
H	-4.47073	2.30567	0.01083
C	-1.64722	2.43408	0.28947
C	-2.05358	3.75808	0.17846
C	0.58706	3.08790	0.41895
C	-1.09808	4.76748	0.18986
H	-3.10970	3.99962	0.08646
C	0.24312	4.42931	0.31229
H	1.62415	2.77113	0.52277
H	-1.40258	5.80799	0.10538
H	1.02190	5.18715	0.32735
N	-0.43371	-1.99139	0.55105
N	-1.97168	0.09651	0.39846
N	-0.32596	2.11058	0.40469
C	1.68910	-0.12262	-1.88993
C	2.06991	-0.16682	-3.23019
C	1.09452	-0.15507	-4.21680
C	-0.24396	-0.09933	-3.84679
C	-0.55479	-0.05857	-2.49660
H	3.11940	-0.20772	-3.50754
H	1.38003	-0.18813	-5.26567
H	-1.04035	-0.08764	-4.58609
H	-1.59137	-0.01324	-2.16352
C	2.64459	-0.12686	-0.77218
C	4.02213	-0.22258	-0.95564
C	2.92653	-0.05060	1.53373
C	4.86367	-0.23039	0.14639
H	4.43869	-0.29429	-1.95630
C	4.30393	-0.14409	1.41482
H	2.45436	0.00936	2.51044
H	5.94022	-0.30665	0.01331
H	4.91829	-0.15081	2.31127
N	0.38231	-0.07034	-1.53905
N	2.10139	-0.03847	0.47167
C	-0.03367	0.33714	2.51452
O	0.42474	1.10311	3.29224
C	-0.05673	-2.23220	3.67531
O	1.09516	-1.92354	3.84049
O	-0.82864	-3.15571	3.62535
O	-0.94482	-0.80647	3.43119
H	-1.72073	-1.09644	2.91675

$[Ru–CO_2H]^+$ C–O bond cleavage TS with H_2O

Ru	0.05978	0.21129	0.56865
C	0.64126	-2.83046	0.76049
C	-1.59487	-2.19018	0.57064
C	-2.00174	-3.51730	0.61842
C	-1.04683	-4.52044	0.73743
C	0.29555	-4.17473	0.80886
H	1.67900	-2.50531	0.82337
H	-3.05838	-3.76685	0.56843
H	-1.35421	-5.56270	0.77715
H	1.07333	-4.92728	0.90564
C	-2.52925	-1.05648	0.43850
C	-3.91106	-1.12457	0.28887
C	-4.62158	0.06303	0.13945
H	-4.42913	-2.07997	0.28145
C	-2.58172	1.30642	0.27442
C	-3.96514	1.28964	0.12400
H	-5.70199	0.03066	0.02170
H	-4.52420	2.21181	-0.01050
C	-1.70236	2.48789	0.23860
C	-2.17587	3.78769	0.11635
C	0.49951	3.24970	0.32995
C	-1.26968	4.84284	0.11458
H	-3.24331	3.97688	0.03512
C	0.08746	4.57229	0.22224
H	1.54982	2.98408	0.42536
H	-1.62608	5.86678	0.02933
H	0.82749	5.36812	0.22561
N	-0.27198	-1.86096	0.64101
N	-1.92193	0.14493	0.43824
N	-0.36605	2.23365	0.33890
C	1.66982	-0.22109	-1.89397
C	2.00490	-0.51450	-3.21379
C	1.00344	-0.58760	-4.17152
C	-0.31442	-0.35966	-3.79496
C	-0.58198	-0.07710	-2.46455
H	3.04026	-0.68131	-3.49729
H	1.25395	-0.81644	-5.20479
H	-1.12853	-0.39929	-4.51349
H	-1.60179	0.10369	-2.12685
C	2.65882	-0.07604	-0.81501
C	4.02980	-0.21640	-1.01032
C	2.99616	0.50819	1.41724
C	4.89581	0.00018	0.05254
H	4.42299	-0.48806	-1.98597
C	4.37148	0.38753	1.27909
H	2.52492	0.89054	2.32827
H	5.96861	-0.11310	-0.08596
H	5.01485	0.60284	2.12839
N	0.38018	-0.01124	-1.53467
N	2.15213	0.24903	0.40301
C	0.01137	0.13431	2.45649
O	0.06975	-0.34002	3.51278
O	1.29104	2.35281	3.24615
H	1.55139	1.98852	4.10290
O	-1.12980	2.16481	3.28634
H	-1.43120	2.88252	2.71367
H	0.12362	2.31369	3.28920

$[Ru–CO_2H]^+$ C–O bond cleavage TS with $TEOAH^+$

Ru	-0.02113	-0.01120	0.55202
C	0.79834	-2.97492	0.81117
C	-1.47882	-2.52370	0.58479
C	-1.77896	-3.87788	0.67253
C	-0.74860	-4.79617	0.83320

C	0.56121	-4.33975	0.90248
H	1.80649	-2.56686	0.86832
H	-2.81086	-4.21558	0.61860
H	-0.97137	-5.85815	0.90483
H	1.39605	-5.02358	1.02957
C	-2.49415	-1.47375	0.39613
C	-3.85827	-1.65746	0.19141
C	-4.65158	-0.54173	-0.05774
H	-4.29802	-2.65104	0.20461
C	-2.72657	0.87013	0.12461
C	-4.09244	0.73165	-0.10578
H	-5.71730	-0.66814	-0.23235
H	-4.71407	1.59499	-0.32624
C	-1.95047	2.12266	0.10700
C	-2.51937	3.37341	-0.10497
C	0.16755	3.07577	0.31235
C	-1.70462	4.49991	-0.11348
H	-3.59046	3.47148	-0.25673
C	-0.33942	4.35050	0.09399
H	1.22859	2.90813	0.49079
H	-2.13686	5.48382	-0.28062
H	0.33371	5.20415	0.09573
N	-0.18785	-2.08389	0.65459
N	-1.98093	-0.22602	0.37327
N	-0.60896	1.98691	0.32174
C	1.63550	0.05724	-1.93440
C	1.99670	0.05470	-3.28058
C	1.01844	-0.11989	-4.24876
C	-0.30306	-0.29142	-3.85452
C	-0.59537	-0.27517	-2.49977
H	3.03289	0.18901	-3.57730
H	1.28905	-0.12336	-5.30206
H	-1.10063	-0.43467	-4.57837
H	-1.61896	-0.40461	-2.14874
C	2.59857	0.21462	-0.83400
C	3.96892	0.35410	-1.04370
C	2.91182	0.30479	1.46523
C	4.82262	0.47059	0.04272
H	4.37207	0.36622	-2.05223
C	4.28304	0.44051	1.32255
H	2.45320	0.29023	2.44934
H	5.89368	0.57868	-0.11090
H	4.90805	0.52090	2.20791
N	0.34447	-0.10317	-1.56037
N	2.07288	0.19839	0.42048
C	-0.16855	-0.01826	2.49840
O	-0.48697	-0.69981	3.41221
O	0.46636	1.52058	3.17885
H	0.93764	1.19539	3.97048
H	-0.48988	2.17294	3.71455
C	-0.58433	4.04787	4.80584
H	-1.23818	4.67366	5.42976
H	0.27922	3.74126	5.41249
C	-0.07418	4.84599	3.62330
H	-0.90724	5.31323	3.07191
H	0.45459	4.17267	2.92371
C	-2.53394	3.11272	3.65236
H	-2.23573	3.57586	2.70094
H	-3.13589	3.84911	4.20628
C	-3.37326	1.89347	3.33118
H	-3.79755	1.44394	4.24317
H	-2.74609	1.11982	2.84309
C	-1.49734	1.91589	5.57896
H	-1.90429	0.96428	5.21507
H	-0.50138	1.70147	5.99027
C	-2.39018	2.46072	6.67491
H	-1.93576	3.35121	7.13945
H	-3.36892	2.76613	6.26496
N	-1.29844	2.80981	4.41117
O	0.78405	5.81904	4.16925
H	1.03965	6.42297	3.45584
O	-4.39300	2.35711	2.47815
H	-5.02481	1.63261	2.35162
O	-2.52245	1.40805	7.60157
H	-3.03847	1.73674	8.35303

[Ru–CO_2H]^0

Ru	0.18108	-0.00006	0.47857
C	0.68581	-3.05041	0.52534
C	-1.53658	-2.35269	0.43592
C	-1.96799	-3.67658	0.42570
C	-1.03864	-4.70579	0.47080
C	0.31568	-4.38580	0.52189
H	1.73396	-2.75467	0.56878
H	-3.03268	-3.89582	0.38403
H	-1.36604	-5.74310	0.46620
H	1.08141	-5.15677	0.56083
C	-2.44642	-1.19951	0.38873
C	-3.83138	-1.24848	0.31873
C	-4.53112	-0.02109	0.26739
H	-4.36451	-2.19563	0.30540
C	-2.44336	1.19805	0.34860
C	-3.85651	1.18115	0.28028
H	-5.61862	-0.02701	0.21564
H	-4.40936	2.11856	0.24055
C	-1.57422	2.32459	0.34548
C	-2.00395	3.67506	0.28324
C	0.66552	3.06707	0.38618
C	-1.08960	4.69777	0.26955
H	-3.07151	3.88939	0.24632
C	0.29307	4.39725	0.31962
H	1.71882	2.78302	0.43800
H	-1.42674	5.73220	0.22139
H	1.05039	5.17707	0.31046
N	-0.20396	-2.04453	0.48303
N	-1.79361	-0.02093	0.39974
N	-0.20248	2.04562	0.40009
C	1.79351	-0.00228	-2.06419
C	2.12944	0.04289	-3.41882
C	1.12044	0.08364	-4.36928
C	-0.20718	0.07670	-3.95093
C	-0.46942	0.03012	-2.59085

H	3.16961	0.05126	-3.73344
H	1.36924	0.12088	-5.42765
H	-1.02800	0.10674	-4.66310
H	-1.49176	0.01898	-2.21026
C	2.78222	-0.04369	-0.97752
C	4.15588	-0.11173	-1.21226
C	3.14801	-0.05377	1.31611
C	5.03856	-0.15431	-0.14528
H	4.53502	-0.13549	-2.23049
C	4.52005	-0.12325	1.14584
H	2.70345	-0.00711	2.30729
H	6.11072	-0.21021	-0.31906
H	5.16689	-0.15137	2.01938
N	0.50011	-0.00766	-1.66629
N	2.27510	-0.01789	0.28834
C	0.05675	0.01921	2.48216
O	-0.58354	-0.72632	3.22380
O	0.78620	1.01527	3.12060
H	0.61773	0.88414	4.07663

$[Ru–CO_2H]^0$ CO_2 attack TS

Ru	0.04642	0.13208	0.53989
C	0.48316	-2.94232	0.60587
C	-1.73934	-2.17052	0.39193
C	-2.18187	-3.51478	0.30848
C	-1.28094	-4.54808	0.36779
C	0.09681	-4.26528	0.51535
H	1.53341	-2.67130	0.72831
H	-3.24539	-3.71622	0.18859
H	-1.62644	-5.57822	0.29840
H	0.84173	-5.05521	0.56415
C	-2.59115	-1.03041	0.29840
C	-3.99289	-0.99787	0.11301
C	-4.64048	0.21020	-0.02113
H	-4.55725	-1.92793	0.07087
C	-2.55482	1.37086	0.20366
C	-3.92232	1.43083	0.01174
H	-5.71888	0.22936	-0.16601
H	-4.43528	2.38025	-0.11780
C	-1.62606	2.51315	0.22513
C	-2.03182	3.83949	0.10574
C	0.60356	3.18204	0.39584
C	-1.08453	4.85320	0.13295
H	-3.08817	4.07366	-0.00469
C	0.25875	4.51991	0.28191
H	1.64061	2.87058	0.51939
H	-1.39190	5.89257	0.04147
H	1.03413	5.28117	0.31155
N	-0.37394	-1.90945	0.55350
N	-1.93146	0.18220	0.36011
N	-0.30355	2.19443	0.36527
C	1.68960	-0.10605	-1.95333
C	2.04817	-0.17975	-3.29984
C	1.05741	-0.15792	-4.27045
C	-0.27412	-0.06169	-3.88006
C	-0.56107	0.00781	-2.52581
H	3.09195	-0.24965	-3.59358
H	1.32477	-0.21402	-5.32333
H	-1.08101	-0.04204	-4.60800
H	-1.58844	0.08335	-2.16829
C	2.66178	-0.10793	-0.84968
C	4.03499	-0.23908	-1.05220
C	2.98731	0.04242	1.44672
C	4.89612	-0.22774	0.03386
H	4.43191	-0.35269	-2.05724
C	4.35975	-0.08160	1.30845
H	2.52978	0.15516	2.42691
H	5.96842	-0.33227	-0.11428
H	4.99040	-0.06650	2.19374
N	0.39065	-0.01451	-1.58355
N	2.14009	0.02863	0.40033
C	0.01423	0.39115	2.46889
O	0.48236	1.12482	3.27983
C	-0.16650	-2.10162	3.86633
O	0.99950	-1.83379	3.99730
O	-0.99254	-2.96994	3.98868
O	-0.98486	-0.70951	3.32235
H	-1.63644	-1.07067	2.69148

$[Ru–CO_2H]^0$ C–O bond cleavage TS with H_2O

Ru	0.02351	0.23463	0.59951
C	0.64415	-2.79934	0.79557
C	-1.62286	-2.17095	0.54875
C	-1.99055	-3.53627	0.60153
C	-1.03302	-4.50985	0.74220
C	0.32838	-4.14165	0.84225
H	1.67725	-2.45818	0.88198
H	-3.04377	-3.80392	0.53427
H	-1.32300	-5.55828	0.78229
H	1.11451	-4.88278	0.95909
C	-2.53932	-1.08611	0.40357
C	-3.93815	-1.14198	0.22933
C	-4.65608	0.02356	0.06267
H	-4.44862	-2.10358	0.21845
C	-2.64074	1.31162	0.22630
C	-4.01005	1.28353	0.05146
H	-5.73447	-0.02371	-0.07418
H	-4.57956	2.19662	-0.10135
C	-1.77688	2.50140	0.18871
C	-2.25407	3.80021	0.02982
C	0.42213	3.28911	0.24817
C	-1.35907	4.85925	-0.01431
H	-3.32353	3.97761	-0.05614
C	0.00581	4.60125	0.08940
H	1.47682	3.03312	0.34300
H	-1.72291	5.87747	-0.13283
H	0.74114	5.40079	0.05293
N	-0.27230	-1.82875	0.64546
N	-1.95195	0.16064	0.40544
N	-0.43700	2.26219	0.31103
C	1.64343	-0.19768	-1.87563
C	1.98170	-0.49586	-3.19463

C	0.98088	-0.57887	-4.15223
C	-0.33920	-0.35771	-3.77785
C	-0.60792	-0.06859	-2.44866
H	3.01767	-0.65946	-3.47797
H	1.23351	-0.81191	-5.18421
H	-1.15215	-0.40885	-4.49715
H	-1.62657	0.10690	-2.10288
C	2.63102	-0.04815	-0.79428
C	4.00226	-0.18731	-0.99410
C	2.97367	0.53280	1.43878
C	4.87210	0.02829	0.06536
H	4.39243	-0.45842	-1.97123
C	4.34920	0.41384	1.29324
H	2.51359	0.91035	2.36640
H	5.94470	-0.08457	-0.07632
H	4.99527	0.62905	2.14100
N	0.35382	0.00927	-1.52107
N	2.12543	0.27324	0.42590
C	-0.07452	0.11948	2.45249
O	-0.10629	-0.36342	3.51136
O	1.62882	2.07612	3.74891
H	1.61027	1.33754	4.37061
O	-0.75231	2.40822	3.37940
H	-0.77905	3.02457	2.63749
H	0.47586	2.27084	3.57805

$[Ru–CO_2H]^0$ C–O bond cleavage TS with $TEOAH^+$

Ru	0.11288	0.14652	0.63083
C	0.60883	-2.89373	0.91604
C	-1.62517	-2.18933	0.62621
C	-2.04557	-3.53912	0.69754
C	-1.12658	-4.54439	0.87309
C	0.24375	-4.22422	0.98732
H	1.65315	-2.58953	1.00727
H	-3.10671	-3.76919	0.61718
H	-1.45555	-5.58063	0.92872
H	1.00093	-4.99079	1.12923
C	-2.49769	-1.07806	0.43257
C	-3.88062	-1.09432	0.15072
C	-4.54630	0.08529	-0.10763
H	-4.41818	-2.04060	0.11796
C	-2.49975	1.31389	0.17391
C	-3.85712	1.32765	-0.09971
H	-5.61130	0.06744	-0.32949
H	-4.37781	2.25231	-0.33579
C	-1.59181	2.47303	0.12563
C	-2.01212	3.76900	-0.16671
C	0.62272	3.19115	0.26765
C	-1.07642	4.79007	-0.25742
H	-3.06771	3.97130	-0.33442
C	0.26742	4.49644	-0.03779
H	1.65939	2.91529	0.45667
H	-1.39228	5.80363	-0.49542
H	1.03502	5.26409	-0.09797
N	-0.26691	-1.89316	0.73565
N	-1.86598	0.15415	0.45631
N	-0.27188	2.19510	0.34922
C	1.67628	-0.06633	-1.91657
C	1.99336	-0.19773	-3.26855
C	0.97218	-0.29760	-4.20169
C	-0.34821	-0.26449	-3.76772
C	-0.59392	-0.13050	-2.41007
H	3.02893	-0.22404	-3.59560
H	1.20787	-0.40151	-5.25846
H	-1.17896	-0.34126	-4.46417
H	-1.61252	-0.09924	-2.02332
C	2.68663	0.04191	-0.85346
C	4.05630	0.04520	-1.11372
C	3.09355	0.23867	1.42425
C	4.95771	0.14683	-0.06608
H	4.41983	-0.03163	-2.13461
C	4.46443	0.24501	1.23000
H	2.67472	0.32009	2.42426
H	6.02764	0.14907	-0.26031
H	5.12658	0.32613	2.08809
N	0.38771	-0.03258	-1.50357
N	2.20615	0.13898	0.41660
C	0.14122	0.13508	2.56279
O	0.10471	-0.58745	3.50696
O	0.52272	1.77364	3.21192
H	1.05335	1.52876	3.99328
H	-0.59291	2.20350	3.78650
C	-1.22160	4.09377	4.55880
H	-1.97165	4.57190	5.20307
H	-0.23618	4.20013	5.03257
C	-1.17242	4.75475	3.19735
H	-2.18843	4.90218	2.79472
H	-0.62659	4.09567	2.49898
C	-2.80554	2.36711	3.81476
H	-2.75244	2.76604	2.79003
H	-3.59397	2.91912	4.34807
C	-3.17142	0.89423	3.72600
H	-3.29761	0.45038	4.72171
H	-2.37081	0.32983	3.21384
C	-1.29530	1.95719	5.76185
H	-1.30882	0.87399	5.58477
H	-0.28333	2.21502	6.10254
C	-2.29455	2.31109	6.84401
H	-2.24442	3.38618	7.08441
H	-3.32459	2.09612	6.51105
N	-1.49476	2.63847	4.45747
O	-0.51479	5.98604	3.37530
H	-0.55694	6.46427	2.53291
O	-4.41064	0.75897	3.07783
H	-4.29289	1.02398	2.14933
O	-1.93434	1.51827	7.95126
H	-2.54035	1.73004	8.67704

$[Ru–CO]^{2+}$

Ru	0.18471	0.00061	0.55575
C	0.67631	-3.06169	0.48002

C	-1.54397	-2.34349	0.41118
C	-1.99242	-3.65508	0.34046
C	-1.06573	-4.69186	0.34122
C	0.28774	-4.39365	0.41026
H	1.72492	-2.77550	0.54146
H	-3.05702	-3.86690	0.28341
H	-1.40381	-5.72382	0.28719
H	1.04367	-5.17412	0.41243
C	-2.44592	-1.17768	0.39037
C	-3.83264	-1.19892	0.28379
C	-4.51245	0.01382	0.22331
H	-4.37661	-2.13845	0.24296
C	-2.43660	1.19243	0.36216
C	-3.82289	1.22215	0.25280
H	-5.59644	0.01719	0.14026
H	-4.35889	2.16485	0.18693
C	-1.52665	2.35210	0.36272
C	-1.96689	3.66538	0.27413
C	0.69769	3.05776	0.42649
C	-1.03404	4.69653	0.26314
H	-3.03015	3.88303	0.21379
C	0.31740	4.39101	0.33886
H	1.74447	2.76661	0.49450
H	-1.36570	5.72981	0.19594
H	1.07817	5.16675	0.33343
N	-0.21023	-2.06184	0.48137
N	-1.80832	0.00568	0.44185
N	-0.19475	2.06313	0.43872
C	1.74838	-0.03944	-1.97905
C	2.06455	-0.07802	-3.33439
C	1.04180	-0.10014	-4.27209
C	-0.27796	-0.08420	-3.83985
C	-0.52654	-0.05035	-2.47685
H	3.09983	-0.09284	-3.66221
H	1.27814	-0.12972	-5.33313
H	-1.10847	-0.09923	-4.54001
H	-1.54737	-0.03988	-2.09835
C	2.75875	-0.00809	-0.91111
C	4.12717	0.01127	-1.16516
C	3.15433	0.02545	1.38035
C	5.02199	0.03552	-0.10583
H	4.49585	0.00909	-2.18649
C	4.52666	0.04096	1.19138
H	2.73456	0.03148	2.38263
H	6.09256	0.05004	-0.29500
H	5.18546	0.05846	2.05513
N	0.45744	-0.02954	-1.56781
N	2.28008	0.00255	0.36046
C	0.12670	0.02143	2.40101
O	0.08766	0.03533	3.55919

[Ru–CO]$^{+}$

Ru	0.18251	-0.00316	0.58829
C	0.66263	-3.07813	0.53471
C	-1.56020	-2.35365	0.39710
C	-1.99917	-3.67655	0.33500
C	-1.07706	-4.70862	0.37289
C	0.28189	-4.40690	0.47241
H	1.70964	-2.78939	0.61963
H	-3.06279	-3.88876	0.25472
H	-1.41210	-5.74224	0.32432
H	1.03790	-5.18694	0.50287
C	-2.45138	-1.19396	0.34760
C	-3.82405	-1.21117	0.21355
C	-4.51144	0.02088	0.14611
H	-4.37020	-2.14949	0.15658
C	-2.42582	1.21643	0.33076
C	-3.82180	1.22004	0.19927
H	-5.59407	0.02511	0.04294
H	-4.36087	2.16342	0.13494
C	-1.54051	2.34201	0.35739
C	-1.95432	3.68866	0.29064
C	0.70780	3.05477	0.46924
C	-1.02457	4.70092	0.30859
H	-3.01687	3.91552	0.22473
C	0.34682	4.38354	0.39669
H	1.75315	2.75558	0.55044
H	-1.34649	5.73907	0.25659
H	1.11170	5.15524	0.41271
N	-0.22323	-2.07021	0.49949
N	-1.79267	-0.00424	0.40940
N	-0.18463	2.04856	0.44997
C	1.73599	-0.03949	-1.98344
C	2.04326	-0.07636	-3.34210
C	1.01303	-0.10562	-4.27142
C	-0.30406	-0.09866	-3.82929
C	-0.54077	-0.06660	-2.46355
H	3.07573	-0.08439	-3.67918
H	1.24130	-0.13353	-5.33446
H	-1.13903	-0.11897	-4.52427
H	-1.55483	-0.06282	-2.06492
C	2.75483	0.00007	-0.92129
C	4.12120	0.02985	-1.19086
C	3.17698	0.03926	1.36324
C	5.02845	0.06265	-0.14296
H	4.47848	0.02973	-2.21646
C	4.54703	0.06568	1.16006
H	2.76566	0.04381	2.36966
H	6.09675	0.08571	-0.34446
H	5.21568	0.08983	2.01629
N	0.44997	-0.03860	-1.56447
N	2.28871	0.00808	0.35507
C	0.14260	0.03313	2.40892
O	0.11774	0.06689	3.57404

[Ru–CO]^{0}

Ru	0.09384	0.00456	0.44576
C	0.60640	-3.06417	0.34249
C	-1.64249	-2.33588	0.41963
C	-2.06028	-3.68661	0.45819
C	-1.13857	-4.70276	0.43409
C	0.23989	-4.38928	0.36337

H	1.65606	-2.76802	0.30579
H	-3.12582	-3.90902	0.49518
H	-1.46590	-5.74059	0.46198
H	1.00046	-5.16538	0.33213
C	-2.50560	-1.20247	0.37511
C	-3.87840	-1.19328	0.55874
C	-4.58087	0.02084	0.57605
H	-4.40901	-2.12858	0.73760
C	-2.49751	1.22504	0.34381
C	-3.87018	1.22930	0.52929
H	-5.65648	0.02646	0.73895
H	-4.39459	2.17209	0.68609
C	-1.62717	2.35376	0.35386
C	-2.03618	3.70776	0.35181
C	0.62616	3.06479	0.24371
C	-1.10814	4.71662	0.29174
H	-3.10019	3.93795	0.38457
C	0.26801	4.39221	0.22466
H	1.67374	2.76091	0.21059
H	-1.42881	5.75689	0.28805
H	1.03317	5.16215	0.16534
N	-0.28058	-2.04620	0.37547
N	-1.84643	0.00512	0.06592
N	-0.26716	2.05423	0.31314
C	1.88929	-0.03852	-2.07511
C	2.29272	-0.05939	-3.41077
C	1.32723	-0.08021	-4.40830
C	-0.01828	-0.07922	-4.05752
C	-0.34411	-0.05549	-2.70897
H	3.34573	-0.06012	-3.67844
H	1.62728	-0.09717	-5.45390
H	-0.80238	-0.09581	-4.81027
H	-1.37714	-0.05128	-2.35283
C	2.82888	-0.01996	-0.93825
C	4.21322	-0.02337	-1.10928
C	3.08560	0.01749	1.36529
C	5.04320	-0.00507	0.00089
H	4.64438	-0.04081	-2.10641
C	4.46737	0.01611	1.26595
H	2.59833	0.03313	2.33849
H	6.12378	-0.00747	-0.12229
H	5.07228	0.03102	2.16886
N	0.58183	-0.03506	-1.74878
N	2.27037	-0.00014	0.29795
C	-0.02377	0.03410	2.23614
O	-0.12866	0.05482	3.40816