Supporting information:

Mechanism and Selectivity of Photocatalyzed CO_2 Reduction by a Function-Integrated Ru Catalyst

Ya-Qiong Zhang[a], Ying-Ying Li[a], Feliu Maseras[b], and Rong-Zhen Liao[a*]

[a]Key Laboratory of Material Chemistry for Energy Conversion and Storage, Ministry of Education, Hubei Key Laboratory of Bioinorganic Chemistry and Materia Medica, Hubei Key Laboratory of Materials Chemistry and Service Failure, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan 430074, China

[b]Institute of Chemical Research of Catalonia (ICIQ), The Barcelona Institute of Science and Technology, Avgda. Països Catalans, 16, 43007 Tarragona, Catalonia, Spain

*Corresponding author: rongzhen@hust.edu.cn

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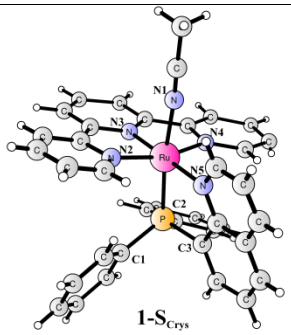
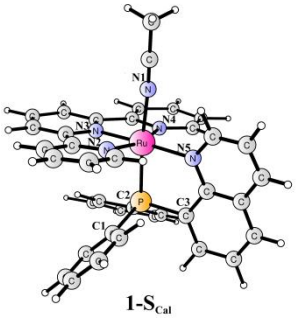
Contents

S1. Comparison of the crystal structure and the calculated structure of 1-S.

Table S1. Comparison of the crystal structure and the calculated structure of **1-S**.

		Crystal structure [S1]	Calculated structure
		 1-S$_{Crys}$	 1-S$_{Cal}$
Bond distance/(Å)	Ru-N1	2.127	2.102
	Ru-N2	2.077	2.103
	Ru-N3	1.967	1.991
	Ru-N4	2.081	2.102
	Ru-N5	2.119	2.156
	Ru-P	2.265	2.305
	P-C1	1.824	1.837
	P-C2	1.812	1.828
	P-C3	1.819	1.826
Angle/(°)	∠N2RuP	99.8	94.5
	∠N3RuP	96.2	95.4
	∠N4RuP	86.7	90.0
	∠N5RuP	83.0	82.3
	∠N1RuN2	86.3	88.7
	∠N1RuN3	88.0	89.4
	∠N1RuN4	88.7	88.5
	∠N1RuN5	92.8	92.9
	∠N2RuN3	79.7	79.2
	∠N3RuN4	79.3	79.4
	∠N4RuN5	100.3	98.4
	∠N5RuN2	100.7	103.0

S2. Energy diagram of ^{3}1-S with the increase of the Ru-N1distance.

The energy diagram of **^{3}1-S** with the increased distance of the Ru-N1 bond is shown in **Figure S1**. With the increase of the Ru-N1distance, the energy of the **^{3}1-S** complex increase gradually. It indicated that the S ligand tends to keep coordinated to Ru^{II} in the excitation process.

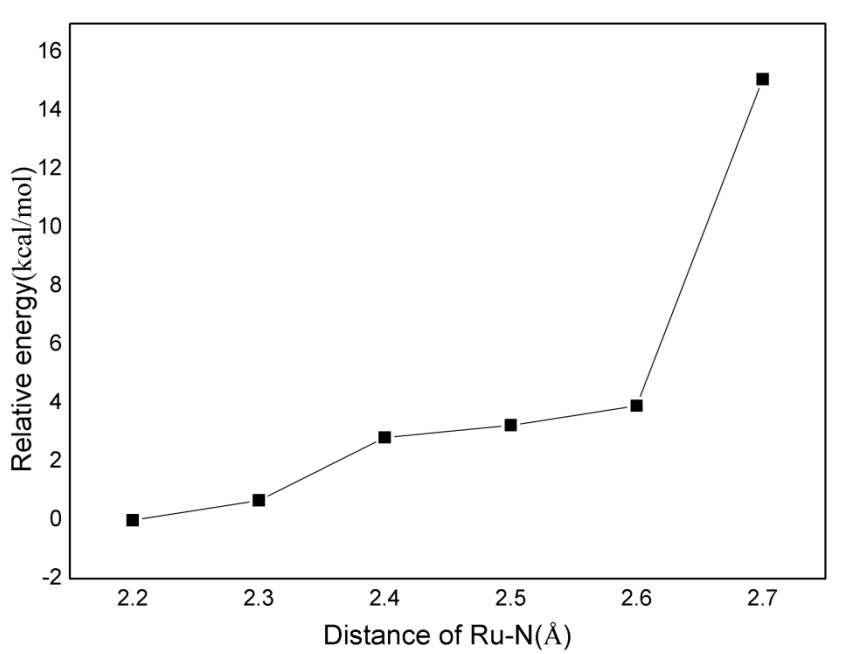


Figure S1. Energy diagram of **^{3}1-S** with the increased distance of Ru-N1.

S3. Computed UV-Vis absorption spectra.

The three smaller absorption peaks at 415, 395, and 382 nm (see **Table S1**) correspond to the excitation from HOMO-2 to LUMO, HOMO-1 to LUMO+1, and HOMO to LUMO+2, respectively.

The computed UV-Vis absorption spectra of ^{2}**2-S** showed a red-shift relative to that of ^{1}**1-S**, which is in good agreement with the experiment results.[S2]

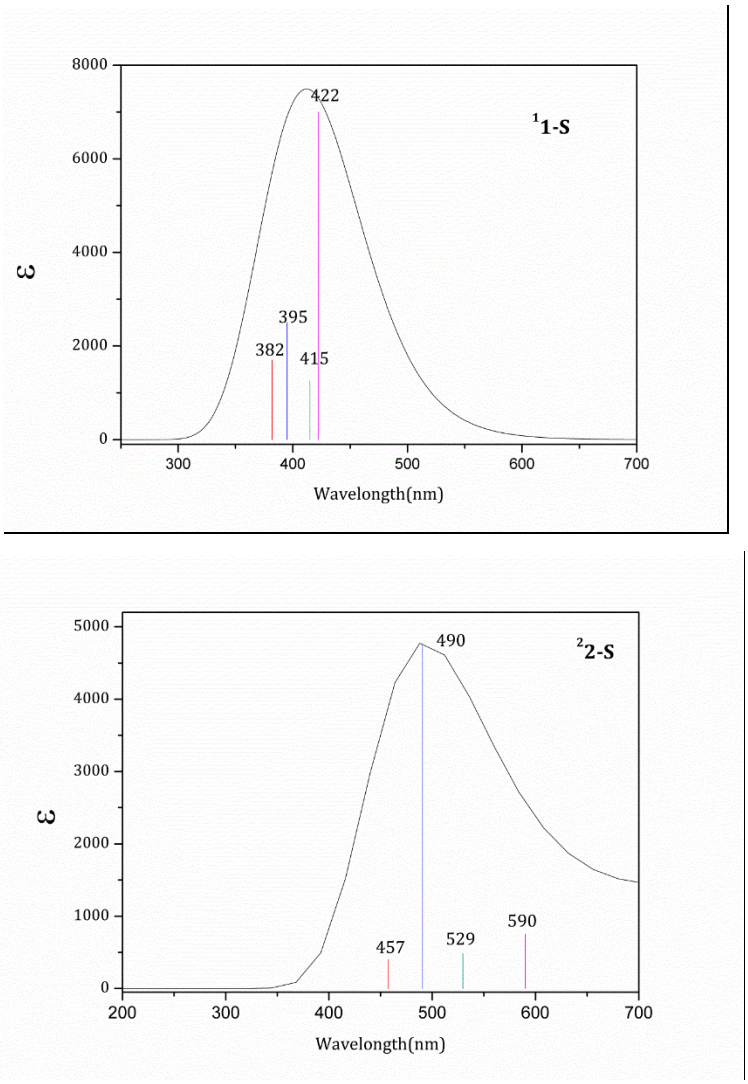


Figure S2. The computed UV-Vis absorption spectra for the ^{1}**1-S** and ^{2}**2-S** complexes in the 250~700 nm region.

S4. Calculated main optical transitions for ^{1}1-S.

Table S2. The calculated main optical transition for the ^{1}**1-S** complex, with oscillator strength f >0.02[a] (nstate=20).

excitation	composition	Energy(eV)	w(nm)	f
161A ->162A	97%(HOMO → LUMO)	2.4926	497.42	0.0011
160A ->162A	97%(HOMO-1 → LUMO)	2.7552	450.01	0.0119
159A ->162A 161A ->163A 161A ->164A	3%(HOMO-2 → LUMO) 25%(HOMO → LUMO+1) 71%(HOMO → LUMO+2)	2.8523	434.68	0.0033
159A ->162A 160A ->164A 161A ->163A 161A ->164A	35%(HOMO-2 → LUMO) 3%(HOMO-1 → LUMO+2) 31%(HOMO → LUMO+1) 21%(HOMO → LUMO+2)	2.9355	422.36	**0.1017**
159A ->162A 160A ->163A 160A ->164A 161A ->163A 161A ->164A	33%(HOMO-2→ LUMO) 7%(HOMO-1 → LUMO+1) 14%(HOMO-1 → LUMO+2) 37%(HOMO → LUMO+1) 6%(HOMO → LUMO+2)	2.9885	414.87	**0.0198**
160A ->163A 160A ->164A	84%(HOMO-1→ LUMO+1) 12%(HOMO-1→ LUMO+2)	3.1329	395.74	0.0018
159A ->163A 159A ->164A	50%(HOMO-2→ LUMO+1) 46%(HOMO-2→ LUMO+2)	3.1423	394.56	**0.0248**
159A->163A 159A->164A 160A ->164A	44%(HOMO-2→ LUMO+1) 50%(HOMO-2→ LUMO+2) 2%(HOMO-1→ LUMO+2)	3.1772	390.23	0.0094
159A ->162A 159A->163A 160A->163A 160A->164A 161A ->163A	16%(HOMO-2→ LUMO) 3%(HOMO-2→ LUMO+1) 6%(HOMO-1→ LUMO+1) 65%(HOMO-1→ LUMO+2) 4%(HOMO→ LUMO+1)	3.2453	382.04	**0.0344**

[a]Only orbitals with a percentage larger than 10% are shown.

S5. Isodensity plots of the frontier orbitals of ^{1}1-S.

The isodensity plots of the frontier orbital of the **^{1}1-S** complex are shown in **Figure S1**. It can be seen that the HOMO is the d_{xy} orbital of Ru. HOMO-1 (d_{xz} of Ru) and HOMO-2 (d_{yz} of Ru) lie at -0.22 eV and -0.27 eV relative to HOMO, respectively. LUMO, LUMO+1, LUMO+2 are all π* orbitals of the ligands. The LUMO orbital is mainly localized on the tpy ligand. LUMO+1 (delocalized over pnq ligand) lies at +0.15 eV relative to the LUMO. LUMO+2 was found +0.19 eV above the LUMO, with contributions from both tpy and pnq groups.

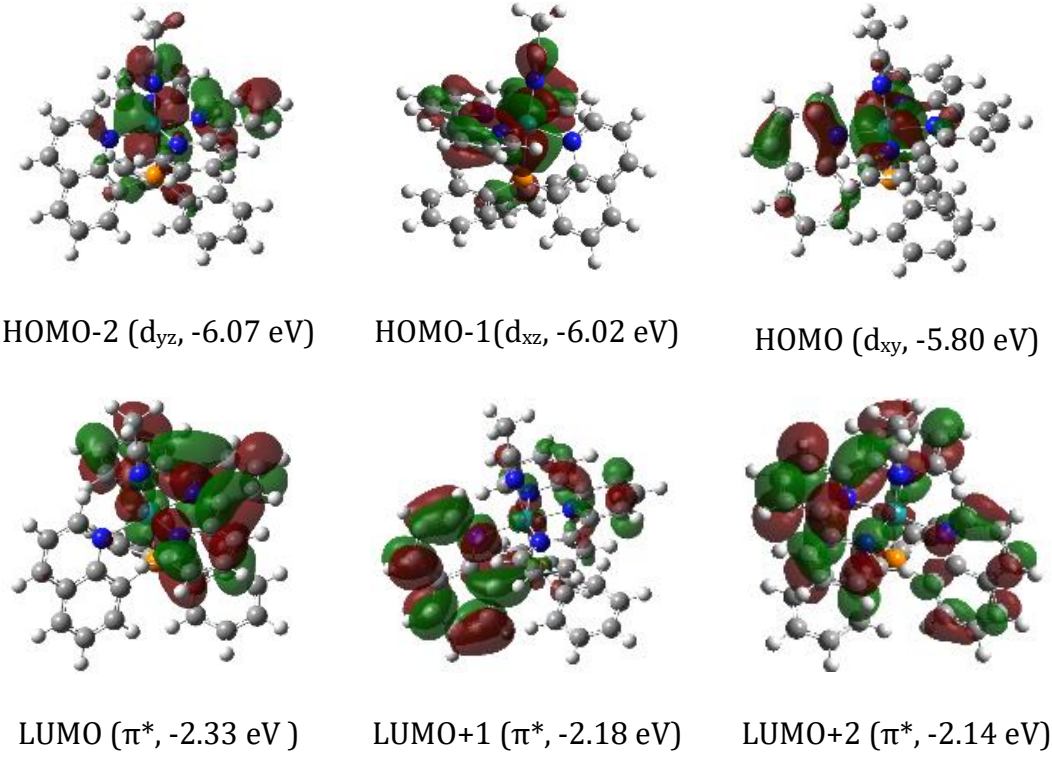


Figure S3. Isodensity plots of the frontier orbitals of **^{1}1-S**.

S6. Optimized structures of ^{2}2', ^{2}2pt and ^{2}2pt'.

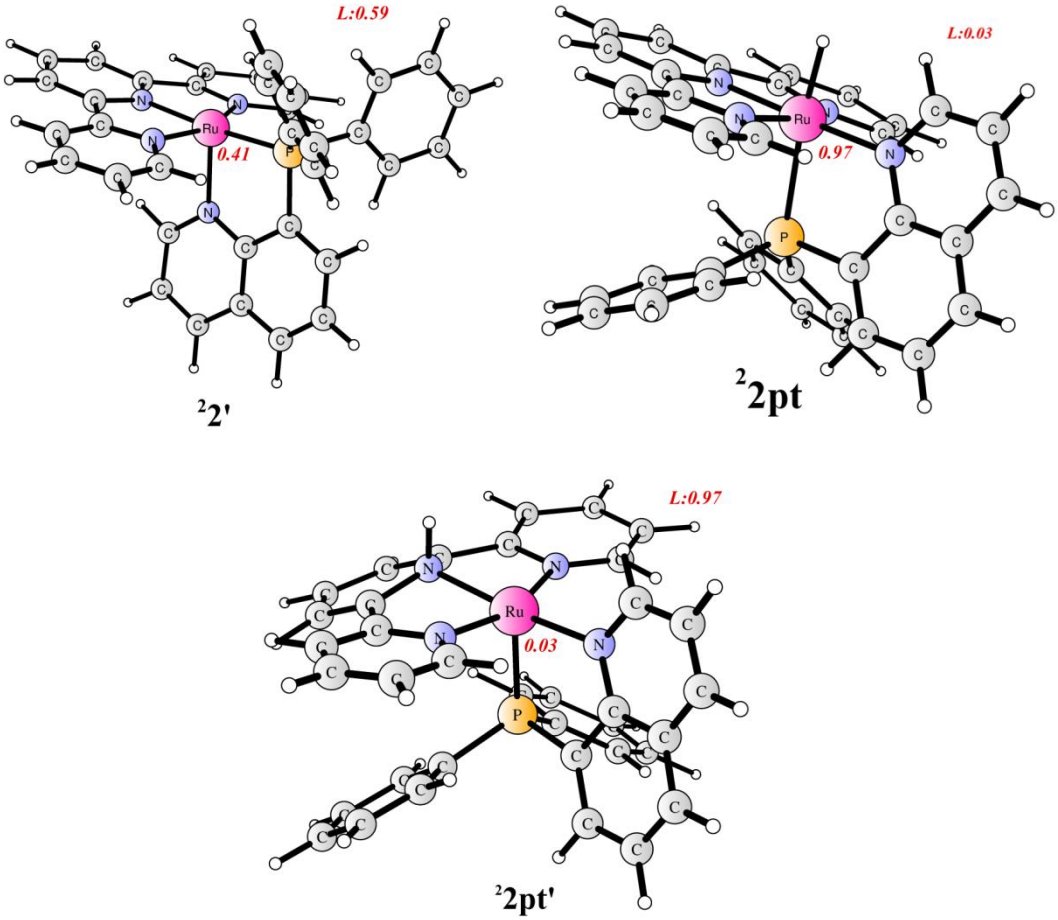


Figure S4. Optimized structures of ^{2}**2'**, ^{2}**2pt**, and ^{2}**2pt'**. The spin densities are shown in red italics.

S7. Possible reactions with ^{2}2.

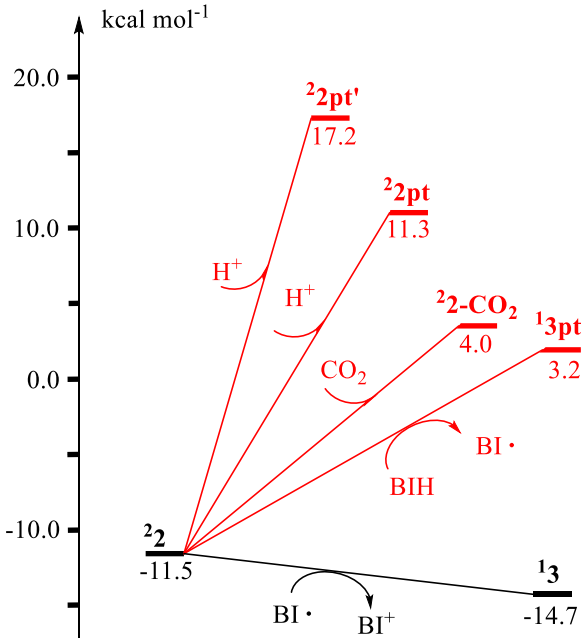


Figure S5. The Gibbs free energy diagram (in kcal mol^{-1}) for the possible reactions with ^{2}**2**.

S8. Electronic structures of ^{1}1, ^{2}2, ^{1}3 and ^{3}3.

Table S3. The calculated Mulliken charges and NBO charges for **^{1}1, ^{2}2, ^{1}3**, **and ^{3}3**.

	Mulliken charges			NBO charges		
	Ru	tpy	pqn	Ru	tpy	pqn
^{1}1	0.80	0.59	0.60	1.85	-0.51	0.66
^{2}2	0.65	-0.02	0.36	1.82	-1.05	0.23
^{1}3	0.44	-0.56	0.11	1.91	-1.60	-0.31
^{3}3	0.57	-0.12	-0.45	1.79	-1.28	-0.51

Table S4. The calculated Mulliken charges and NBO charges for **1, 2, 3,** and $Ru^0(NH_3)_5$.

	Mulliken charges			NBO charges		
	Ru	L(+)	L(-)	Ru	L(+)	L(-)
^{1}1	0.80	6.2	-5.0	1.85	9.27	-9.12
^{3}1	0.85	6.3	-5.2	1.79	9.35	-9.13
^{2}2	0.65	5.65	-5.31	1.82	8.74	-9.56
^{4}2	0.84	5.83	-5.67	1.74	8.95	-9.69
^{1}3	0.44	5.12	-5.56	1.91	8.26	-10.17
^{3}3	0.57	5.17	-5.75	1.79	8.38	-10.17
$^1Ru^0(NH_3)_5$	-1.04	4.44	-3.40	-0.60	6.66	-6.06
$^3Ru^0(NH_3)_5$	-1.03	4.41	-3.40	-0.69	6.75	-6.06

Table S5. The structural differences for **1, 2, 3,** and free tpy, singlet-reduced tpy^- and double-reduced tpy^{2-}.

	Average C=C bond (Å)	Average N-C_o bond (Å)	Average N-C_p bond (Å)	Average C-C bond (Å)
tpy	1.397	1.343	2.797	1.494
tpy^-	1.405	1.366	2.807	1.470
tpy^{2-}	1.414	1.367	2.820	1.450
^{1}1	1.394	1.357	2.769	1.482
^{2}2	1.395	1.372	2.789	1.461
^{1}3	1.397	1.387	2.810	1.442

o and *p* in the right superscript stand for ortho- and para-.

S9. Relationship between the reaction energy of Equation (11) and the percentage of water.

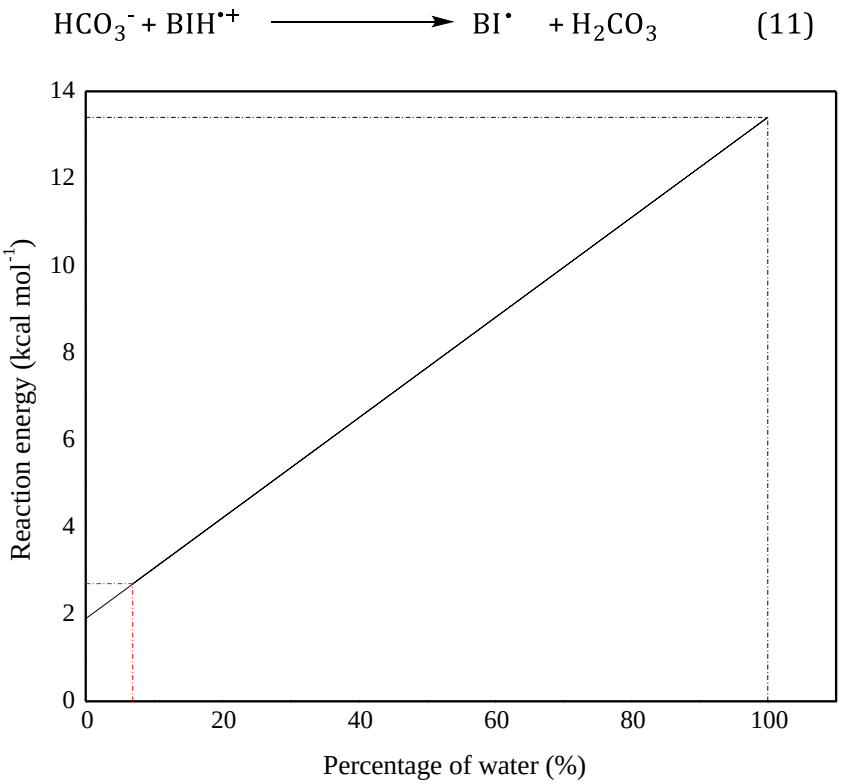


Figure S6. The relationship between the reaction energy of Equation (11) and the percentage of water in the working solution.

S10. Calculated UV-Vis absorption spectra and COPASI simulations.

Table S6. The calculated UV-Vis absorption spectra (nm) of Ru-contained species.

Species	UV-Vis absorption spectra (nm)
Ru^{II}-S	422.36
Ru^{II}	431.24
Ru^{I}-S	490.62
Ru^{I}	499.60
$^{1}Ru^{0}$	568.8
$^{3}Ru^{0}$	690.14
$^{2}Ru^{3}$-CO_2	458.78
$^{1}Ru^{2}$-CO_2	542.34
$^{1}Ru^{2}$-COOH	464.22
$^{1}Ru^{2}$-CO	368.50

As shown in Equation (5) in the paper, the reaction between the one-electron reduced species and CO_2 is endothermic by 15.5 kcal mol^{-1}, which is thermodynamically unfavorable. In contrast, the reaction of CO_2 with the two-electron reduced species of the catalyst is a thermally neutral process.

After light excitation, the first step of the catalyst reduction is very rapid (exergonic by 11.0 kcal mol^{-1}). However, due to the low concentration of H_2CO_3 and H_2CO_3-, the deprotonation of $BIH^{\cdot+}$ to produce $BI^{\cdot}$ is restricted. The second reduction process is relatively slow with the single-electron reduction species accumulated. According to our proposed mechanism, taking into account the influence of concentration, the COPASI simulation shows that the concentration of Ru^0 is also much lower than that of Ru^1. This verifies the accumulation of Ru^1, which is consistent with the spectroscopic experiment phenomenon. These results explained why the spectra in the experiment (FigureS5 and S11 in Ref. 49) and the calculations show the presence of Ru^{I}/ Ru^{I}-S.

This issue is now explained at the end of manuscript Section 3.1. In addition, this is similar to the proposal of using the two-electron reduced catalyst for the reaction with CO_2 in the literature. (ref 77-79)

The UV−vis absorption spectra of Ru^{II}-S has a maximum absorption wavelength of 422 nm, which is consistent with 440 nm measured in the experiment (Fig 5, in gray, Ref 49). After photoirradiation, the catalyst will first be reduced to Ru^{I}-S/Ru^{I}, which is a thermodynamically favorable process. The maximum absorption wavelengths of the UV−vis absorption spectra for Ru^{I}-S and Ru^{I} were calculated to be 490.62 nm and 499.60 nm, respectively. The values are very close to the experimental value of 490 nm (Fig 5, in red, Ref. 49). This confirms that Ru^{I}-S/Ru^{I} exists in the reaction process.

After adding CO_2, it is found that the maximum absorption wavelength of UV analysis has returned to about 440 nm, with a minor difference with Ru^{II}-S. According to our calculations, the two-electron reduction catalyst reacts with CO_2, and then becomes protonated to generate Ru^{II}-COOH species. We deem that the detected UV absorption peak in blue under CO_2 may correspond to Ru^{II}-COOH. The calculated maximum absorption wavelength of the spectrum for Ru^{II}-COOH is 464.22 nm, which is consistent with 440 nm in the experiment. Moreover, our calculated value (368 nm, Fig. S15) agrees with the experimental value for Ru^{II}-CO (360 nm, see Fig. S10 in Ref. 49).

The simulated concentrations of Ru^{II}-COOH by COPASI are shown in the Figures below:

Details of the COPASI simulations for the fixation of CO_2.

Duration： 500 s

Intervals: 10000

Interval size: 0005

The initial concentrations are :

BIH: 0.1 mol L^{-1},

Ru^{II}-CO: 4×10^{-5} mol L^{-1},

CH_3CN: 19.2 mol L^{-1},

H_2O: 1.4 mol L^{-1}

CO_2: 0.245 mol L^{-1}.

Table S7. All possible elementary reactions in the dissociation of CO are shown below.

Reactions	k_1	k_{-1}
[a] $H_2CO_3 \rightleftharpoons HCO_3^- + H^+$	5.25292×10^{-5}	1.68448×10^{10}
[a] $H_2O + CO_2 \rightleftharpoons H_2CO_3$	2.75207×10^{7}	1.68448×10^{10}
[a] $HCO_3^- + BIH^{\cdot+} \rightleftharpoons BI^{\cdot} + H_2CO_3$	6.80867×10^{8}	1.68448×10^{10}
[a] $^3Ru^{II}\text{-}S + BIH \rightleftharpoons {}^2Ru^{I}\text{-}S + BIH^{\cdot+}$	1.68448×10^{10}	1.44342×10^{2}
[a] $^2Ru^{I} + BI^{\cdot} \rightleftharpoons {}^3Ru^{0} + BI^{+}$	1.68448×10^{10}	3.06392×10^{6}
[a] $^2Ru^{I}\text{-}S = {}^2Ru^{I} + S$	1.68448×10^{10}	7.24070×10^{9}
[b] $^1Ru^{0} + CO_2 = {}^1Ru^{II}\text{-}CO_2^-$	1.40059×10^{7}	9.99163×10^{6}
[a] $^1Ru^{II}\text{-}S \longrightarrow {}^3Ru^{II}\text{-}S$	1.0×10^{15}	
[a] $^1Ru^{II}\text{-}S \rightleftharpoons {}^1Ru^{II} + S$	2.7092×10^{4}	1.68448×10^{10}

$\rightleftharpoons$: means reversible reaction.

$\longrightarrow$: means irreversible reactions

[a]: rate constant k is from ΔG .

[b]: rate constant k is from $\Delta G^{\neq}$.

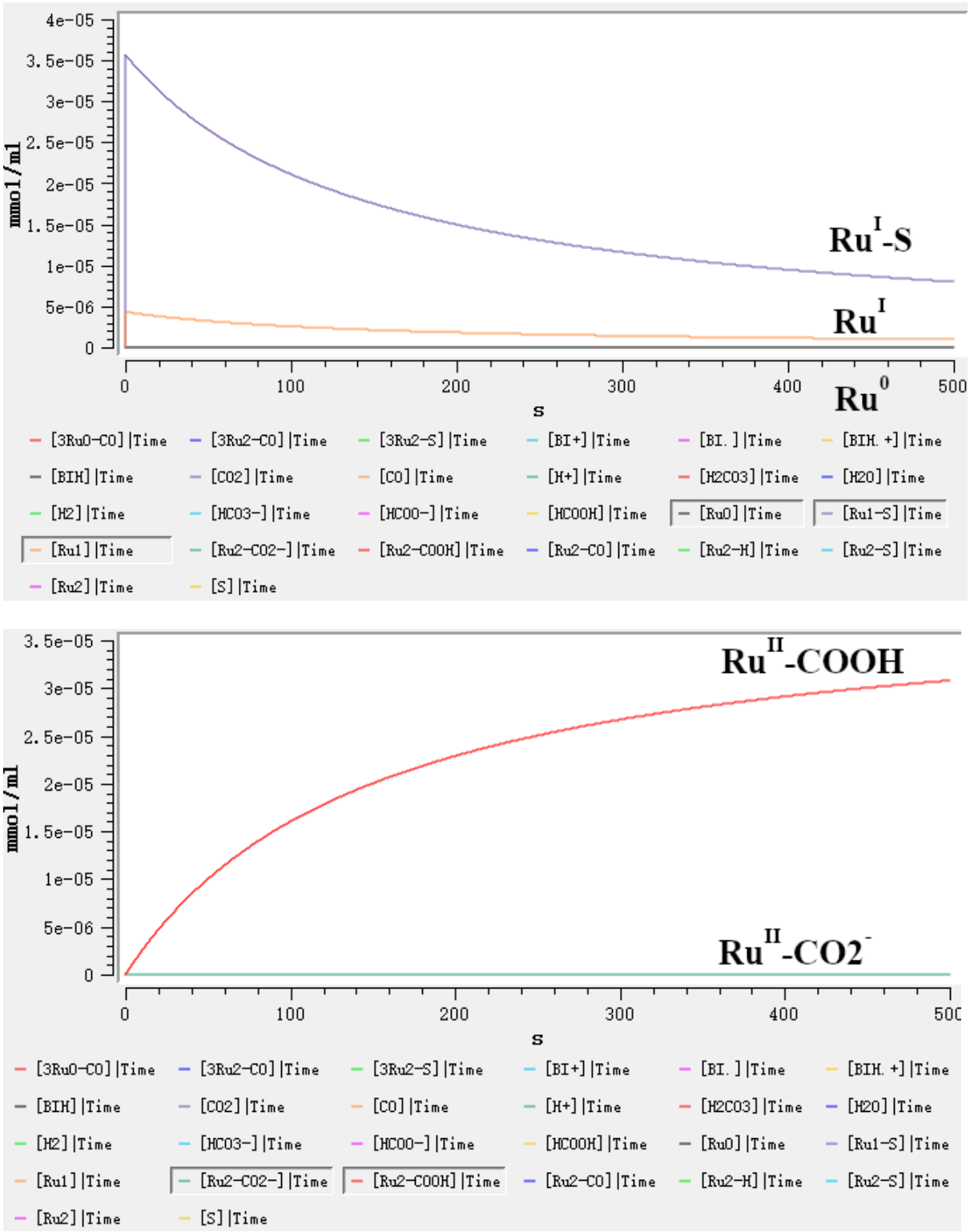


Figure S7. The microkinetic model outcome of $^{2}Ru^{I}$-S, $^{2}Ru^{I}$, $^{1}Ru^{0}$, $^{1}Ru^{II}$-CO_2^- and $^{1}Ru^{0}$-COOH, over the beginning 500 s.

S11. Results of principal interacting orbital (PIO) analysis.

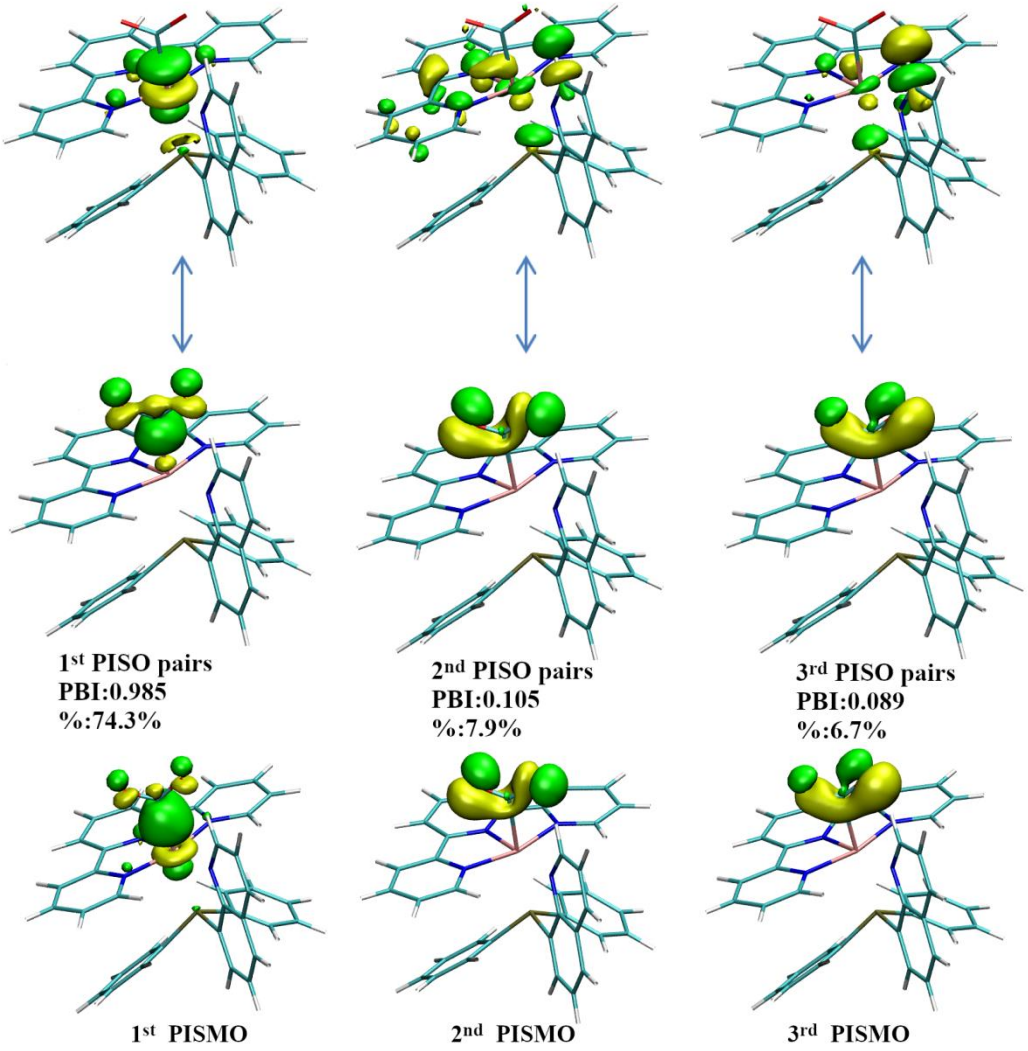


Figure S8. Dominant PISO pairs on **^{1}3-CO_2 (Ru^{II}-CO_2^-)** between the CO_2 and the catalyst moieties (up). The PISMOs (down) shown here correspond to the dominant interactions between the two fragments, with an overall contribution of 88.9%, indicating that these orbitals captured most of the CO_2-catalyst interactions. The third interration is H-bond intreration between pqn and the CO_2^- moiety.

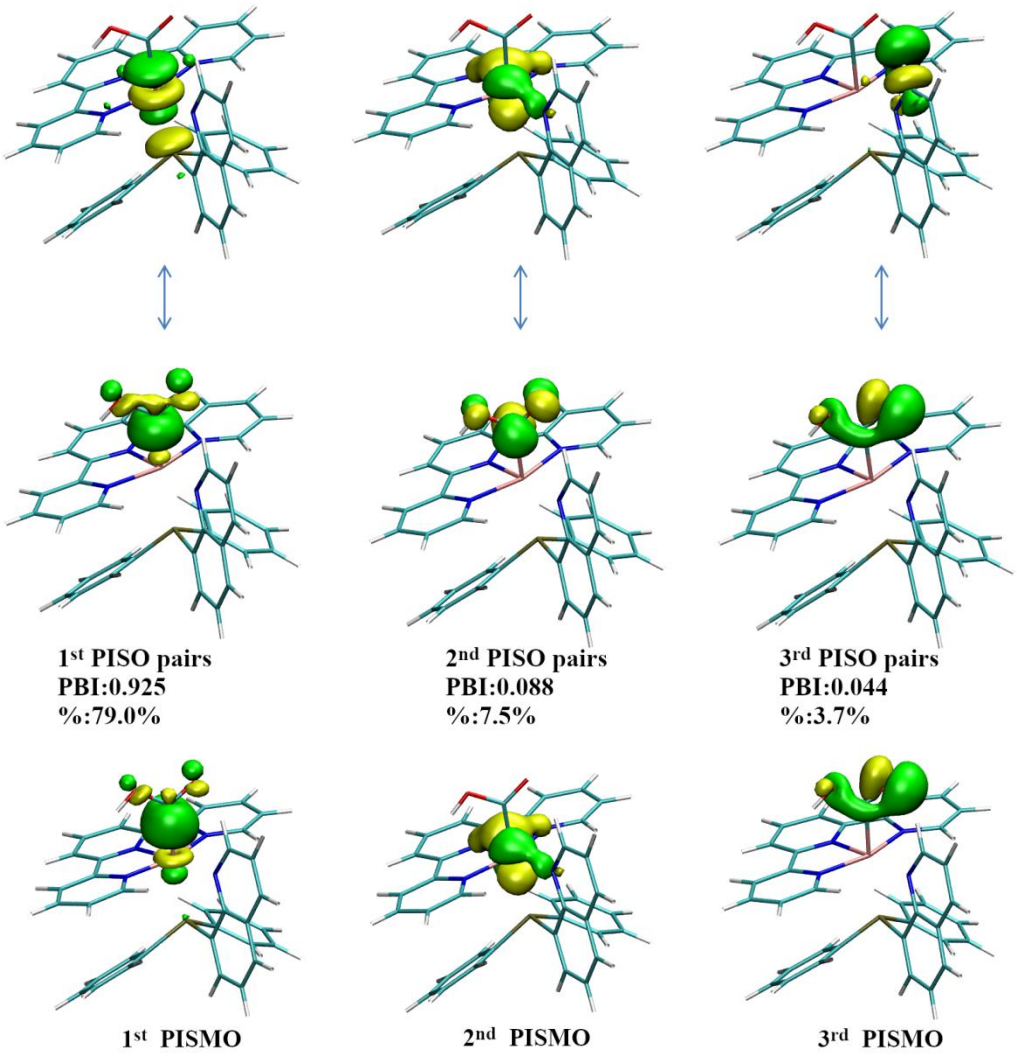


Figure S9. Dominant PISO pairs on **4 (Ru^{II}-COOH)** between the COOH and the catalyst moieties (up). The PISMOs (down) shown here correspond to the dominant interactions, with an overall contribution of 90.2%, indicating that these orbitals captured most of the COOH-catalyst interactions. The third interration is H-bond intreration between pqn and the COOH moiety.

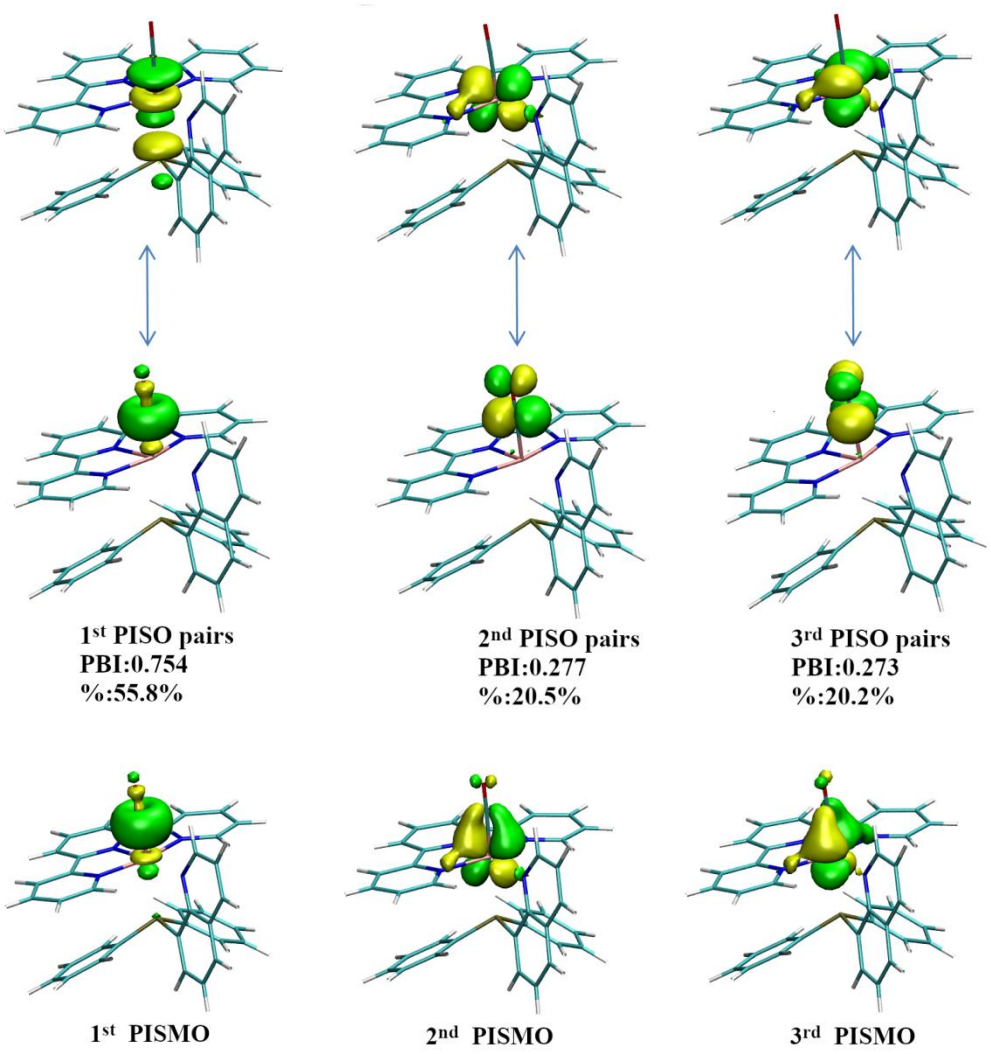


Figure S10. Dominant PISO pairs on **1-CO (Ru^{II}-CO)** between the CO and the catalyst moieties (up). The PISMOs (down) shown here correspond to the dominant interactions in the α and β spaces, respectively, with an overall contribution of 96.5%, indicating that these orbitals captured most of the CO-catalyst interactions.

Table S8. PISO analysis with the two fragments being the catalyst (fragment A) and the substrate (fragment B).

Species	Pop A	Pop B	PBI	Total	Recovered contribution
	1.12	0.88	0.99		
3-CO_2(Ru^{II}-CO_2^-)	0.05	1.95	0.11	1.22	88.9%
	0.05	1.95	0.09		
	0.73	1.27	0.93		
4(Ru^{II}-COOH)	1.96	0.04	0.09	1.06	90.2%
	0.023	1.98	0.04		
	0.50	1.50	0.75		
1-CO(Ru^{II}-CO)	1.85	0.15	0.28	1.30	96.8%
	1.85	0.15	0.27		

The interactions (recovered contribution > 3%) are shown for each species with corresponding PISO populations and PBI values. The recovered contribution indicates the total percentage contributions to the overall interaction between the substrate and the catalyst.

S12. Optimized structures of ^{1}TS1' and ^{1}1-CO.

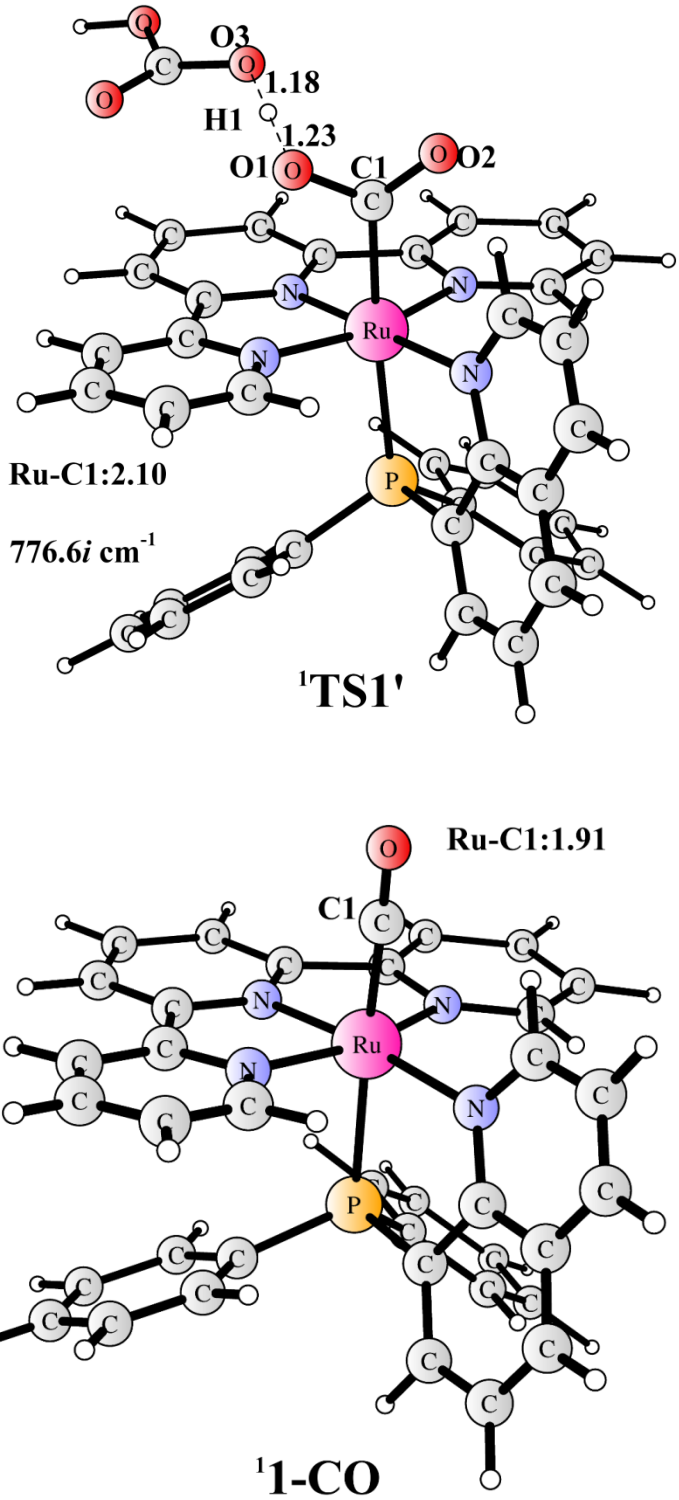


Figure S11. Optimized structures of **^{1}TS1'** and **^{1}1-CO**.

S13. Reaction between 3-CO_2 and $BIH^{\bullet+}$.

$BIH^{\bullet+}$ + **3-CO_2** ⟶ **2-CO_2** + BIH ΔG= -19.4 kcal mol^{-1} (S1)

2-CO_2 + BIH $\xrightarrow{\text{TS2'}}$ **4** + $BI^{\bullet}$ ΔG= +0.6 kcal mol^{-1} (S2)

3-CO_2 + **CO_2** ⟶ **1-CO** + **CO_3^{2-}** ΔG= +18.5 kcal mol^{-1} (S3)

^{2}TS2' prefers to be a doublet, with a barrier of 13.8 kcal mol^{-1} relative to the energy of **2-CO_2** plus BIH, and the quartet state is 32.8 kcal mol^{-1} higher. The nature of **^{2}TS2'** was proved by vibration analysis, with only one imaginary frequency of 1223.6*i* cm^{-1}, which corresponds to the transfer of H1' atom from BIH to **2-CO_2**. The H1'-C2 and H1'-O1 bonds are 1.34 Å and 1.27 Å, respectively. Downhill the transition state **TS2'**, **4** and a $BI^{\bullet}$ radical are generated.

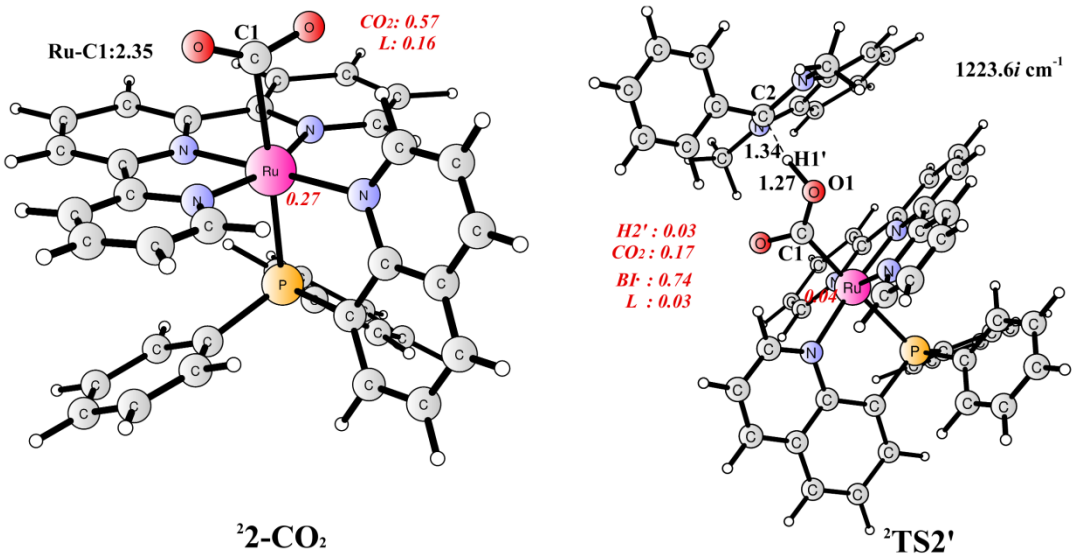


Figure S12. Optimized structures of **^{2}2-CO_2** and **^{2}TS2'**. The spin densities are given in red italics. Distances are given in Ångström, and the imaginary frequency for **^{2}TS2'** is shown.

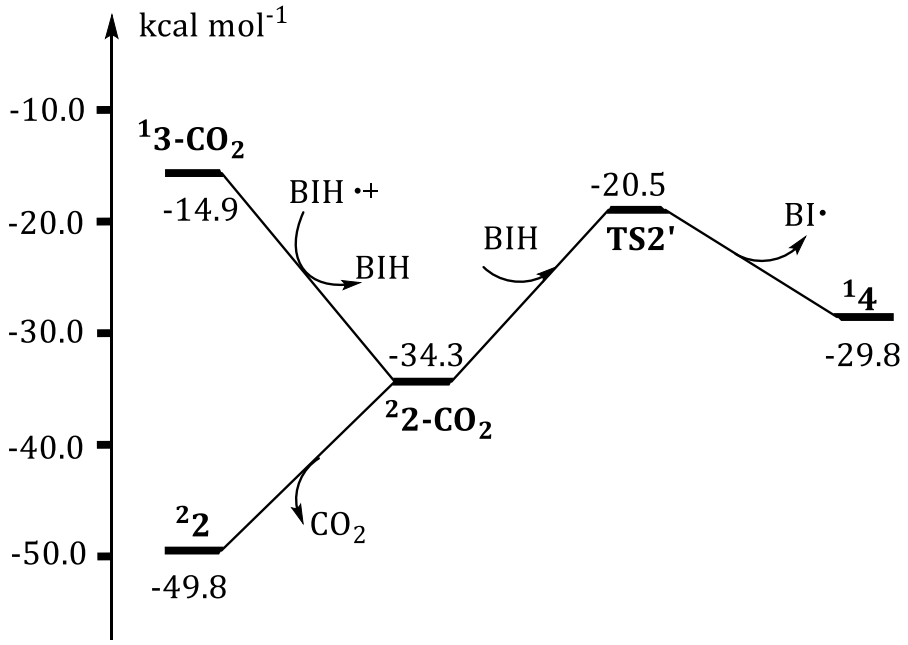


Figure S13. The Gibbs energy diagram of the reactions of ^{2}**3-CO$_2$** with BIH$^{\bullet+}$.

S14. pK_as of all possible proton donors.

Table S9. The calculated pK_as of all possible proton donors.

Specie	pK_a
BIH_2^+	6.1
H_2CO_3	14.5
$BIH^{\bullet+}$	15.9
$(H_2O)_4$	27.5

S15. Gibbs free energy diagram for the reactions with ^{1}4.

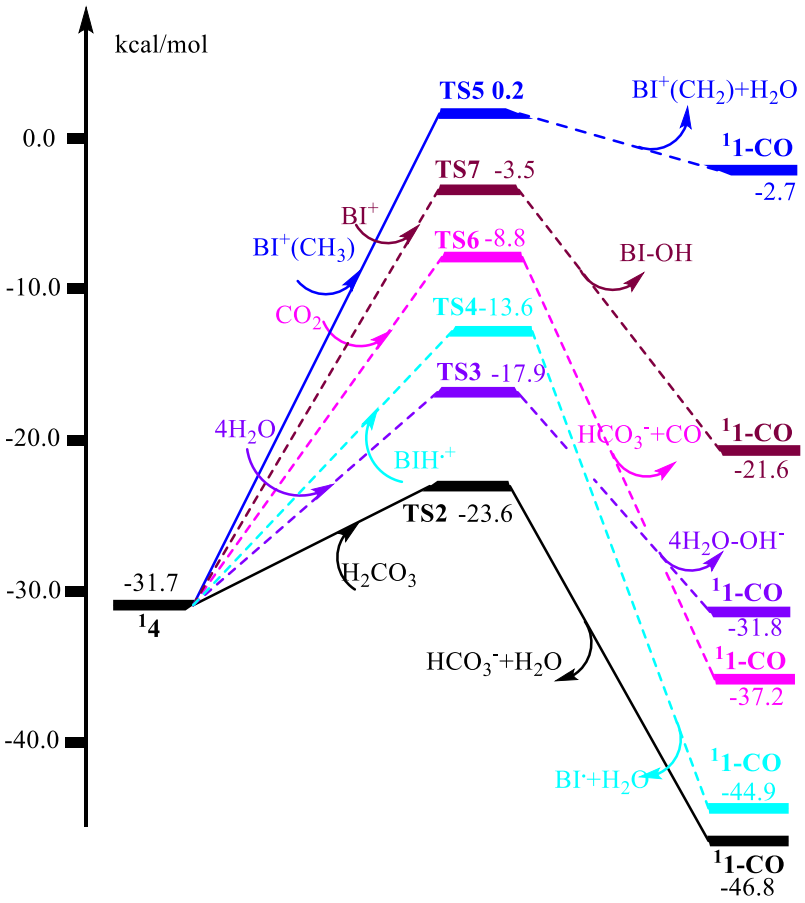


Figure S14. The Gibbs free energy diagram (in kcal mol^{-1}) for the reactions with **^{1}4**.

S16. Transition state structures for C-O bond cleavage and COPASI simulations.

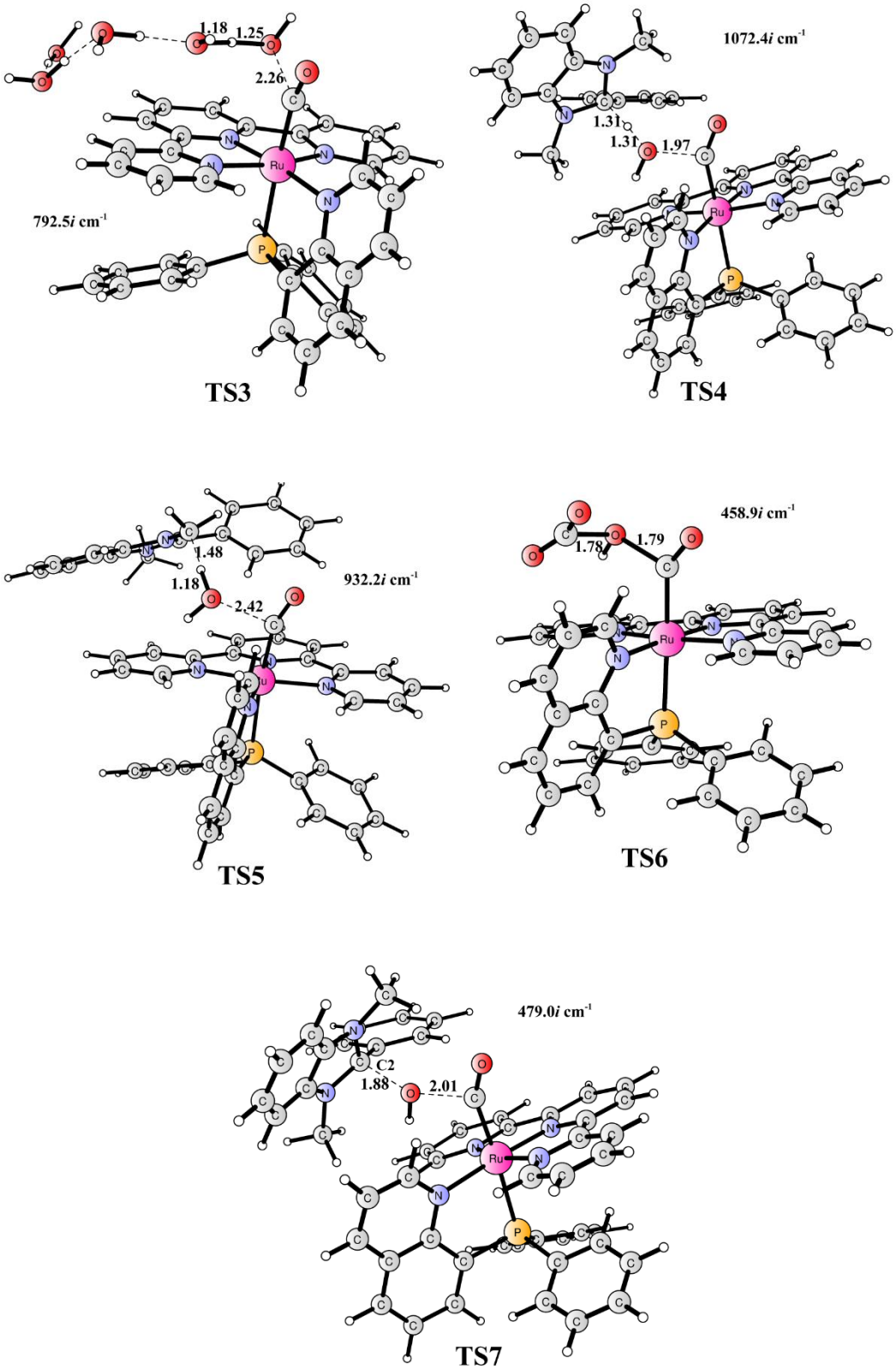


Figure S15. Optimized structures of **TS3**, **TS4**, **TS5**, **TS6,** and **TS7.** The spin densities are shown in red italic. Distances are given in Ångström, and the imaginary frequencies (in cm^{-1}) are shown.

We used COPASI to simulate the protonating process of Ru^{II}-COOH with two proton sources (H_2CO_3 and $4H_2O$) to make Ru^{II}-CO. The Ru^{II}-CO generated with the proton source of H_2CO_3 is marked as *Ru^{II}-CO. The final concentrations of *Ru^{II}-CO and Ru^{II}-CO are 3.98×10^{-5} mol L^{-1} and 1.32×10^{-7} mol L^{-1}, respectively. H_2CO_3 is the primary proton source.

Details of the COPASI simulations are shown below:

Duration： 14400 s (4 h)

Intervals: 1000000

Interval size: 0.0144

The initial concentrations are :

Ru^{II}-COOH: 4×10^{-5} mol L^{-1},

H_2O:1.4 mol L^{-1}

H_2CO_3:5.6×10^{-4} mol L^{-1},

$4H_2O$: 0.35 (1.4/4) mol L^{-1}

Table S10. The protonation of Ru^{II}-COOH by H_2CO_3 and $4H_2O$.

Reactions	k_1	k_{-1}
Ru^{II}-COOH + H_2CO_3 = *Ru^{II}-CO + H_2O +HCO_3^-	7.12791×10^{6}	6.01272×10^{-5}
Ru^{II}-COOH + $4H_2O$ = Ru^{II}-CO + $4H_2O$-OH	9.24911×10^{2}	5.57300×10^{2}

The rate constant k is from $\Delta G^{\neq}$.

Table S11. The final concentrations of the products.

Species	concentration (mol L^{-1})
*Ru^{II}-CO	3.98×10^{-5}
Ru^{II}-CO	6.93×10^{-15}

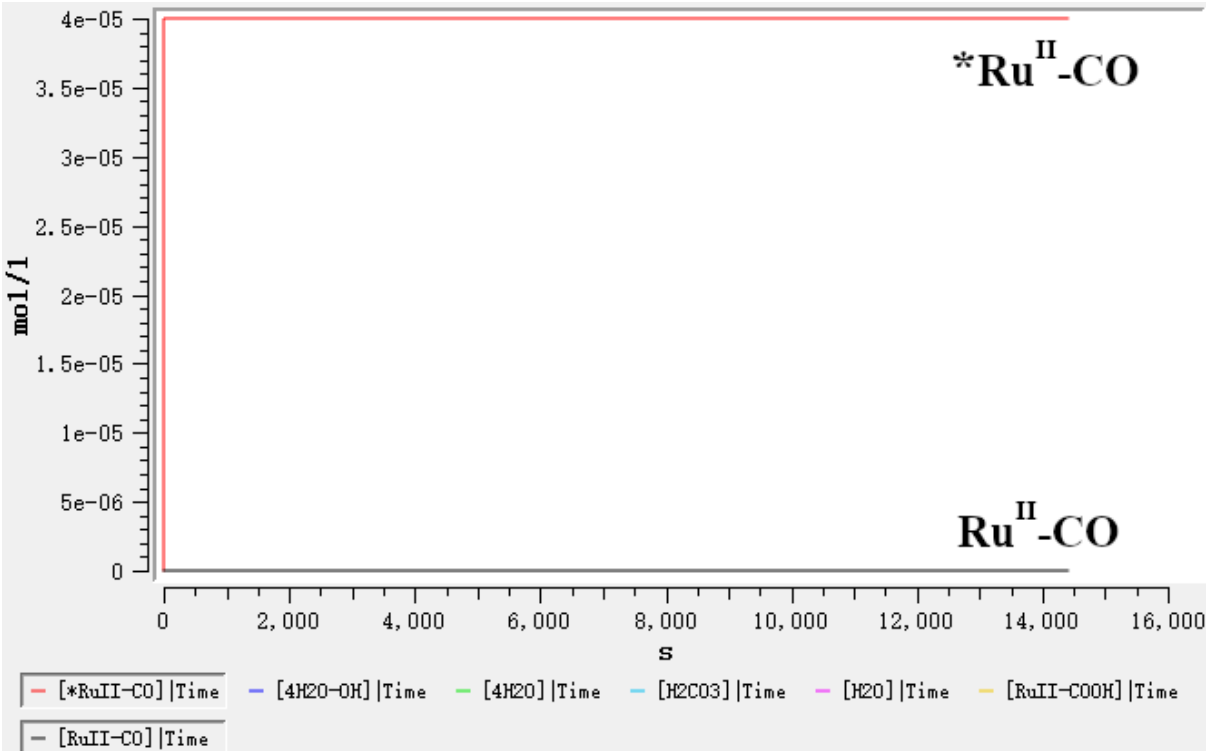


Figure S16. The microkinetic model outcome of *Ru^{II}-CO and Ru^{II}-CO, over the whole 4 h (14400 s).

S17. Protonation of Ru^{II}-CO_2^- by H_2CO_3.

The Gibbs energy change of the protonation of Ru^{II}-CO_2^- to produce Ru^{II}-COOH depends on the acidity of the proton source. The pK_a of H_2CO_3 is much smaller than that of H_2O, so the protonation process is more exergonic when using H_2CO_3 as the proton source.

In the COPASI simulations, the protonation process was also considered, being either reversible or irreversible. Compared with the irreversible reaction, the results for the reversible protonation are very similar.

Reversible: $Ru^{II}\text{-}CO_2^- + H_2CO_3 \rightleftharpoons Ru^{II}\text{-}COOH + HCO_3^-$

Irreversible: $Ru^{II}\text{-}CO_2^- + H_2CO_3 \longrightarrow Ru^{II}\text{-}COOH + HCO_3^-$

Details of the COPASI simulations for the protonation of Ru^{II}-CO_2^- by H_2CO_3.

Duration： 14400 (4 h)

Intervals: 1000000

Interval size: 0.0144

The initial concentrations are :

Ru^{II}-CO_2^-: 4×10^{-5} mol L^{-1},

H_2CO_3:5.6×10^{-4} mol L^{-1}

Table S12. Rate constants for the protonation of Ru^{II}-CO_2^- by H_2CO_3.

Reactions	k_1	k_{-1}
$Ru^{II}\text{-}CO_2^- + H_2CO_3 \rightleftharpoons Ru^{II}\text{-}COOH + HCO_3^-$	1.68448×10^{10}	8.05090×10^{-3}
$Ru^{II}\text{-}CO_2^- + H_2CO_3 \longrightarrow Ru^{II}\text{-}COOH + HCO_3^-$	1.76797×10^{30}	

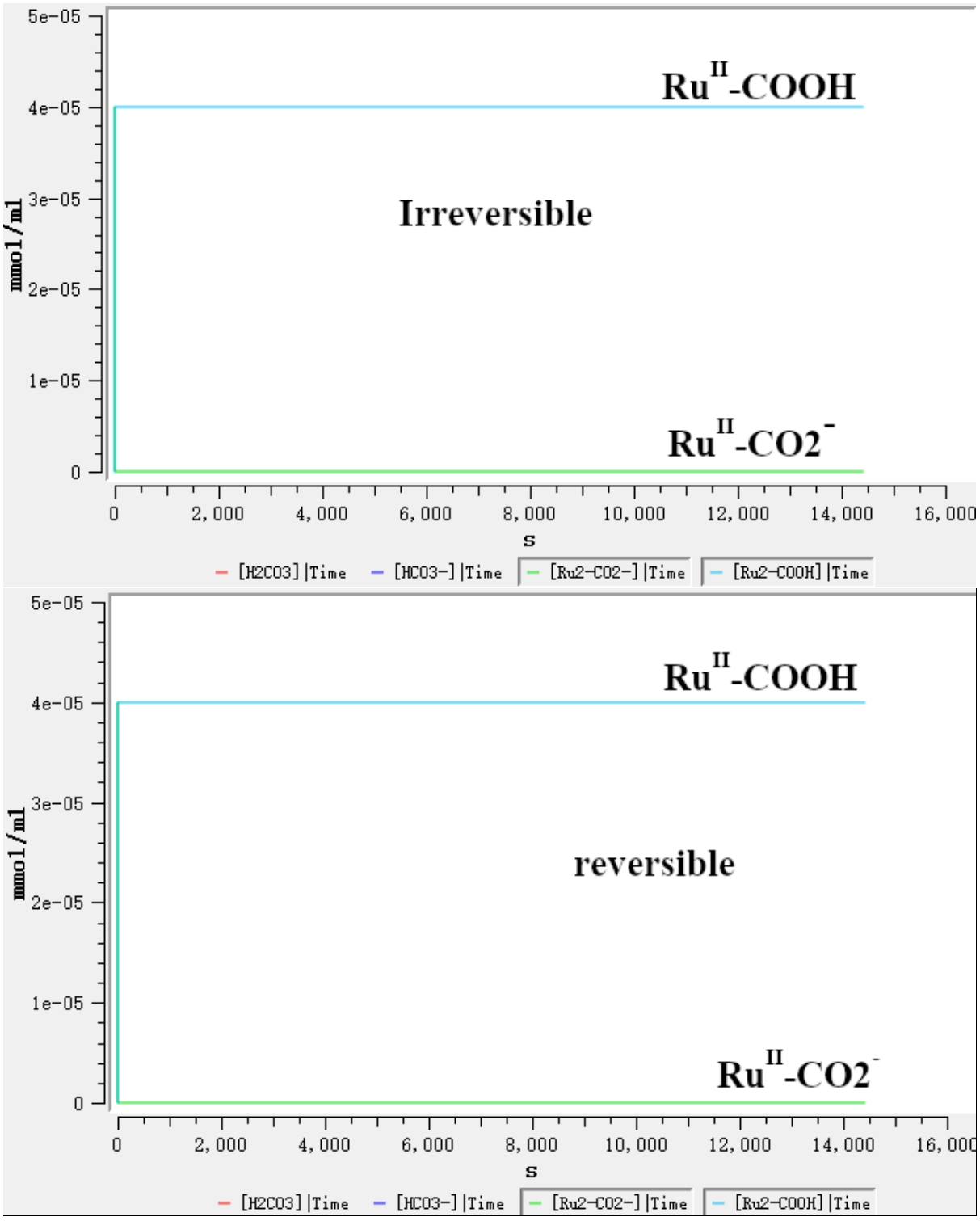


Figure S17. The microkinetic model outcome for the protonation of Ru^{II}-CO_2^- by H_2CO_3 reversibly and irreversibly, over the whole 4 h (14400 s).

S18. Comparison of the two catalysts.

The Gibbs energy change for the reaction of CO_2 and the reduced catalyst depends on the property of the catalyst. Cat. 1 (Ru^{II}(tpy)(pqn)) contains two redox non-innocent ligands. During the reduction process of the catalyst, the tpy and pqn ligands could be reduced, and the oxidation state of Ru keeps +2. For Cat. 2 ([Ru^{II}(bpy)$_2$(CO)]),[S3] the bpy ligands are more difficult to be reduced. As shown in Table S11, in the one-electron reduced form of Cat.1 (formally Ru(I)), the spin density on the ligand is 0.70, which is much higher than that for Cat. 2 (0.19). In the double-reduced form of Cat.1 (formally Ru(0)), the spin density on the ligand is 1.72, which is also bigger than 1.38 (for ^{3}double-reduced Cat. 2).

We calculated the CO_2 reduction by **Cat. 2** in water solution, which is exergonic by 20.7 kcal mol^{-1}. While in acetonitrile, it is exergonic by 10.9 kcal mol^{-1}. The CO_2 reduction by **Cat. 1** in water is exergonic by 12.7 kcal mol^{-1}, while 0.3 kcal mol^{-1} in acetonitrile. In addition, we also calculated the ΔG of the Ru^{II}-CO_2^- protonation process both in acetonitrile and in water. The proton source could be H_2CO_3 or $4H_2O$. It is an exergonic process when H_2CO_3 acts as the proton source both in acetonitrile and in water. However, it could be considered as a thermal equilibrium process, if water is the proton source. This process is the same both for **Cat. 1** and **Cat. 2**. Our calculations are thus fully consistent with the previous experimental results. It shows that acidity of the proton donor and the solvent has an important influence on the thermodynamics of the CO_2 reduction.

Table S13. Spin densities on Cat. 1 and Cat. 2 The number in the upper left corner represents multiplicity.

	Species	Spin density	
		Ru	Ligand
Cat.1	$^{1}Ru^{II}$	0.0	0.0
	$^{2}Ru^{I}$	0.30	0.70
	$^{3}Ru^{0}$	0.28	1.72
Cat.2	$^{1}Ru^{II}$	0.0	0.0
	$^{2}Ru^{I}$	0.81	0.19
	$^{3}Ru^{0}$	0.62	1.38

Note: For Ru^{0}, the energies for singlet and triplet are very similar. Triplet is about 1.0 kcal mol^{-1} higher than singlet, and only the triplet data is listed in Table S13.

Table S14. Gibbs energies for the reaction with Cat. 1 and Cat. 2.

Reactions	ΔG with Cat. 1 in CH_3CN (in H_2O)	ΔG with Cat. 2 in CH_3CN (in H_2O)
$Cat + CO_2 \rightleftharpoons Cat\text{-}CO_2$	-0.3(-12.7)	-10.9 (-20.7)
$Cat\text{-}CO_2 + H_2CO_3 \rightleftharpoons Cat\text{-}COOH + HCO_3^-$	-16.8 (-14.0[a])	-16.1 (-12.5[a])
$Cat\text{-}CO_2 + 4H_2O \rightleftharpoons Cat\text{-}COOH + 3H_2O\text{-}OH^-$	+1.0 (+1.4[a])	+1.6 (+1.3[a])

[a] The pK_a of carbonic acid (6.4) and water (15.7) used here is from the experiment.

We calculated the CO_2 fixation process with **Cat.2** in water; it is exergonic by 20.7 kcal mol^{-1}. While in acetonitrile, it is exergonic by 10.9 kcal mol^{-1}. The CO_2 fixation process with **Cat.1** in water is exergonic by 12.7 kcal mol^{-1}. Similarly, we also calculated the ΔG of the Ru^{II}-CO_2^- protonation process in acetonitrile and water. The proton source could be H_2CO_3 or $4H_2O$. It is an exergonic process in acetonitrile or water when H_2CO_3 acts as the proton source. However, it is almost a thermal equilibrium process if water is the proton

source. This process is the same for **Cat. 1** (we studied) and **Cat. 2** (reported by Okazaki). Our study is not inconsistent with previous experimental results. It shows that solvent has an important influence on the thermodynamic changes of the CO_2 fixation process.

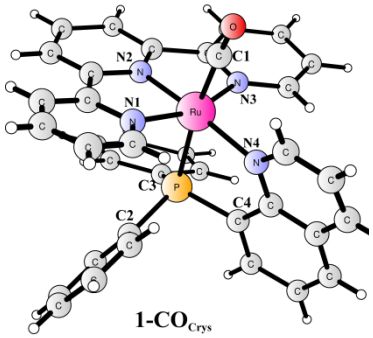
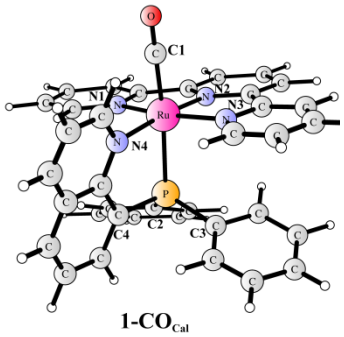
Table S15. The pK_a of several species used in the protonation process.

	pK_a	
	In water	In CH_3CN
H_2CO_3	3.7 (6.4 [a])	14.5
$4H_2O$	19.1 (15.7 [a])	27.5
Cal. 1-COOH	16.7	26.8
Cal. 2-COOH	15.6	26.3

[a] data from the experiment.

S19. Comparison of crystal structure and calculated structure of 1-CO.

Table S16. The comparison of the crystal structure and the calculated structure of **1-CO**.

		Crystal structure[S3]	Calculated structure
		 1-CO$_{Crys}$	 1-CO$_{Cal}$
Bond distance/(Å)	Ru-N1	2.099	2.114
	Ru-N2	1.988	2.006
	Ru-N3	2.104	2.111
	Ru-N4	2.148	2.174
	Ru-P	2.368	2.411
	Ru-C1	1.938	1.905
	C1-O	1.129	1.155
	P-C2	1.806	1.832
	P-C3	1.824	1.833
	P-C4	1.807	1.818
Angle/(°)	∠N1RuP	88.6	87.8
	∠N2 RuP	91.0	93.1
	∠N3 RuP	94.3	91.5
	∠N4 RuP	80.2	80.6
	∠C1RuN1	87.5	91.0
	∠C1RuN2	96.9	92.2
	∠C1RuN3	92.6	91.7
	∠C1RuN4	91.9	94.1
	∠N1RuN2	78.7	79.6
	∠N2RuN3	79.2	79.2
	∠N3RuN4	95.8	101.6
	∠N4RuN1	106.4	99.7

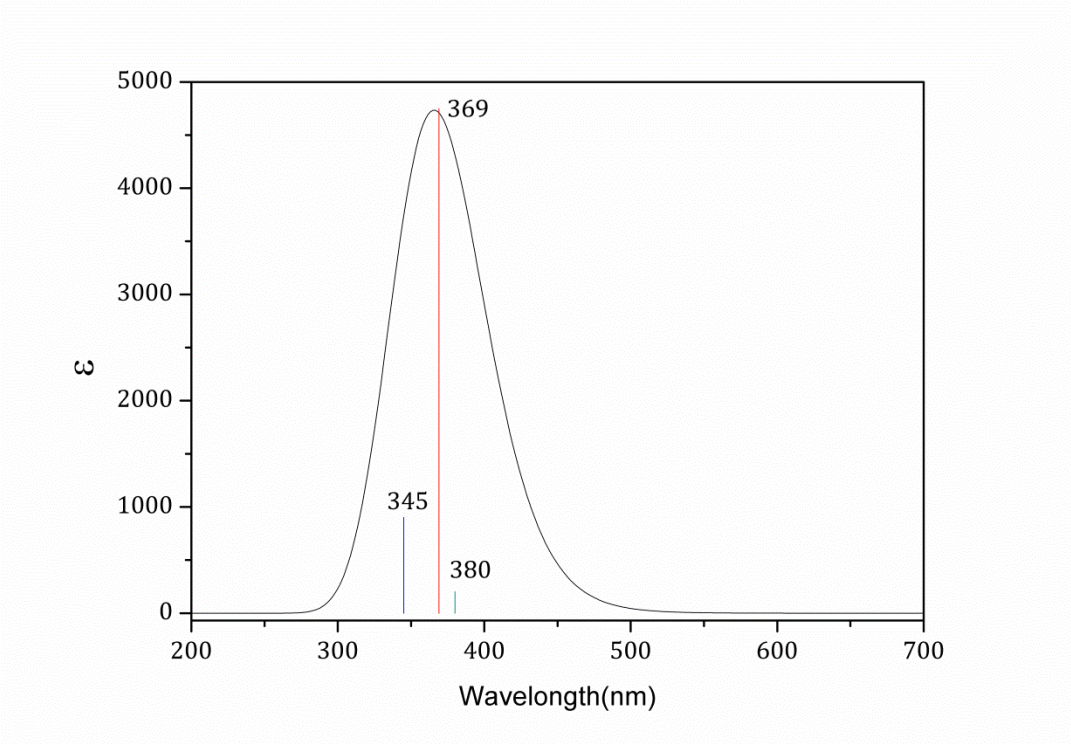


Figure S18. The computed UV-Vis absorption spectra for **^{1}1-CO** complex in 200~700 nm region.

S20. Optimized structures of ^{1}1, ^{2}2-CO, ^{2}2, ^{3}3-CO, ^{3}3, and ^{1}3.

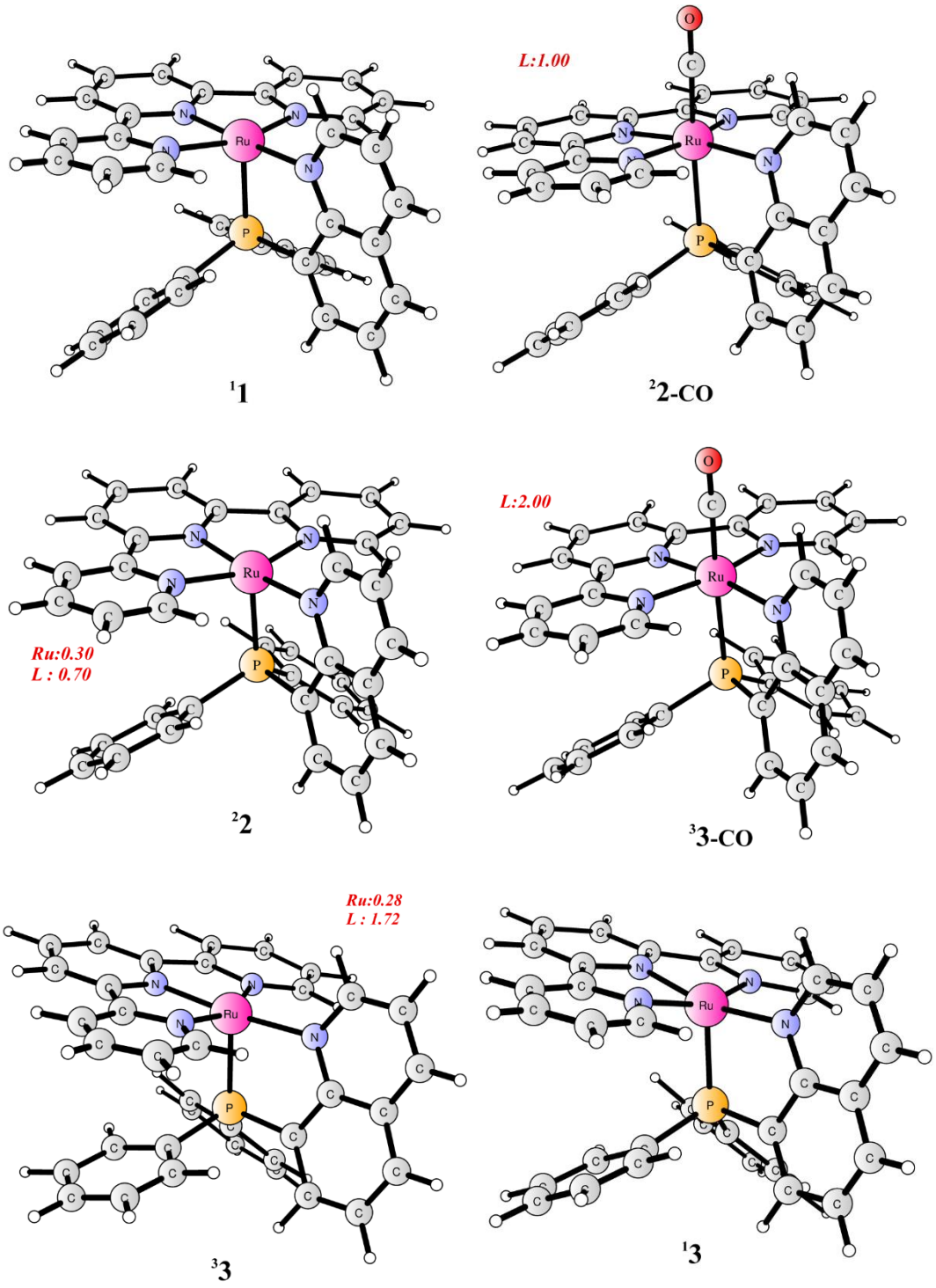


Figure S19. The optimized structures of **^{1}1**, **^{2}2-CO**, **^{2}2**, **^{3}3-CO**, **^{3}3**, and **^{1}3**. The spin densities are shown in red italic.

S21. Dissociation of CO.

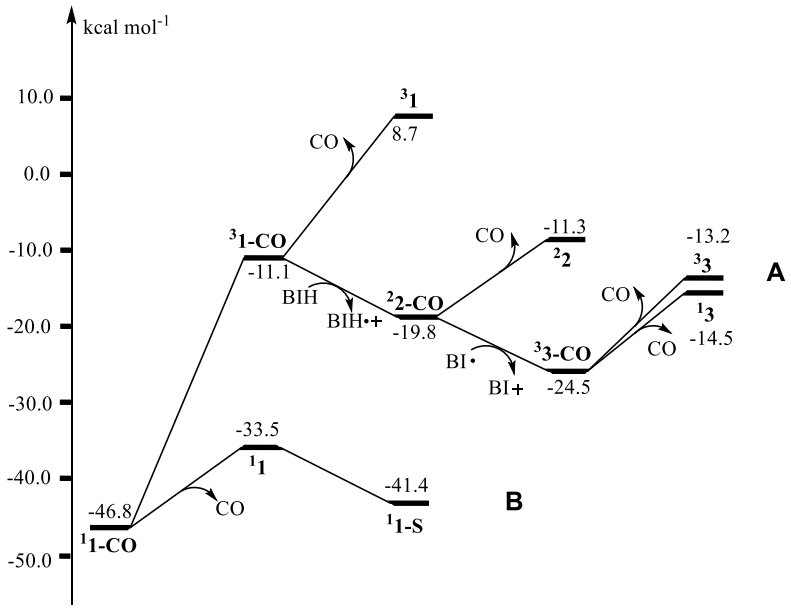


Figure S20. The Gibbs energy profile of CO dissociation process.

S22. Potential energy scan for the dissociation of CO from ^{2}2-CO and ^{3}3-CO.

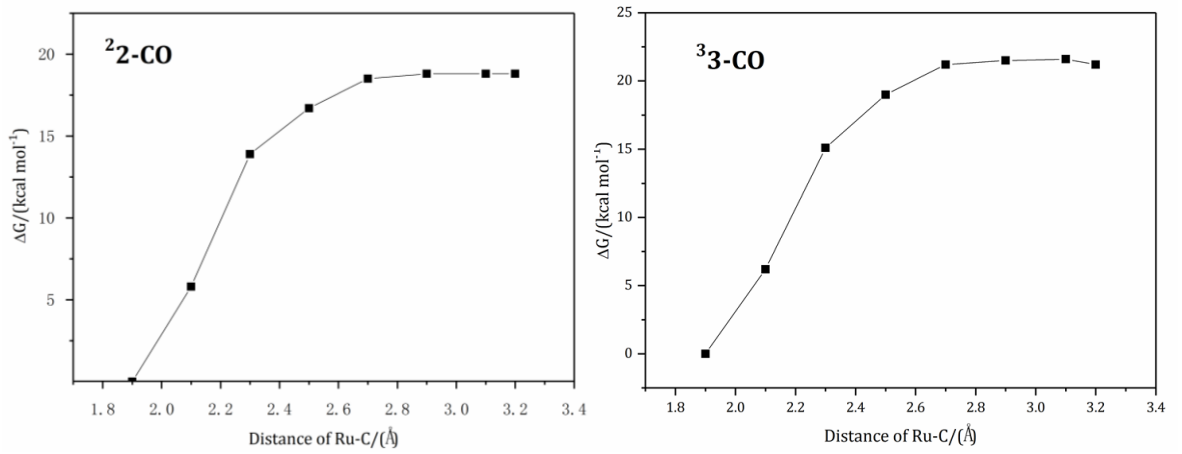


Figure S21. Potential energy scan along the Ru-C distance (in kcal mol^{-1}) for the dissociation of CO from **^{2}2-CO and ^{3}3-CO.**

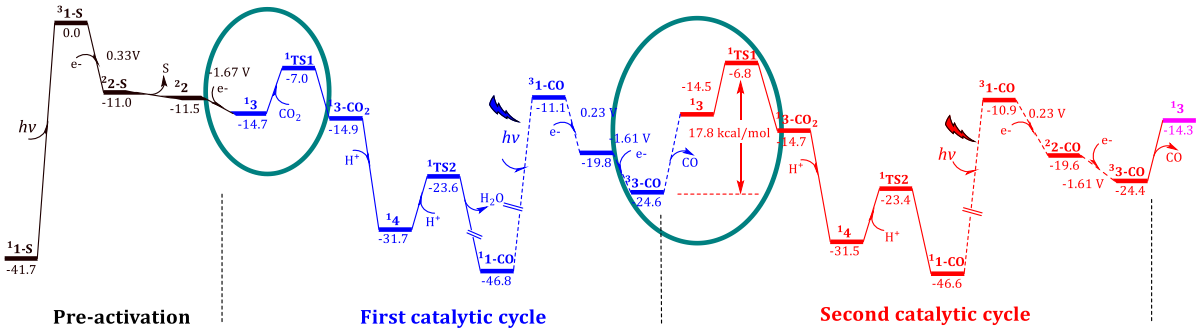


Figure 22. Gibbs free energy diagram for the catalytic reaction. For clarity, the pre-activation part is shown in black, the first catalytic cycle is shown in blue, and the second catalytic cycle is shown in red.

S23. Optimized structures of ^{1}TS11 and ^{2}TS12.

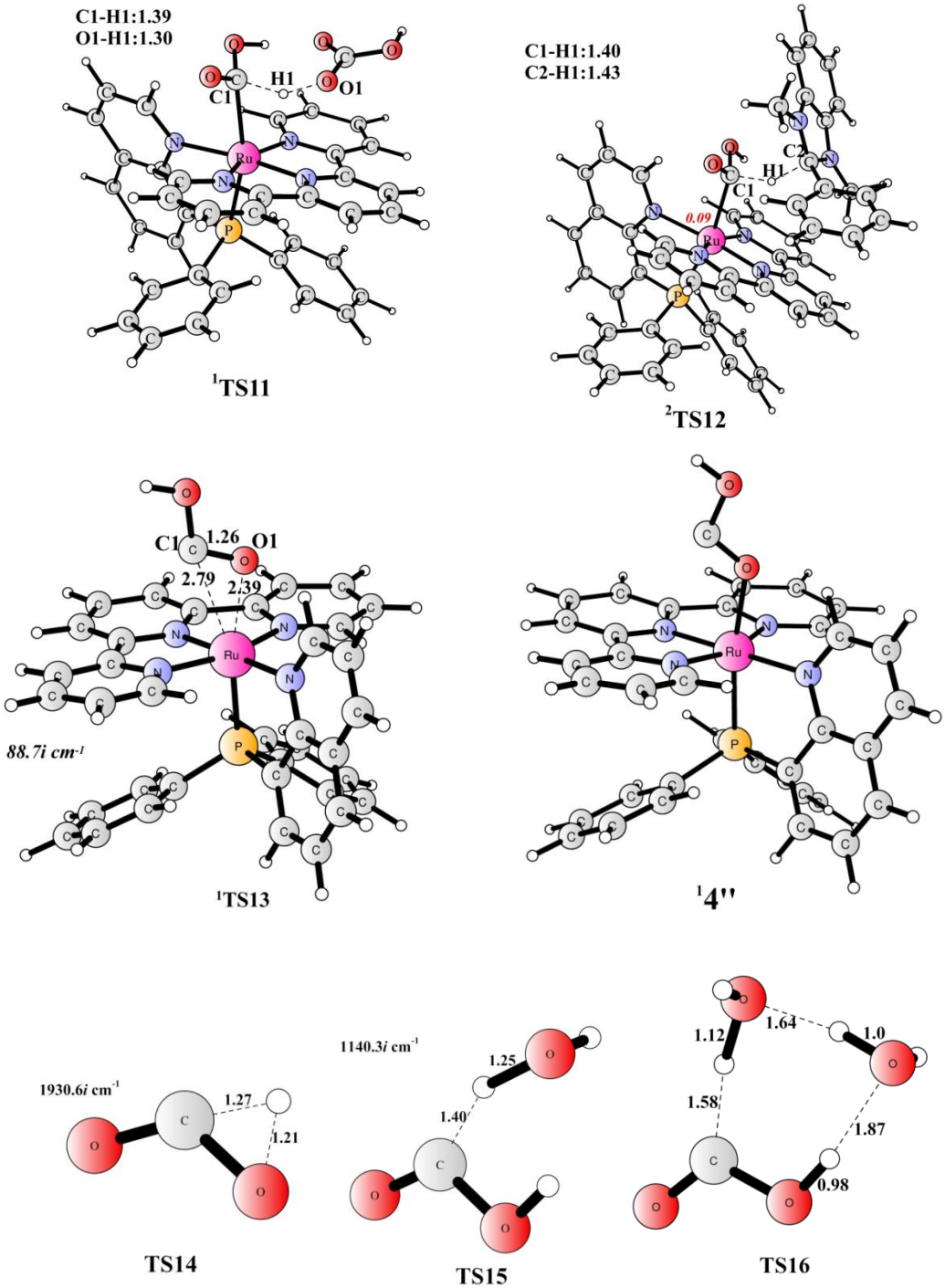


Figure S23. Optimized structures of ^{1}**TS11**, ^{2}**TS12**, ^{1}**TS13**, ^{1}**4''**, ^{1}**TS14**, ^{1}**TS15**, **and** ^{1}**TS16**. The spin density of Ru is shown in red italic.

S24. Gibbs free energy diagram for the formation of HCOOH.

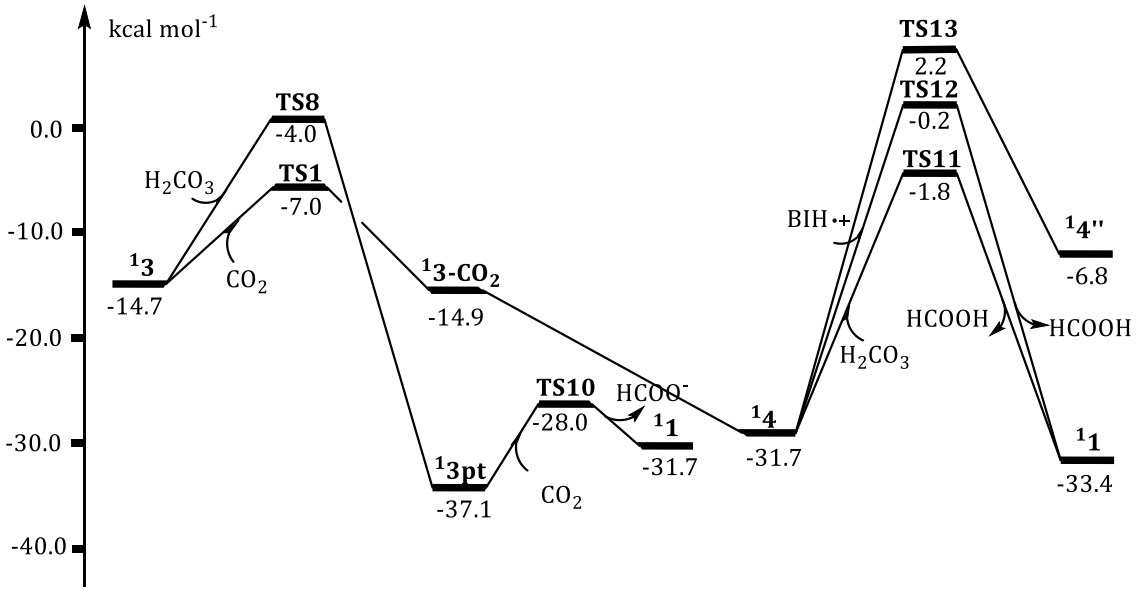


Figure S24. Gibbs free energy diagram (in kcal mol^{-1}) for the formation of HCOOH.

S25. Calculated results with different density functionals.

Table S17. Comparison of redox potentials (in V) and barriers (in kcal mol^{-1}) for selectivity-determining steps (**TS1** and **TS8**) with different methods.

Method	Reduction potential (V)		Barrier (kcal mol^{-1})	
	^{2}**2-S**/ ^{3}**1-S**	^{1}**3**/ ^{2}**2**	**TS1**	**TS8**
B3LYP-D3	0.33	-1.67	7.7	10.7
MN15	0.61	-1.57	9.8	13.2
MN15L	0.34	-1.55	9.9	17.7

To evaluate the sensitivity of the redox potentials and barriers to the choice of density functionals, the MN15 and MN15L functionals have been used for single-point calculations. The Gibbs free energy diagrams are shown in **Figure S25**. The redox potentials of the first and second reduction processes for the catalyst and the barriers were found to be somewhat sensitive to the functionals. The redox potentials and barriers for the selectivity-determining steps with different methods are summarized in **Table S17**. The redox potentials all show that the first reduction of the catalyst is easy after photoexcitation (0.33 V using B3LYP-D3, 0.61 V using MN15, and 0.34 V using MN15L). However, the second reduction needs a more negative potential, all about -1.60 V for these three methods. This confirms that BIH needs to be converted to BI· to provide sufficient reduction power.

The barriers for the bonding of CO_2 and the formation of Ru^{II}-H using the three functionals all show that the barrier of the reaction with CO_2 (7.7 kcal mol^{-1} using B3LYP-D3, 9.8 kcal mol^{-1} using MN15, and 9.9 kcal mol^{-1} using MN15L) is lower than that for the formation of Ru^{II}-H (10.7 kcal mol^{-1} using B3LYP-D3, 13.2 kcal mol^{-1} using MN15 and 17.7 kcal mol^{-1} using MN15L), which can explain the selectivity of this reaction.

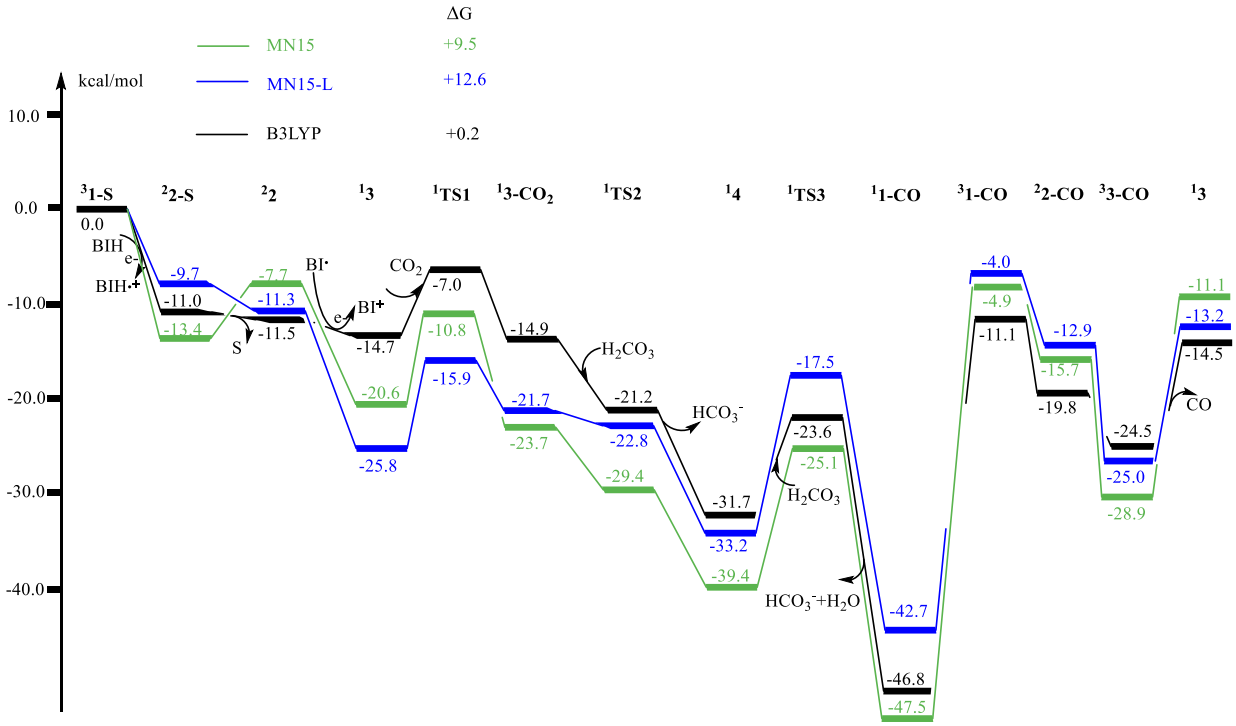


Figure S25. Gibbs free energy diagram (in kcal mol^{-1}) for the whole reaction calculated at levels of B3LYP-D3 (in black), MN15(in green), and MN15-L (in blue).

To further validate the density functional results, domain-based local pair natural orbital coupled cluster (DLPNO-CCSD(T)) [S4] two-point complete basis set (CBS) limit extrapolations [S5] calculations (def2-SVP and def2-TZVP) [S6] in the gas phase were performed to check the reaction free energy (ΔG) of the uncatalyzed reaction using ORCA 4.2. [S7, S8] Equation (1) was calculated to be endergonic by 3.9 kcal mol^{-1}.

In **Table S18**, the ΔG obtained using the four DFT methods all showed that Equation (1) is an endergonic reaction. The ΔG is slightly underestimated with the B3LYP-D3 method, while they are overestimated using MN15L-D3 and MN15L-D3 methods.

$$H_2CO_3 + CO_2 + BIH \longrightarrow BI^+ + HCO_3^- + CO + H_2O \qquad (1)$$

Table S18. The reaction free energy (ΔG) calculated by diffierent methods.

Method	ΔG (kcal mol^{-1})
B3LYP-D3	+0.2
MN15-D3	+9.5
MN15L-D3	+12.6
DLPNO-CCSD(T)	+3.9

The total energy barriers obtained using three DFT methods are 27.6 kcal mol^{-1} (by MN15-D3), 21.7 (by MN15L-D3), and 17.8 kcal mol^{-1}(by B3LYP-D3), respectively. The TON (42 in 4 h) of CO measured experimentally can be approximately converted to a barrier of 20.9 kcal mol^{-1} using classical transition state theory. This suggested that the barrier calculated by MN15-D3 is overestimated, that MN15L-D3 is in line with the experimental data, and the barrier calculated by B3LYP-D3 is somewhat underestimated. However, the rate-determining intermediate and the rate-determining transition state are the same for these three methods.

S26. Details of the COPASI simulations for the whole reaction.

Duration： 14400 s (4 h)

Intervals: 1000000

Interval size: 0.0144

The initial concentrations are :

BIH: 0.1 mol L^{-1},

Ru^{II}-S: 4×10^{-5} mol L^{-1},

CH_3CN: 19.2 mol L^{-1},

H_2O: 1.4 mol L^{-1}

CO_2: 0.245 mol L^{-1}.

The final concertions of the products are:

CO: 0.1 mol L^{-1},

HCOOH: 4.2×10^{-4} mol L^{-1},

H_2: 7.1×10^{-3} mol L^{-1}.

The corresponding TON_{CO}=2500, TON_{HCOOH}=0.1, $TON_{H2}=1.2\times10^{-3}$.

For all species in COPASI, a concentration correction of 1.9 kcal mol^{-1}, which originates from the free energy change for 1atm (24.5 L mol^{-1} for the ideal gas) to 1 mol L^{-1} (in acetonitrile) was used.

Table S19. All possible elementary reactions in this system are shown below

Reactions	k_1	k_{-1}
[a] $H_2O + CO_2 \rightleftharpoons H_2CO_3$	2.75207×10^{7}	1.68448×10^{10}
$Ru^{II}\text{-}S \longrightarrow {}^3Ru^{II}\text{-}S$	1.0×10^{15}	
[a] ${}^3Ru^{II}\text{-}S + BIH \rightleftharpoons Ru^{I}\text{-}S + BIH^{\cdot+}$	1.68448×10^{10}	1.44342×10^{2}
[a] $HCO_3^- + BIH^{\cdot+} \rightleftharpoons BI^{\cdot} + H_2CO_3$	6.80867×10^{8}	1.68448×10^{10}
[a] $Ru^{I}\text{-}S \rightleftharpoons Ru^{I} + S$	1.68448×10^{10}	7.24070×10^{9}
[a] $Ru^{I} + BI^{\cdot} \rightleftharpoons Ru^{0} + BI^{+}$	1.68448×10^{10}	3.06392×10^{6}
[b] $Ru^{0} + CO_2 \rightleftharpoons Ru^{II}\text{-}CO_2^-$	1.40059×10^{7}	9.99163×10^{6}
[b] $Ru^{II}\text{-}CO_2^- + H_2CO_3 \rightleftharpoons Ru^{II}\text{-}COOH + HCO_3^-$	1.68448×10^{10}	8.05090×10^{-3}
[b] $Ru^{II}\text{-}COOH + H_2CO_3 \rightleftharpoons Ru^{II}\text{-}CO + H_2O + HCO_3^-$	7.12791×10^{6}	6.01272×10^{-5}
[b] $Ru^{II}\text{-}H + H_2CO_3 \rightleftharpoons Ru^{II} + HCO_3^- + H_2$	6.02040×10^{6}	6.59820×10^{2}
[b] $Ru^{II}\text{-}H + CO_2 \rightleftharpoons Ru^{II} + HCOO^-$	1.31702×10^{6}	1.20169×10^{10}
[a] $Ru^{II}\text{-}CO \rightleftharpoons Ru^{II} + CO$	2.96921	1.68448×10^{10}
[a] $H_2CO_3 \rightleftharpoons HCO_3^- + H+$	5.25292×10^{-5}	1.68448×10^{10}
[b] $Ru^{0} + H_2CO_3 \rightleftharpoons Ru^{II}\text{-}H + HCO_3^-$	8.83486×10^{4}	3.30145×10^{-12}
[a] $Ru^{II}\text{-}CO \longrightarrow {}^3Ru^{II}\text{-}CO$	1.0×10^{15}	
[a] ${}^3Ru^{II}\text{-}CO + BIH \rightleftharpoons Ru^{I}\text{-}CO + BIH.+$	1.68448×10^{10}	7.01688×10^{3}
[a] $Ru^{I}\text{-}CO + BI. \rightleftharpoons {}^3Ru^{0}\text{-}CO + BI+$	1.68448×10^{10}	2.05535×10^{5}
[a] ${}^3Ru^{0}\text{-}CO \rightleftharpoons {}^1Ru^{0} + CO$	6.59820×10^{2}	1.68448×10^{10}
$Ru^{II} + S = Ru^{II}\text{-}S$	1.68448×10^{10}	2.70920×10^{4}

$\rightleftharpoons$: means reversible reaction.

$\longrightarrow$: means irreversible reactions

[a]: rate constant k is from ΔG .

[b]: rate constant k is from $\Delta G^{\neq}$.

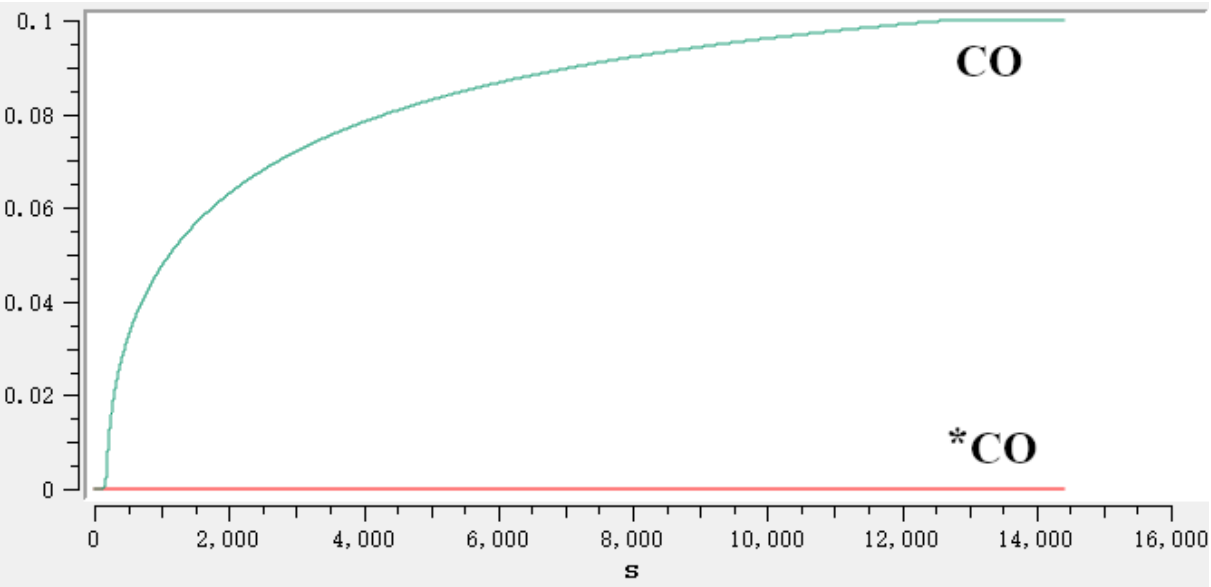


Figure S26. The microkinetic model outcome of CO and *CO over the whole 4 h (14400 s).

Table S20. The final concentrations of the products.

Species	Concentration (mol L^{-1})
*CO (B)	2.97×10^{-16}
CO (A)	9.99×10^{-2}
CO	9.99×10^{-2}

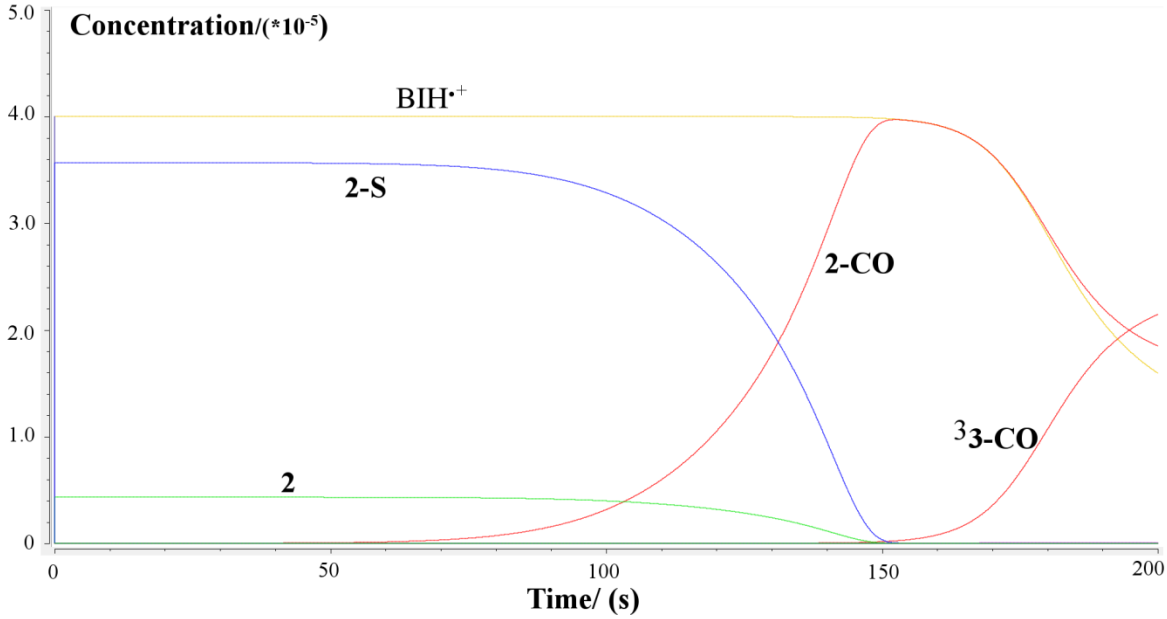


Figure S27. The microkinetic model outcome with the concentrations of $BIH^{\cdot+}$ in yellow, **2-S** in blue, **2** in green, **2-CO,** and **3-CO** in red (in mol L^{-1}) over the beginning 200 seconds.

It should be pointed out that at the beginning of this reaction, it is difficult to generate HCO_3^- from the dissociation of H_2CO_3 as it is an endergonic process. Therefore, in the initial stage of the reaction, there will be an accumulation of $BIH^{\cdot+}$ and **2-S**. After 150 s, with the formation of 1-CO, one HCO_3^- is also formed, thus starting the following catalytic cycles.

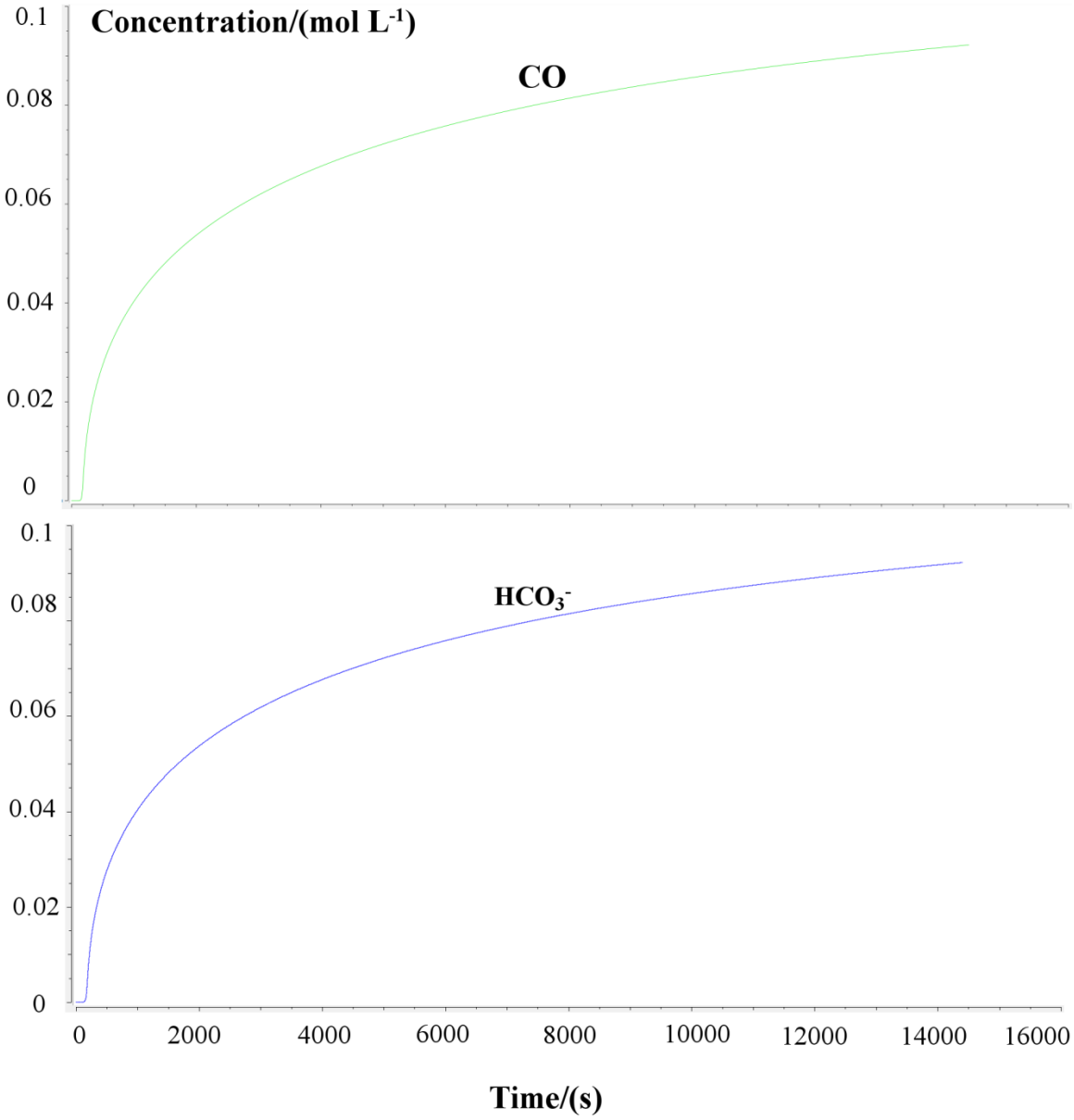


Figure S28. The microkinetic model outcome with the concentrations of **CO** in green and **HCO_3^-** in blue (in mol L^{-1}) over 4 h.

After four hours, the concentrations of HCO_3^- and CO become the same, which confirms that the total reaction for the formation of CO is:

$$H_2CO_3 + CO_2 + BIH \longrightarrow BI^+ + HCO_3^- + CO + H_2O$$

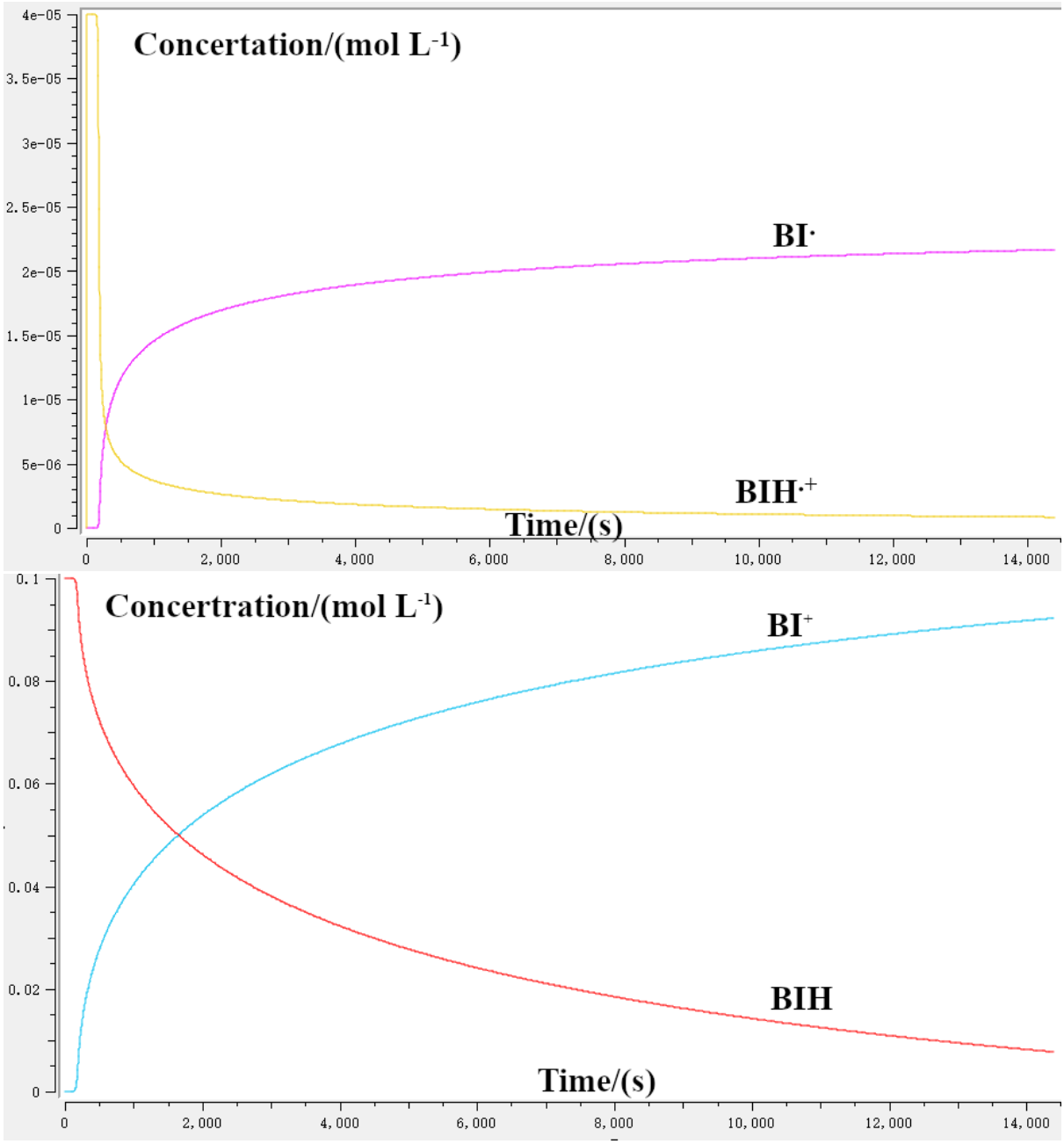
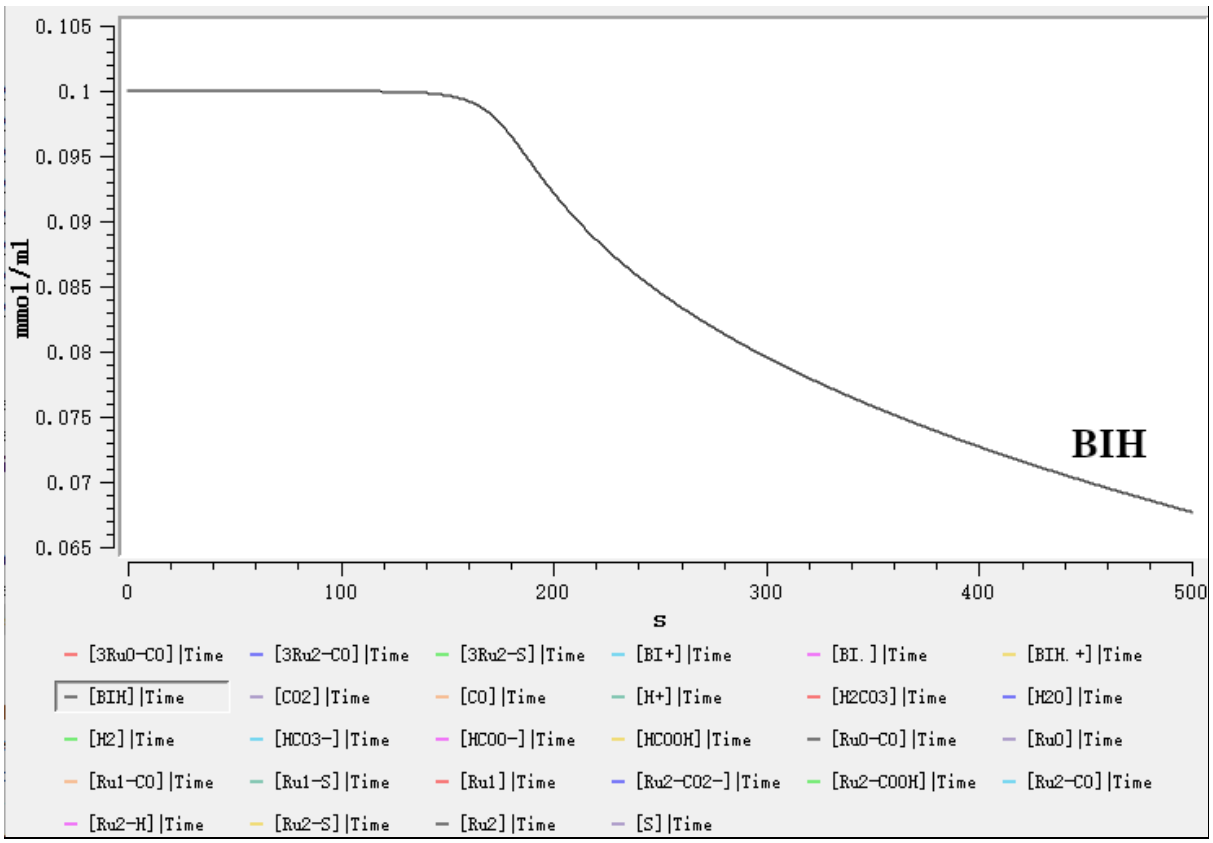
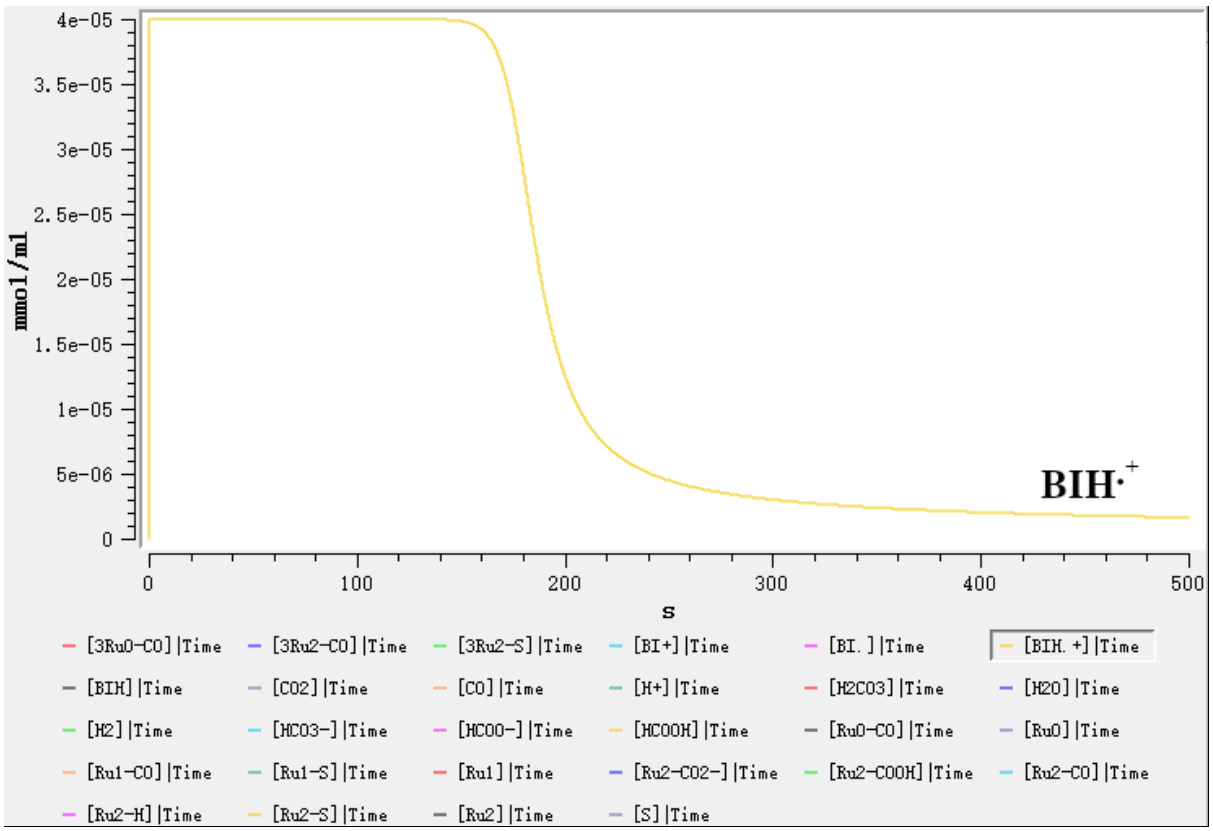
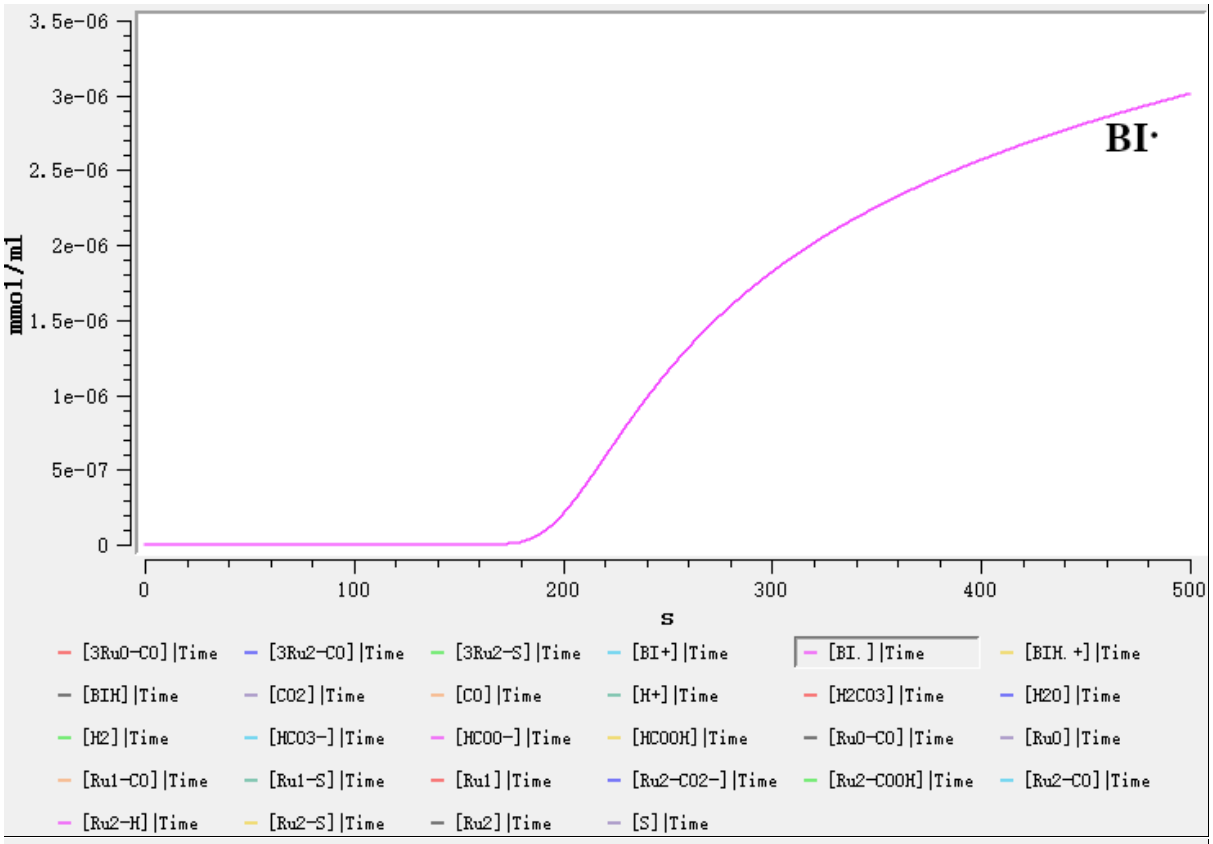


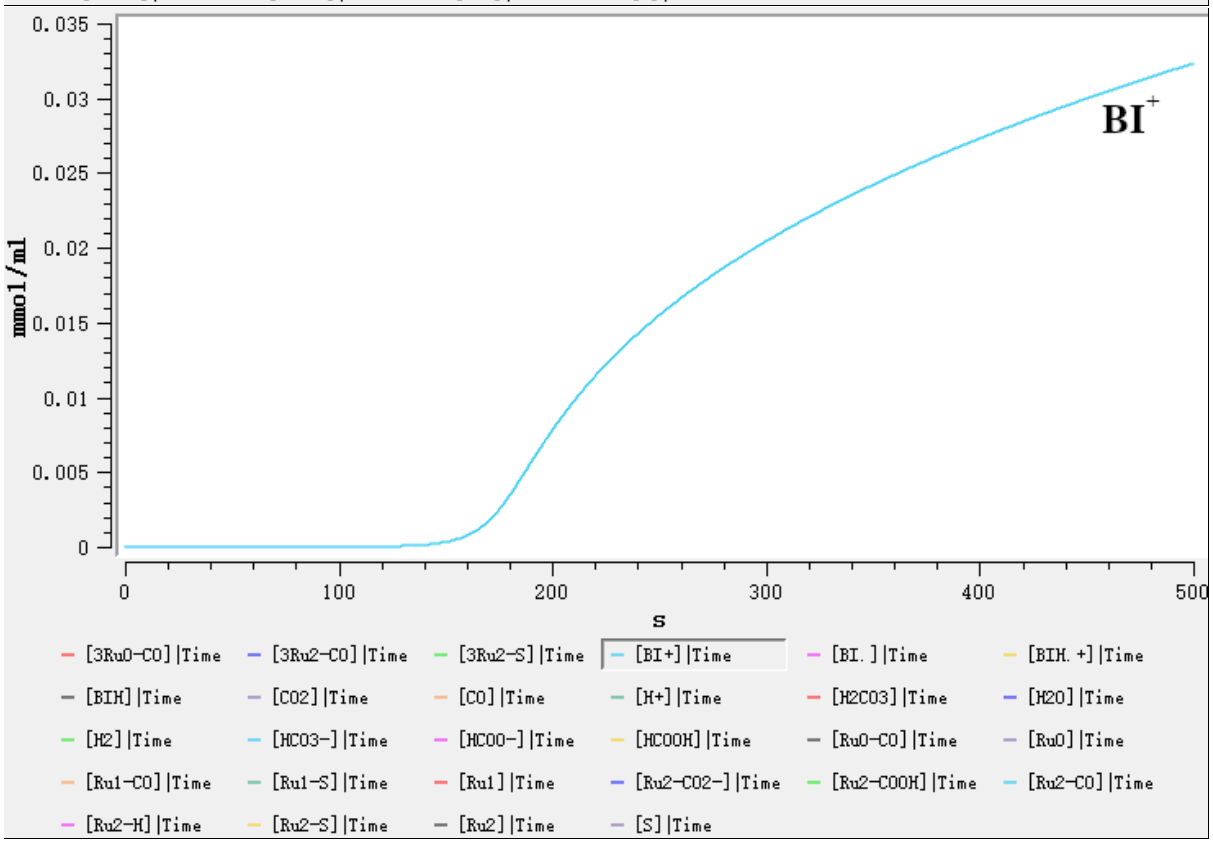
Figure S29. The microkinetic model outcome with the concentrations of BIH in red, $BIH^{\cdot+}$ in yellow, **BI**· in purple and **BI**$^{+}$ in blue (in mol L^{-1}) over 4 h.

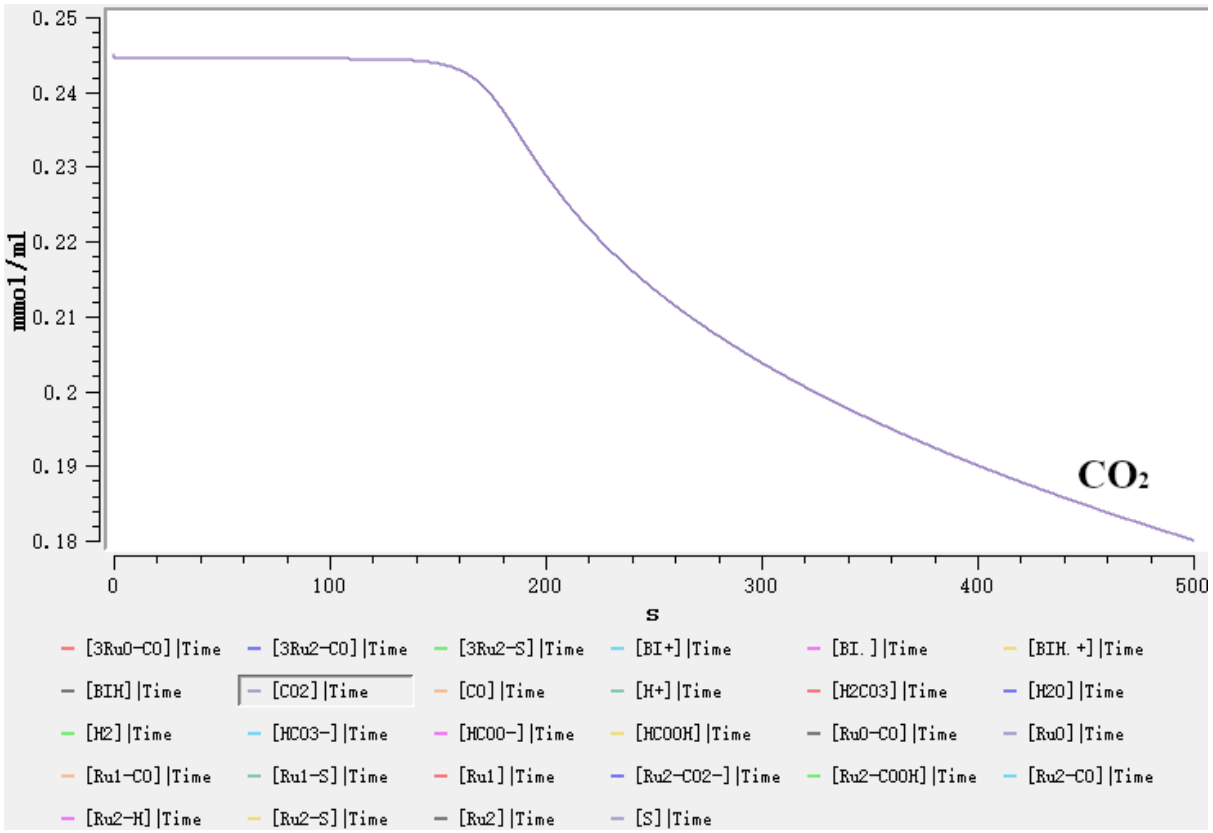
S27. The microkinetic model outcome for all species, over the beginning 500 s.

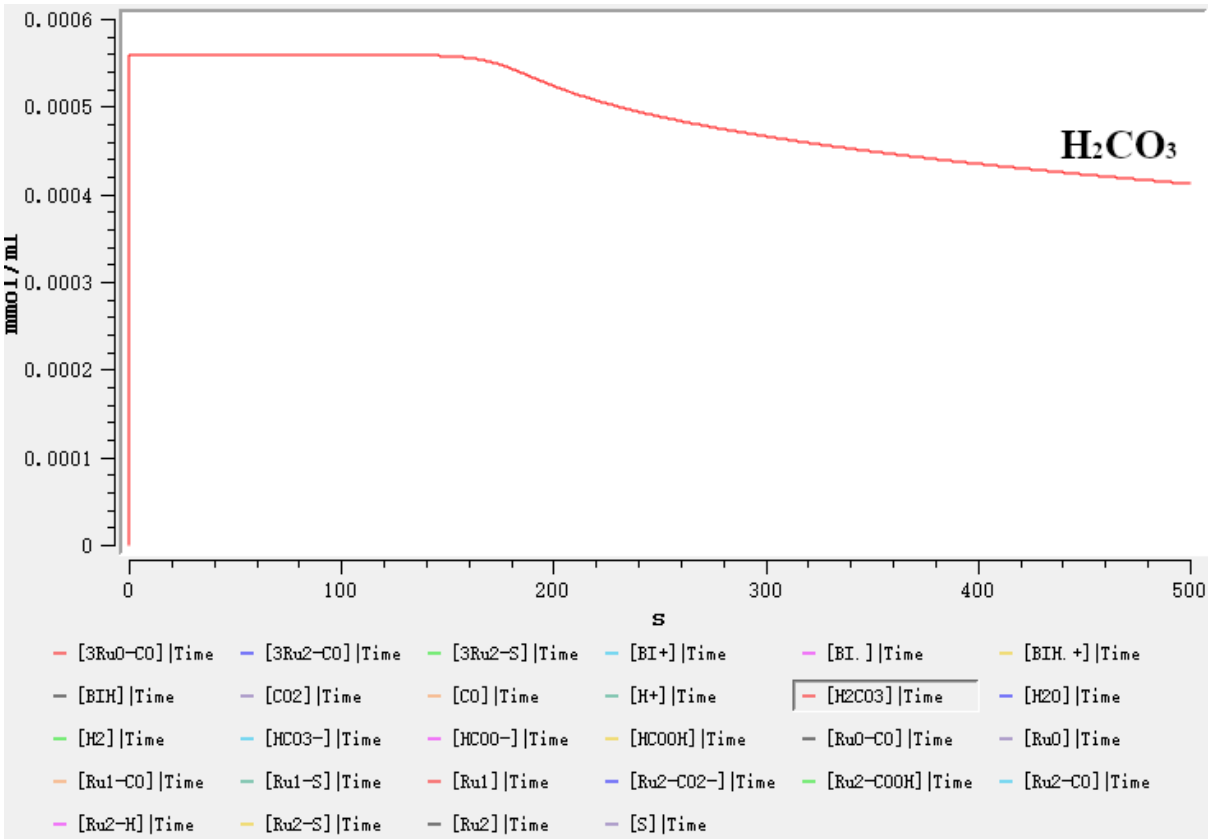


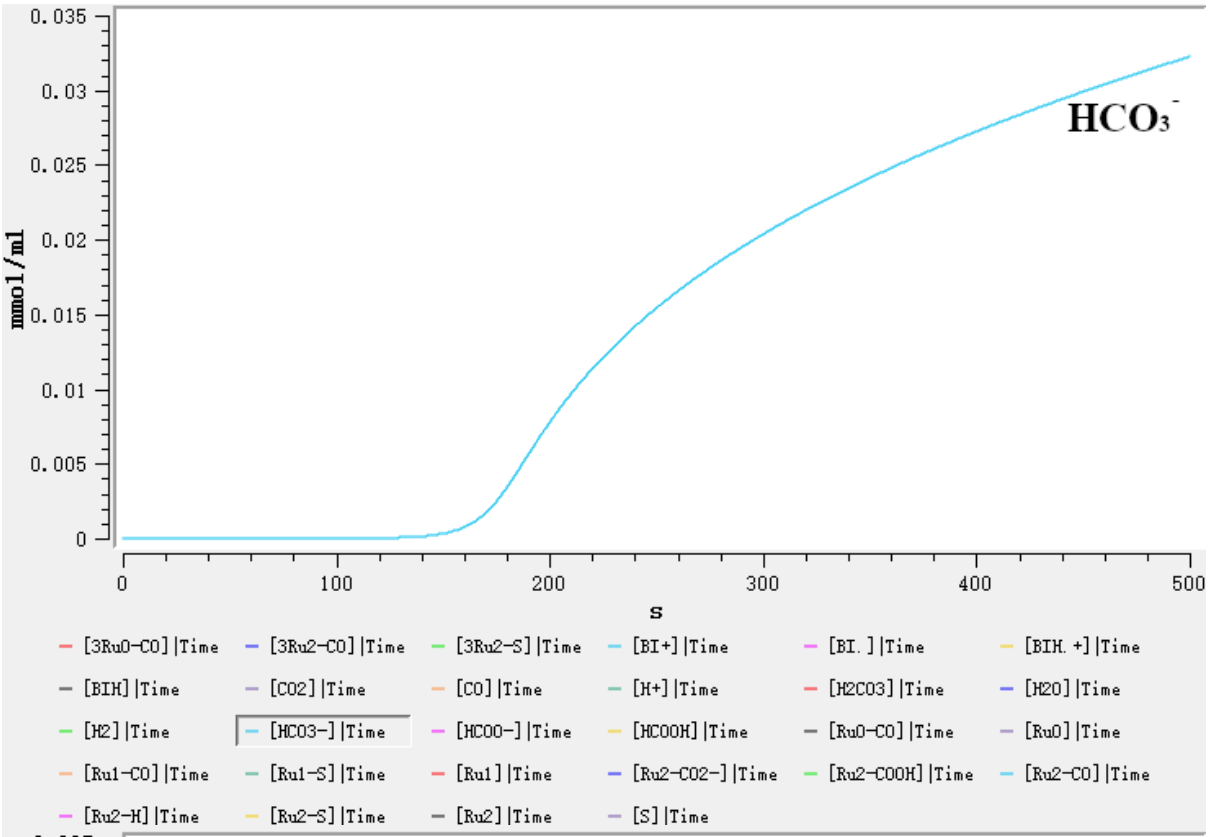


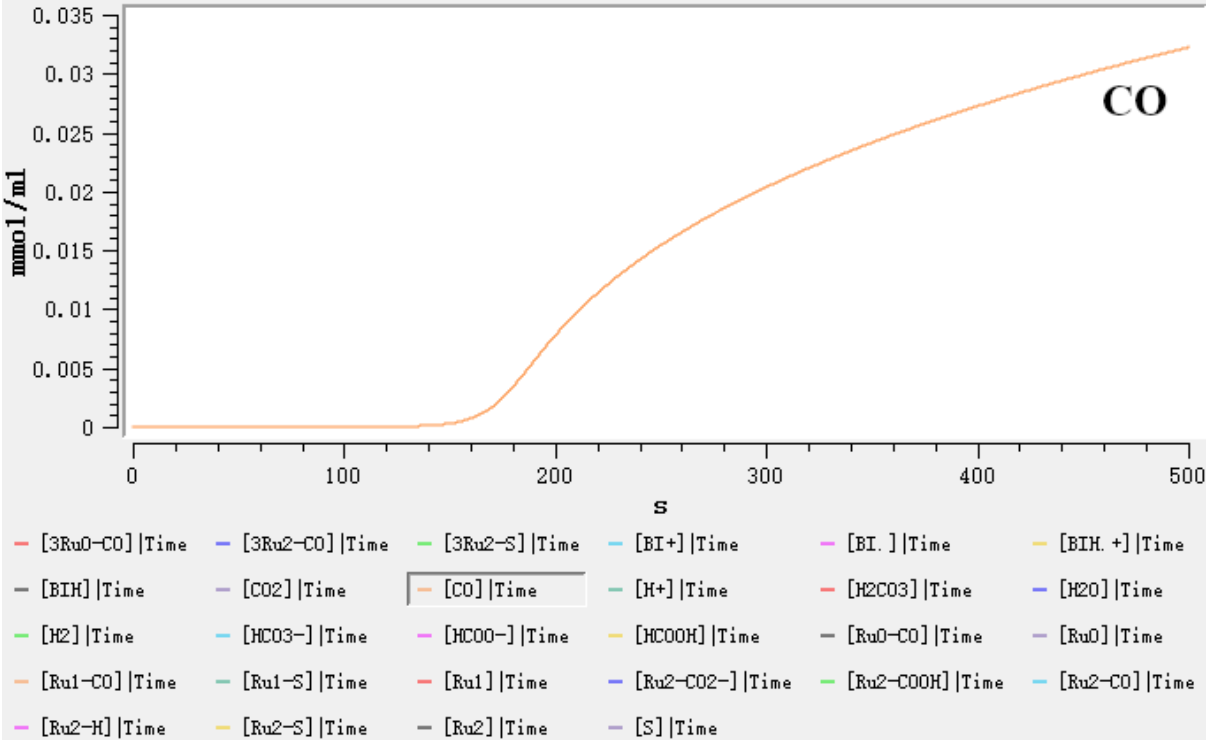

3.5e-06
3e-06
2.5e-06
2e-06
1.5e-06
1e-06
5e-07
0
mmol/ml
0
100
200
300
400
500
s
BI·
[3Ru0-C0]|Time
[3Ru2-C0]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[C02]|Time
[C0]|Time
[H+]|Time
[H2C03]|Time
[H20]|Time
[H2]|Time
[HC03-]|Time
[HC00-]|Time
[HC00H]|Time
[Ru0-C0]|Time
[Ru0]|Time
[Ru1-C0]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-C02-]|Time
[Ru2-C00H]|Time
[Ru2-C0]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

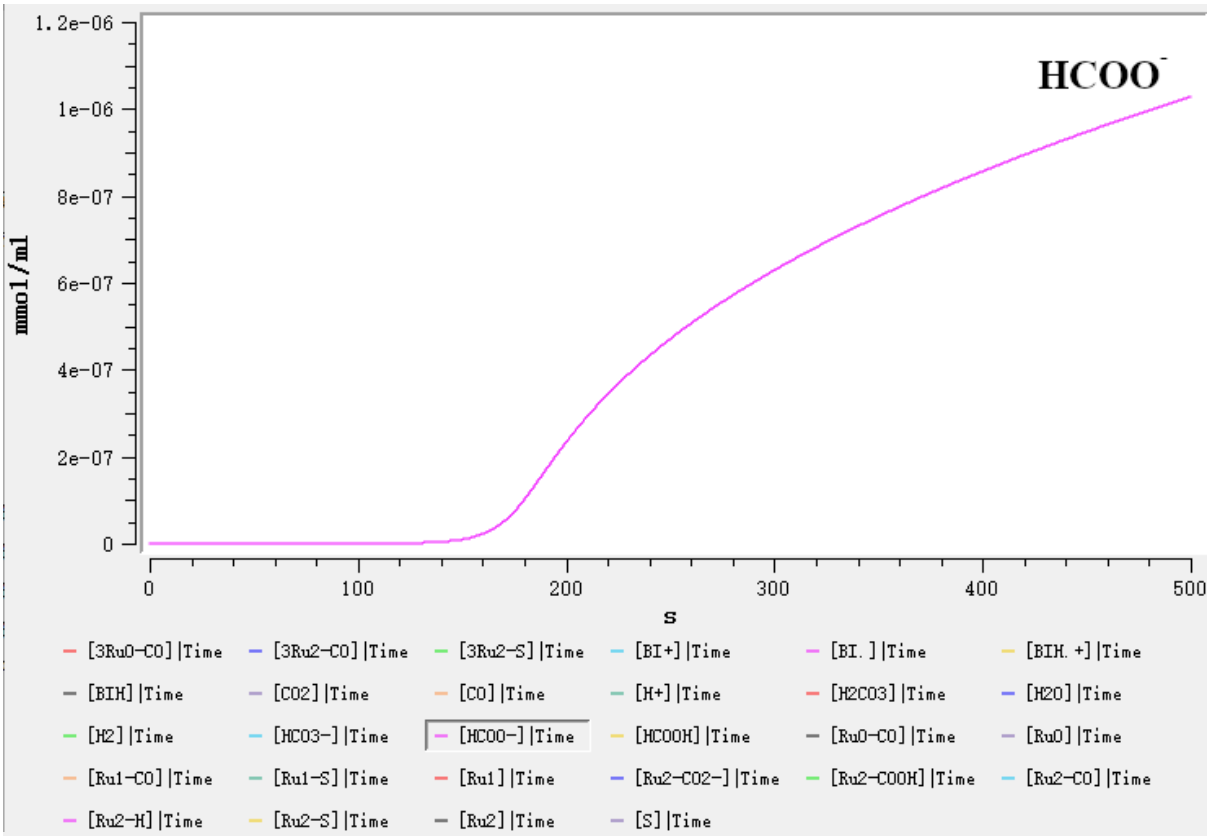

0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
mmol/ml
0
100
200
300
400
500
s
BI+
[3Ru0-C0]|Time
[3Ru2-C0]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[C02]|Time
[C0]|Time
[H+]|Time
[H2C03]|Time
[H20]|Time
[H2]|Time
[HC03-]|Time
[HC00-]|Time
[HC00H]|Time
[Ru0-C0]|Time
[Ru0]|Time
[Ru1-C0]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-C02-]|Time
[Ru2-C00H]|Time
[Ru2-C0]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

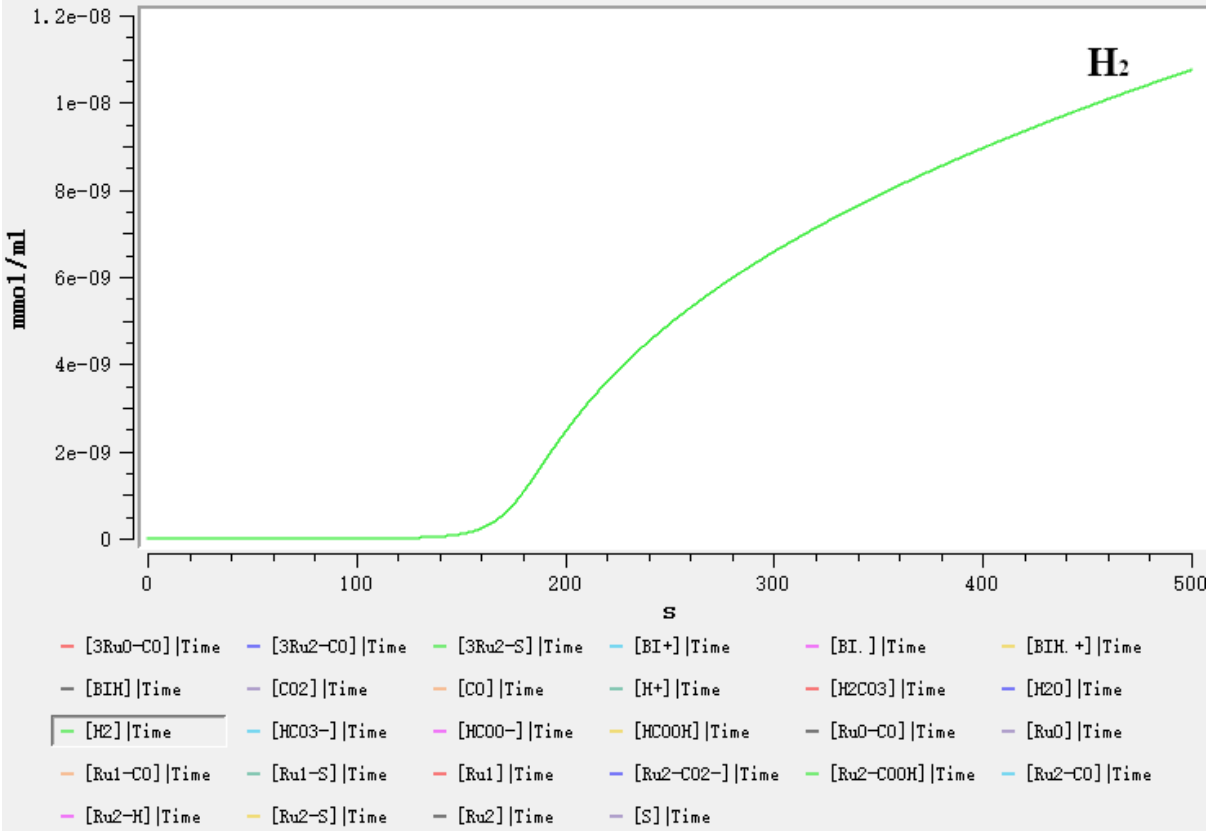

0.25
0.24
0.23
0.22
0.21
0.2
0.19
0.18
mmol/ml
0
100
200
300
400
500
s
CO2
[3RuO-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[RuO-CO]|Time
[RuO]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

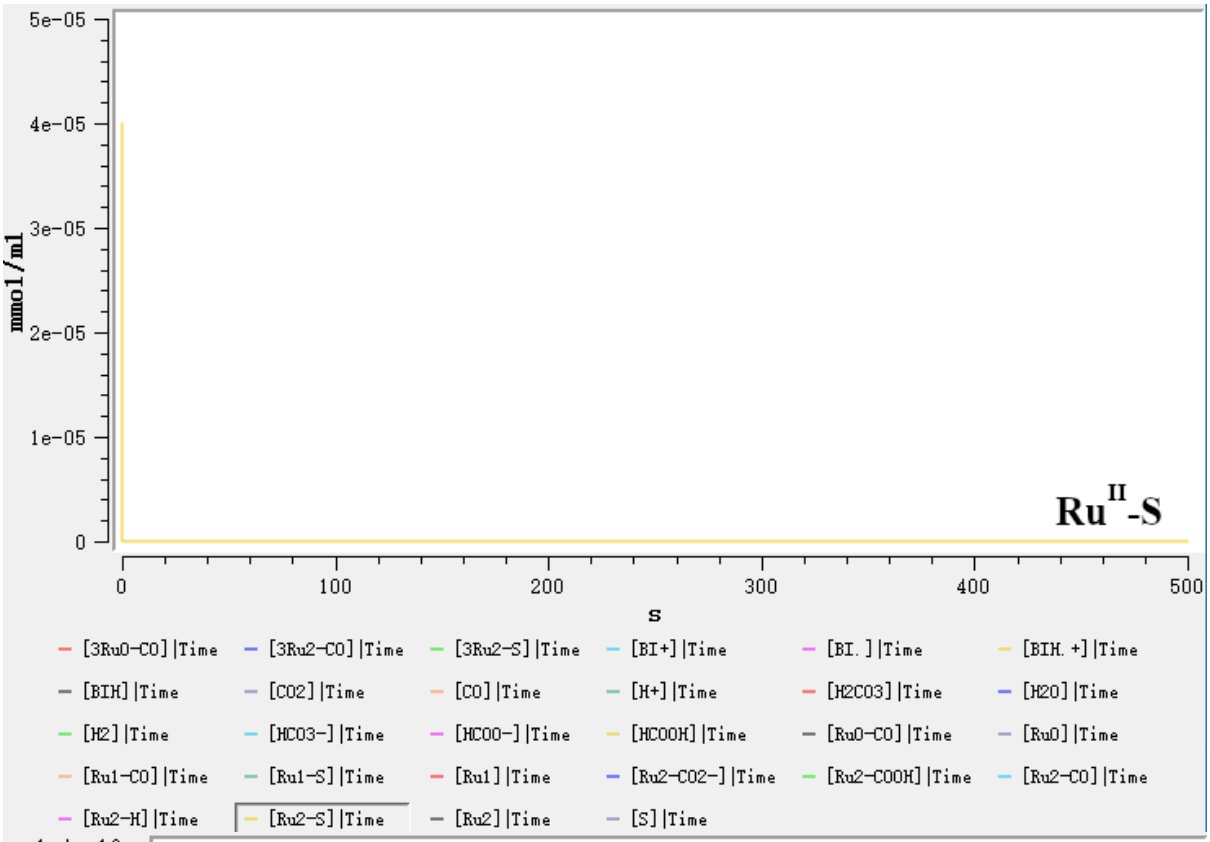

0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0
mmol/ml
0
100
200
300
400
500
s
H2CO3
[3RuO-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[RuO-CO]|Time
[RuO]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

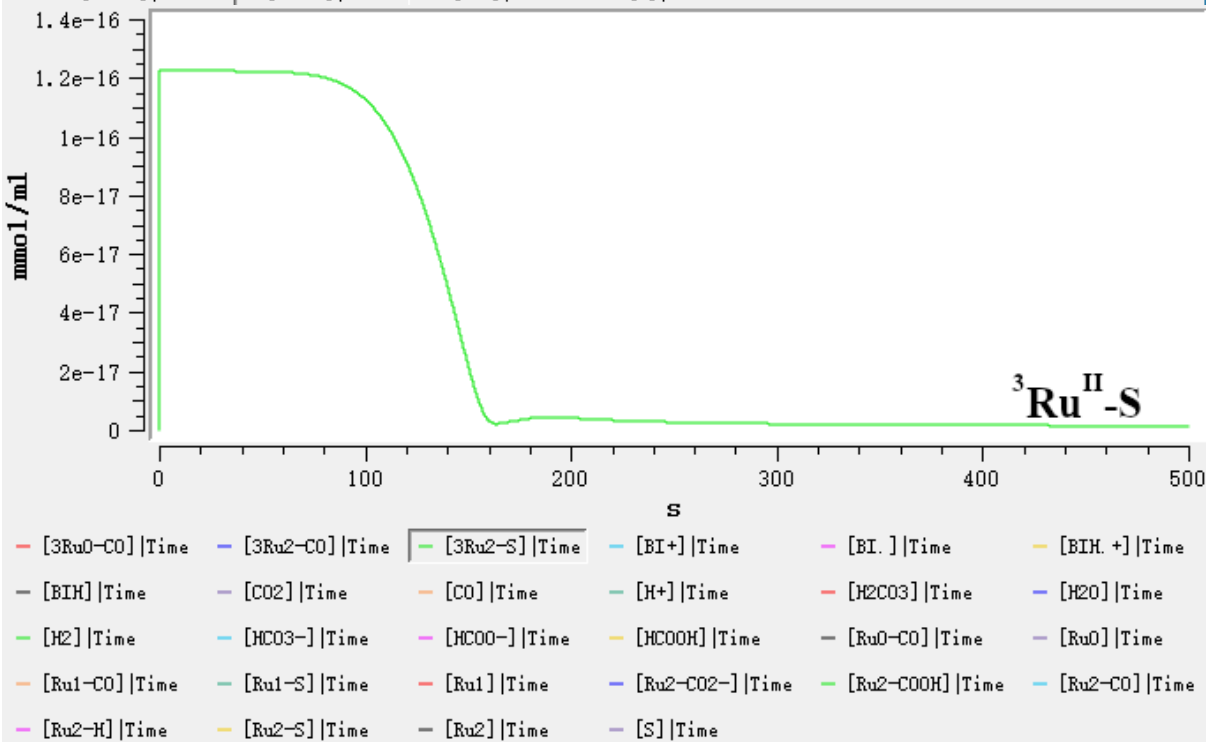

0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
mmol/ml
HCO3-
0
100
200
300
400
500
s
[3Ru0-C0]|Time
[3Ru2-C0]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[C02]|Time
[C0]|Time
[H+]|Time
[H2C03]|Time
[H20]|Time
[H2]|Time
[HC03-]|Time
[HC00-]|Time
[HC00H]|Time
[Ru0-C0]|Time
[Ru0]|Time
[Ru1-C0]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-C02-]|Time
[Ru2-C00H]|Time
[Ru2-C0]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

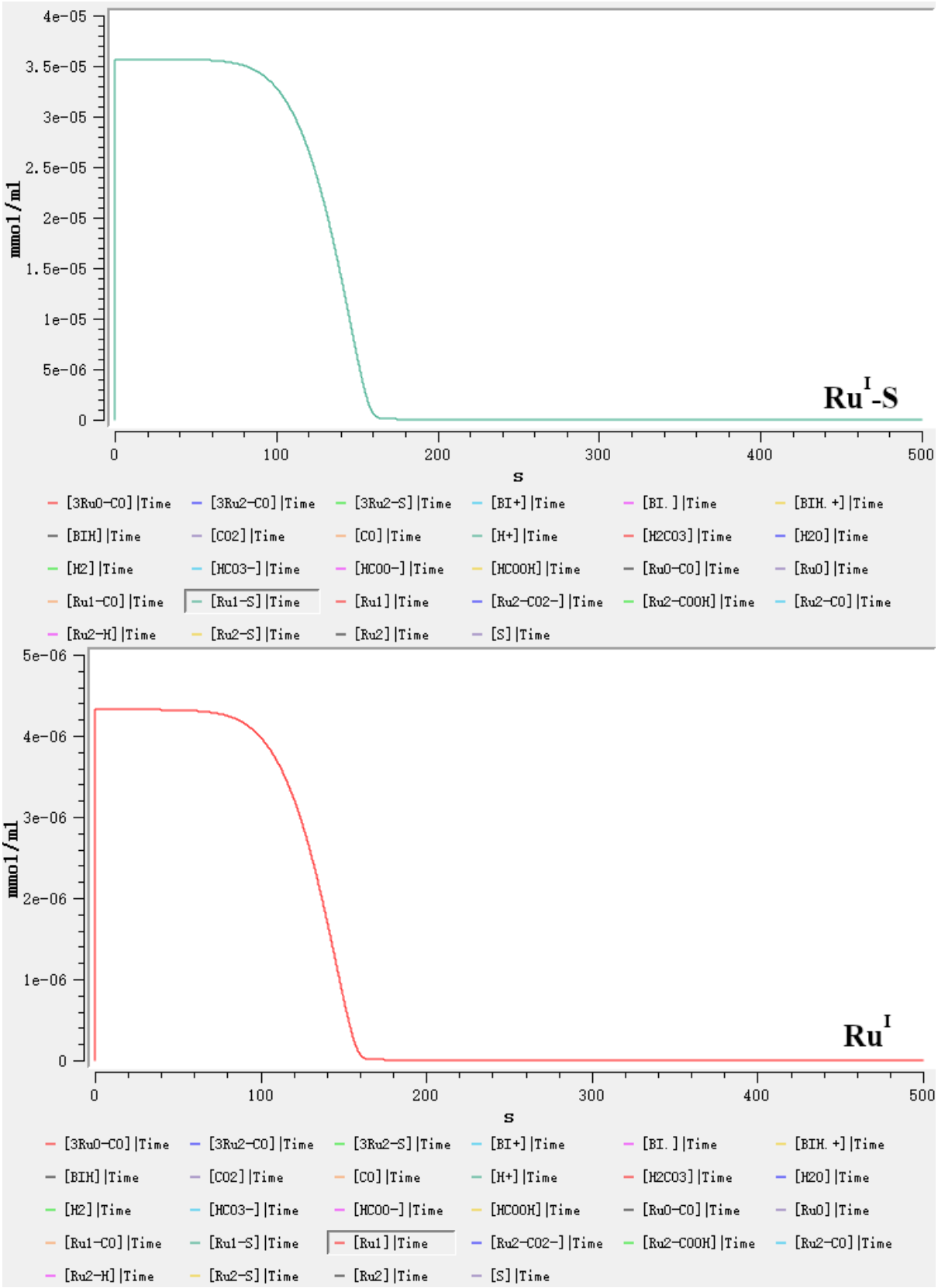

0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
mmol/ml
CO
0
100
200
300
400
500
s
[3Ru0-C0]|Time
[3Ru2-C0]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[C02]|Time
[C0]|Time
[H+]|Time
[H2C03]|Time
[H20]|Time
[H2]|Time
[HC03-]|Time
[HC00-]|Time
[HC00H]|Time
[Ru0-C0]|Time
[Ru0]|Time
[Ru1-C0]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-C02-]|Time
[Ru2-C00H]|Time
[Ru2-C0]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

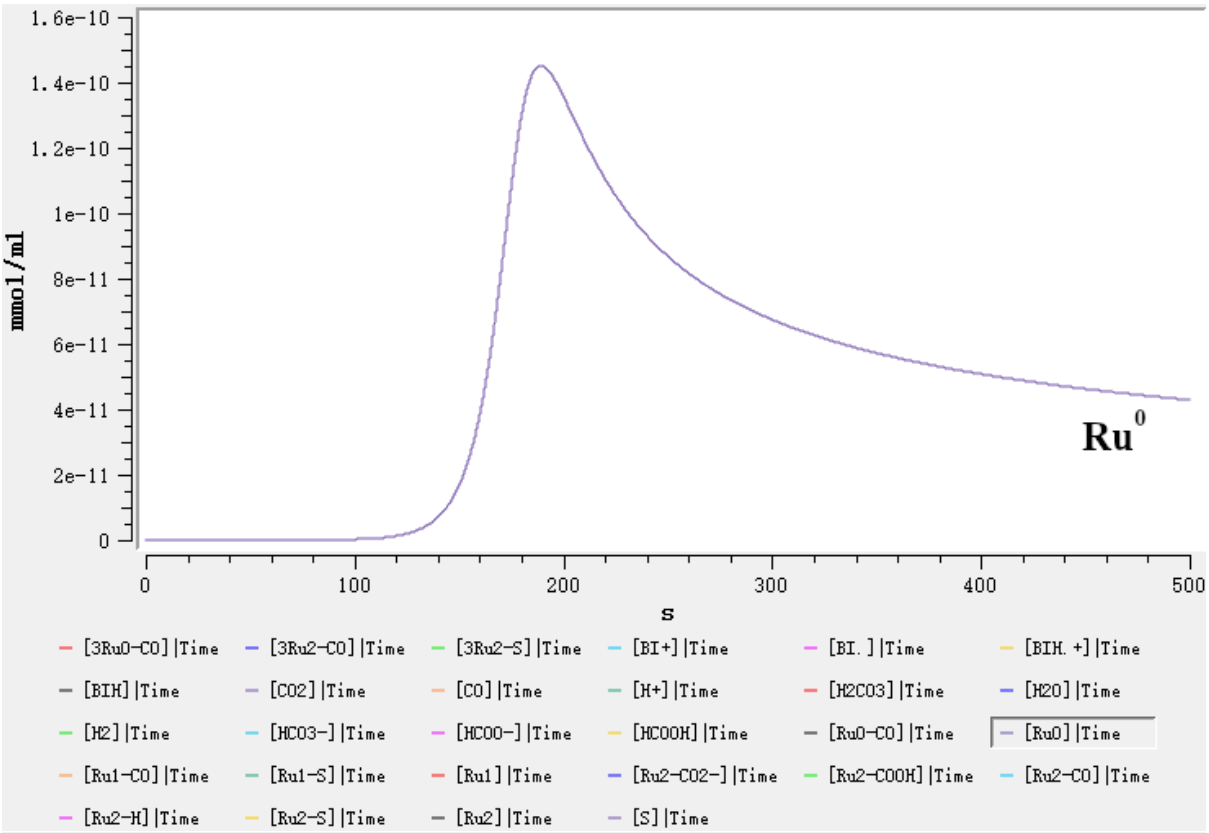

HCOO-
mmol/ml
1.2e-06
1e-06
8e-07
6e-07
4e-07
2e-07
0
0
100
200
300
400
500
s
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

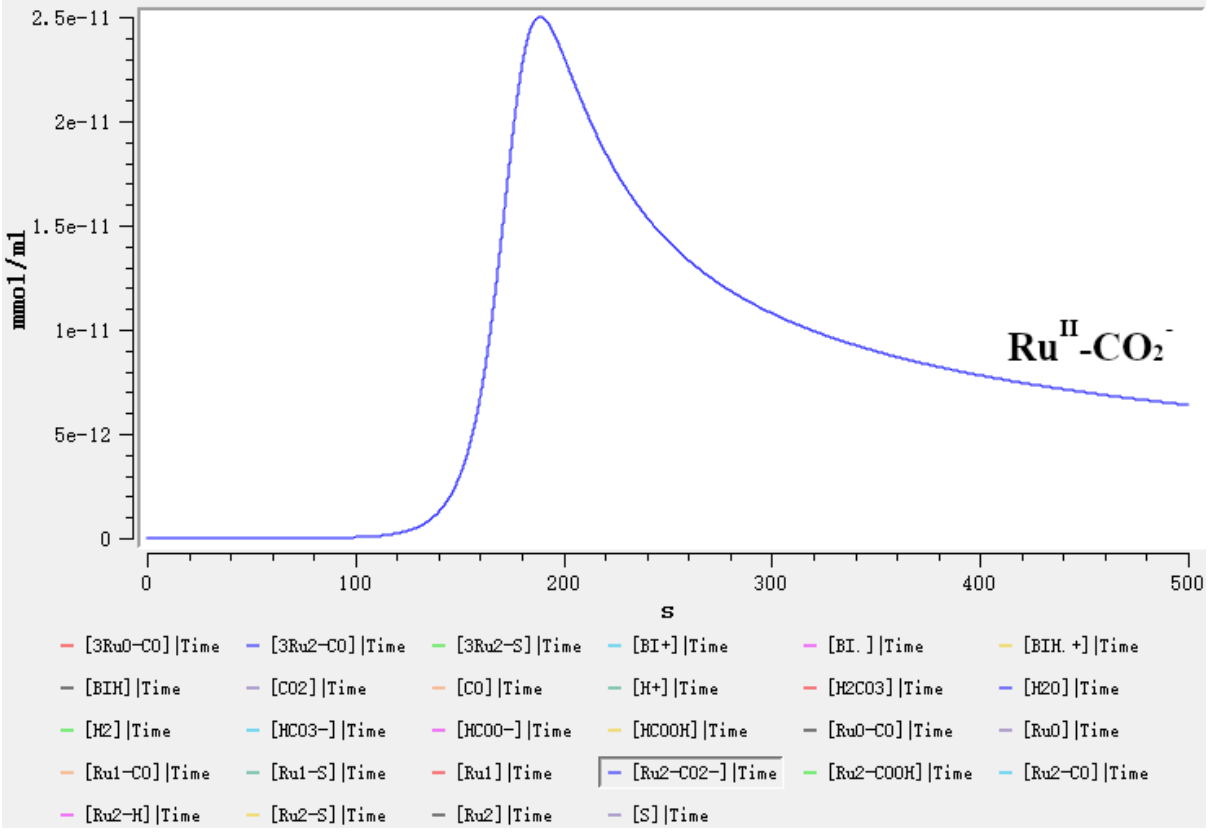

H2
mmol/ml
1.2e-08
1e-08
8e-09
6e-09
4e-09
2e-09
0
0
100
200
300
400
500
s
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

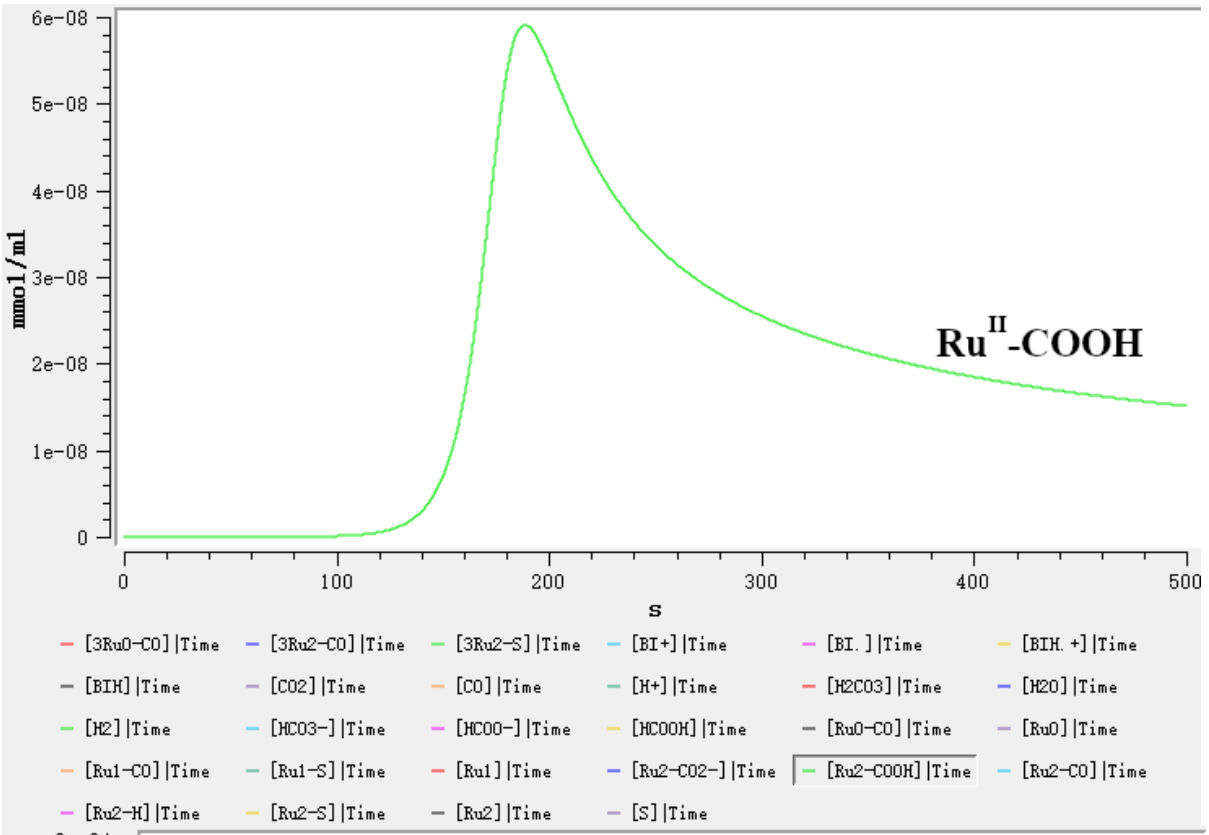

5e-05
4e-05
3e-05
2e-05
1e-05
0
mmol/ml
0
100
200
300
400
500
s
Ru^{II}-S
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

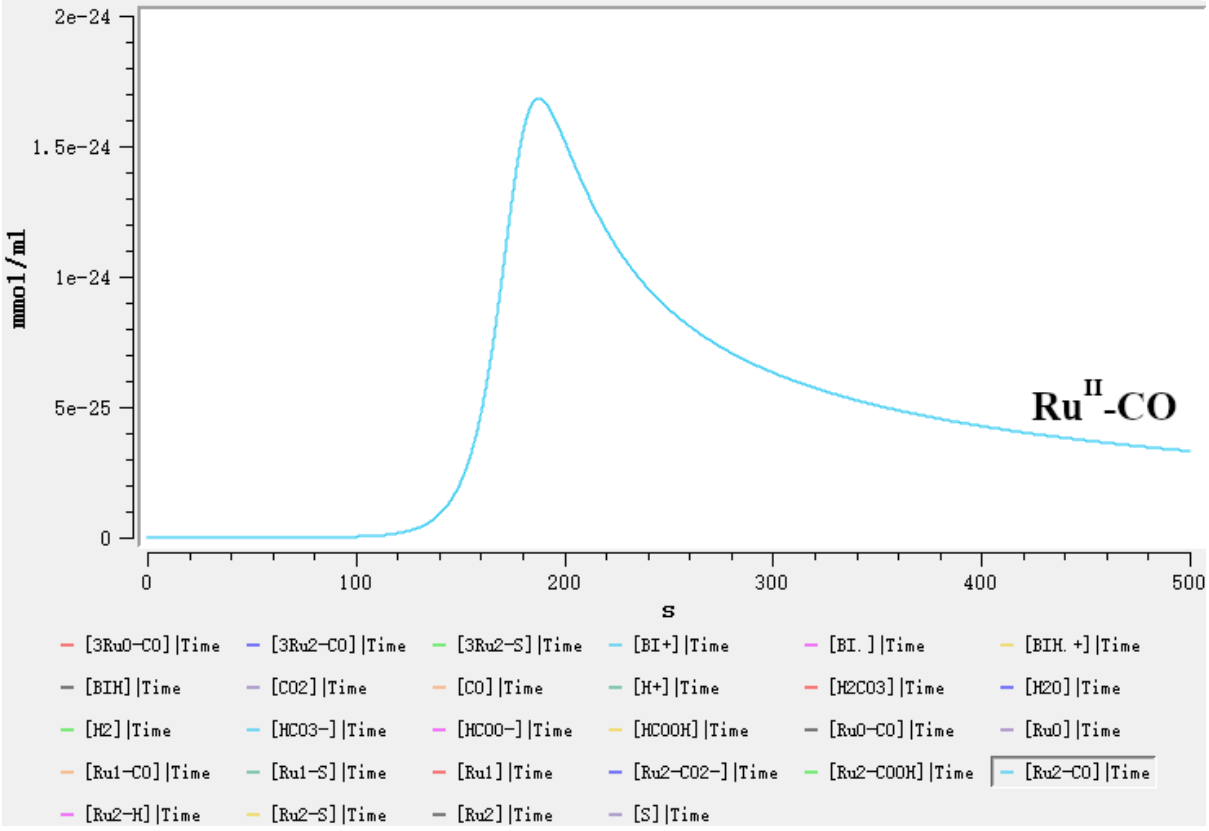

1.4e-16
1.2e-16
1e-16
8e-17
6e-17
4e-17
2e-17
0
mmol/ml
0
100
200
300
400
500
s
$^{3}Ru^{II}$-S
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

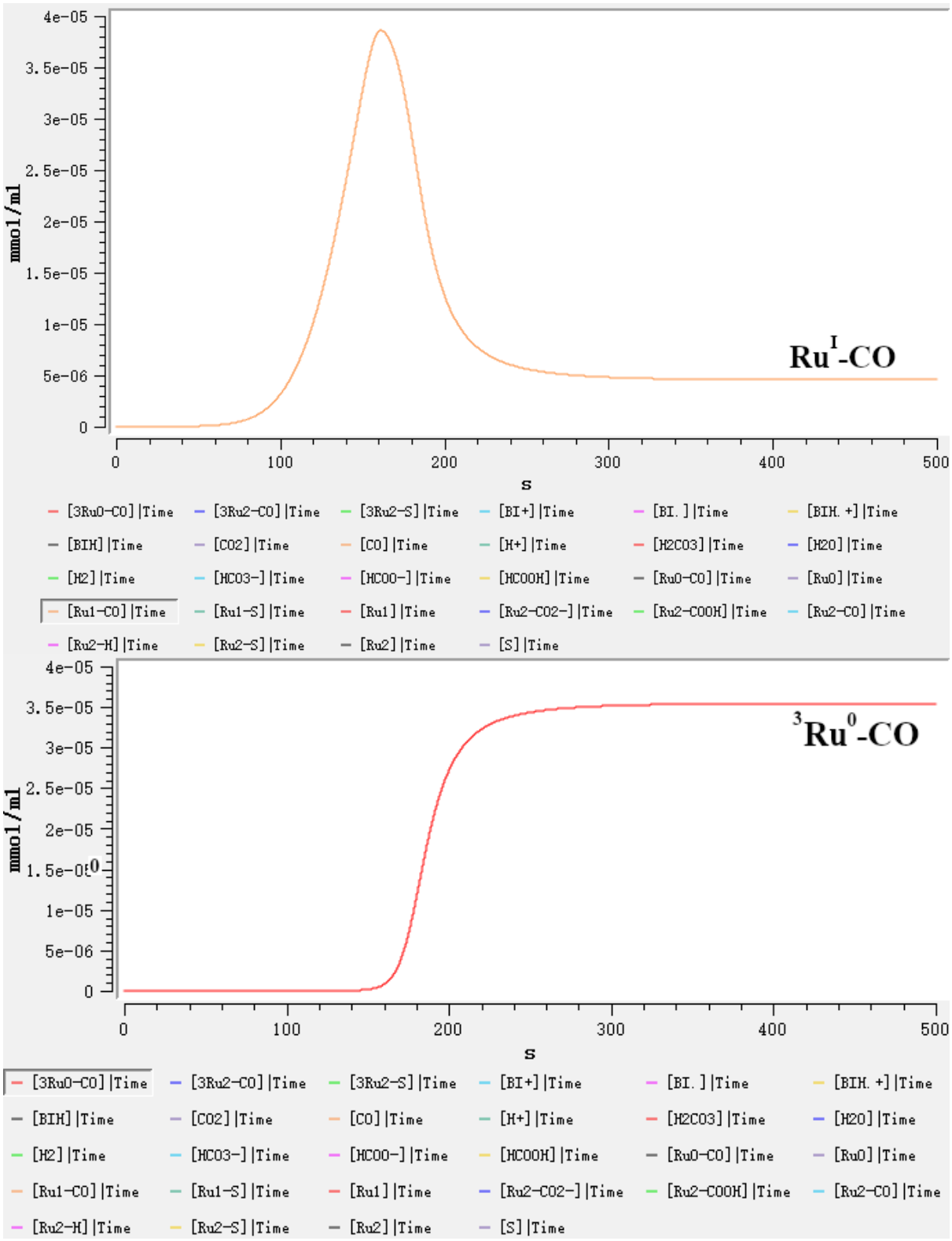

4e-05
3.5e-05
3e-05
2.5e-05
2e-05
1.5e-05
1e-05
5e-06
0
mmol/ml
0
100
200
300
400
500
s
Ru^I-S
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time
5e-06
4e-06
3e-06
2e-06
1e-06
0
mmol/ml
0
100
200
300
400
500
s
Ru^I
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time


1.6e-10
1.4e-10
1.2e-10
1e-10
8e-11
6e-11
4e-11
2e-11
0
mmol/ml
0
100
200
300
400
500
s
Ru0
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time


2.5e-11
2e-11
1.5e-11
1e-11
5e-12
0
mmol/ml
0
100
200
300
400
500
s
RuII-CO2-
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time


6e-08
5e-08
4e-08
3e-08
2e-08
1e-08
0
mmol/ml
0
100
200
300
400
500
s
Ru^II-COOH
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time


2e-24
1.5e-24
1e-24
5e-25
0
mmol/ml
0
100
200
300
400
500
s
Ru^II-CO
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time


4e-05
3.5e-05
3e-05
2.5e-05
2e-05
1.5e-05
1e-05
5e-06
0
mmol/ml
0
100
200
300
400
500
s
Ru^I-CO
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time
4e-05
3.5e-05
3e-05
2.5e-05
2e-05
1.5e-05
1e-05
5e-06
0
mmol/ml
0
100
200
300
400
500
s
3Ru^0-CO
[3Ru0-CO]|Time
[3Ru2-CO]|Time
[3Ru2-S]|Time
[BI+]|Time
[BI.]|Time
[BIH.+]|Time
[BIH]|Time
[CO2]|Time
[CO]|Time
[H+]|Time
[H2CO3]|Time
[H2O]|Time
[H2]|Time
[HCO3-]|Time
[HCOO-]|Time
[HCOOH]|Time
[Ru0-CO]|Time
[Ru0]|Time
[Ru1-CO]|Time
[Ru1-S]|Time
[Ru1]|Time
[Ru2-CO2-]|Time
[Ru2-COOH]|Time
[Ru2-CO]|Time
[Ru2-H]|Time
[Ru2-S]|Time
[Ru2]|Time
[S]|Time

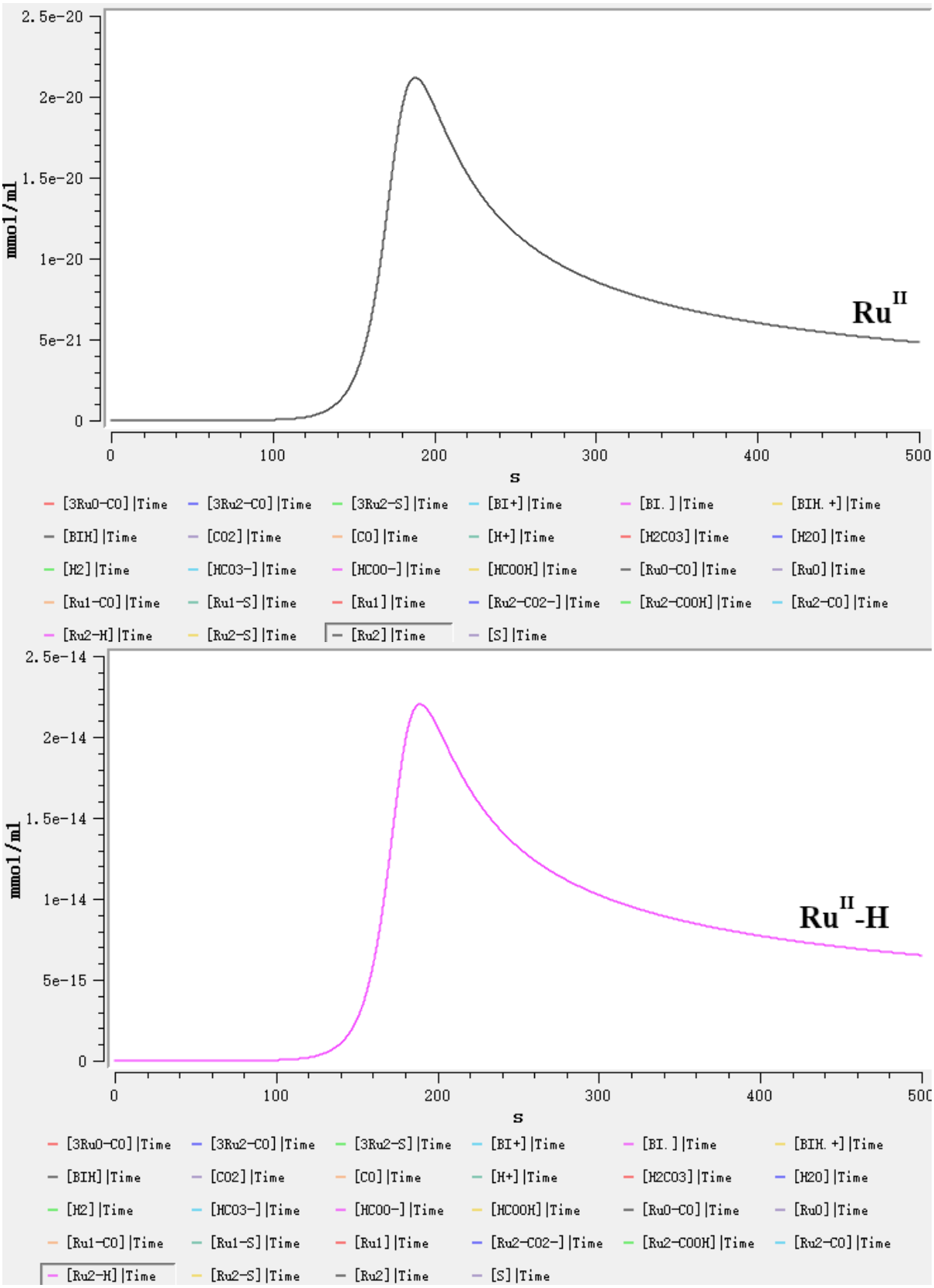


Figure S30. The microkinetic model outcome for all species, over the beginning 500 s.

S28. Table of energies and Cartesian coordinates for all stationary points.

Table S21. Calculated energies for all species (in Hartree).

Species	Geometry optimization energy	Gibbs free energy correction	B3LYP-D3 large basis set Single-point energy
BIH	-690.78518	0.23567	-690.99695
$BIH^{\cdot+}$	-690.63451	0.23738	-690.83800
BI·	-690.15562	0.22411	-690.36832
BI^{+}	-690.07320	0.22884	-690.27663
BI-OH	-766.01598	0.23985	-766.25830
H_2CO_3	-265.01233	0.01340	-265.12439
HCO_3^-	-264.52057	0.00056	-264.65820
^{1}1-S	-2176.23803	0.52132	-2176.75278
^{1}S	-132.76618	0.02230	-132.81572
^{1}1	-2043.44128	0.48393	-2043.91509
^{3}1-S	-2176.16375	0.51691	-2176.68196
^{2}2-S	-2176.33589	0.51535	-2176.85852
^{2}2	-2043.55276	0.47623	-2044.03252
^{1}3	-2043.64776	0.47353	-2044.13442
^{3}3	-2043.64026	0.47000	-2044.12879
^{1}TS1	-2232.23624	0.48058	-2232.79542
^{1}3-CO_2	-2232.25714	0.48464	-2232.81212
^{1}4	-2232.76127	0.49871	-2233.30629

^{1}TS2	-2497.78365	0.52678	-2498.43641
^{1}TS3	-2538.50542	0.57808	-2539.20168
^{2}TS4	-2923.38333	0.75192	-2924.12829
^{1}TS5	-2922.79580	0.74433	-2923.54549
^{1}TS6	-2421.32134	0.50525	-2421.94250
^{1}TS7	-2922.81273	0.74928	-2923.55673
^{1}1-CO	-2156.79657	0.48661	-2157.30748
^{3}1-CO	-2156.73333	0.48154	-2157.24543
^{2}2-CO	-2156.90063	0.48024	-2157.41869
^{3}3-CO	-2156.99249	0.47380	-2157.51930
^{1}TS8	-2308.67008	0.50011	-2309.25896
^{1}3pt	-2044.16099	0.48574	-2044.63574
^{1}TS9	-2309.17880	0.51521	-2309.76710
^{1}TS10	-2232.74402	0.49248	-2233.29406
^{1}TS11	-2497.76205	0.53183	-2498.41167
^{2}TS12	-2923.37128	0.75911	-2924.11426
^{1}TS13	-2232.70041	0.49503	-2233.24855
^{1}TS14	-189.15039	-0.00977	-189.26395
^{1}TS15	-265.64774	0.01395	-265.79039
^{1}TS16	-342.10614	0.03658	-342.28360
$HCOO^-$	-189.26974	-0.00355	-189.37572
H_2	-1.17854	-0.00131	-1.18001
CO_2	-188.57776	-0.00910	-188.65707

CO	-113.30691	-0.01410	-113.35447
H_2O	-76.42571	0.00300	-76.47047
H_2O-OH	-152.31819	0.00484	-152.43985
$4H_2O$	-305.74227	0.06306	-305.90380
$4H_2O$-OH	-381.68272	0.07089	-381.89877

Cartesian coordinates for all stationary points.

BIH E_{opt}= -690.785177852 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.137684	-0.696604	0.422468
2	6	0	2.942770	-1.420664	0.226575
3	6	0	1.766535	-0.706397	0.045543
4	6	0	1.766546	0.706387	0.045571
5	6	0	2.942784	1.420641	0.226663
6	6	0	4.137692	0.696561	0.422513
7	1	0	5.068706	-1.239015	0.561665
8	1	0	2.946390	-2.505989	0.206769
9	1	0	2.946402	2.505967	0.206913
10	1	0	5.068719	1.238953	0.561747
11	6	0	-2.047343	-0.000016	1.195950
12	6	0	-3.369228	-0.000026	1.638212
13	6	0	-4.419230	-0.000017	0.711341
14	6	0	-4.139330	0.000017	-0.656257
15	6	0	-2.811556	0.000029	-1.097190
16	6	0	-1.760733	0.000016	-0.176094
17	1	0	-1.226078	-0.000005	1.906684
18	1	0	-3.584564	-0.000050	2.703277
19	1	0	-5.449376	-0.000029	1.056788
20	1	0	-4.950091	0.000034	-1.379534
21	1	0	-2.589112	0.000034	-2.161545
22	7	0	0.449171	1.147166	-0.131113
23	7	0	0.449135	-1.147140	-0.131122

24	6	0	-0.319876	0.000023	-0.647911
25	1	0	-0.308180	0.000051	-1.759955
26	6	0	0.183009	-2.438595	-0.739393
27	1	0	0.685048	-3.225464	-0.170950
28	1	0	-0.892024	-2.634720	-0.711812
29	1	0	0.523070	-2.487280	-1.786603
30	6	0	0.183058	2.438612	-0.739391
31	1	0	-0.891980	2.634709	-0.711869
32	1	0	0.685058	3.225502	-0.170944
33	1	0	0.523182	2.487310	-1.786585

$BIH^{\cdot+}$ E_{opt}=-690.634505814 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.934940	-0.711332	0.702213
2	6	0	2.832222	-1.442235	0.292590
3	6	0	1.700007	-0.718634	-0.121267
4	6	0	1.700007	0.718634	-0.121266
5	6	0	2.832220	1.442236	0.292592
6	6	0	3.934939	0.711334	0.702214
7	1	0	4.828199	-1.234705	1.027675
8	1	0	2.834428	-2.525814	0.282200
9	1	0	2.834424	2.525815	0.282204
10	1	0	4.828198	1.234708	1.027677
11	6	0	-1.756596	-0.000004	1.159971
12	6	0	-2.994956	-0.000004	1.799040
13	6	0	-4.173866	0.000000	1.043825
14	6	0	-4.112076	0.000003	-0.350779

15	6	0	-2.871277	0.000003	-0.994828
16	6	0	-1.695797	-0.000001	-0.239763
17	1	0	-0.838543	-0.000007	1.740702
18	1	0	-3.043172	-0.000007	2.884009
19	1	0	-5.137694	0.000000	1.544670
20	1	0	-5.025097	0.000006	-0.938733
21	1	0	-2.815664	0.000006	-2.080136
22	7	0	0.497344	1.140094	-0.563245
23	7	0	0.497345	-1.140095	-0.563246
24	6	0	-0.346087	0.000000	-0.937147
25	1	0	-0.495503	0.000000	-2.027277
26	6	0	0.099751	-2.512400	-0.824994
27	1	0	0.559896	-3.171076	-0.086693
28	1	0	-0.985616	-2.588542	-0.743378
29	1	0	0.409980	-2.816188	-1.830951
30	6	0	0.099750	2.512400	-0.824990
31	1	0	-0.985619	2.588537	-0.743395
32	1	0	0.559879	3.171073	-0.086676
33	1	0	0.409998	2.816196	-1.830940

BI· E_{opt}= -690.15561697 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.237934	-0.698347	-0.022803
2	6	0	3.035171	-1.428811	-0.039859
3	6	0	1.845050	-0.705189	-0.017699
4	6	0	1.845083	0.705120	0.017695
5	6	0	3.035259	1.428686	0.039781

6	6	0	4.237972	0.698163	0.022587
7	1	0	5.181597	-1.235937	-0.039842
8	1	0	3.034397	-2.513388	-0.058488
9	1	0	3.034493	2.513263	0.058463
10	1	0	5.181673	1.235690	0.039546
11	6	0	-2.494805	-1.077896	0.572489
12	6	0	-3.881012	-1.068856	0.562526
13	6	0	-4.601210	-0.000085	-0.000206
14	6	0	-3.881063	1.068804	-0.562664
15	6	0	-2.494817	1.078076	-0.572278
16	6	0	-1.739077	0.000119	0.000101
17	1	0	-1.976299	-1.895336	1.061443
18	1	0	-4.415200	-1.899616	1.018221
19	1	0	-5.686867	-0.000248	-0.000375
20	1	0	-4.415209	1.899566	-1.018403
21	1	0	-1.976390	1.895717	-1.060979
22	7	0	0.521369	1.120592	0.033994
23	7	0	0.521229	-1.120557	-0.033832
24	6	0	-0.319747	0.000071	0.000160
25	6	0	0.131289	-2.469884	-0.419866
26	1	0	-0.002948	-3.119172	0.451365
27	1	0	-0.800229	-2.437100	-0.986056
28	1	0	0.909696	-2.894898	-1.058639
29	6	0	0.131566	2.469985	0.419911
30	1	0	-0.800038	2.437337	0.985938
31	1	0	0.909949	2.894883	1.058805
32	1	0	-0.002366	3.119253	-0.451387

BI^+ E_{opt} = -690.0731999 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.209594	-0.700274	-0.085696
2	6	0	3.025343	-1.426895	-0.174178
3	6	0	1.839061	-0.695986	-0.085759
4	6	0	1.839054	0.695966	0.085893
5	6	0	3.025323	1.426900	0.174286
6	6	0	4.209586	0.700316	0.085650
7	1	0	5.157597	-1.224950	-0.148932
8	1	0	3.019878	-2.503217	-0.303073
9	1	0	3.019841	2.503226	0.303143
10	1	0	5.157583	1.225016	0.148766
11	6	0	-2.449045	-0.860086	0.861645
12	6	0	-3.842743	-0.854713	0.858706
13	6	0	-4.539708	0.000016	-0.000003
14	6	0	-3.842691	0.854739	-0.858695
15	6	0	-2.449005	0.860050	-0.861625
16	6	0	-1.746924	-0.000036	0.000021
17	1	0	-1.906226	-1.512852	1.537652
18	1	0	-4.383067	-1.514955	1.529968
19	1	0	-5.625716	0.000033	-0.000010
20	1	0	-4.382987	1.515008	-1.529952
21	1	0	-1.906142	1.512815	-1.537596
22	7	0	0.505759	1.091092	0.141653
23	7	0	0.505759	-1.091121	-0.141541
24	6	0	-0.279059	-0.000007	0.000030
25	6	0	0.076769	-2.469245	-0.386469
26	1	0	0.186236	-3.059057	0.526162
27	1	0	-0.962441	-2.475206	-0.708623

28	1	0	0.703769	-2.889509	-1.174703
29	6	0	0.076722	2.469253	0.386227
30	1	0	-0.962469	2.475270	0.708445
31	1	0	0.703739	2.889753	1.174319
32	1	0	0.186126	3.058856	-0.526549

BI-OH E_{opt} = -766.015976344 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.255970	0.366889	1.980940
2	1	0	0.873275	-0.227613	2.436133
3	6	0	-4.120762	0.672153	-0.710575
4	6	0	-2.913662	1.394202	-0.603408
5	6	0	-1.764388	0.693499	-0.265886
6	6	0	-1.801906	-0.697964	-0.030067
7	6	0	-2.990419	-1.407685	-0.118914
8	6	0	-4.159095	-0.700589	-0.471855
9	1	0	-5.032594	1.202419	-0.970949
10	1	0	-2.887869	2.466780	-0.767595
11	1	0	-3.022072	-2.473670	0.083351
12	1	0	-5.100324	-1.237834	-0.547619
13	6	0	2.788043	0.581883	0.761574
14	6	0	4.092945	0.516354	0.264123
15	6	0	4.358104	-0.174235	-0.919630
16	6	0	3.310751	-0.794791	-1.608773
17	6	0	2.007867	-0.723949	-1.115893
18	6	0	1.737173	-0.041816	0.077996
19	1	0	2.586022	1.121985	1.680492

20	1	0	4.899154	1.004951	0.804046
21	1	0	5.372570	-0.228970	-1.304540
22	1	0	3.509479	-1.333727	-2.531019
23	1	0	1.191981	-1.201514	-1.648554
24	7	0	-0.500229	-1.120196	0.251551
25	7	0	-0.444492	1.119553	-0.112525
26	6	0	0.295228	0.069154	0.579759
27	6	0	-0.118038	2.511926	0.134908
28	1	0	-0.498923	2.869219	1.100781
29	1	0	0.966587	2.638883	0.115309
30	1	0	-0.544736	3.127084	-0.662107
31	6	0	-0.254668	-2.340529	1.000108
32	1	0	0.821508	-2.527605	1.042569
33	1	0	-0.650318	-2.293544	2.024559
34	1	0	-0.721472	-3.183128	0.483642

H_2 E_{opt} = -1.17853938133 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	0.371397
2	1	0	0.000000	0.000000	-0.371397

CO_2 E_{opt}= -188.5777595 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000

2	8	0	0.000000	0.000000	1.169716
3	8	0	0.000000	0.000000	-1.169716

CO E_{opt} = -113.3069132 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.650135
2	8	0	0.000000	0.000000	0.487601

S E_{opt} = -132.766178791 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.277523
2	7	0	0.000000	0.000000	1.438621
3	6	0	0.000000	0.000000	-1.179340
4	1	0	0.000000	1.028569	-1.553149
5	1	0	0.890766	-0.514284	-1.553149
6	1	0	-0.890766	-0.514284	-1.553149

$HCOO^-$ E_{opt} = -189.269740639 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000092	0.317058	-0.000234
2	8	0	-1.138150	-0.210303	0.000080

3	1	0	0.000663	1.463227	0.000103
4	8	0	1.138136	-0.210393	0.000083

H_2O E_{opt} =-76.4257098 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118840
2	1	0	0.000000	0.760114	-0.475358
3	1	0	0.000000	-0.760114	-0.475358

H_2O-OH E_{opt} = -152.3181904 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.413872	0.663360	0.518257
2	8	0	1.220794	-0.076022	-0.075007
3	1	0	0.001114	-0.110390	-0.000147
4	8	0	-1.220954	-0.076052	0.075000
5	1	0	-1.413705	0.663624	-0.518054

$4H_2O$ E_{opt} = -305.742266776 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.238303	1.116677	-0.157952
2	8	0	-2.342438	1.154498	0.222181

3	1	0	-1.602114	-0.468427	-0.098651
4	8	0	-1.201534	-1.346573	-0.272250
5	1	0	0.550162	-1.261907	-0.055566
6	8	0	1.529352	-1.219014	0.061459
7	1	0	2.081321	0.465141	0.019532
8	8	0	2.310867	1.420887	-0.026806
9	1	0	-1.854554	1.780556	-0.360811
10	1	0	1.666906	-1.597066	0.948961
11	1	0	1.615213	1.783402	-0.597378
12	1	0	-1.588601	-1.896764	0.425198

$4H_2O$-OH E_{opt} = -381.68271519 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.781688	-0.522199	-0.228728
2	8	0	1.164504	1.776907	0.414980
3	1	0	1.046354	1.445872	1.315869
4	8	0	1.941950	-0.381786	-0.688491
5	1	0	1.108433	-1.182887	-0.051467
6	8	0	0.382851	-1.842716	0.504347
7	1	0	-1.066309	-1.365539	0.064420
8	8	0	-2.003391	-1.069939	-0.193769
9	1	0	-1.734215	0.779164	-0.287037
10	8	0	-1.607880	1.746328	-0.215753
11	1	0	1.483197	0.921482	-0.089708
12	1	0	-2.457399	-1.040122	0.658479
13	1	0	-0.648640	1.835352	-0.019023
14	1	0	0.462625	-2.701467	0.066677

H_2CO_3 E_{opt} =-265.0123292 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000077	0.100718	0.000087
2	8	0	0.000493	1.314281	-0.000076
3	8	0	-1.086110	-0.682342	0.000533
4	8	0	1.085546	-0.682988	-0.000695
5	1	0	1.863838	-0.098683	0.003555
6	1	0	-1.863739	-0.097241	-0.002171

HCO_3^- E_{opt} = -264.52057481 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.146167	0.063313	-0.000074
2	8	0	0.065073	1.299925	0.000014
3	8	0	1.032210	-0.744948	-0.000006
4	8	0	-1.206648	-0.590407	0.000029
5	1	0	1.751922	-0.096438	0.000145

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^{1}**1-S** E_{opt} = -2176.23802836 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.221723	2.227208	1.274375

2	1	0	-2.749173	1.367155	1.671030
3	6	0	-2.834027	3.472772	1.162250
4	1	0	-3.861729	3.595602	1.485142
5	6	0	-2.106048	4.530951	0.622474
6	1	0	-2.554908	5.512056	0.507984
7	6	0	-0.783158	4.318427	0.236163
8	1	0	-0.195931	5.132816	-0.170881
9	6	0	-0.218360	3.051526	0.385986
10	6	0	1.190864	2.736633	0.059206
11	6	0	2.152006	3.610303	-0.453732
12	1	0	1.902692	4.639595	-0.681386
13	6	0	3.448323	3.134566	-0.663558
14	1	0	4.206270	3.800361	-1.062140
15	6	0	3.777876	1.812682	-0.362112
16	1	0	4.784310	1.446513	-0.523282
17	6	0	2.782028	0.970781	0.137766
18	6	0	2.921826	-0.463303	0.472953
19	6	0	4.115673	-1.172354	0.342014
20	1	0	5.009730	-0.670512	-0.007973
21	6	0	4.145990	-2.529662	0.657749
22	1	0	5.067922	-3.092029	0.553871
23	6	0	2.979616	-3.149293	1.103155
24	1	0	2.957777	-4.202968	1.357825
25	6	0	1.817365	-2.390843	1.213668
26	1	0	0.882596	-2.827096	1.546483
27	6	0	-1.727151	-1.352604	2.886888
28	1	0	-1.290354	-0.654265	3.589820
29	6	0	-2.620318	-2.341161	3.346429
30	1	0	-2.857663	-2.382485	4.403580
31	6	0	-3.161743	-3.228364	2.447572

32	1	0	-3.847223	-4.008891	2.763939
33	6	0	-2.824031	-3.111642	1.075661
34	6	0	-3.368372	-3.970617	0.085249
35	1	0	-4.049533	-4.755900	0.399731
36	6	0	-3.050755	-3.802859	-1.244968
37	1	0	-3.476588	-4.457601	-1.998471
38	6	0	-2.176508	-2.764914	-1.637489
39	1	0	-1.953421	-2.625054	-2.691389
40	6	0	-1.603238	-1.925005	-0.697424
41	6	0	-1.918243	-2.080714	0.681437
42	6	0	0.844655	-1.092582	-2.164149
43	6	0	1.753270	-0.136232	-2.654973
44	1	0	1.581869	0.921700	-2.483041
45	6	0	2.895004	-0.537748	-3.348144
46	1	0	3.586186	0.211970	-3.721581
47	6	0	3.154974	-1.896788	-3.542586
48	1	0	4.048385	-2.209677	-4.074965
49	6	0	2.266991	-2.852088	-3.042437
50	1	0	2.468203	-3.910181	-3.182247
51	6	0	1.117206	-2.455998	-2.354834
52	1	0	0.446338	-3.211809	-1.962157
53	6	0	-1.608987	0.559292	-2.149449
54	6	0	-1.239007	1.072247	-3.401127
55	1	0	-0.289183	0.807991	-3.850719
56	6	0	-2.103574	1.926681	-4.092298
57	1	0	-1.806538	2.315406	-5.062059
58	6	0	-3.340369	2.273412	-3.545889
59	1	0	-4.007600	2.939245	-4.085411
60	6	0	-3.721217	1.753294	-2.304949
61	1	0	-4.684922	2.010947	-1.875464

62	6	0	-2.863375	0.901305	-1.611644
63	1	0	-3.173148	0.497016	-0.653376
64	7	0	-0.956359	2.009501	0.884472
65	7	0	1.532215	1.453844	0.318739
66	7	0	1.779941	-1.085132	0.904236
67	7	0	-1.363031	-1.216801	1.612888
68	15	0	-0.530621	-0.506498	-1.111377
69	44	0	0.125098	0.208870	0.978836
70	7	0	0.659648	0.689576	2.954023
71	6	0	1.015901	0.997614	4.011980
72	6	0	1.452925	1.378027	5.343587
73	1	0	1.754873	0.485416	5.899460
74	1	0	2.302452	2.063329	5.269398
75	1	0	0.632682	1.873915	5.870841

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^{1}1 E_{opt} = -2043.44127569 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.734568	-1.563354	-1.497365
2	1	0	-3.130308	-0.563955	-1.637288
3	6	0	-3.563093	-2.682627	-1.495921
4	1	0	-4.629340	-2.560421	-1.649456
5	6	0	-2.994403	-3.935766	-1.282310
6	1	0	-3.610223	-4.828773	-1.261870
7	6	0	-1.614742	-4.034507	-1.101474
8	1	0	-1.151277	-5.001972	-0.949536
9	6	0	-0.833859	-2.879978	-1.126311
10	6	0	0.642441	-2.886493	-0.997404

11	6	0	1.458978	-4.007124	-0.834737
12	1	0	1.030675	-4.999081	-0.758720
13	6	0	2.842202	-3.828476	-0.775171
14	1	0	3.490337	-4.688739	-0.647394
15	6	0	3.397669	-2.553311	-0.885181
16	1	0	4.471179	-2.416027	-0.845694
17	6	0	2.544121	-1.459263	-1.035619
18	6	0	2.950293	-0.037150	-1.126799
19	6	0	4.275876	0.389194	-1.063120
20	1	0	5.075707	-0.334171	-0.960061
21	6	0	4.562898	1.752383	-1.122528
22	1	0	5.591089	2.093974	-1.066077
23	6	0	3.515789	2.662962	-1.250025
24	1	0	3.694582	3.731331	-1.295752
25	6	0	2.211645	2.179478	-1.310275
26	1	0	1.360653	2.845713	-1.397184
27	6	0	-1.568259	2.161493	-2.675741
28	1	0	-1.268307	1.555271	-3.525859
29	6	0	-2.303333	3.349344	-2.866831
30	1	0	-2.566695	3.648874	-3.874957
31	6	0	-2.669062	4.097519	-1.771337
32	1	0	-3.235727	5.017343	-1.880887
33	6	0	-2.301974	3.655701	-0.474391
34	6	0	-2.651345	4.356617	0.709837
35	1	0	-3.215955	5.279914	0.619479
36	6	0	-2.289876	3.869009	1.947666
37	1	0	-2.566662	4.405808	2.849320
38	6	0	-1.559032	2.662913	2.055723
39	1	0	-1.294417	2.284614	3.038807
40	6	0	-1.179397	1.964939	0.922465

41	6	0	-1.556150	2.446824	-0.360089
42	6	0	1.272556	0.577611	1.881303
43	6	0	2.112026	-0.540016	2.046508
44	1	0	1.811172	-1.514870	1.677501
45	6	0	3.352441	-0.403959	2.668832
46	1	0	3.988357	-1.275675	2.790750
47	6	0	3.778719	0.849146	3.117010
48	1	0	4.747828	0.955964	3.595347
49	6	0	2.958676	1.965461	2.939636
50	1	0	3.287908	2.943928	3.276744
51	6	0	1.711801	1.835194	2.323144
52	1	0	1.096473	2.716408	2.182133
53	6	0	-1.381952	-0.739639	1.897016
54	6	0	-0.925778	-1.646453	2.865338
55	1	0	0.120339	-1.683277	3.143840
56	6	0	-1.826077	-2.509487	3.496449
57	1	0	-1.461672	-3.204253	4.247447
58	6	0	-3.182915	-2.476771	3.169464
59	1	0	-3.878410	-3.150993	3.660633
60	6	0	-3.645179	-1.567909	2.212787
61	1	0	-4.699868	-1.531872	1.956571
62	6	0	-2.752562	-0.703968	1.581083
63	1	0	-3.122222	-0.001029	0.841293
64	7	0	-1.407761	-1.646993	-1.305791
65	7	0	1.202692	-1.654505	-1.072740
66	7	0	1.927155	0.867670	-1.248152
67	7	0	-1.199741	1.716880	-1.477045
68	15	0	-0.278558	0.368484	0.932823
69	44	0	0.005893	-0.048861	-1.251936

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^{3}1-S E_{opt} = -2176.16374826 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.049553	2.707331	1.618463
2	1	0	-1.854480	2.066481	1.960193
3	6	0	-1.133072	4.086617	1.684975
4	1	0	-2.020701	4.550014	2.099699
5	6	0	-0.060843	4.852783	1.194214
6	1	0	-0.105050	5.936648	1.216528
7	6	0	1.057423	4.213843	0.683799
8	1	0	1.898355	4.786713	0.310695
9	6	0	1.109848	2.810523	0.659778
10	6	0	2.223825	2.009239	0.191827
11	6	0	3.411696	2.467501	-0.362967
12	1	0	3.578593	3.530880	-0.492307
13	6	0	4.391461	1.540835	-0.757384
14	1	0	5.321717	1.890279	-1.191055
15	6	0	4.161886	0.171722	-0.608435
16	1	0	4.906355	-0.545930	-0.933342
17	6	0	2.956650	-0.274014	-0.063712
18	6	0	2.517000	-1.639757	0.069921
19	6	0	3.272340	-2.777262	-0.274763
20	1	0	4.282630	-2.650512	-0.646348
21	6	0	2.724269	-4.038681	-0.144901
22	1	0	3.303923	-4.915845	-0.413000
23	6	0	1.403389	-4.173464	0.332511
24	1	0	0.936800	-5.144881	0.448559
25	6	0	0.691093	-3.034090	0.650377

26	1	0	-0.328911	-3.089410	1.009809
27	6	0	-1.830359	-1.216825	2.918175
28	1	0	-1.064730	-0.915604	3.622492
29	6	0	-2.987466	-1.877148	3.364821
30	1	0	-3.104213	-2.077410	4.423533
31	6	0	-3.940005	-2.256035	2.445601
32	1	0	-4.843878	-2.773065	2.754071
33	6	0	-3.743378	-1.965516	1.072500
34	6	0	-4.692390	-2.312474	0.076125
35	1	0	-5.597179	-2.830090	0.380264
36	6	0	-4.472167	-1.990229	-1.245534
37	1	0	-5.203174	-2.250576	-2.003694
38	6	0	-3.292651	-1.311313	-1.622511
39	1	0	-3.137404	-1.049848	-2.664997
40	6	0	-2.332742	-0.977611	-0.680365
41	6	0	-2.548080	-1.289967	0.687083
42	6	0	0.143473	-0.972684	-2.326490
43	6	0	1.359414	-0.425222	-2.776776
44	1	0	1.694990	0.543218	-2.421315
45	6	0	2.160510	-1.136871	-3.669267
46	1	0	3.096632	-0.703749	-4.008394
47	6	0	1.770496	-2.405622	-4.104506
48	1	0	2.400558	-2.962673	-4.791606
49	6	0	0.572996	-2.960867	-3.646537
50	1	0	0.269363	-3.950730	-3.974025
51	6	0	-0.239945	-2.251758	-2.760298
52	1	0	-1.158923	-2.704146	-2.405523
53	6	0	-1.384838	1.516014	-1.792286
54	6	0	-0.769620	2.121231	-2.898905
55	1	0	0.053091	1.638819	-3.411650

56	6	0	-1.226930	3.356778	-3.363566
57	1	0	-0.745994	3.813782	-4.223304
58	6	0	-2.296375	3.996341	-2.733885
59	1	0	-2.647267	4.957309	-3.098241
60	6	0	-2.919316	3.392899	-1.637822
61	1	0	-3.755341	3.880773	-1.145794
62	6	0	-2.468083	2.160913	-1.167302
63	1	0	-2.962640	1.702355	-0.317396
64	7	0	0.036719	2.081977	1.117052
65	7	0	2.021853	0.655882	0.339773
66	7	0	1.221634	-1.794075	0.530020
67	7	0	-1.602806	-0.930301	1.634033
68	15	0	-0.805131	-0.060761	-1.064775
69	44	0	0.222442	-0.010038	1.000099
70	7	0	1.163843	-0.054860	2.983453
71	6	0	1.769930	-0.016702	3.968417
72	6	0	2.528591	0.030078	5.204370
73	1	0	2.620255	-0.979810	5.614513
74	1	0	3.524829	0.435775	5.005202
75	1	0	2.011747	0.670743	5.924925

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^{2}2-S E_{opt} = -2176.33589097 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.218779	2.088812	1.220347
2	1	0	-2.661206	1.228505	1.713939
3	6	0	-2.938117	3.256158	1.032422
4	1	0	-3.957697	3.330076	1.393718

5	6	0	-2.310055	4.326901	0.345420
6	1	0	-2.849110	5.250777	0.158100
7	6	0	-1.007497	4.186584	-0.081945
8	1	0	-0.512591	4.998996	-0.603828
9	6	0	-0.295446	2.982810	0.157811
10	6	0	1.075003	2.756477	-0.200304
11	6	0	1.977889	3.654726	-0.810909
12	1	0	1.646553	4.647977	-1.095239
13	6	0	3.290614	3.270078	-1.037122
14	1	0	3.982017	3.964525	-1.503647
15	6	0	3.746552	1.982407	-0.656846
16	1	0	4.776359	1.690319	-0.824175
17	6	0	2.838016	1.111693	-0.071840
18	6	0	3.097167	-0.278594	0.350640
19	6	0	4.335837	-0.915965	0.222173
20	1	0	5.184344	-0.368265	-0.171258
21	6	0	4.469565	-2.251013	0.587101
22	1	0	5.426004	-2.752967	0.483064
23	6	0	3.353078	-2.935419	1.080692
24	1	0	3.409181	-3.978856	1.370901
25	6	0	2.149973	-2.251854	1.197663
26	1	0	1.254985	-2.736420	1.572936
27	6	0	-1.232867	-1.398225	3.116625
28	1	0	-0.471399	-0.932335	3.730169
29	6	0	-2.226827	-2.196520	3.718336
30	1	0	-2.203529	-2.341435	4.792829
31	6	0	-3.208373	-2.755379	2.934958
32	1	0	-4.002902	-3.358726	3.364028
33	6	0	-3.175917	-2.537525	1.534035
34	6	0	-4.155341	-3.075150	0.657689

35	1	0	-4.959356	-3.669559	1.082125
36	6	0	-4.089471	-2.843956	-0.699014
37	1	0	-4.845415	-3.251242	-1.362951
38	6	0	-3.025069	-2.085422	-1.236789
39	1	0	-2.973258	-1.924078	-2.309536
40	6	0	-2.046207	-1.551347	-0.415806
41	6	0	-2.119574	-1.744555	0.992113
42	6	0	0.450961	-1.801162	-1.935666
43	6	0	1.716714	-1.365791	-2.369018
44	1	0	2.027227	-0.340355	-2.199323
45	6	0	2.590170	-2.246955	-3.005521
46	1	0	3.564563	-1.894560	-3.331204
47	6	0	2.217868	-3.579087	-3.207963
48	1	0	2.901259	-4.268007	-3.695952
49	6	0	0.967038	-4.022191	-2.773437
50	1	0	0.672578	-5.057122	-2.922740
51	6	0	0.086335	-3.140615	-2.139665
52	1	0	-0.876383	-3.506898	-1.800625
53	6	0	-1.269652	0.559224	-2.259623
54	6	0	-0.545182	0.922526	-3.405746
55	1	0	0.397091	0.440334	-3.640167
56	6	0	-1.032549	1.911041	-4.265001
57	1	0	-0.462376	2.178386	-5.150162
58	6	0	-2.244060	2.549038	-3.990514
59	1	0	-2.618880	3.319416	-4.658238
60	6	0	-2.973774	2.188534	-2.854147
61	1	0	-3.917134	2.678580	-2.630963
62	6	0	-2.492412	1.200913	-1.995160
63	1	0	-3.068011	0.937398	-1.115202
64	7	0	-0.951324	1.919511	0.795013

65	7	0	1.550143	1.496414	0.118863
66	7	0	2.010178	-0.958457	0.848169
67	7	0	-1.168466	-1.151401	1.808718
68	15	0	-0.595275	-0.608072	-1.007701
69	44	0	0.262508	0.214498	0.942734
70	7	0	0.896957	0.915085	2.833670
71	6	0	1.272809	1.368142	3.831709
72	6	0	1.736675	1.931724	5.088535
73	1	0	1.871897	1.132579	5.823377
74	1	0	2.690719	2.443783	4.932055
75	1	0	1.000248	2.647916	5.464734

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^{2}2 E_{opt} = -2043.55275596 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.617350	1.667980	-1.421477
2	1	0	3.034237	0.681179	-1.591447
3	6	0	3.426631	2.788554	-1.340985
4	1	0	4.499540	2.685442	-1.461448
5	6	0	2.832144	4.037314	-1.096674
6	1	0	3.437743	4.934306	-1.018165
7	6	0	1.454006	4.108366	-0.956360
8	1	0	0.970983	5.061196	-0.770401
9	6	0	0.675225	2.945511	-1.057120
10	6	0	-0.781693	2.921183	-0.951190
11	6	0	-1.628974	4.012497	-0.768724
12	1	0	-1.221557	5.012496	-0.672380
13	6	0	-3.013016	3.808031	-0.714540

14	1	0	-3.679021	4.652685	-0.574846
15	6	0	-3.540141	2.518015	-0.843444
16	1	0	-4.611873	2.359444	-0.804085
17	6	0	-2.675184	1.439097	-1.017925
18	6	0	-3.040653	0.029586	-1.126656
19	6	0	-4.357004	-0.450457	-1.046381
20	1	0	-5.174612	0.250845	-0.923262
21	6	0	-4.605123	-1.812714	-1.106673
22	1	0	-5.620570	-2.188991	-1.037820
23	6	0	-3.520252	-2.695763	-1.248604
24	1	0	-3.666863	-3.769412	-1.294038
25	6	0	-2.240891	-2.174702	-1.330562
26	1	0	-1.372871	-2.817031	-1.434528
27	6	0	1.465878	-2.022003	-2.816858
28	1	0	0.959874	-1.492465	-3.618588
29	6	0	2.339093	-3.091018	-3.107491
30	1	0	2.490940	-3.379637	-4.141705
31	6	0	2.984363	-3.733241	-2.076122
32	1	0	3.672811	-4.552150	-2.262810
33	6	0	2.745655	-3.312083	-0.742495
34	6	0	3.382072	-3.906306	0.379335
35	1	0	4.078499	-4.722503	0.210106
36	6	0	3.128808	-3.449194	1.654816
37	1	0	3.626287	-3.901357	2.507022
38	6	0	2.213998	-2.390869	1.865256
39	1	0	2.025069	-2.042949	2.876619
40	6	0	1.558368	-1.799180	0.799367
41	6	0	1.832422	-2.238817	-0.525584
42	6	0	-1.083725	-1.062365	1.897340
43	6	0	-2.219549	-0.237353	2.005196

44	1	0	-2.216371	0.754328	1.565430
45	6	0	-3.365985	-0.691344	2.656408
46	1	0	-4.233233	-0.041600	2.730136
47	6	0	-3.403691	-1.981313	3.193443
48	1	0	-4.299842	-2.338472	3.692535
49	6	0	-2.287498	-2.812652	3.076238
50	1	0	-2.311830	-3.819438	3.483467
51	6	0	-1.132991	-2.359515	2.431963
52	1	0	-0.281930	-3.025210	2.343116
53	6	0	1.173067	0.828822	1.973260
54	6	0	0.459073	1.670345	2.842459
55	1	0	-0.601115	1.518331	3.010771
56	6	0	1.109142	2.711919	3.509142
57	1	0	0.544243	3.350437	4.182442
58	6	0	2.474949	2.930823	3.314484
59	1	0	2.976984	3.743203	3.831814
60	6	0	3.193166	2.096614	2.452872
61	1	0	4.255525	2.258646	2.294567
62	6	0	2.549372	1.054686	1.785747
63	1	0	3.119002	0.421077	1.114357
64	7	0	1.271925	1.715678	-1.282630
65	7	0	-1.317244	1.658835	-1.066133
66	7	0	-1.978986	-0.846337	-1.279599
67	7	0	1.212941	-1.593498	-1.581816
68	15	0	0.340030	-0.430451	0.925259
69	44	0	-0.093896	0.096157	-1.202119

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13 E_{opt} = -2043.64775646 Hartree

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.575169	2.649934	-1.325137
2	1	0	2.361241	1.922228	-1.499676
3	6	0	1.859334	3.993079	-1.201831
4	1	0	2.885420	4.334559	-1.292061
5	6	0	0.801039	4.898382	-0.952859
6	1	0	0.993920	5.960695	-0.841491
7	6	0	-0.483720	4.401607	-0.847256
8	1	0	-1.314037	5.071308	-0.647602
9	6	0	-0.734736	3.020631	-0.987779
10	6	0	-2.035040	2.402311	-0.898671
11	6	0	-3.261994	3.029932	-0.698503
12	1	0	-3.309949	4.109463	-0.596855
13	6	0	-4.436818	2.267290	-0.626107
14	1	0	-5.393116	2.757350	-0.475395
15	6	0	-4.373549	0.870112	-0.731382
16	1	0	-5.280167	0.278568	-0.654563
17	6	0	-3.146897	0.241573	-0.928174
18	6	0	-2.890897	-1.174869	-1.018707
19	6	0	-3.872696	-2.181653	-0.899911
20	1	0	-4.906999	-1.892735	-0.742981
21	6	0	-3.523285	-3.515519	-0.962274
22	1	0	-4.276660	-4.290615	-0.863560
23	6	0	-2.159437	-3.850641	-1.145904
24	1	0	-1.834225	-4.884820	-1.195008
25	6	0	-1.231761	-2.839185	-1.264621
26	1	0	-0.176635	-3.055842	-1.399572
27	6	0	1.921074	-1.101787	-2.991223
28	1	0	1.178178	-0.776651	-3.712527

29	6	0	3.114831	-1.715183	-3.427576
30	1	0	3.269907	-1.864798	-4.490668
31	6	0	4.057748	-2.093111	-2.500590
32	1	0	4.995258	-2.553175	-2.799251
33	6	0	3.795794	-1.869780	-1.124003
34	6	0	4.723648	-2.208314	-0.103425
35	1	0	5.668940	-2.660583	-0.390169
36	6	0	4.434334	-1.959373	1.220919
37	1	0	5.152625	-2.210933	1.995243
38	6	0	3.194926	-1.380590	1.581578
39	1	0	2.981266	-1.191349	2.629641
40	6	0	2.254764	-1.054419	0.619026
41	6	0	2.553695	-1.270717	-0.756753
42	6	0	-0.353831	-1.497770	1.933996
43	6	0	-1.732613	-1.248754	2.082778
44	1	0	-2.172712	-0.362747	1.636323
45	6	0	-2.548491	-2.147519	2.769285
46	1	0	-3.609518	-1.937940	2.872891
47	6	0	-2.007665	-3.322699	3.299757
48	1	0	-2.644518	-4.028888	3.824928
49	6	0	-0.645926	-3.589742	3.139136
50	1	0	-0.219238	-4.505550	3.539113
51	6	0	0.177669	-2.685153	2.462170
52	1	0	1.229839	-2.918106	2.340968
53	6	0	0.939903	1.134354	2.006155
54	6	0	-0.049766	1.638336	2.870819
55	1	0	-0.980472	1.098816	3.012159
56	6	0	0.151854	2.835362	3.560683
57	1	0	-0.621216	3.204525	4.229198
58	6	0	1.338504	3.555824	3.394437

59	1	0	1.492259	4.488131	3.930222
60	6	0	2.325752	3.066909	2.534469
61	1	0	3.250840	3.619593	2.395202
62	6	0	2.128788	1.870871	1.842373
63	1	0	2.901618	1.513058	1.170264
64	7	0	0.318429	2.130240	-1.229353
65	7	0	-1.989290	1.014288	-1.049831
66	7	0	-1.547932	-1.512110	-1.218215
67	7	0	1.626874	-0.872344	-1.711589
68	15	0	0.599596	-0.302490	0.909506
69	44	0	-0.241604	0.113066	-1.106905

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^{3}3 E_{opt} = -2043.640256 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.257617	2.058782	-1.347335
2	1	0	2.841713	1.159223	-1.510873
3	6	0	2.856450	3.300226	-1.223224
4	1	0	3.934912	3.386727	-1.301128
5	6	0	2.045350	4.424206	-0.985160
6	1	0	2.483987	5.410060	-0.869324
7	6	0	0.672584	4.252747	-0.892420
8	1	0	0.026444	5.102037	-0.699758
9	6	0	0.109482	2.974678	-1.036834
10	6	0	-1.320213	2.692613	-0.960399
11	6	0	-2.353614	3.616682	-0.812533
12	1	0	-2.134107	4.675623	-0.730790
13	6	0	-3.679350	3.167940	-0.778046

14	1	0	-4.488872	3.881556	-0.666821
15	6	0	-3.964787	1.800930	-0.891815
16	1	0	-4.992172	1.454944	-0.868780
17	6	0	-2.918138	0.891934	-1.033254
18	6	0	-3.019614	-0.562217	-1.126026
19	6	0	-4.227244	-1.273955	-1.046566
20	1	0	-5.160792	-0.731865	-0.943084
21	6	0	-4.223015	-2.659534	-1.081776
22	1	0	-5.153760	-3.213395	-1.013763
23	6	0	-2.993075	-3.332386	-1.195660
24	1	0	-2.940539	-4.415590	-1.219462
25	6	0	-1.829628	-2.587977	-1.280394
26	1	0	-0.857350	-3.061810	-1.366203
27	6	0	1.817060	-1.740666	-2.857246
28	1	0	1.157496	-1.374792	-3.639187
29	6	0	2.903821	-2.547659	-3.142268
30	1	0	3.104891	-2.826246	-4.172729
31	6	0	3.733271	-2.993644	-2.098586
32	1	0	4.596695	-3.622175	-2.298252
33	6	0	3.435659	-2.618646	-0.763190
34	6	0	4.210039	-3.008502	0.359899
35	1	0	5.085105	-3.632100	0.193692
36	6	0	3.873448	-2.597078	1.659501
37	1	0	4.494671	-2.903873	2.497470
38	6	0	2.754984	-1.802789	1.882707
39	1	0	2.499855	-1.482350	2.888844
40	6	0	1.941513	-1.399316	0.789419
41	6	0	2.278290	-1.784262	-0.538007
42	6	0	-0.790670	-1.309173	1.923232
43	6	0	-2.108356	-0.820109	1.995578

44	1	0	-2.370865	0.109685	1.503296
45	6	0	-3.099509	-1.537610	2.665506
46	1	0	-4.112227	-1.146093	2.704172
47	6	0	-2.795166	-2.763050	3.265307
48	1	0	-3.568438	-3.325947	3.780405
49	6	0	-1.493914	-3.265155	3.187711
50	1	0	-1.250153	-4.220959	3.643517
51	6	0	-0.498309	-2.546751	2.519257
52	1	0	0.503792	-2.957128	2.457321
53	6	0	0.891184	1.094959	1.925179
54	6	0	-0.101975	1.891423	2.523213
55	1	0	-1.140982	1.582850	2.502726
56	6	0	0.231810	3.094511	3.148242
57	1	0	-0.549180	3.694458	3.607334
58	6	0	1.560231	3.528301	3.178787
59	1	0	1.817957	4.466131	3.662644
60	6	0	2.553839	2.747714	2.582723
61	1	0	3.589074	3.077143	2.597713
62	6	0	2.223572	1.543326	1.958001
63	1	0	3.002892	0.952723	1.488846
64	7	0	0.919362	1.869816	-1.259731
65	7	0	-1.619371	1.351041	-1.064243
66	7	0	-1.812353	-1.232931	-1.256184
67	7	0	1.499243	-1.344196	-1.585185
68	15	0	0.454423	-0.387924	0.919275
69	44	0	-0.130598	0.038431	-1.197743

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^{1}1-CO E_{opt} = -2156.796566 Hartree

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-3.042018	0.107031	-1.306417
2	1	0	-2.867379	1.158862	-1.500580
3	6	0	-4.328283	-0.416044	-1.202145
4	1	0	-5.183423	0.239370	-1.321589
5	6	0	-4.480143	-1.774367	-0.934420
6	1	0	-5.467749	-2.212348	-0.836391
7	6	0	-3.346006	-2.573072	-0.791384
8	1	0	-3.446710	-3.631313	-0.583628
9	6	0	-2.082264	-1.997207	-0.914922
10	6	0	-0.817278	-2.757547	-0.790794
11	6	0	-0.682612	-4.124870	-0.538465
12	1	0	-1.553608	-4.754608	-0.407516
13	6	0	0.600386	-4.666954	-0.454850
14	1	0	0.722668	-5.726626	-0.258003
15	6	0	1.728860	-3.860492	-0.614819
16	1	0	2.722122	-4.285013	-0.537979
17	6	0	1.548539	-2.498558	-0.862856
18	6	0	2.608669	-1.472771	-0.994632
19	6	0	3.971055	-1.758230	-0.918187
20	1	0	4.308479	-2.781528	-0.807388
21	6	0	4.893497	-0.714173	-0.970824
22	1	0	5.955720	-0.924389	-0.904199
23	6	0	4.434266	0.594779	-1.100662
24	1	0	5.117250	1.435988	-1.135753
25	6	0	3.062552	0.819208	-1.188389
26	1	0	2.651818	1.816636	-1.295208
27	6	0	-0.087228	2.801288	-2.474374
28	1	0	0.258608	2.249300	-3.338903

29	6	0	-0.387476	4.169195	-2.611747
30	1	0	-0.258913	4.638706	-3.580315
31	6	0	-0.853129	4.864722	-1.522517
32	1	0	-1.119260	5.915196	-1.591664
33	6	0	-0.980175	4.194828	-0.280926
34	6	0	-1.447334	4.857588	0.884340
35	1	0	-1.725861	5.904319	0.805654
36	6	0	-1.543112	4.190031	2.084709
37	1	0	-1.905094	4.699305	2.971791
38	6	0	-1.148256	2.837280	2.169801
39	1	0	-1.199923	2.325694	3.126100
40	6	0	-0.689469	2.155284	1.054192
41	6	0	-0.622000	2.813259	-0.206216
42	6	0	1.498819	0.479028	2.050712
43	6	0	2.259725	-0.700648	2.146852
44	1	0	1.894767	-1.628425	1.721784
45	6	0	3.503916	-0.689816	2.776124
46	1	0	4.079205	-1.608648	2.838511
47	6	0	4.011515	0.498589	3.307641
48	1	0	4.983923	0.507672	3.791018
49	6	0	3.267040	1.675472	3.207985
50	1	0	3.656245	2.604354	3.614342
51	6	0	2.018245	1.670724	2.581787
52	1	0	1.462726	2.598298	2.505622
53	6	0	-1.307418	-0.521078	2.069063
54	6	0	-0.945211	-1.713479	2.717296
55	1	0	0.090804	-2.026936	2.766208
56	6	0	-1.921923	-2.515541	3.310798
57	1	0	-1.627081	-3.432159	3.813104
58	6	0	-3.267276	-2.144351	3.257060

59	1	0	-4.025113	-2.773068	3.715056
60	6	0	-3.633883	-0.960205	2.612741
61	1	0	-4.677342	-0.663590	2.564070
62	6	0	-2.663258	-0.151999	2.020533
63	1	0	-2.967303	0.758635	1.517618
64	7	0	-1.948978	-0.656161	-1.160656
65	7	0	0.293556	-2.004742	-0.942007
66	7	0	2.172775	-0.182767	-1.140116
67	7	0	-0.212126	2.119716	-1.334184
68	15	0	-0.077001	0.444521	1.115253
69	44	0	0.069980	-0.034448	-1.243567
70	6	0	0.092600	-0.248632	-3.136528
71	8	0	0.089514	-0.412217	-4.279780

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^{3}1-CO E_{opt} = -2156.73333472 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.646263	1.969924	-0.920653
2	1	0	3.131519	1.085017	-1.313408
3	6	0	3.391112	3.086866	-0.551250
4	1	0	4.470423	3.075449	-0.655027
5	6	0	2.713750	4.198907	-0.053984
6	1	0	3.255025	5.089374	0.248849
7	6	0	1.326154	4.156910	0.048941
8	1	0	0.788863	5.015072	0.431385
9	6	0	0.645223	2.996738	-0.339184
10	6	0	-0.830437	2.866241	-0.250339
11	6	0	-1.656424	3.881623	0.247666

12	1	0	-1.240292	4.817934	0.595506
13	6	0	-3.030568	3.672344	0.294363
14	1	0	-3.686025	4.444755	0.682514
15	6	0	-3.560542	2.468437	-0.159874
16	1	0	-4.628880	2.295487	-0.128228
17	6	0	-2.685459	1.493121	-0.647635
18	6	0	-3.130689	0.171087	-1.143989
19	6	0	-4.469229	-0.226390	-1.215978
20	1	0	-5.262025	0.450786	-0.925125
21	6	0	-4.775319	-1.508988	-1.664626
22	1	0	-5.809705	-1.831606	-1.720743
23	6	0	-3.741556	-2.367982	-2.036719
24	1	0	-3.936030	-3.374712	-2.388643
25	6	0	-2.431910	-1.907091	-1.945617
26	1	0	-1.587889	-2.532490	-2.218340
27	6	0	2.557911	-1.320602	-2.580390
28	1	0	2.047717	-0.988315	-3.475652
29	6	0	3.826999	-1.915611	-2.686782
30	1	0	4.266414	-2.044694	-3.669120
31	6	0	4.485451	-2.293517	-1.540061
32	1	0	5.478413	-2.731518	-1.578205
33	6	0	3.857233	-2.109718	-0.283798
34	6	0	4.489338	-2.473356	0.934217
35	1	0	5.487002	-2.899846	0.891443
36	6	0	3.852380	-2.284443	2.140234
37	1	0	4.341462	-2.555471	3.070080
38	6	0	2.546536	-1.747986	2.170657
39	1	0	2.044650	-1.620694	3.125161
40	6	0	1.893567	-1.388561	1.002702
41	6	0	2.548802	-1.537018	-0.250636

42	6	0	-0.910335	-2.127521	1.483112
43	6	0	-2.302593	-1.924419	1.454040
44	1	0	-2.713056	-0.961279	1.174442
45	6	0	-3.174013	-2.963380	1.777946
46	1	0	-4.245434	-2.789007	1.752429
47	6	0	-2.670043	-4.221665	2.118025
48	1	0	-3.349475	-5.032614	2.363199
49	6	0	-1.290068	-4.434643	2.135239
50	1	0	-0.891265	-5.410859	2.394933
51	6	0	-0.410527	-3.395807	1.819918
52	1	0	0.657229	-3.583161	1.836079
53	6	0	0.120058	0.550305	2.256019
54	6	0	-1.039865	0.793926	3.008118
55	1	0	-1.904526	0.147086	2.920548
56	6	0	-1.089638	1.877413	3.887822
57	1	0	-1.992495	2.055606	4.464454
58	6	0	0.012232	2.724424	4.027490
59	1	0	-0.031612	3.567873	4.710209
60	6	0	1.172830	2.479704	3.289164
61	1	0	2.035194	3.131544	3.391091
62	6	0	1.228685	1.402089	2.405642
63	1	0	2.132455	1.233368	1.830199
64	7	0	1.312138	1.922160	-0.808221
65	7	0	-1.354878	1.702328	-0.675510
66	7	0	-2.142341	-0.673339	-1.507201
67	7	0	1.931814	-1.115615	-1.418240
68	15	0	0.186580	-0.753704	0.970959
69	44	0	0.001708	-0.067172	-1.327875
70	6	0	-0.021792	0.556603	-3.144457
71	8	0	-0.064968	1.021440	-4.199470

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^{2}2-CO E_{opt} = -2156.90062793 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.014005	-0.463207	-1.355328
2	1	0	-3.038070	0.606124	-1.538834
3	6	0	-4.176209	-1.208703	-1.278231
4	1	0	-5.138554	-0.726931	-1.408130
5	6	0	-4.067186	-2.597673	-1.019217
6	1	0	-4.958393	-3.212815	-0.942099
7	6	0	-2.820031	-3.165473	-0.870235
8	1	0	-2.720537	-4.228367	-0.677925
9	6	0	-1.652225	-2.368967	-0.966173
10	6	0	-0.310278	-2.862507	-0.836246
11	6	0	0.106357	-4.181232	-0.564251
12	1	0	-0.631229	-4.965729	-0.433200
13	6	0	1.458779	-4.471652	-0.456174
14	1	0	1.776134	-5.486738	-0.241640
15	6	0	2.434043	-3.455326	-0.614659
16	1	0	3.488173	-3.684399	-0.514108
17	6	0	2.006098	-2.164884	-0.882511
18	6	0	2.852716	-0.967568	-1.020672
19	6	0	4.250924	-0.983175	-0.955744
20	1	0	4.773607	-1.926116	-0.845023
21	6	0	4.959215	0.210470	-1.020600
22	1	0	6.042774	0.205059	-0.962481
23	6	0	4.258406	1.415106	-1.154689
24	1	0	4.771646	2.368995	-1.200868

25	6	0	2.872935	1.373966	-1.230873
26	1	0	2.280081	2.275696	-1.337944
27	6	0	-0.632100	2.787042	-2.414203
28	1	0	-0.136060	2.358948	-3.276536
29	6	0	-1.239795	4.052057	-2.527294
30	1	0	-1.189010	4.575450	-3.475353
31	6	0	-1.901715	4.575769	-1.443200
32	1	0	-2.409481	5.534166	-1.496707
33	6	0	-1.911972	3.849458	-0.226783
34	6	0	-2.568951	4.337149	0.933683
35	1	0	-3.089859	5.288043	0.870660
36	6	0	-2.544875	3.621629	2.109615
37	1	0	-3.052980	3.995409	2.992699
38	6	0	-1.833385	2.403214	2.177587
39	1	0	-1.791858	1.863374	3.118726
40	6	0	-1.181822	1.892494	1.067186
41	6	0	-1.235548	2.591325	-0.173286
42	6	0	1.376886	0.844909	2.014774
43	6	0	2.423000	-0.094523	2.067900
44	1	0	2.294856	-1.080954	1.634855
45	6	0	3.640455	0.235968	2.661927
46	1	0	4.438896	-0.499539	2.692057
47	6	0	3.835398	1.511447	3.199387
48	1	0	4.786788	1.771343	3.654319
49	6	0	2.805103	2.452300	3.143156
50	1	0	2.950329	3.446562	3.555732
51	6	0	1.580964	2.124855	2.553919
52	1	0	0.796061	2.872127	2.513118
53	6	0	-1.066114	-0.818121	2.145639
54	6	0	-0.399494	-1.729510	2.980657

55	1	0	0.674264	-1.672754	3.117138
56	6	0	-1.116664	-2.721815	3.652861
57	1	0	-0.588364	-3.417905	4.298014
58	6	0	-2.501715	-2.817899	3.500119
59	1	0	-3.055596	-3.592983	4.021723
60	6	0	-3.171488	-1.909668	2.675702
61	1	0	-4.248225	-1.974834	2.549640
62	6	0	-2.461508	-0.916580	2.001566
63	1	0	-2.996355	-0.225903	1.359883
64	7	0	-1.786160	-0.995818	-1.191262
65	7	0	0.673854	-1.902500	-0.985433
66	7	0	2.180195	0.222005	-1.168783
67	7	0	-0.637492	2.051990	-1.301363
68	15	0	-0.152905	0.389060	1.113224
69	44	0	0.077163	-0.016658	-1.276377
70	6	0	0.110406	-0.180062	-3.146589
71	8	0	0.108620	-0.300212	-4.301239

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^{2}2-CO-fix-210 E_{opt} = -2156.89133711 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.977175	-0.677273	-1.335096
2	1	0	-3.070127	0.386393	-1.531397
3	6	0	-4.089364	-1.497175	-1.267197
4	1	0	-5.079289	-1.082509	-1.419738
5	6	0	-3.892425	-2.872852	-0.984378
6	1	0	-4.742043	-3.544715	-0.909739
7	6	0	-2.613257	-3.353937	-0.808292

8	1	0	-2.447751	-4.405266	-0.598332
9	6	0	-1.497374	-2.483719	-0.903199
10	6	0	-0.128103	-2.887994	-0.762125
11	6	0	0.376111	-4.179669	-0.497139
12	1	0	-0.307998	-5.010317	-0.360072
13	6	0	1.744506	-4.385141	-0.412237
14	1	0	2.127591	-5.379625	-0.207957
15	6	0	2.653467	-3.311105	-0.590089
16	1	0	3.722004	-3.477200	-0.524300
17	6	0	2.137725	-2.048039	-0.837253
18	6	0	2.906394	-0.798988	-0.994226
19	6	0	4.302771	-0.729200	-0.944474
20	1	0	4.882332	-1.637378	-0.826873
21	6	0	4.937534	0.504335	-1.032161
22	1	0	6.020005	0.565470	-0.987020
23	6	0	4.162515	1.661370	-1.171114
24	1	0	4.615641	2.644330	-1.235385
25	6	0	2.780797	1.535017	-1.227001
26	1	0	2.133082	2.398369	-1.334124
27	6	0	-0.804021	2.679007	-2.476121
28	1	0	-0.307044	2.238117	-3.331470
29	6	0	-1.465211	3.914035	-2.623535
30	1	0	-1.455991	4.400700	-3.592347
31	6	0	-2.121581	4.457245	-1.545316
32	1	0	-2.664758	5.394234	-1.624275
33	6	0	-2.079397	3.777810	-0.302339
34	6	0	-2.726752	4.280474	0.857215
35	1	0	-3.281232	5.210905	0.776986
36	6	0	-2.653901	3.603466	2.054432
37	1	0	-3.155929	3.989111	2.935893

38	6	0	-1.903811	2.409573	2.145758
39	1	0	-1.828566	1.898517	3.100814
40	6	0	-1.257311	1.889260	1.037309
41	6	0	-1.356956	2.548414	-0.220004
42	6	0	1.328216	0.909669	1.995807
43	6	0	2.392040	-0.007601	2.073438
44	1	0	2.291727	-0.999939	1.647774
45	6	0	3.593957	0.353262	2.681262
46	1	0	4.406261	-0.365912	2.729648
47	6	0	3.755341	1.637209	3.209467
48	1	0	4.694236	1.920341	3.676262
49	6	0	2.707654	2.556609	3.128080
50	1	0	2.826944	3.557807	3.532004
51	6	0	1.499250	2.198989	2.523827
52	1	0	0.701560	2.931085	2.462675
53	6	0	-1.069102	-0.813505	2.121931
54	6	0	-0.381484	-1.719759	2.944796
55	1	0	0.692705	-1.651007	3.069287
56	6	0	-1.077885	-2.723735	3.621800
57	1	0	-0.533012	-3.415824	4.257306
58	6	0	-2.463178	-2.836359	3.485385
59	1	0	-3.000954	-3.620673	4.010025
60	6	0	-3.154327	-1.932949	2.673525
61	1	0	-4.231534	-2.011244	2.559881
62	6	0	-2.464717	-0.928092	1.995815
63	1	0	-3.016054	-0.242188	1.363473
64	7	0	-1.719054	-1.122833	-1.148060
65	7	0	0.792677	-1.865021	-0.903794
66	7	0	2.158642	0.344271	-1.144850
67	7	0	-0.755721	1.988804	-1.336121

68	15	0	-0.185821	0.415597	1.085285
69	44	0	0.075007	-0.020564	-1.201987
70	6	0	0.124618	-0.303775	-3.282211
71	8	0	0.100752	-0.498318	-4.413387

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^{2}2-CO-fix-230 E_{opt} = -2156.87854357 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.945755	-0.789604	-1.315958
2	1	0	-3.060259	0.264850	-1.547392
3	6	0	-4.040323	-1.630526	-1.227419
4	1	0	-5.037309	-1.242389	-1.403139
5	6	0	-3.819722	-2.988438	-0.891528
6	1	0	-4.655924	-3.674059	-0.795561
7	6	0	-2.530300	-3.434426	-0.687772
8	1	0	-2.344019	-4.472499	-0.433979
9	6	0	-1.435917	-2.545794	-0.811667
10	6	0	-0.053766	-2.918402	-0.656327
11	6	0	0.473311	-4.193133	-0.383674
12	1	0	-0.192594	-5.036660	-0.235587
13	6	0	1.850533	-4.371729	-0.311652
14	1	0	2.255959	-5.356491	-0.104141
15	6	0	2.731091	-3.283540	-0.514315
16	1	0	3.803825	-3.430040	-0.467501
17	6	0	2.191460	-2.030187	-0.766097
18	6	0	2.931168	-0.771937	-0.946767
19	6	0	4.327432	-0.668919	-0.895348
20	1	0	4.926295	-1.561371	-0.754794

21	6	0	4.936084	0.573951	-1.008398
22	1	0	6.016937	0.659207	-0.963133
23	6	0	4.135175	1.713089	-1.172175
24	1	0	4.567742	2.703712	-1.258224
25	6	0	2.757688	1.556543	-1.223166
26	1	0	2.092703	2.404850	-1.345311
27	6	0	-0.802685	2.545652	-2.590266
28	1	0	-0.303543	2.051549	-3.415075
29	6	0	-1.457121	3.774409	-2.809516
30	1	0	-1.445726	4.203495	-3.805232
31	6	0	-2.108498	4.385819	-1.764868
32	1	0	-2.644077	5.320912	-1.899022
33	6	0	-2.071192	3.780067	-0.483645
34	6	0	-2.712835	4.350746	0.647274
35	1	0	-3.260783	5.279544	0.517475
36	6	0	-2.644010	3.738835	1.879815
37	1	0	-3.142155	4.176561	2.738898
38	6	0	-1.905402	2.544224	2.036911
39	1	0	-1.836513	2.083576	3.017825
40	6	0	-1.262924	1.960359	0.958188
41	6	0	-1.358737	2.552749	-0.331429
42	6	0	1.292121	0.963267	1.998256
43	6	0	2.343136	0.034944	2.111268
44	1	0	2.241380	-0.960888	1.695167
45	6	0	3.534795	0.388549	2.743100
46	1	0	4.336995	-0.339629	2.818767
47	6	0	3.699705	1.676586	3.259884
48	1	0	4.630893	1.953933	3.745289
49	6	0	2.665640	2.607410	3.142759
50	1	0	2.787763	3.612051	3.537202

51	6	0	1.467362	2.256846	2.514486
52	1	0	0.680730	2.997929	2.426689
53	6	0	-1.136162	-0.714686	2.117343
54	6	0	-0.477836	-1.643940	2.937903
55	1	0	0.598999	-1.613811	3.056075
56	6	0	-1.206771	-2.621457	3.619929
57	1	0	-0.684610	-3.331928	4.254227
58	6	0	-2.595575	-2.684632	3.489108
59	1	0	-3.158819	-3.448783	4.016824
60	6	0	-3.257769	-1.758723	2.678229
61	1	0	-4.337459	-1.799803	2.568761
62	6	0	-2.535323	-0.780272	1.996187
63	1	0	-3.063806	-0.075829	1.364404
64	7	0	-1.677912	-1.201388	-1.107903
65	7	0	0.837728	-1.874414	-0.813350
66	7	0	2.156708	0.354655	-1.118902
67	7	0	-0.760000	1.924386	-1.411255
68	15	0	-0.211542	0.472345	1.065833
69	44	0	0.085260	-0.049720	-1.138447
70	6	0	0.169547	-0.523708	-3.387498
71	8	0	0.108455	-0.873512	-4.471549

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^{2}2-CO-fix-250 E_{opt} = -2156.87403637 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.079847	2.250922	-1.130133
2	1	0	2.707016	1.418435	-1.429717
3	6	0	2.601347	3.522189	-0.942504

4	1	0	3.658490	3.697998	-1.108979
5	6	0	1.744297	4.550323	-0.526227
6	1	0	2.123588	5.552176	-0.353678
7	6	0	0.397726	4.268715	-0.337684
8	1	0	-0.285909	5.046986	-0.018206
9	6	0	-0.082695	2.971582	-0.562592
10	6	0	-1.489614	2.581624	-0.430801
11	6	0	-2.571514	3.411030	-0.129121
12	1	0	-2.418902	4.467172	0.061212
13	6	0	-3.857089	2.864722	-0.085345
14	1	0	-4.705629	3.499953	0.145019
15	6	0	-4.058187	1.504973	-0.349272
16	1	0	-5.057350	1.085643	-0.326587
17	6	0	-2.957335	0.700920	-0.642821
18	6	0	-2.958245	-0.740077	-0.918273
19	6	0	-4.105601	-1.542590	-0.882341
20	1	0	-5.068772	-1.094015	-0.667654
21	6	0	-4.001793	-2.908964	-1.106771
22	1	0	-4.885244	-3.538063	-1.075412
23	6	0	-2.738749	-3.459839	-1.364944
24	1	0	-2.609920	-4.522111	-1.541870
25	6	0	-1.634488	-2.621398	-1.391420
26	1	0	-0.636549	-3.002491	-1.579459
27	6	0	1.800453	-1.435888	-2.876103
28	1	0	1.096153	-1.073290	-3.616847
29	6	0	2.938005	-2.166528	-3.276352
30	1	0	3.087477	-2.368159	-4.331417
31	6	0	3.835557	-2.590865	-2.325242
32	1	0	4.732216	-3.140464	-2.596058
33	6	0	3.579425	-2.303527	-0.959996

34	6	0	4.459976	-2.698934	0.081387
35	1	0	5.365133	-3.238415	-0.182375
36	6	0	4.174675	-2.400679	1.396074
37	1	0	4.855674	-2.698903	2.186848
38	6	0	2.983436	-1.714405	1.725407
39	1	0	2.764001	-1.497161	2.766603
40	6	0	2.094264	-1.320518	0.739469
41	6	0	2.391828	-1.585915	-0.627419
42	6	0	-0.570119	-1.638142	1.955362
43	6	0	-1.922182	-1.289123	2.133690
44	1	0	-2.292503	-0.335368	1.774411
45	6	0	-2.806556	-2.171800	2.752835
46	1	0	-3.846833	-1.886570	2.879930
47	6	0	-2.359866	-3.422302	3.189054
48	1	0	-3.050568	-4.113232	3.663622
49	6	0	-1.023595	-3.783267	3.002576
50	1	0	-0.669866	-4.756152	3.331834
51	6	0	-0.131697	-2.899854	2.388503
52	1	0	0.898758	-3.204706	2.244357
53	6	0	0.883639	0.922353	2.173339
54	6	0	-0.111879	1.482488	2.992560
55	1	0	-1.089056	1.019687	3.070619
56	6	0	0.144326	2.645937	3.721273
57	1	0	-0.634261	3.062431	4.354001
58	6	0	1.390388	3.271860	3.636091
59	1	0	1.585289	4.179513	4.199824
60	6	0	2.384883	2.722864	2.822263
61	1	0	3.356241	3.203014	2.746738
62	6	0	2.135781	1.558891	2.094438
63	1	0	2.915299	1.153796	1.458873

64	7	0	0.776303	1.960361	-0.939477
65	7	0	-1.709106	1.254557	-0.664347
66	7	0	-1.720802	-1.290491	-1.179438
67	7	0	1.524231	-1.133014	-1.608565
68	15	0	0.503660	-0.467813	1.036718
69	44	0	-0.154983	0.090096	-1.057174
70	6	0	-0.591947	0.916104	-3.375961
71	8	0	-0.875523	1.984762	-3.715742

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^{2}2-CO-fix-270 E_{opt} = -2156.87117857 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.246333	-2.829614	-1.105240
2	1	0	-2.094796	-2.237829	-1.430917
3	6	0	-1.350009	-4.197355	-0.905380
4	1	0	-2.295697	-4.695789	-1.088411
5	6	0	-0.224550	-4.903167	-0.456185
6	1	0	-0.276103	-5.971681	-0.274596
7	6	0	0.961767	-4.213268	-0.246737
8	1	0	1.846614	-4.736817	0.097140
9	6	0	1.019505	-2.832707	-0.483268
10	6	0	2.230313	-2.022352	-0.332702
11	6	0	3.509787	-2.468145	0.003994
12	1	0	3.689691	-3.516207	0.214114
13	6	0	4.560528	-1.548250	0.057360
14	1	0	5.559262	-1.884051	0.315051
15	6	0	4.334129	-0.197912	-0.234033
16	1	0	5.153165	0.511397	-0.206711

17	6	0	3.044738	0.219530	-0.561215
18	6	0	2.605610	1.582966	-0.873862
19	6	0	3.445382	2.703953	-0.843609
20	1	0	4.495136	2.583336	-0.601757
21	6	0	2.927449	3.964755	-1.107478
22	1	0	3.570577	4.838207	-1.079795
23	6	0	1.561838	4.089240	-1.401054
24	1	0	1.113012	5.054469	-1.609010
25	6	0	0.774503	2.948559	-1.422274
26	1	0	-0.287280	2.995377	-1.638405
27	6	0	-2.052095	0.685772	-2.957833
28	1	0	-1.247067	0.496927	-3.660314
29	6	0	-3.337464	1.033144	-3.422569
30	1	0	-3.504419	1.118505	-4.490714
31	6	0	-4.349908	1.240402	-2.514968
32	1	0	-5.355848	1.493886	-2.836292
33	6	0	-4.070026	1.117879	-1.129644
34	6	0	-5.059606	1.299140	-0.127463
35	1	0	-6.072062	1.543133	-0.436162
36	6	0	-4.743507	1.160692	1.206913
37	1	0	-5.506951	1.291312	1.967308
38	6	0	-3.418441	0.856781	1.596603
39	1	0	-3.181563	0.759459	2.652081
40	6	0	-2.422651	0.686714	0.649871
41	6	0	-2.739683	0.789998	-0.733497
42	6	0	0.011407	1.778687	1.904815
43	6	0	1.398724	1.814787	2.141627
44	1	0	2.023842	0.978435	1.847603
45	6	0	1.987112	2.930793	2.735580
46	1	0	3.059029	2.942585	2.910380

47	6	0	1.203709	4.034198	3.085889
48	1	0	1.663339	4.907171	3.540091
49	6	0	-0.170989	4.013314	2.840142
50	1	0	-0.785333	4.869901	3.102646
51	6	0	-0.766959	2.894323	2.252062
52	1	0	-1.834117	2.902663	2.060428
53	6	0	-0.696322	-1.067881	2.211071
54	6	0	0.322939	-1.248672	3.161267
55	1	0	1.090184	-0.495200	3.298709
56	6	0	0.358561	-2.402506	3.947933
57	1	0	1.149636	-2.524222	4.682396
58	6	0	-0.614795	-3.392394	3.793282
59	1	0	-0.581856	-4.290640	4.402938
60	6	0	-1.633352	-3.219374	2.851789
61	1	0	-2.394768	-3.983326	2.723706
62	6	0	-1.675718	-2.068045	2.065543
63	1	0	-2.468621	-1.953107	1.334730
64	7	0	-0.102793	-2.142797	-0.896200
65	7	0	2.028699	-0.694909	-0.588383
66	7	0	1.264595	1.714569	-1.170905
67	7	0	-1.745846	0.554834	-1.668053
68	15	0	-0.665942	0.324558	1.015719
69	44	0	0.199188	-0.077362	-1.027025
70	6	0	1.103727	-0.876631	-3.442181
71	8	0	1.731168	-1.828544	-3.600681

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^{2}2-CO-fix-290 E_{opt} = -2156.87070109 Hartree

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-0.209254	-3.150611	-1.006256
2	1	0	-1.195677	-2.879561	-1.366881
3	6	0	0.129156	-4.468515	-0.743427
4	1	0	-0.600253	-5.253517	-0.910456
5	6	0	1.411516	-4.751940	-0.250610
6	1	0	1.703217	-5.770928	-0.018141
7	6	0	2.305971	-3.707709	-0.062599
8	1	0	3.302504	-3.902509	0.317540
9	6	0	1.921457	-2.392793	-0.363263
10	6	0	2.801840	-1.229557	-0.231636
11	6	0	4.150363	-1.241253	0.127070
12	1	0	4.646284	-2.176567	0.359860
13	6	0	4.859884	-0.038952	0.171001
14	1	0	5.909410	-0.039419	0.444826
15	6	0	4.223159	1.165309	-0.150178
16	1	0	4.776210	2.097186	-0.128118
17	6	0	2.875075	1.153108	-0.501817
18	6	0	2.052056	2.317387	-0.847804
19	6	0	2.515411	3.639639	-0.818466
20	1	0	3.546072	3.842770	-0.551757
21	6	0	1.650072	4.683857	-1.114186
22	1	0	2.001196	5.710143	-1.086831
23	6	0	0.317539	4.391499	-1.439187
24	1	0	-0.394090	5.176093	-1.671969
25	6	0	-0.089570	3.066825	-1.460750
26	1	0	-1.110286	2.789856	-1.701880
27	6	0	-2.115020	-0.097005	-3.054378
28	1	0	-1.266554	-0.066547	-3.731182
29	6	0	-3.430411	-0.179550	-3.557721

30	1	0	-3.583265	-0.201738	-4.631024
31	6	0	-4.485112	-0.243871	-2.677088
32	1	0	-5.510017	-0.322915	-3.027393
33	6	0	-4.226377	-0.209714	-1.282401
34	6	0	-5.255128	-0.292991	-0.307100
35	1	0	-6.284266	-0.380637	-0.643417
36	6	0	-4.952231	-0.270446	1.037187
37	1	0	-5.742173	-0.343040	1.778153
38	6	0	-3.609278	-0.145579	1.463343
39	1	0	-3.387443	-0.125908	2.526345
40	6	0	-2.579043	-0.046224	0.543980
41	6	0	-2.872072	-0.099862	-0.848612
42	6	0	-0.621225	1.747724	1.832586
43	6	0	0.684452	2.193539	2.112849
44	1	0	1.537035	1.569468	1.866637
45	6	0	0.898148	3.447110	2.684670
46	1	0	1.912347	3.775816	2.892221
47	6	0	-0.186251	4.281940	2.970080
48	1	0	-0.019691	5.262237	3.407113
49	6	0	-1.483907	3.854190	2.681084
50	1	0	-2.331188	4.500294	2.892617
51	6	0	-1.703917	2.595495	2.114295
52	1	0	-2.718501	2.288244	1.886820
53	6	0	-0.485183	-1.168537	2.223465
54	6	0	0.479913	-1.007636	3.231804
55	1	0	0.975193	-0.053824	3.374611
56	6	0	0.812311	-2.076302	4.067763
57	1	0	1.556692	-1.934766	4.846164
58	6	0	0.192527	-3.317859	3.906312
59	1	0	0.455896	-4.148052	4.555187

60	6	0	-0.770705	-3.485353	2.907309
61	1	0	-1.259060	-4.446455	2.774308
62	6	0	-1.107945	-2.421186	2.070998
63	1	0	-1.852416	-2.568996	1.296148
64	7	0	0.645460	-2.120867	-0.819951
65	7	0	2.188312	-0.036711	-0.526945
66	7	0	0.741773	2.038748	-1.179880
67	7	0	-1.827935	-0.063762	-1.755413
68	15	0	-0.802126	0.136492	0.970440
69	44	0	0.249933	-0.034355	-1.010095
70	6	0	1.566106	-0.783516	-3.483240
71	8	0	2.468548	-1.489792	-3.444636

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^{2}2-CO-fix-310 E_{opt} = -2156.87064549 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.911863	-3.028657	-0.983450
2	1	0	-0.100563	-3.124144	-1.360774
3	6	0	1.689126	-4.141807	-0.708110
4	1	0	1.286510	-5.133862	-0.881035
5	6	0	2.982834	-3.954438	-0.197005
6	1	0	3.611731	-4.805038	0.044641
7	6	0	3.448509	-2.661782	-0.005145
8	1	0	4.445714	-2.490474	0.384431
9	6	0	2.629540	-1.567105	-0.319173
10	6	0	3.043436	-0.169761	-0.193440
11	6	0	4.302019	0.299057	0.183751
12	1	0	5.089386	-0.398756	0.445038

13	6	0	4.542263	1.675509	0.212036
14	1	0	5.519391	2.048676	0.499237
15	6	0	3.527875	2.573966	-0.139065
16	1	0	3.715359	3.641489	-0.127131
17	6	0	2.276019	2.083167	-0.503607
18	6	0	1.097972	2.874223	-0.867540
19	6	0	1.058861	4.275367	-0.845411
20	1	0	1.946890	4.831605	-0.567464
21	6	0	-0.116983	4.941652	-1.159106
22	1	0	-0.155757	6.025793	-1.136450
23	6	0	-1.253803	4.190726	-1.495700
24	1	0	-2.195326	4.668575	-1.743714
25	6	0	-1.163030	2.808382	-1.507652
26	1	0	-2.016645	2.186364	-1.754949
27	6	0	-1.905891	-0.834488	-3.054295
28	1	0	-1.101067	-0.537588	-3.720405
29	6	0	-3.112456	-1.348642	-3.573836
30	1	0	-3.228790	-1.432120	-4.648756
31	6	0	-4.104919	-1.743393	-2.706955
32	1	0	-5.041471	-2.156154	-3.070158
33	6	0	-3.895952	-1.612287	-1.309614
34	6	0	-4.856639	-2.017035	-0.345424
35	1	0	-5.795105	-2.439560	-0.692650
36	6	0	-4.598278	-1.885442	1.002175
37	1	0	-5.332666	-2.206777	1.734035
38	6	0	-3.376449	-1.325450	1.443462
39	1	0	-3.189427	-1.225784	2.508669
40	6	0	-2.422059	-0.901822	0.534706
41	6	0	-2.660213	-1.061569	-0.859385
42	6	0	-1.170610	1.439939	1.827204

43	6	0	-0.084410	2.286510	2.118883
44	1	0	0.927623	1.973957	1.883189
45	6	0	-0.296736	3.540643	2.690156
46	1	0	0.552991	4.181009	2.908341
47	6	0	-1.596867	3.976955	2.961249
48	1	0	-1.763202	4.957604	3.397547
49	6	0	-2.681525	3.150555	2.658948
50	1	0	-3.695296	3.485717	2.859061
51	6	0	-2.473568	1.889035	2.094217
52	1	0	-3.330292	1.268080	1.857499
53	6	0	-0.083737	-1.269407	2.224973
54	6	0	0.747661	-0.801259	3.256243
55	1	0	0.886834	0.262428	3.413340
56	6	0	1.402417	-1.702875	4.098949
57	1	0	2.037179	-1.325526	4.895669
58	6	0	1.242509	-3.079179	3.920747
59	1	0	1.755859	-3.777814	4.575009
60	6	0	0.415826	-3.552820	2.897886
61	1	0	0.285190	-4.621076	2.750756
62	6	0	-0.241691	-2.657180	2.054831
63	1	0	-0.873942	-3.040051	1.260868
64	7	0	1.344853	-1.762209	-0.792689
65	7	0	2.054961	0.726862	-0.519913
66	7	0	-0.024022	2.142648	-1.208230
67	7	0	-1.669019	-0.692555	-1.751935
68	15	0	-0.807302	-0.141417	0.968684
69	44	0	0.245009	0.045657	-1.003272
70	6	0	1.944659	-0.345872	-3.566063
71	8	0	3.016898	-0.708492	-3.404176

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^{2}2-CO-fix-400-opt E_{opt} = -2156.87062328 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.551746	-3.116098	-1.009670
2	1	0	-1.489115	-2.738723	-1.403804
3	6	0	-0.371336	-4.462958	-0.742294
4	1	0	-1.176062	-5.162058	-0.941723
5	6	0	0.854523	-4.888692	-0.206610
6	1	0	1.023993	-5.934471	0.028201
7	6	0	1.850265	-3.949840	0.019376
8	1	0	2.806577	-4.255670	0.428135
9	6	0	1.624902	-2.598540	-0.284311
10	6	0	2.623197	-1.542147	-0.119273
11	6	0	3.943052	-1.692099	0.306747
12	1	0	4.321980	-2.668595	0.585967
13	6	0	4.778387	-0.572145	0.364040
14	1	0	5.806136	-0.680199	0.693616
15	6	0	4.296653	0.686015	-0.015325
16	1	0	4.947118	1.552478	0.015863
17	6	0	2.973278	0.813407	-0.432468
18	6	0	2.297590	2.043704	-0.847308
19	6	0	2.903592	3.308430	-0.852919
20	1	0	3.941874	3.406328	-0.556175
21	6	0	2.171520	4.427274	-1.221740
22	1	0	2.633153	5.409245	-1.221740
23	6	0	0.825007	4.267895	-1.586341
24	1	0	0.213174	5.114737	-1.877641
25	6	0	0.273703	2.997577	-1.570229

26	1	0	-0.763292	2.827268	-1.838859
27	6	0	-2.057740	0.050017	-3.055160
28	1	0	-1.200751	-0.032912	-3.716081
29	6	0	-3.365625	0.090299	-3.581896
30	1	0	-3.501824	0.047792	-4.656813
31	6	0	-4.435949	0.169128	-2.721349
32	1	0	-5.457254	0.188297	-3.089831
33	6	0	-4.197365	0.221734	-1.323779
34	6	0	-5.243315	0.285137	-0.365253
35	1	0	-6.270860	0.299073	-0.717025
36	6	0	-4.959514	0.315555	0.983185
37	1	0	-5.763890	0.352451	1.711227
38	6	0	-3.617466	0.303643	1.430451
39	1	0	-3.409936	0.330521	2.496177
40	6	0	-2.570103	0.262262	0.526798
41	6	0	-2.846723	0.199768	-0.867385
42	6	0	-0.432941	1.857812	1.789249
43	6	0	0.909059	2.148165	2.100690
44	1	0	1.683443	1.412523	1.908694
45	6	0	1.259753	3.388382	2.632913
46	1	0	2.299760	3.597567	2.865927
47	6	0	0.280582	4.363479	2.844942
48	1	0	0.555700	5.333252	3.249389
49	6	0	-1.050802	4.089369	2.524280
50	1	0	-1.815853	4.845253	2.677811
51	6	0	-1.409127	2.844930	1.998441
52	1	0	-2.446357	2.657040	1.744612
53	6	0	-0.642485	-1.044937	2.260937
54	6	0	0.249974	-0.941265	3.340256
55	1	0	0.804727	-0.025475	3.511629

56	6	0	0.428510	-2.017256	4.214125
57	1	0	1.117773	-1.919526	5.048046
58	6	0	-0.273466	-3.208765	4.019542
59	1	0	-0.129557	-4.044123	4.698598
60	6	0	-1.166117	-3.319091	2.948918
61	1	0	-1.717463	-4.241332	2.789403
62	6	0	-1.349440	-2.247906	2.075470
63	1	0	-2.041507	-2.350595	1.246762
64	7	0	0.403598	-2.184697	-0.788133
65	7	0	2.160648	-0.294068	-0.459818
66	7	0	0.973715	1.893959	-1.217765
67	7	0	-1.788239	0.094257	-1.752101
68	15	0	-0.787759	0.254821	0.969477
69	44	0	0.249348	-0.082777	-0.984067
70	6	0	1.777268	-0.966225	-3.711683
71	8	0	2.368498	-1.932819	-3.573885

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^{3}3-CO E_{opt} = -2156.99249439 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.982466	-0.689120	-1.319690
2	1	0	-3.091235	0.378112	-1.486078
3	6	0	-4.080644	-1.527601	-1.241577
4	1	0	-5.080830	-1.124819	-1.353779
5	6	0	-3.854048	-2.907075	-1.002889
6	1	0	-4.691028	-3.594628	-0.925978
7	6	0	-2.563918	-3.372835	-0.871079
8	1	0	-2.377923	-4.426926	-0.694254

9	6	0	-1.463292	-2.482300	-0.967910
10	6	0	-0.086269	-2.864947	-0.853859
11	6	0	0.444774	-4.148886	-0.594082
12	1	0	-0.222371	-4.993224	-0.456379
13	6	0	1.816049	-4.326060	-0.507281
14	1	0	2.218984	-5.313076	-0.304197
15	6	0	2.704907	-3.231432	-0.672803
16	1	0	3.775963	-3.373125	-0.593642
17	6	0	2.162069	-1.980116	-0.921585
18	6	0	2.904811	-0.710473	-1.056608
19	6	0	4.298900	-0.612823	-1.003634
20	1	0	4.897507	-1.510971	-0.906028
21	6	0	4.906986	0.636504	-1.061276
22	1	0	5.987857	0.719804	-1.012529
23	6	0	4.108257	1.779267	-1.173957
24	1	0	4.540185	2.773108	-1.212308
25	6	0	2.729184	1.624612	-1.237592
26	1	0	2.060620	2.473926	-1.326499
27	6	0	-0.908162	2.747422	-2.437435
28	1	0	-0.402222	2.340670	-3.303848
29	6	0	-1.597243	3.940864	-2.522376
30	1	0	-1.626992	4.467816	-3.471674
31	6	0	-2.250763	4.450175	-1.390620
32	1	0	-2.813242	5.378431	-1.432820
33	6	0	-2.156509	3.745636	-0.163628
34	6	0	-2.771713	4.195933	1.031363
35	1	0	-3.352415	5.114352	0.994815
36	6	0	-2.646979	3.488237	2.234959
37	1	0	-3.137959	3.856096	3.132307
38	6	0	-1.890200	2.325666	2.282841

39	1	0	-1.777936	1.778748	3.214631
40	6	0	-1.256021	1.836802	1.108816
41	6	0	-1.395803	2.513025	-0.134359
42	6	0	1.350245	0.840785	2.030723
43	6	0	2.426993	-0.064147	2.056874
44	1	0	2.330326	-1.041323	1.596230
45	6	0	3.637221	0.288666	2.654825
46	1	0	4.459755	-0.420881	2.660182
47	6	0	3.794376	1.553531	3.228362
48	1	0	4.738915	1.830540	3.687852
49	6	0	2.733709	2.462132	3.200882
50	1	0	2.849044	3.448784	3.640941
51	6	0	1.519930	2.111567	2.603422
52	1	0	0.707702	2.830504	2.579641
53	6	0	-1.027385	-0.893194	2.117018
54	6	0	-0.326396	-1.829959	2.894155
55	1	0	0.748643	-1.756518	3.011297
56	6	0	-1.005850	-2.870636	3.532670
57	1	0	-0.447686	-3.585109	4.131339
58	6	0	-2.391427	-2.992549	3.404628
59	1	0	-2.916456	-3.805099	3.898624
60	6	0	-3.098090	-2.059340	2.641011
61	1	0	-4.176046	-2.142126	2.535107
62	6	0	-2.423704	-1.017514	2.004316
63	1	0	-2.983917	-0.303753	1.411346
64	7	0	-1.714785	-1.120751	-1.178591
65	7	0	0.816225	-1.826342	-1.002785
66	7	0	2.134760	0.419131	-1.184824
67	7	0	-0.819818	2.004329	-1.282592
68	15	0	-0.183958	0.398892	1.115544

69	44	0	0.056266	0.009511	-1.278157
70	6	0	0.074601	-0.122111	-3.146048
71	8	0	0.066868	-0.220249	-4.305805

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^{3}3-CO-fix-210 E_{opt} = -2156.98262354 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.721457	1.383373	-1.233198
2	1	0	3.073908	0.374210	-1.415537
3	6	0	3.596277	2.457016	-1.119433
4	1	0	4.663573	2.293534	-1.220318
5	6	0	3.070249	3.726848	-0.866576
6	1	0	3.724032	4.586901	-0.764273
7	6	0	1.692207	3.877266	-0.743539
8	1	0	1.262433	4.852246	-0.546249
9	6	0	0.856923	2.763725	-0.871662
10	6	0	-0.616547	2.820964	-0.760027
11	6	0	-1.382777	3.956456	-0.534744
12	1	0	-0.924200	4.929806	-0.410343
13	6	0	-2.792714	3.805755	-0.467090
14	1	0	-3.412962	4.677886	-0.285434
15	6	0	-3.385645	2.565673	-0.631091
16	1	0	-4.464879	2.467628	-0.576867
17	6	0	-2.582195	1.422776	-0.863122
18	6	0	-2.999393	0.059781	-1.007164
19	6	0	-4.347854	-0.383786	-0.947443
20	1	0	-5.141209	0.349364	-0.844993
21	6	0	-4.646442	-1.726960	-1.004967

22	1	0	-5.679378	-2.058286	-0.952789
23	6	0	-3.595836	-2.673221	-1.126650
24	1	0	-3.789489	-3.739125	-1.167892
25	6	0	-2.295488	-2.200403	-1.191347
26	1	0	-1.450828	-2.877040	-1.282758
27	6	0	1.462536	-2.403401	-2.525590
28	1	0	0.852273	-2.097106	-3.366081
29	6	0	2.408593	-3.400209	-2.667842
30	1	0	2.538425	-3.871857	-3.637603
31	6	0	3.188094	-3.784073	-1.566393
32	1	0	3.948583	-4.554688	-1.654439
33	6	0	2.960685	-3.166361	-0.310686
34	6	0	3.685793	-3.500918	0.861075
35	1	0	4.462717	-4.257774	0.786280
36	6	0	3.421393	-2.880639	2.090795
37	1	0	4.000493	-3.154171	2.969132
38	6	0	2.417543	-1.926899	2.190914
39	1	0	2.201747	-1.451205	3.143206
40	6	0	1.667956	-1.557891	1.040867
41	6	0	1.937257	-2.146427	-0.225626
42	6	0	-1.072912	-1.176868	2.042460
43	6	0	-2.334395	-0.557223	2.087705
44	1	0	-2.494706	0.391389	1.589255
45	6	0	-3.404013	-1.170155	2.740898
46	1	0	-4.373257	-0.680027	2.757621
47	6	0	-3.233436	-2.415058	3.352789
48	1	0	-4.068275	-2.895179	3.855361
49	6	0	-1.986906	-3.043204	3.305631
50	1	0	-1.846463	-4.013738	3.773368
51	6	0	-0.913381	-2.431724	2.652172

52	1	0	0.045314	-2.937606	2.613657
53	6	0	0.832346	1.068439	2.048949
54	6	0	-0.099659	1.953648	2.616229
55	1	0	-1.159727	1.730764	2.591334
56	6	0	0.323735	3.142884	3.213823
57	1	0	-0.411707	3.815500	3.646137
58	6	0	1.681563	3.469269	3.249385
59	1	0	2.008645	4.396937	3.710244
60	6	0	2.615960	2.595486	2.687850
61	1	0	3.674125	2.840356	2.706883
62	6	0	2.196318	1.405559	2.090943
63	1	0	2.931182	0.742973	1.648276
64	7	0	1.388859	1.520719	-1.111395
65	7	0	-1.211388	1.612690	-0.902471
66	7	0	-1.978542	-0.893571	-1.141405
67	7	0	1.232372	-1.743887	-1.341890
68	15	0	0.295818	-0.404199	1.079965
69	44	0	-0.071555	-0.011482	-1.202019
70	6	0	-0.221703	0.196235	-3.286320
71	8	0	-0.303979	0.310057	-4.428446

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^{3}3-CO-fix-230 E_{opt} = -2156.96842426 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.674155	1.445228	-1.255251
2	1	0	3.045009	0.441578	-1.439611
3	6	0	3.531462	2.528124	-1.166640
4	1	0	4.599007	2.386678	-1.293490

5	6	0	2.975826	3.803869	-0.896753
6	1	0	3.617771	4.674834	-0.805161
7	6	0	1.610983	3.929898	-0.745911
8	1	0	1.170766	4.899053	-0.535862
9	6	0	0.765824	2.798175	-0.863173
10	6	0	-0.665131	2.826051	-0.727989
11	6	0	-1.493964	3.939932	-0.485923
12	1	0	-1.058018	4.926259	-0.365617
13	6	0	-2.870492	3.774833	-0.406666
14	1	0	-3.506333	4.634779	-0.222409
15	6	0	-3.457400	2.496062	-0.571970
16	1	0	-4.532869	2.373837	-0.521690
17	6	0	-2.621367	1.410701	-0.792797
18	6	0	-3.027949	0.001724	-0.942677
19	6	0	-4.355129	-0.439272	-0.879701
20	1	0	-5.155154	0.281745	-0.756546
21	6	0	-4.639764	-1.797103	-0.959271
22	1	0	-5.666298	-2.144752	-0.904446
23	6	0	-3.583356	-2.706073	-1.101234
24	1	0	-3.757936	-3.774925	-1.158232
25	6	0	-2.286642	-2.215449	-1.168938
26	1	0	-1.432172	-2.874953	-1.276754
27	6	0	1.472010	-2.308668	-2.584442
28	1	0	0.849705	-1.980984	-3.408352
29	6	0	2.428580	-3.289518	-2.768088
30	1	0	2.554848	-3.727933	-3.753836
31	6	0	3.222993	-3.700617	-1.686792
32	1	0	3.990368	-4.460008	-1.807448
33	6	0	3.004726	-3.123038	-0.410274
34	6	0	3.745662	-3.480887	0.744793

35	1	0	4.528500	-4.228503	0.643163
36	6	0	3.490315	-2.892255	1.992608
37	1	0	4.082180	-3.182523	2.857046
38	6	0	2.481690	-1.947598	2.128396
39	1	0	2.274971	-1.495856	3.094404
40	6	0	1.714619	-1.559336	0.996822
41	6	0	1.972669	-2.117164	-0.285317
42	6	0	-1.017999	-1.211178	2.031001
43	6	0	-2.278611	-0.593610	2.122288
44	1	0	-2.446208	0.377922	1.672344
45	6	0	-3.339246	-1.231965	2.765579
46	1	0	-4.307056	-0.741479	2.818416
47	6	0	-3.161350	-2.501297	3.322819
48	1	0	-3.989090	-3.000890	3.818045
49	6	0	-1.916346	-3.127299	3.231093
50	1	0	-1.769951	-4.116218	3.656584
51	6	0	-0.852132	-2.490108	2.586709
52	1	0	0.105332	-2.994406	2.512854
53	6	0	0.880097	1.038611	2.068231
54	6	0	-0.038579	1.877713	2.719968
55	1	0	-1.093763	1.633957	2.738865
56	6	0	0.391774	3.047227	3.351182
57	1	0	-0.333600	3.683657	3.850301
58	6	0	1.743437	3.398919	3.336910
59	1	0	2.075866	4.311025	3.824329
60	6	0	2.664986	2.570228	2.691749
61	1	0	3.718162	2.835604	2.670720
62	6	0	2.238235	1.400146	2.062128
63	1	0	2.962076	0.773398	1.554078
64	7	0	1.337827	1.543538	-1.109693

65	7	0	-1.274048	1.589094	-0.844763
66	7	0	-1.999579	-0.900706	-1.098716
67	7	0	1.246559	-1.691939	-1.378478
68	15	0	0.337778	-0.411432	1.067627
69	44	0	-0.089439	0.001309	-1.144556
70	6	0	-0.313137	0.306445	-3.413224
71	8	0	-0.422684	0.456799	-4.541193

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^{3}3-CO-fix-250 E_{opt} = -2156.9621744 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.272511	1.936721	-1.445725
2	1	0	2.788491	1.016252	-1.696436
3	6	0	2.937022	3.151997	-1.385287
4	1	0	3.998627	3.194371	-1.603820
5	6	0	2.216919	4.300890	-1.026770
6	1	0	2.709896	5.264836	-0.954778
7	6	0	0.858490	4.186329	-0.760804
8	1	0	0.280348	5.059438	-0.479806
9	6	0	0.230024	2.937194	-0.851747
10	6	0	-1.198617	2.715037	-0.611038
11	6	0	-2.169908	3.677149	-0.334455
12	1	0	-1.902105	4.724870	-0.258208
13	6	0	-3.500359	3.274795	-0.167426
14	1	0	-4.264890	4.014806	0.043978
15	6	0	-3.851677	1.926092	-0.284288
16	1	0	-4.884359	1.618175	-0.165393
17	6	0	-2.857521	0.984484	-0.555585

18	6	0	-3.017256	-0.466853	-0.678978
19	6	0	-4.236096	-1.140138	-0.510210
20	1	0	-5.137226	-0.574283	-0.302213
21	6	0	-4.281205	-2.524076	-0.594414
22	1	0	-5.220084	-3.051252	-0.459522
23	6	0	-3.093498	-3.228241	-0.848791
24	1	0	-3.080682	-4.310580	-0.918750
25	6	0	-1.915368	-2.516278	-1.010026
26	1	0	-0.970441	-3.012751	-1.203248
27	6	0	1.581977	-1.781889	-2.875776
28	1	0	0.908246	-1.361215	-3.613783
29	6	0	2.594621	-2.650633	-3.238804
30	1	0	2.712863	-2.920883	-4.284306
31	6	0	3.457024	-3.165730	-2.257369
32	1	0	4.266132	-3.842323	-2.518098
33	6	0	3.266493	-2.794025	-0.902799
34	6	0	4.089990	-3.251931	0.158399
35	1	0	4.911104	-3.923942	-0.079030
36	6	0	3.871120	-2.846170	1.483880
37	1	0	4.528042	-3.205441	2.272262
38	6	0	2.821299	-1.990897	1.793080
39	1	0	2.653160	-1.673856	2.818511
40	6	0	1.959353	-1.521099	0.764332
41	6	0	2.177873	-1.894340	-0.591631
42	6	0	-0.648997	-1.253222	2.138263
43	6	0	-1.903732	-0.653376	2.355847
44	1	0	-2.129985	0.311834	1.916485
45	6	0	-2.882987	-1.302288	3.108516
46	1	0	-3.846875	-0.824509	3.260301
47	6	0	-2.631657	-2.567558	3.646254

48	1	0	-3.396564	-3.076299	4.226045
49	6	0	-1.395286	-3.178984	3.423927
50	1	0	-1.194000	-4.165977	3.831295
51	6	0	-0.411164	-2.529991	2.673157
52	1	0	0.539047	-3.023668	2.500323
53	6	0	1.196256	1.028640	1.983977
54	6	0	0.344717	1.857997	2.735062
55	1	0	-0.696745	1.594322	2.878308
56	6	0	0.825553	3.036323	3.310606
57	1	0	0.152332	3.662127	3.890068
58	6	0	2.160700	3.411380	3.139887
59	1	0	2.531878	4.330252	3.584665
60	6	0	3.015586	2.594672	2.394893
61	1	0	4.055465	2.876555	2.254925
62	6	0	2.538872	1.415615	1.819721
63	1	0	3.209935	0.795919	1.234686
64	7	0	0.953897	1.807799	-1.183800
65	7	0	-1.562754	1.400070	-0.698872
66	7	0	-1.855925	-1.168986	-0.933338
67	7	0	1.362157	-1.387645	-1.581158
68	15	0	0.566724	-0.419545	1.033859
69	44	0	-0.161814	0.045804	-1.064742
70	6	0	-1.063677	0.318232	-3.380432
71	8	0	-2.166080	0.405921	-3.719775

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^{3}3-CO-fix-270 E_{opt} = -2156.9587861 Hartree

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	1.991196	2.200650	-1.448123
2	1	0	2.608035	1.349053	-1.713843
3	6	0	2.506187	3.486626	-1.396596
4	1	0	3.550266	3.656306	-1.636839
5	6	0	1.661009	4.540518	-1.019569
6	1	0	2.035544	5.556943	-0.956047
7	6	0	0.332613	4.263064	-0.723784
8	1	0	-0.339492	5.060236	-0.426904
9	6	0	-0.143108	2.947480	-0.804189
10	6	0	-1.527937	2.553288	-0.530752
11	6	0	-2.601408	3.387778	-0.220961
12	1	0	-2.460681	4.459456	-0.136227
13	6	0	-3.869650	2.825904	-0.028781
14	1	0	-4.711997	3.465724	0.212009
15	6	0	-4.059362	1.446556	-0.159964
16	1	0	-5.044674	1.015035	-0.023644
17	6	0	-2.966461	0.634367	-0.467576
18	6	0	-2.955065	-0.821310	-0.624465
19	6	0	-4.081739	-1.639711	-0.455455
20	1	0	-5.040083	-1.189856	-0.221124
21	6	0	-3.963838	-3.016498	-0.575572
22	1	0	-4.830664	-3.655303	-0.440946
23	6	0	-2.704873	-3.567344	-0.866164
24	1	0	-2.564507	-4.638498	-0.964113
25	6	0	-1.623504	-2.716711	-1.028428
26	1	0	-0.630057	-3.091851	-1.250006
27	6	0	1.662154	-1.575386	-2.925031
28	1	0	0.895326	-1.252240	-3.621174
29	6	0	2.759389	-2.305849	-3.343739
30	1	0	2.855285	-2.566875	-4.393829

31	6	0	3.734957	-2.695583	-2.410780
32	1	0	4.610413	-3.261667	-2.716645
33	6	0	3.571788	-2.344893	-1.046594
34	6	0	4.501811	-2.683421	-0.029570
35	1	0	5.392284	-3.241408	-0.308679
36	6	0	4.296873	-2.303971	1.306365
37	1	0	5.035352	-2.567745	2.059513
38	6	0	3.158469	-1.596460	1.671812
39	1	0	3.001652	-1.302166	2.705745
40	6	0	2.191371	-1.248752	0.689138
41	6	0	2.392567	-1.595613	-0.676502
42	6	0	-0.381530	-1.394554	2.142648
43	6	0	-1.713281	-1.009768	2.386418
44	1	0	-2.103592	-0.094631	1.955981
45	6	0	-2.557828	-1.812103	3.154260
46	1	0	-3.584309	-1.500163	3.325850
47	6	0	-2.091016	-3.018875	3.682736
48	1	0	-2.750187	-3.647082	4.275122
49	6	0	-0.775131	-3.417668	3.435346
50	1	0	-0.405802	-4.357844	3.835686
51	6	0	0.073852	-2.614924	2.668277
52	1	0	1.089018	-2.945002	2.475920
53	6	0	1.083787	1.146407	1.980252
54	6	0	0.108342	1.855845	2.703822
55	1	0	-0.892343	1.455542	2.819053
56	6	0	0.409866	3.090642	3.282180
57	1	0	-0.357030	3.622513	3.838600
58	6	0	1.685772	3.643118	3.140730
59	1	0	1.917156	4.606099	3.586954
60	6	0	2.661556	2.947925	2.421685

61	1	0	3.656227	3.368824	2.303727
62	6	0	2.364168	1.712423	1.843397
63	1	0	3.127138	1.188989	1.277430
64	7	0	0.702843	1.913559	-1.159601
65	7	0	-1.731743	1.203524	-0.625950
66	7	0	-1.722306	-1.372529	-0.918786
67	7	0	1.468187	-1.205456	-1.620013
68	15	0	0.660228	-0.368236	1.021536
69	44	0	-0.189171	0.032409	-1.031589
70	6	0	-1.310397	0.379300	-3.463155
71	8	0	-2.448327	0.342061	-3.638016

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^{3}3-CO-fix-290 E_{opt} = -2156.9583112 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.865427	2.329511	-1.532998
2	1	0	2.515582	1.506524	-1.809944
3	6	0	2.323393	3.636795	-1.493728
4	1	0	3.353949	3.852759	-1.754059
5	6	0	1.437777	4.652291	-1.102829
6	1	0	1.767231	5.684732	-1.047640
7	6	0	0.129507	4.316512	-0.781712
8	1	0	-0.570967	5.083699	-0.471883
9	6	0	-0.289038	2.980117	-0.849475
10	6	0	-1.648818	2.527815	-0.542530
11	6	0	-2.741959	3.330005	-0.220324
12	1	0	-2.633735	4.407212	-0.162792
13	6	0	-3.985227	2.733412	0.020346

14	1	0	-4.841801	3.350299	0.270374
15	6	0	-4.128188	1.345701	-0.070846
16	1	0	-5.092644	0.883712	0.108375
17	6	0	-3.020086	0.561451	-0.392579
18	6	0	-2.979705	-0.898023	-0.503677
19	6	0	-4.081873	-1.734458	-0.270210
20	1	0	-5.041238	-1.297368	-0.017264
21	6	0	-3.939012	-3.111132	-0.352076
22	1	0	-4.787141	-3.762422	-0.167287
23	6	0	-2.679668	-3.645987	-0.670553
24	1	0	-2.520087	-4.716544	-0.741112
25	6	0	-1.623690	-2.778914	-0.897668
26	1	0	-0.631480	-3.142251	-1.143896
27	6	0	1.693673	-1.597093	-2.966997
28	1	0	0.907518	-1.302798	-3.655144
29	6	0	2.800807	-2.309977	-3.390278
30	1	0	2.888267	-2.586225	-4.437198
31	6	0	3.798015	-2.662571	-2.464861
32	1	0	4.681099	-3.214524	-2.774704
33	6	0	3.648431	-2.292879	-1.103631
34	6	0	4.601253	-2.592246	-0.095935
35	1	0	5.499447	-3.135863	-0.378751
36	6	0	4.408853	-2.191835	1.235778
37	1	0	5.164541	-2.425088	1.981885
38	6	0	3.261394	-1.501407	1.606098
39	1	0	3.115682	-1.190100	2.636671
40	6	0	2.270410	-1.194753	0.633978
41	6	0	2.458325	-1.563491	-0.728126
42	6	0	-0.258624	-1.353601	2.162918
43	6	0	-1.587265	-0.982448	2.442228

44	1	0	-2.002897	-0.080793	2.006839
45	6	0	-2.396175	-1.782068	3.249887
46	1	0	-3.421135	-1.481090	3.448069
47	6	0	-1.896432	-2.973560	3.783234
48	1	0	-2.528246	-3.600543	4.405966
49	6	0	-0.583682	-3.359013	3.501080
50	1	0	-0.189347	-4.287562	3.904713
51	6	0	0.229878	-2.558325	2.694169
52	1	0	1.242760	-2.878504	2.475209
53	6	0	1.167818	1.200982	1.917323
54	6	0	0.219326	1.892305	2.692388
55	1	0	-0.764248	1.470680	2.865065
56	6	0	0.526611	3.134916	3.250629
57	1	0	-0.218808	3.652169	3.848508
58	6	0	1.781169	3.713057	3.038120
59	1	0	2.017049	4.681622	3.469673
60	6	0	2.729885	3.036056	2.267436
61	1	0	3.707669	3.476961	2.094189
62	6	0	2.426412	1.793056	1.708692
63	1	0	3.167645	1.283403	1.102494
64	7	0	0.596599	1.983344	-1.218932
65	7	0	-1.802323	1.162830	-0.611639
66	7	0	-1.745429	-1.433260	-0.826059
67	7	0	1.512258	-1.212210	-1.664983
68	15	0	0.728826	-0.330143	0.988087
69	44	0	-0.216241	0.023761	-1.028338
70	6	0	-1.614509	0.008190	-3.568929
71	8	0	-2.759587	-0.060088	-3.575697

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^{3}3-CO-fix-310 E_{opt} = -2156.9581351 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.740977	2.420499	-1.514618
2	1	0	2.420336	1.629613	-1.814045
3	6	0	2.142390	3.745820	-1.471868
4	1	0	3.156608	4.008880	-1.752354
5	6	0	1.222133	4.718660	-1.051709
6	1	0	1.507547	5.763977	-0.993261
7	6	0	-0.062778	4.322827	-0.706815
8	1	0	-0.790337	5.054997	-0.375233
9	6	0	-0.425229	2.970188	-0.780529
10	6	0	-1.758365	2.457405	-0.458006
11	6	0	-2.880627	3.205934	-0.108428
12	1	0	-2.818710	4.285937	-0.034353
13	6	0	-4.093877	2.551413	0.137564
14	1	0	-4.973376	3.126317	0.407399
15	6	0	-4.177975	1.160195	0.024117
16	1	0	-5.120345	0.654700	0.203576
17	6	0	-3.041104	0.430122	-0.323146
18	6	0	-2.937113	-1.021886	-0.466056
19	6	0	-3.992679	-1.914393	-0.222556
20	1	0	-4.963572	-1.528388	0.067362
21	6	0	-3.788562	-3.280695	-0.337577
22	1	0	-4.600047	-3.974844	-0.144375
23	6	0	-2.513859	-3.749426	-0.699485
24	1	0	-2.306868	-4.809801	-0.796528
25	6	0	-1.505564	-2.829891	-0.933443
26	1	0	-0.503817	-3.141238	-1.210373

27	6	0	1.652043	-1.465531	-3.023954
28	1	0	0.829039	-1.187664	-3.675971
29	6	0	2.770026	-2.124675	-3.502378
30	1	0	2.829815	-2.375623	-4.557552
31	6	0	3.813867	-2.456214	-2.621160
32	1	0	4.705981	-2.965390	-2.975183
33	6	0	3.699223	-2.122767	-1.247081
34	6	0	4.697538	-2.403670	-0.278813
35	1	0	5.606995	-2.903415	-0.603450
36	6	0	4.534885	-2.039296	1.067369
37	1	0	5.325299	-2.256459	1.781703
38	6	0	3.373464	-1.405646	1.492852
39	1	0	3.251414	-1.122717	2.534611
40	6	0	2.338348	-1.120275	0.561630
41	6	0	2.496103	-1.450570	-0.813529
42	6	0	-0.142041	-1.411906	2.151646
43	6	0	-1.481478	-1.106978	2.457134
44	1	0	-1.945892	-0.221732	2.037356
45	6	0	-2.235890	-1.950044	3.273423
46	1	0	-3.270035	-1.699978	3.493435
47	6	0	-1.669253	-3.119461	3.788551
48	1	0	-2.258254	-3.780069	4.418461
49	6	0	-0.344917	-3.439528	3.479614
50	1	0	0.101003	-4.350520	3.869354
51	6	0	0.414130	-2.595033	2.664387
52	1	0	1.437315	-2.863626	2.424758
53	6	0	1.175181	1.199627	1.926909
54	6	0	0.227909	1.825394	2.756827
55	1	0	-0.725895	1.351347	2.959217
56	6	0	0.498695	3.068446	3.332981

57	1	0	-0.244651	3.535091	3.973557
58	6	0	1.714634	3.711300	3.084691
59	1	0	1.921772	4.680149	3.530170
60	6	0	2.662254	3.098694	2.260579
61	1	0	3.609964	3.590456	2.059259
62	6	0	2.395335	1.855603	1.683938
63	1	0	3.133947	1.396155	1.035853
64	7	0	0.495000	2.015475	-1.178043
65	7	0	-1.853961	1.088240	-0.547500
66	7	0	-1.686619	-1.491986	-0.830183
67	7	0	1.504739	-1.114484	-1.707915
68	15	0	0.772885	-0.326997	0.974350
69	44	0	-0.228589	0.027961	-1.007180
70	6	0	-1.869035	0.227125	-3.630016
71	8	0	-2.994682	0.066202	-3.504437

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^{3}3-CO-fix-400-opt E_{opt} = -2156.9586941 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.017787	-2.131203	-1.585330
2	1	0	-2.592992	-1.251629	-1.853921
3	6	0	-2.584410	-3.394697	-1.576125
4	1	0	-3.625815	-3.518185	-1.853299
5	6	0	-1.792234	-4.489735	-1.194262
6	1	0	-2.207942	-5.491650	-1.164636
7	6	0	-0.466838	-4.270822	-0.846829
8	1	0	0.160629	-5.100254	-0.540461
9	6	0	0.065269	-2.973130	-0.880494

10	6	0	1.447838	-2.640220	-0.535360
11	6	0	2.468542	-3.529597	-0.203181
12	1	0	2.278014	-4.596359	-0.167484
13	6	0	3.748960	-3.035005	0.074104
14	1	0	4.549210	-3.720875	0.330952
15	6	0	4.002436	-1.660531	0.010459
16	1	0	4.996188	-1.278860	0.216300
17	6	0	2.966547	-0.787438	-0.320237
18	6	0	3.039244	0.669708	-0.412261
19	6	0	4.196034	1.418458	-0.144970
20	1	0	5.113443	0.907200	0.125328
21	6	0	4.161083	2.802188	-0.218039
22	1	0	5.051925	3.385524	-0.008620
23	6	0	2.952324	3.434322	-0.559335
24	1	0	2.876631	4.514536	-0.622850
25	6	0	1.839634	2.652545	-0.818608
26	1	0	0.883745	3.093382	-1.081554
27	6	0	-1.473304	1.711166	-2.974659
28	1	0	-0.669929	1.387723	-3.630005
29	6	0	-2.526529	2.478935	-3.438188
30	1	0	-2.553919	2.769071	-4.484620
31	6	0	-3.546272	2.870831	-2.553806
32	1	0	-4.386969	3.467682	-2.896428
33	6	0	-3.474674	2.482594	-1.191165
34	6	0	-4.453236	2.819211	-0.220658
35	1	0	-5.311179	3.409366	-0.533538
36	6	0	-4.335095	2.399507	1.114005
37	1	0	-5.108226	2.665085	1.830861
38	6	0	-3.240111	1.648683	1.524493
39	1	0	-3.152859	1.322652	2.557093

40	6	0	-2.228507	1.297863	0.589637
41	6	0	-2.340144	1.691734	-0.773339
42	6	0	0.262440	1.348123	2.180740
43	6	0	1.571298	0.931147	2.486624
44	1	0	1.964624	0.016575	2.057740
45	6	0	2.391334	1.702555	3.310322
46	1	0	3.401490	1.367063	3.528171
47	6	0	1.922717	2.910803	3.834427
48	1	0	2.563674	3.515948	4.469307
49	6	0	0.630008	3.341363	3.526638
50	1	0	0.260163	4.283393	3.922226
51	6	0	-0.194448	2.569032	2.703230
52	1	0	-1.190653	2.924705	2.463538
53	6	0	-1.259074	-1.148364	1.899263
54	6	0	-0.334701	-1.904391	2.642768
55	1	0	0.677259	-1.545520	2.791827
56	6	0	-0.701064	-3.133574	3.194467
57	1	0	0.026901	-3.701924	3.766905
58	6	0	-1.992360	-3.634172	3.005776
59	1	0	-2.274788	-4.592725	3.431638
60	6	0	-2.916959	-2.893604	2.265052
61	1	0	-3.922700	-3.274403	2.110430
62	6	0	-2.554210	-1.663228	1.712840
63	1	0	-3.278184	-1.104589	1.129717
64	7	0	-0.727613	-1.897356	-1.249341
65	7	0	1.711408	-1.290025	-0.575654
66	7	0	1.855930	1.299838	-0.759579
67	7	0	-1.369936	1.304570	-1.670420
68	15	0	-0.737788	0.363503	0.982037
69	44	0	0.229340	-0.028394	-1.003204

70	6	0	1.988334	0.127307	-3.722177
71	8	0	3.103385	-0.010687	-3.516768

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^{1}TS1 E_{opt} = -2232.236239 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.017079	-3.133197	-0.850726
2	1	0	-0.960430	-2.841021	-1.300196
3	6	0	0.280665	-4.459579	-0.606246
4	1	0	-0.436147	-5.229165	-0.872815
5	6	0	1.516213	-4.780435	-0.006824
6	1	0	1.777729	-5.812069	0.206849
7	6	0	2.388909	-3.755082	0.309228
8	1	0	3.344292	-3.973339	0.774574
9	6	0	2.047670	-2.416848	0.031372
10	6	0	2.898097	-1.277317	0.303467
11	6	0	4.181991	-1.287995	0.843093
12	1	0	4.646616	-2.229097	1.119109
13	6	0	4.874913	-0.084738	1.029049
14	1	0	5.877280	-0.093490	1.444010
15	6	0	4.265218	1.132097	0.691782
16	1	0	4.794134	2.067017	0.845734
17	6	0	2.980816	1.139853	0.156841
18	6	0	2.199450	2.291412	-0.243695
19	6	0	2.613225	3.630018	-0.102986
20	1	0	3.583583	3.840952	0.333992
21	6	0	1.785907	4.663334	-0.503264
22	1	0	2.099331	5.696422	-0.391383

23	6	0	0.524716	4.347549	-1.051504
24	1	0	-0.160123	5.123686	-1.377008
25	6	0	0.159817	3.021180	-1.170428
26	1	0	-0.805098	2.735253	-1.576573
27	6	0	-1.308889	-0.045136	-3.336659
28	1	0	-0.310714	-0.021176	-3.759648
29	6	0	-2.439483	-0.083888	-4.180904
30	1	0	-2.292858	-0.086935	-5.255569
31	6	0	-3.695226	-0.131163	-3.622990
32	1	0	-4.588570	-0.177340	-4.239182
33	6	0	-3.822248	-0.120698	-2.209910
34	6	0	-5.080715	-0.184465	-1.555026
35	1	0	-5.979969	-0.239480	-2.162107
36	6	0	-5.156948	-0.185728	-0.179128
37	1	0	-6.121121	-0.245857	0.316348
38	6	0	-3.977986	-0.102086	0.598309
39	1	0	-4.055127	-0.104055	1.681732
40	6	0	-2.732470	-0.019874	-0.000582
41	6	0	-2.633528	-0.053928	-1.421871
42	6	0	-1.145341	1.680177	1.817483
43	6	0	0.079445	2.116385	2.359913
44	1	0	0.968687	1.504641	2.243078
45	6	0	0.170364	3.342414	3.017694
46	1	0	1.123934	3.662363	3.428311
47	6	0	-0.954921	4.165776	3.125716
48	1	0	-0.882348	5.126559	3.627334
49	6	0	-2.169379	3.751358	2.574474
50	1	0	-3.046062	4.389447	2.645092
51	6	0	-2.267128	2.516799	1.924769
52	1	0	-3.217607	2.219922	1.495292

53	6	0	-1.200471	-1.229517	2.143695
54	6	0	-0.505676	-1.120540	3.362042
55	1	0	-0.016311	-0.190519	3.632606
56	6	0	-0.438942	-2.203529	4.241310
57	1	0	0.095789	-2.097298	5.181264
58	6	0	-1.056519	-3.415212	3.918106
59	1	0	-1.002293	-4.256708	4.602832
60	6	0	-1.745542	-3.535557	2.708012
61	1	0	-2.228405	-4.472930	2.445673
62	6	0	-1.815815	-2.455635	1.826532
63	1	0	-2.349435	-2.569358	0.888921
64	7	0	0.822142	-2.108316	-0.552042
65	7	0	2.318807	-0.065935	-0.068046
66	7	0	0.955370	1.987007	-0.787608
67	7	0	-1.377108	-0.038357	-2.007040
68	15	0	-1.115715	0.099263	0.873127
69	44	0	0.468776	-0.047618	-0.716513
70	6	0	2.367903	-0.427262	-3.004099
71	8	0	2.211891	0.606675	-3.577584
72	8	0	2.811894	-1.516006	-2.830132

$^{1}3\text{-}CO_2$ E_{opt} = -2043.64775646 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.091433	2.205537	-1.129496
2	1	0	2.682487	1.346429	-1.426766
3	6	0	2.664154	3.461731	-0.976591
4	1	0	3.723661	3.594772	-1.167508

5	6	0	1.854379	4.527673	-0.572361
6	1	0	2.269845	5.520584	-0.433875
7	6	0	0.502299	4.294263	-0.345980
8	1	0	-0.146188	5.102743	-0.028542
9	6	0	-0.022985	3.010074	-0.530614
10	6	0	-1.435502	2.666834	-0.318606
11	6	0	-2.464992	3.536519	0.051195
12	1	0	-2.263865	4.589074	0.214109
13	6	0	-3.759989	3.037096	0.198037
14	1	0	-4.568631	3.702977	0.480243
15	6	0	-4.019356	1.681646	-0.027838
16	1	0	-5.026211	1.291887	0.067905
17	6	0	-2.966197	0.842437	-0.389633
18	6	0	-3.035129	-0.600438	-0.667704
19	6	0	-4.199573	-1.365444	-0.554322
20	1	0	-5.132404	-0.890319	-0.272948
21	6	0	-4.149701	-2.735616	-0.792549
22	1	0	-5.045854	-3.340799	-0.702699
23	6	0	-2.925843	-3.315076	-1.139732
24	1	0	-2.836926	-4.379776	-1.327679
25	6	0	-1.802914	-2.503122	-1.244889
26	1	0	-0.831851	-2.905890	-1.510293
27	6	0	1.712121	-1.443219	-2.883473
28	1	0	0.930953	-1.138706	-3.577896
29	6	0	2.868372	-2.126520	-3.319275
30	1	0	2.982445	-2.338723	-4.377238
31	6	0	3.824732	-2.492449	-2.405054
32	1	0	4.736458	-3.002092	-2.703896
33	6	0	3.605520	-2.202548	-1.033928
34	6	0	4.545123	-2.559174	-0.031429

35	1	0	5.460196	-3.059975	-0.335298
36	6	0	4.302952	-2.276620	1.294948
37	1	0	5.027394	-2.546630	2.057030
38	6	0	3.096929	-1.643763	1.669042
39	1	0	2.906499	-1.439042	2.718660
40	6	0	2.153535	-1.280690	0.721370
41	6	0	2.399262	-1.531544	-0.660058
42	6	0	-0.424972	-1.751241	2.024237
43	6	0	-1.780614	-1.458778	2.270793
44	1	0	-2.188675	-0.495838	1.981023
45	6	0	-2.616955	-2.403835	2.864203
46	1	0	-3.659986	-2.159756	3.044673
47	6	0	-2.119738	-3.665883	3.203163
48	1	0	-2.773129	-4.406677	3.655073
49	6	0	-0.781418	-3.972692	2.947327
50	1	0	-0.388763	-4.953481	3.201325
51	6	0	0.062235	-3.024313	2.361285
52	1	0	1.095997	-3.286203	2.162753
53	6	0	0.956262	0.828430	2.316478
54	6	0	0.019375	1.265874	3.269541
55	1	0	-0.909129	0.724863	3.416846
56	6	0	0.269263	2.402348	4.042776
57	1	0	-0.464271	2.719399	4.778997
58	6	0	1.450601	3.128501	3.871547
59	1	0	1.640069	4.015090	4.469734
60	6	0	2.388498	2.702555	2.926682
61	1	0	3.311519	3.257636	2.783910
62	6	0	2.146159	1.564698	2.156656
63	1	0	2.883621	1.253169	1.425488
64	7	0	0.784343	1.965810	-0.910568

65	7	0	-1.705703	1.345813	-0.507438
66	7	0	-1.839315	-1.175847	-1.018536
67	7	0	1.473109	-1.123504	-1.611306
68	15	0	0.550610	-0.493544	1.104148
69	44	0	-0.238553	0.163053	-1.032571
70	6	0	-0.729937	0.613122	-3.079086
71	8	0	-0.815510	-0.343819	-3.907477
72	8	0	-0.963171	1.827565	-3.330933

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^{1}4 E_{opt} =-2232.761266 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.875870	-0.702244	-1.427982
2	1	0	-2.933466	0.343530	-1.707852
3	6	0	-4.010241	-1.502201	-1.348777
4	1	0	-4.981614	-1.077228	-1.576306
5	6	0	-3.868918	-2.838155	-0.970054
6	1	0	-4.734714	-3.487199	-0.891910
7	6	0	-2.596857	-3.332125	-0.693489
8	1	0	-2.462277	-4.366512	-0.400526
9	6	0	-1.491549	-2.484208	-0.793142
10	6	0	-0.100468	-2.913522	-0.548873
11	6	0	0.331945	-4.195326	-0.199887
12	1	0	-0.379749	-5.001961	-0.071544
13	6	0	1.696783	-4.420917	-0.018977
14	1	0	2.048676	-5.410141	0.253343
15	6	0	2.612623	-3.378695	-0.182955
16	1	0	3.672228	-3.550074	-0.034379

17	6	0	2.140494	-2.112774	-0.531017
18	6	0	2.939708	-0.880902	-0.691752
19	6	0	4.329499	-0.836623	-0.571059
20	1	0	4.887510	-1.747591	-0.388457
21	6	0	4.988610	0.386040	-0.679429
22	1	0	6.068068	0.434703	-0.581329
23	6	0	4.240358	1.540431	-0.910160
24	1	0	4.711386	2.513404	-0.996602
25	6	0	2.858048	1.431761	-1.033815
26	1	0	2.231980	2.297216	-1.218597
27	6	0	-0.598167	2.549133	-2.576511
28	1	0	-0.042130	2.044230	-3.355976
29	6	0	-1.231907	3.779378	-2.846771
30	1	0	-1.154573	4.198903	-3.843863
31	6	0	-1.943342	4.403457	-1.852284
32	1	0	-2.465106	5.340020	-2.026416
33	6	0	-1.985783	3.810360	-0.565392
34	6	0	-2.692401	4.406403	0.512114
35	1	0	-3.223177	5.336498	0.329591
36	6	0	-2.704080	3.819924	1.758136
37	1	0	-3.249767	4.277168	2.577372
38	6	0	-1.985052	2.624428	1.978117
39	1	0	-1.978817	2.180944	2.969471
40	6	0	-1.284238	2.011144	0.952372
41	6	0	-1.291849	2.578259	-0.354575
42	6	0	1.161708	0.998829	2.198192
43	6	0	2.201718	0.064361	2.360510
44	1	0	2.112227	-0.930001	1.936681
45	6	0	3.362721	0.406323	3.053218
46	1	0	4.155143	-0.327717	3.167335

47	6	0	3.510891	1.692177	3.581020
48	1	0	4.418749	1.962247	4.112653
49	6	0	2.489956	2.630285	3.414528
50	1	0	2.599726	3.633358	3.816971
51	6	0	1.321454	2.289184	2.727244
52	1	0	0.545002	3.035741	2.600987
53	6	0	-1.300315	-0.629136	2.180059
54	6	0	-0.717147	-1.575403	3.039273
55	1	0	0.349947	-1.562404	3.231910
56	6	0	-1.505723	-2.545998	3.662423
57	1	0	-1.039278	-3.266507	4.328319
58	6	0	-2.882540	-2.591458	3.431985
59	1	0	-3.492338	-3.350264	3.913651
60	6	0	-3.471099	-1.652515	2.580411
61	1	0	-4.540787	-1.678061	2.393434
62	6	0	-2.688695	-0.679496	1.958358
63	1	0	-3.161537	0.035842	1.294832
64	7	0	-1.642250	-1.165864	-1.152212
65	7	0	0.807787	-1.916381	-0.700798
66	7	0	2.215900	0.257952	-0.926500
67	7	0	-0.631206	1.935522	-1.393494
68	15	0	-0.274496	0.507546	1.163184
69	44	0	0.161885	-0.089836	-1.098176
70	6	0	0.518565	-0.331078	-3.140462
71	8	0	1.244661	0.365091	-3.843340
72	8	0	-0.050603	-1.410431	-3.813268
73	1	0	-0.643924	-1.869038	-3.200488

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^{1}TS2 E_{opt} =-2497.78364787 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567537	-2.954901	-0.866901
2	1	0	-0.226086	-2.951097	-1.605238
3	6	0	1.141934	-4.138369	-0.415354
4	1	0	0.795893	-5.086705	-0.810905
5	6	0	2.146407	-4.072400	0.550201
6	1	0	2.607889	-4.976940	0.932091
7	6	0	2.555583	-2.827384	1.020317
8	1	0	3.340172	-2.752771	1.762458
9	6	0	1.952224	-1.672559	0.523309
10	6	0	2.336778	-0.306521	0.934425
11	6	0	3.360400	0.044553	1.818041
12	1	0	3.969721	-0.716113	2.289063
13	6	0	3.598336	1.395641	2.065776
14	1	0	4.396086	1.686024	2.740690
15	6	0	2.817935	2.379779	1.453720
16	1	0	2.997909	3.428415	1.657066
17	6	0	1.801272	1.984745	0.584082
18	6	0	0.825495	2.861587	-0.101279
19	6	0	0.827384	4.252477	0.005173
20	1	0	1.602475	4.753229	0.572707
21	6	0	-0.180766	4.989210	-0.613757
22	1	0	-0.192771	6.070985	-0.531730
23	6	0	-1.171097	4.318270	-1.329575
24	1	0	-1.977636	4.851663	-1.820036
25	6	0	-1.112073	2.929831	-1.415084
26	1	0	-1.850755	2.358700	-1.966182
27	6	0	-1.571105	-0.550487	-3.384850

28	1	0	-0.701654	-0.122154	-3.864147
29	6	0	-2.597314	-1.087530	-4.186187
30	1	0	-2.490170	-1.053041	-5.264540
31	6	0	-3.693200	-1.653098	-3.582706
32	1	0	-4.497750	-2.095129	-4.162842
33	6	0	-3.771646	-1.655342	-2.167953
34	6	0	-4.874157	-2.227610	-1.480917
35	1	0	-5.670481	-2.677071	-2.066937
36	6	0	-4.930471	-2.216500	-0.105211
37	1	0	-5.771868	-2.661485	0.415990
38	6	0	-3.891604	-1.611225	0.634779
39	1	0	-3.950616	-1.593880	1.718953
40	6	0	-2.801068	-1.037385	0.001081
41	6	0	-2.705405	-1.066605	-1.419231
42	6	0	-2.181505	1.318881	1.631749
43	6	0	-1.320952	2.239049	2.258930
44	1	0	-0.261658	2.026552	2.349885
45	6	0	-1.812983	3.445367	2.756207
46	1	0	-1.132971	4.144165	3.234411
47	6	0	-3.168364	3.758721	2.623028
48	1	0	-3.549815	4.702152	3.002439
49	6	0	-4.027741	2.857290	1.992038
50	1	0	-5.081538	3.095159	1.878878
51	6	0	-3.540517	1.644730	1.496780
52	1	0	-4.224042	0.965585	0.999977
53	6	0	-0.975331	-1.318347	2.257721
54	6	0	-0.363026	-0.828718	3.423665
55	1	0	-0.275218	0.237016	3.598654
56	6	0	0.143069	-1.712088	4.379855
57	1	0	0.608738	-1.316900	5.278048

58	6	0	0.054601	-3.091848	4.182381
59	1	0	0.453868	-3.776570	4.924848
60	6	0	-0.550954	-3.586444	3.024512
61	1	0	-0.622665	-4.657453	2.859130
62	6	0	-1.061471	-2.709062	2.067441
63	1	0	-1.518707	-3.111953	1.170808
64	7	0	0.951192	-1.749020	-0.410610
65	7	0	1.602241	0.665927	0.351077
66	7	0	-0.144149	2.215494	-0.821188
67	7	0	-1.588417	-0.537628	-2.051222
68	15	0	-1.451744	-0.192496	0.886313
69	44	0	0.116759	0.130536	-0.864309
70	6	0	1.222495	0.496272	-2.520907
71	8	0	1.313487	1.267372	-3.404869
72	8	0	2.635462	-0.655094	-2.773962
73	1	0	2.591530	-1.356239	-2.105051
74	6	0	5.015878	-0.086306	-0.985177
75	8	0	4.754796	-1.266295	-0.718161
76	8	0	5.993145	0.575151	-0.293384
77	8	0	4.461366	0.655282	-1.878802
78	1	0	3.537890	-0.017956	-2.393832
79	1	0	6.333433	-0.061073	0.356561

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^{1}TS3 E_{opt} = -2538.505418 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.623026	-2.862974	-0.897512
2	1	0	-0.341347	-3.066753	-1.348920

3	6	0	1.521010	-3.881097	-0.591736
4	1	0	1.261314	-4.910213	-0.813386
5	6	0	2.734798	-3.545125	0.007408
6	1	0	3.453508	-4.315147	0.268438
7	6	0	3.021045	-2.206932	0.269876
8	1	0	3.966138	-1.925144	0.718317
9	6	0	2.086852	-1.229428	-0.075163
10	6	0	2.301185	0.217497	0.137106
11	6	0	3.429173	0.818668	0.695841
12	1	0	4.266444	0.225496	1.037060
13	6	0	3.464565	2.209082	0.799928
14	1	0	4.351701	2.671205	1.219199
15	6	0	2.388093	2.982501	0.361443
16	1	0	2.415529	4.061794	0.448631
17	6	0	1.282146	2.335818	-0.192124
18	6	0	0.038064	2.969005	-0.678209
19	6	0	-0.178928	4.347200	-0.685531
20	1	0	0.603736	5.023773	-0.364454
21	6	0	-1.411359	4.846699	-1.101453
22	1	0	-1.590874	5.916775	-1.107655
23	6	0	-2.407657	3.955885	-1.498992
24	1	0	-3.383380	4.301013	-1.822195
25	6	0	-2.131763	2.591944	-1.477441
26	1	0	-2.868530	1.855410	-1.777700
27	6	0	-2.623444	-0.980198	-2.864959
28	1	0	-2.073816	-0.399776	-3.593094
29	6	0	-3.718607	-1.754974	-3.295325
30	1	0	-3.986515	-1.743724	-4.345805
31	6	0	-4.399435	-2.519885	-2.380487
32	1	0	-5.230330	-3.153889	-2.675260

33	6	0	-4.014794	-2.463400	-1.017784
34	6	0	-4.691946	-3.205400	-0.014595
35	1	0	-5.511259	-3.851653	-0.315750
36	6	0	-4.324062	-3.101619	1.308369
37	1	0	-4.843751	-3.671680	2.071614
38	6	0	-3.280812	-2.225892	1.680998
39	1	0	-3.022546	-2.120491	2.730354
40	6	0	-2.589096	-1.493558	0.729782
41	6	0	-2.920598	-1.621580	-0.648806
42	6	0	-2.180618	1.148449	1.915538
43	6	0	-1.453121	2.324568	2.174759
44	1	0	-0.391038	2.371056	1.964781
45	6	0	-2.090718	3.452395	2.690451
46	1	0	-1.513955	4.352325	2.882574
47	6	0	-3.465107	3.427768	2.942501
48	1	0	-3.962903	4.308975	3.336501
49	6	0	-4.196745	2.268238	2.678317
50	1	0	-5.266062	2.242309	2.867238
51	6	0	-3.562021	1.133554	2.166128
52	1	0	-4.150712	0.246944	1.958848
53	6	0	-0.217420	-1.029155	2.387481
54	6	0	0.585367	-0.227033	3.215831
55	1	0	0.479755	0.851425	3.215040
56	6	0	1.540102	-0.809938	4.051485
57	1	0	2.151374	-0.176215	4.687342
58	6	0	1.713124	-2.195828	4.064533
59	1	0	2.460900	-2.646288	4.710589
60	6	0	0.921236	-2.999282	3.240474
61	1	0	1.051612	-4.077441	3.238973
62	6	0	-0.036337	-2.423113	2.405019

63	1	0	-0.629799	-3.061872	1.761254
64	7	0	0.890795	-1.573048	-0.640754
65	7	0	1.275710	0.989026	-0.274951
66	7	0	-0.944212	2.107348	-1.082737
67	7	0	-2.195763	-0.923036	-1.603784
68	15	0	-1.310653	-0.263228	1.129129
69	44	0	-0.343256	0.098796	-1.014966
70	6	0	0.270167	0.123190	-2.878452
71	8	0	0.316063	-0.237526	-3.983478
72	1	0	2.925211	-0.842319	-3.295070
73	8	0	1.856493	1.727095	-2.954613
74	1	0	1.819309	1.849742	-3.913921
75	8	0	3.266954	-0.219897	-2.641280
76	1	0	4.591842	-0.806770	-2.060744
77	8	0	5.407068	-1.317119	-1.725120
78	1	0	5.900188	-1.021313	-0.182950
79	8	0	6.125071	-0.901787	0.785529
80	1	0	6.522770	0.821064	1.124806
81	8	0	6.629120	1.790071	1.239688
82	1	0	2.633358	0.766811	-2.794337
83	1	0	6.820219	-1.545572	0.976785
84	1	0	6.604671	2.122561	0.332393
85	1	0	5.106271	-2.236062	-1.716340

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^{2}TS4 E_{opt} = -2923.37127594 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034424	-2.724919	1.297908

2	1	0	-0.314660	-3.234784	0.382736
3	6	0	0.243042	-3.425984	2.467314
4	1	0	0.194816	-4.509199	2.465455
5	6	0	0.564709	-2.710709	3.620741
6	1	0	0.776641	-3.225584	4.551789
7	6	0	0.606891	-1.319556	3.564043
8	1	0	0.854988	-0.742386	4.446601
9	6	0	0.332679	-0.669525	2.360231
10	6	0	0.362329	0.797516	2.198602
11	6	0	0.671419	1.740790	3.180864
12	1	0	0.920890	1.428713	4.187588
13	6	0	0.655211	3.094804	2.842983
14	1	0	0.898131	3.840076	3.592471
15	6	0	0.319897	3.496892	1.548313
16	1	0	0.300787	4.547966	1.288560
17	6	0	0.012664	2.522670	0.597984
18	6	0	-0.404164	2.746457	-0.800995
19	6	0	-0.511690	4.008485	-1.386370
20	1	0	-0.259584	4.894976	-0.817423
21	6	0	-0.948811	4.117390	-2.704643
22	1	0	-1.040136	5.093183	-3.169980
23	6	0	-1.269679	2.957669	-3.410218
24	1	0	-1.618008	2.996467	-4.436358
25	6	0	-1.140059	1.726659	-2.774107
26	1	0	-1.377601	0.797268	-3.278220
27	6	0	-0.673141	-2.090920	-2.882628
28	1	0	0.214180	-1.547034	-3.173574
29	6	0	-1.095252	-3.195494	-3.651947
30	1	0	-0.516389	-3.472462	-4.526142
31	6	0	-2.204876	-3.904829	-3.264502

32	1	0	-2.541372	-4.780931	-3.811066
33	6	0	-2.938455	-3.460504	-2.135727
34	6	0	-4.123418	-4.108958	-1.699129
35	1	0	-4.452297	-4.997041	-2.230943
36	6	0	-4.846561	-3.615936	-0.635071
37	1	0	-5.752874	-4.114675	-0.307152
38	6	0	-4.426268	-2.434467	0.014827
39	1	0	-5.028331	-2.024854	0.820106
40	6	0	-3.263924	-1.787508	-0.370790
41	6	0	-2.475311	-2.306164	-1.434223
42	6	0	-3.824982	1.071976	-0.396824
43	6	0	-3.565102	2.432077	-0.146729
44	1	0	-2.744493	2.725121	0.497185
45	6	0	-4.346228	3.423956	-0.738125
46	1	0	-4.128267	4.468375	-0.535425
47	6	0	-5.391459	3.075040	-1.597994
48	1	0	-5.994836	3.848174	-2.064580
49	6	0	-5.651170	1.728513	-1.859942
50	1	0	-6.459364	1.448189	-2.529275
51	6	0	-4.873586	0.730315	-1.266566
52	1	0	-5.087835	-0.308605	-1.490763
53	6	0	-2.986942	-0.263225	2.111730
54	6	0	-3.150568	0.912050	2.864653
55	1	0	-3.224978	1.877102	2.378270
56	6	0	-3.220318	0.854378	4.257996
57	1	0	-3.350185	1.772097	4.824206
58	6	0	-3.122453	-0.372329	4.918907
59	1	0	-3.173259	-0.413870	6.002974
60	6	0	-2.957800	-1.545063	4.177800
61	1	0	-2.875451	-2.503753	4.681283

62	6	0	-2.886284	-1.493508	2.785577
63	1	0	-2.740687	-2.412797	2.230287
64	7	0	0.008297	-1.380300	1.232301
65	7	0	0.056024	1.211923	0.944663
66	7	0	-0.720691	1.614286	-1.503669
67	7	0	-1.294290	-1.666784	-1.782388
68	15	0	-2.693730	-0.196695	0.301108
69	44	0	-0.492323	-0.139243	-0.392100
70	6	0	1.552800	-0.530306	-1.442419
71	8	0	1.631111	-0.029310	-2.570505
72	8	0	1.971501	-1.856946	-1.334595
73	1	0	1.862482	-2.134121	-0.410486
74	6	0	6.052916	-3.527699	-1.057592
75	6	0	5.667147	-2.364223	-1.724627
76	6	0	4.996616	-1.395118	-0.974029
77	6	0	4.720699	-1.591859	0.397433
78	6	0	5.103120	-2.758206	1.062777
79	6	0	5.775780	-3.722541	0.310034
80	1	0	6.574665	-4.304320	-1.608107
81	1	0	5.871394	-2.217846	-2.779196
82	1	0	4.888425	-2.901505	2.115987
83	1	0	6.091306	-4.643799	0.789637
84	6	0	2.919930	2.651208	-0.883563
85	6	0	2.932469	4.041149	-0.761781
86	6	0	3.731928	4.654553	0.204894
87	6	0	4.534796	3.873998	1.041610
88	6	0	4.546579	2.485298	0.907865
89	6	0	3.732635	1.867333	-0.053227
90	1	0	2.281459	2.172808	-1.618978
91	1	0	2.303331	4.639898	-1.412367

92	1	0	3.730501	5.735824	0.306601
93	1	0	5.161738	4.345352	1.792690
94	1	0	5.192539	1.886465	1.541075
95	7	0	4.062250	-0.470665	0.846982
96	7	0	4.507993	-0.157281	-1.317779
97	6	0	3.769333	0.377694	-0.236505
98	6	0	4.618520	0.400933	-2.656257
99	1	0	3.904019	-0.080435	-3.329324
100	1	0	4.418734	1.470547	-2.627262
101	1	0	5.637685	0.240069	-3.015959
102	6	0	3.651900	-0.290787	2.229551
103	1	0	3.041391	0.603314	2.317839
104	1	0	3.079640	-1.160254	2.556854
105	1	0	4.535032	-0.184850	2.866308
106	1	0	2.397501	0.115203	-0.536768

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[1] TS5 E_{opt} = -2922.79579725 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.801519	-2.363499	-0.125928
2	1	0	0.192500	-2.848398	-0.880442
3	6	0	1.763499	-3.065854	0.594665
4	1	0	1.930934	-4.115768	0.383972
5	6	0	2.475053	-2.398658	1.588319
6	1	0	3.221991	-2.916437	2.178144
7	6	0	2.220830	-1.046855	1.813999
8	1	0	2.756784	-0.512218	2.587533
9	6	0	1.263729	-0.388745	1.043110

10	6	0	0.924753	1.041624	1.208649
11	6	0	1.522726	1.946386	2.089552
12	1	0	2.327346	1.634433	2.743433
13	6	0	1.065959	3.264156	2.108658
14	1	0	1.524059	3.981560	2.780740
15	6	0	0.024969	3.669458	1.270906
16	1	0	-0.332998	4.691043	1.294143
17	6	0	-0.546539	2.730978	0.410005
18	6	0	-1.696520	2.941323	-0.498468
19	6	0	-2.345385	4.165733	-0.651565
20	1	0	-1.983919	5.042181	-0.127130
21	6	0	-3.469873	4.247529	-1.471399
22	1	0	-3.986721	5.193657	-1.592514
23	6	0	-3.921600	3.101819	-2.123686
24	1	0	-4.796526	3.119735	-2.763656
25	6	0	-3.222538	1.910173	-1.948214
26	1	0	-3.522771	0.992082	-2.440330
27	6	0	-1.627412	-1.706448	-3.201998
28	1	0	-0.887497	-1.066096	-3.661870
29	6	0	-2.175964	-2.770244	-3.944511
30	1	0	-1.877363	-2.892277	-4.979663
31	6	0	-3.057035	-3.630348	-3.337417
32	1	0	-3.491682	-4.470218	-3.871217
33	6	0	-3.397725	-3.418274	-1.978269
34	6	0	-4.278873	-4.287442	-1.283994
35	1	0	-4.702059	-5.130188	-1.822808
36	6	0	-4.583093	-4.072936	0.041994
37	1	0	-5.250717	-4.745272	0.570855
38	6	0	-4.028392	-2.965419	0.717831
39	1	0	-4.276987	-2.798450	1.761694

40	6	0	-3.174154	-2.086046	0.070568
41	6	0	-2.823717	-2.303073	-1.291978
42	6	0	-3.852561	0.499968	1.280483
43	6	0	-3.570412	1.759944	1.839618
44	1	0	-2.550198	2.044492	2.070607
45	6	0	-4.596396	2.672526	2.082734
46	1	0	-4.359438	3.641128	2.512799
47	6	0	-5.916316	2.347952	1.759099
48	1	0	-6.713899	3.062020	1.941667
49	6	0	-6.203514	1.105570	1.190624
50	1	0	-7.225535	0.847516	0.928955
51	6	0	-5.180440	0.185228	0.949381
52	1	0	-5.425499	-0.767991	0.495529
53	6	0	-1.719027	-1.211080	2.449409
54	6	0	-1.490778	-0.328835	3.518960
55	1	0	-1.858174	0.689505	3.488661
56	6	0	-0.781256	-0.753656	4.643964
57	1	0	-0.617377	-0.060844	5.464171
58	6	0	-0.282698	-2.056486	4.712774
59	1	0	0.273509	-2.382633	5.586652
60	6	0	-0.503178	-2.937891	3.651723
61	1	0	-0.117329	-3.952114	3.693722
62	6	0	-1.213851	-2.520911	2.525678
63	1	0	-1.363834	-3.215885	1.707253
64	7	0	0.554037	-1.061561	0.084247
65	7	0	-0.074794	1.464750	0.404277
66	7	0	-2.139415	1.827208	-1.161368
67	7	0	-1.925622	-1.456857	-1.925438
68	15	0	-2.458877	-0.621828	0.876912
69	44	0	-0.938948	0.125222	-0.808918

70	6	0	0.051667	0.757753	-2.366236
71	8	0	0.344132	1.457412	-3.239454
72	8	0	1.479995	-1.059814	-3.085827
73	1	0	1.390827	-1.827181	-2.505293
74	6	0	5.973013	-3.436636	0.778761
75	6	0	5.902950	-2.153951	1.315630
76	6	0	5.372611	-1.155388	0.493276
77	6	0	4.947838	-1.431341	-0.817278
78	6	0	5.012941	-2.719702	-1.353964
79	6	0	5.530618	-3.717148	-0.532193
80	1	0	6.376222	-4.242025	1.384812
81	1	0	6.237742	-1.937731	2.324039
82	1	0	4.665672	-2.928553	-2.359225
83	1	0	5.596424	-4.733654	-0.907217
84	6	0	4.915600	3.180955	-0.121687
85	6	0	4.442629	4.487554	-0.244678
86	6	0	3.189877	4.734666	-0.813244
87	6	0	2.404331	3.668403	-1.261561
88	6	0	2.868601	2.362086	-1.135656
89	6	0	4.126664	2.105796	-0.564851
90	1	0	5.897760	2.997318	0.300980
91	1	0	5.058591	5.313906	0.096906
92	1	0	2.827573	5.754128	-0.907238
93	1	0	1.427703	3.851034	-1.698301
94	1	0	2.259131	1.530345	-1.459497
95	7	0	4.474100	-0.240058	-1.365709
96	7	0	5.112942	0.183670	0.721509
97	6	0	4.575566	0.719077	-0.420538
98	6	0	5.298840	0.849973	2.007460
99	1	0	6.323039	1.217695	2.108554

100	1	0	4.601797	1.682445	2.090532
101	1	0	5.090890	0.132252	2.802582
102	6	0	3.944975	-0.155799	-2.721289
103	1	0	3.974783	0.890712	-3.033171
104	1	0	4.634685	-0.721528	-3.357156
105	1	0	2.570618	-0.670745	-2.877252

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^{1}TS6 E_{opt} = -2421.32133475 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.449776	1.669330	0.631826
2	1	0	2.919988	0.715599	0.832674
3	6	0	2.984190	2.863581	1.106926
4	1	0	3.888747	2.844214	1.704262
5	6	0	2.334452	4.058013	0.804264
6	1	0	2.720719	5.006134	1.163065
7	6	0	1.171218	4.023447	0.036362
8	1	0	0.647258	4.940718	-0.203232
9	6	0	0.681268	2.798425	-0.415237
10	6	0	-0.552942	2.656387	-1.218251
11	6	0	-1.378173	3.687804	-1.673390
12	1	0	-1.144448	4.722549	-1.453693
13	6	0	-2.513317	3.361883	-2.416410
14	1	0	-3.163564	4.150865	-2.778758
15	6	0	-2.821338	2.028750	-2.695100
16	1	0	-3.705943	1.778908	-3.268273
17	6	0	-1.972621	1.028556	-2.216815
18	6	0	-2.153321	-0.433697	-2.356752

19	6	0	-3.232771	-1.021030	-3.017496
20	1	0	-3.978107	-0.401073	-3.501051
21	6	0	-3.351296	-2.409452	-3.038510
22	1	0	-4.189698	-2.876742	-3.544201
23	6	0	-2.385080	-3.183136	-2.397090
24	1	0	-2.441876	-4.265849	-2.383473
25	6	0	-1.325810	-2.541900	-1.760915
26	1	0	-0.547043	-3.096167	-1.249448
27	6	0	2.386909	-2.364860	-0.655930
28	1	0	2.363964	-2.225513	-1.727974
29	6	0	3.324426	-3.257610	-0.100787
30	1	0	3.995586	-3.788938	-0.766014
31	6	0	3.383424	-3.405330	1.263222
32	1	0	4.110031	-4.061361	1.733326
33	6	0	2.463815	-2.691008	2.071732
34	6	0	2.450709	-2.813926	3.486049
35	1	0	3.185404	-3.461975	3.954978
36	6	0	1.524662	-2.132779	4.244300
37	1	0	1.519673	-2.229369	5.325191
38	6	0	0.556963	-1.320721	3.612279
39	1	0	-0.190871	-0.815530	4.215947
40	6	0	0.543341	-1.165803	2.235496
41	6	0	1.518509	-1.828904	1.436261
42	6	0	-2.279348	-1.179958	1.465372
43	6	0	-3.375536	-0.792555	0.672977
44	1	0	-3.307946	0.077502	0.030555
45	6	0	-4.556839	-1.533461	0.684933
46	1	0	-5.391073	-1.221201	0.063578
47	6	0	-4.657848	-2.679936	1.477909
48	1	0	-5.574558	-3.262346	1.480369

49	6	0	-3.571715	-3.078051	2.259751
50	1	0	-3.639537	-3.970633	2.875032
51	6	0	-2.387618	-2.335685	2.255010
52	1	0	-1.553466	-2.668901	2.862209
53	6	0	-0.960194	1.363431	2.211431
54	6	0	-2.106163	2.138598	1.959305
55	1	0	-2.910171	1.755771	1.341724
56	6	0	-2.223749	3.422113	2.495360
57	1	0	-3.117255	4.005579	2.292895
58	6	0	-1.197397	3.955351	3.279002
59	1	0	-1.288020	4.956580	3.689884
60	6	0	-0.052852	3.194803	3.527796
61	1	0	0.753845	3.601527	4.130647
62	6	0	0.068985	1.909085	2.997619
63	1	0	0.972303	1.342395	3.190667
64	7	0	1.331420	1.627421	-0.114368
65	7	0	-0.875889	1.373599	-1.501769
66	7	0	-1.206203	-1.205425	-1.736825
67	7	0	1.529880	-1.639024	0.061938
68	15	0	-0.717781	-0.222829	1.318437
69	44	0	0.298675	-0.081844	-0.816622
70	6	0	1.261399	-0.162913	-2.617684
71	8	0	1.115292	-0.619376	-3.694160
72	8	0	2.805271	0.735753	-2.636413
73	1	0	2.734134	1.345430	-1.885462
74	6	0	4.201520	-0.262961	-2.166716
75	8	0	4.304751	-1.140021	-2.982817
76	8	0	4.650264	0.219409	-1.154362

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^{1}TS7 E_{opt} = -2922.812727 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745643	1.530582	1.615173
2	1	0	1.041646	0.564760	2.008877
3	6	0	1.122859	2.711293	2.247998
4	1	0	1.741645	2.667851	3.136866
5	6	0	0.684128	3.922353	1.719508
6	1	0	0.954828	4.863108	2.186514
7	6	0	-0.115463	3.912802	0.577911
8	1	0	-0.475319	4.842913	0.156193
9	6	0	-0.448989	2.698336	-0.021472
10	6	0	-1.295005	2.592162	-1.230972
11	6	0	-1.857118	3.648231	-1.952591
12	1	0	-1.689643	4.675998	-1.653911
13	6	0	-2.639827	3.355845	-3.070366
14	1	0	-3.085047	4.163898	-3.640747
15	6	0	-2.854737	2.033201	-3.461705
16	1	0	-3.464003	1.809355	-4.328801
17	6	0	-2.271310	1.008462	-2.713597
18	6	0	-2.408130	-0.447098	-2.943890
19	6	0	-3.165870	-0.999535	-3.976499
20	1	0	-3.661396	-0.355918	-4.693242
21	6	0	-3.290325	-2.384405	-4.070884
22	1	0	-3.882764	-2.824471	-4.866065
23	6	0	-2.651453	-3.189933	-3.129770
24	1	0	-2.727897	-4.270936	-3.162129
25	6	0	-1.898445	-2.583730	-2.127936
26	1	0	-1.380453	-3.163379	-1.372482

27	6	0	1.096882	-2.536975	0.288382
28	1	0	1.473848	-2.385404	-0.712518
29	6	0	1.739567	-3.457075	1.141125
30	1	0	2.594097	-4.008319	0.766108
31	6	0	1.293134	-3.600082	2.432458
32	1	0	1.782155	-4.273202	3.130385
33	6	0	0.159218	-2.861357	2.855605
34	6	0	-0.376357	-2.982774	4.164637
35	1	0	0.118368	-3.648730	4.865657
36	6	0	-1.502368	-2.280330	4.533442
37	1	0	-1.908047	-2.377188	5.535257
38	6	0	-2.152195	-1.447242	3.595945
39	1	0	-3.061011	-0.927752	3.884539
40	6	0	-1.652799	-1.290921	2.312721
41	6	0	-0.464528	-1.975266	1.925075
42	6	0	-3.968592	-1.269800	0.518955
43	6	0	-4.688140	-0.845779	-0.613190
44	1	0	-4.388853	0.047251	-1.149799
45	6	0	-5.782577	-1.578050	-1.071532
46	1	0	-6.324607	-1.238725	-1.949262
47	6	0	-6.166657	-2.750359	-0.414334
48	1	0	-7.013909	-3.325371	-0.776331
49	6	0	-5.451969	-3.183590	0.704210
50	1	0	-5.741543	-4.095821	1.217788
51	6	0	-4.357204	-2.450812	1.170718
52	1	0	-3.809842	-2.809876	2.035092
53	6	0	-3.025483	1.254766	1.756328
54	6	0	-4.017980	2.025602	1.126326
55	1	0	-4.556181	1.641989	0.267320
56	6	0	-4.323123	3.304003	1.597046

57	1	0	-5.095469	3.885172	1.101719
58	6	0	-3.637495	3.834017	2.692714
59	1	0	-3.872655	4.831026	3.053411
60	6	0	-2.647284	3.075413	3.321216
61	1	0	-2.106051	3.479071	4.171858
62	6	0	-2.340035	1.795185	2.857796
63	1	0	-1.560004	1.227432	3.351231
64	7	0	-0.008731	1.512297	0.504065
65	7	0	-1.522304	1.321081	-1.630996
66	7	0	-1.775633	-1.250703	-2.032106
67	7	0	0.058737	-1.784430	0.655677
68	15	0	-2.473200	-0.324338	1.003301
69	44	0	-0.713594	-0.173355	-0.581866
70	6	0	0.831582	-0.165093	-1.859924
71	8	0	1.224145	-0.163175	-2.957828
72	8	0	2.483974	-0.118779	-0.708314
73	1	0	2.058601	0.008737	0.149991
74	6	0	6.153471	-3.685778	-1.125852
75	6	0	5.850822	-2.494500	-1.801038
76	6	0	5.323478	-1.451199	-1.047217
77	6	0	5.103066	-1.589565	0.334438
78	6	0	5.395915	-2.769575	1.007991
79	6	0	5.930456	-3.822348	0.251212
80	1	0	6.561427	-4.521018	-1.687104
81	1	0	6.010962	-2.395271	-2.869205
82	1	0	5.208144	-2.872104	2.071415
83	1	0	6.169367	-4.760414	0.743047
84	6	0	3.213937	2.616893	-0.954056
85	6	0	3.159156	4.004958	-0.832173
86	6	0	3.993666	4.667211	0.072544

87	6	0	4.898684	3.935218	0.844596
88	6	0	4.970610	2.547416	0.712635
89	6	0	4.120288	1.878272	-0.180539
90	1	0	2.550563	2.096981	-1.632205
91	1	0	2.451508	4.567027	-1.434198
92	1	0	3.938455	5.747102	0.175240
93	1	0	5.554033	4.441864	1.546910
94	1	0	5.685611	1.981792	1.301744
95	7	0	4.568674	-0.383761	0.787625
96	7	0	4.926769	-0.159414	-1.395076
97	6	0	4.252001	0.392283	-0.317818
98	6	0	4.736063	0.290659	-2.762470
99	1	0	3.752290	-0.017490	-3.136123
100	1	0	4.812976	1.377847	-2.806959
101	1	0	5.520369	-0.138310	-3.387715
102	6	0	3.939039	-0.255369	2.095638
103	1	0	3.549531	0.753807	2.218879
104	1	0	3.119982	-0.976473	2.197182
105	1	0	4.679647	-0.445739	2.875849

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^{1}TS8 E_{opt} = -2308.670077 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.687170	-3.047222	0.870779
2	1	0	0.135825	-3.270283	-0.035795
3	6	0	0.930119	-4.017111	1.825042
4	1	0	0.563137	-5.025919	1.666480
5	6	0	1.646217	-3.673341	2.986197

6	1	0	1.845072	-4.411561	3.756254
7	6	0	2.091219	-2.368558	3.128340
8	1	0	2.643268	-2.069483	4.012962
9	6	0	1.826713	-1.418074	2.128561
10	6	0	2.254306	-0.031118	2.175433
11	6	0	3.030252	0.588462	3.155547
12	1	0	3.383288	0.019478	4.008949
13	6	0	3.354959	1.942270	3.029299
14	1	0	3.961092	2.428508	3.786267
15	6	0	2.900631	2.669616	1.922056
16	1	0	3.154215	3.718842	1.818338
17	6	0	2.126167	2.036246	0.953049
18	6	0	1.567532	2.624044	-0.257164
19	6	0	1.701809	3.973592	-0.620986
20	1	0	2.254340	4.648784	0.022981
21	6	0	1.118032	4.439681	-1.788608
22	1	0	1.212180	5.482801	-2.072763
23	6	0	0.400127	3.537789	-2.591651
24	1	0	-0.076674	3.856389	-3.512653
25	6	0	0.298602	2.217087	-2.190605
26	1	0	-0.252072	1.487756	-2.775063
27	6	0	0.452064	-1.891221	-2.804663
28	1	0	1.518194	-1.949347	-2.618371
29	6	0	-0.095885	-2.536806	-3.934379
30	1	0	0.572707	-3.059918	-4.609934
31	6	0	-1.450778	-2.490011	-4.153280
32	1	0	-1.907444	-2.971065	-5.013456
33	6	0	-2.269929	-1.812979	-3.214057
34	6	0	-3.683566	-1.771303	-3.337532
35	1	0	-4.142100	-2.249142	-4.198788

36	6	0	-4.457659	-1.158379	-2.376337
37	1	0	-5.539204	-1.142518	-2.469370
38	6	0	-3.843440	-0.557157	-1.254894
39	1	0	-4.464184	-0.101944	-0.488435
40	6	0	-2.465062	-0.543839	-1.117153
41	6	0	-1.647071	-1.180897	-2.093851
42	6	0	-2.029899	1.917297	0.472781
43	6	0	-1.326039	2.671276	1.433568
44	1	0	-0.595693	2.183659	2.073285
45	6	0	-1.537460	4.044135	1.554708
46	1	0	-0.989430	4.607886	2.304473
47	6	0	-2.430918	4.694751	0.697792
48	1	0	-2.586537	5.766436	0.782571
49	6	0	-3.112549	3.961178	-0.275792
50	1	0	-3.799804	4.460913	-0.952968
51	6	0	-2.915879	2.581649	-0.390041
52	1	0	-3.448316	2.033235	-1.159217
53	6	0	-2.295338	-0.709646	1.750443
54	6	0	-2.598705	-0.069758	2.964680
55	1	0	-2.516762	1.008511	3.051897
56	6	0	-3.018170	-0.812977	4.071236
57	1	0	-3.255944	-0.300465	4.999510
58	6	0	-3.138194	-2.202564	3.986980
59	1	0	-3.463416	-2.776823	4.849690
60	6	0	-2.839141	-2.848553	2.783122
61	1	0	-2.930246	-3.928490	2.705565
62	6	0	-2.417823	-2.112168	1.676230
63	1	0	-2.183845	-2.627933	0.750015
64	7	0	1.108281	-1.760523	0.991309
65	7	0	1.814762	0.698764	1.088486

66	7	0	0.860683	1.744096	-1.052307
67	7	0	-0.268856	-1.209798	-1.912289
68	15	0	-1.553950	0.154579	0.307717
69	44	0	0.678592	-0.156877	-0.236824
70	6	0	3.969970	-1.225168	-2.052695
71	8	0	3.591334	-2.392370	-1.911235
72	8	0	5.290158	-0.954020	-2.295800
73	8	0	3.261084	-0.146365	-2.005236
74	1	0	2.184181	-0.304900	-1.317529
75	1	0	5.736396	-1.816559	-2.341567

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^{1}3pt E_{opt} =-2044.160986 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.807949	1.236676	-1.416430
2	1	0	3.077673	0.202844	-1.600776
3	6	0	3.772356	2.232517	-1.309569
4	1	0	4.820362	1.976463	-1.420312
5	6	0	3.364198	3.541340	-1.048695
6	1	0	4.090816	4.340816	-0.948197
7	6	0	2.004210	3.809311	-0.918913
8	1	0	1.660804	4.817711	-0.719730
9	6	0	1.079135	2.769823	-1.046019
10	6	0	-0.379808	2.954724	-0.947551
11	6	0	-1.060595	4.158727	-0.757152
12	1	0	-0.514622	5.088639	-0.651230
13	6	0	-2.455771	4.148043	-0.710455
14	1	0	-2.998754	5.075679	-0.564625

15	6	0	-3.154943	2.948000	-0.853843
16	1	0	-4.237937	2.937527	-0.820546
17	6	0	-2.438584	1.763923	-1.038159
18	6	0	-2.991948	0.403631	-1.162389
19	6	0	-4.356575	0.111013	-1.095755
20	1	0	-5.077765	0.912292	-0.984575
21	6	0	-4.780732	-1.213213	-1.152949
22	1	0	-5.837427	-1.452076	-1.093322
23	6	0	-3.825249	-2.223447	-1.278521
24	1	0	-4.108139	-3.269666	-1.318271
25	6	0	-2.482012	-1.872774	-1.353239
26	1	0	-1.704055	-2.621353	-1.453416
27	6	0	1.221548	-2.264316	-2.777541
28	1	0	0.754512	-1.745214	-3.604738
29	6	0	1.997911	-3.416022	-3.016709
30	1	0	2.106209	-3.771919	-4.035355
31	6	0	2.608402	-4.047570	-1.960529
32	1	0	3.228703	-4.927246	-2.105058
33	6	0	2.421070	-3.533245	-0.652898
34	6	0	3.032584	-4.126147	0.483116
35	1	0	3.661064	-4.999641	0.334863
36	6	0	2.838792	-3.601845	1.741762
37	1	0	3.316181	-4.053273	2.605707
38	6	0	2.004215	-2.475070	1.914070
39	1	0	1.849485	-2.075092	2.911929
40	6	0	1.378116	-1.875448	0.833630
41	6	0	1.596085	-2.378609	-0.481540
42	6	0	-1.211528	-1.011368	1.923178
43	6	0	-2.310718	-0.134879	1.997853
44	1	0	-2.249263	0.854007	1.554863

45	6	0	-3.492211	-0.528390	2.625874
46	1	0	-4.330118	0.161132	2.673643
47	6	0	-3.601321	-1.809756	3.173491
48	1	0	-4.524295	-2.120614	3.654390
49	6	0	-2.521486	-2.691549	3.091697
50	1	0	-2.601154	-3.691461	3.508863
51	6	0	-1.332744	-2.298239	2.470265
52	1	0	-0.510395	-3.002471	2.409040
53	6	0	1.141614	0.756857	2.041100
54	6	0	0.456975	1.643449	2.888950
55	1	0	-0.612824	1.547446	3.039049
56	6	0	1.146643	2.659353	3.555717
57	1	0	0.602946	3.331815	4.213327
58	6	0	2.523966	2.811175	3.379439
59	1	0	3.056500	3.605159	3.894877
60	6	0	3.213263	1.932776	2.538960
61	1	0	4.284563	2.040788	2.395139
62	6	0	2.530047	0.913405	1.875074
63	1	0	3.080012	0.242283	1.224446
64	7	0	1.491357	1.482111	-1.281995
65	7	0	-1.079713	1.796474	-1.075392
66	7	0	-2.060790	-0.594951	-1.300743
67	7	0	1.018384	-1.736131	-1.568832
68	15	0	0.251294	-0.442409	0.967608
69	44	0	-0.089486	0.104816	-1.304384
70	1	0	-0.156896	0.229998	-2.964411

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^{1}TS9 E_{opt} = -2309.178803 Hartree

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.398580	1.894481	0.016117
2	1	0	-1.818854	2.604895	-0.561390
3	6	0	-3.525757	2.282291	0.733516
4	1	0	-3.842431	3.319064	0.714089
5	6	0	-4.216633	1.321589	1.469362
6	1	0	-5.094097	1.590924	2.047923
7	6	0	-3.769789	0.002228	1.450336
8	1	0	-4.296779	-0.764487	2.005276
9	6	0	-2.637894	-0.328310	0.706365
10	6	0	-2.102172	-1.701106	0.595894
11	6	0	-2.634330	-2.855916	1.172930
12	1	0	-3.521403	-2.806527	1.792692
13	6	0	-2.007619	-4.078571	0.930291
14	1	0	-2.410048	-4.985808	1.368017
15	6	0	-0.865872	-4.144137	0.128560
16	1	0	-0.378273	-5.093336	-0.057141
17	6	0	-0.361407	-2.963318	-0.418729
18	6	0	0.866300	-2.815923	-1.231276
19	6	0	1.689861	-3.884031	-1.589297
20	1	0	1.419720	-4.896198	-1.311941
21	6	0	2.868750	-3.636922	-2.289922
22	1	0	3.520063	-4.459379	-2.566421
23	6	0	3.199974	-2.323557	-2.620321
24	1	0	4.111532	-2.085457	-3.157095
25	6	0	2.332660	-1.299838	-2.249292
26	1	0	2.540524	-0.262028	-2.484341
27	6	0	0.387029	2.120512	-2.947907
28	1	0	-0.117846	1.418456	-3.600245

29	6	0	0.789092	3.376271	-3.444914
30	1	0	0.592791	3.615267	-4.484114
31	6	0	1.402348	4.270021	-2.599820
32	1	0	1.709666	5.254086	-2.941187
33	6	0	1.638237	3.894081	-1.253424
34	6	0	2.260481	4.763621	-0.319300
35	1	0	2.561366	5.752300	-0.653525
36	6	0	2.473464	4.364037	0.981793
37	1	0	2.942765	5.035756	1.693309
38	6	0	2.091077	3.068094	1.395351
39	1	0	2.275786	2.758590	2.419749
40	6	0	1.487279	2.188947	0.512011
41	6	0	1.228258	2.594917	-0.827163
42	6	0	2.564440	-0.450525	1.216695
43	6	0	2.489811	-1.844292	1.395048
44	1	0	1.528588	-2.345611	1.406724
45	6	0	3.650626	-2.603360	1.538250
46	1	0	3.574176	-3.678410	1.671799
47	6	0	4.903171	-1.985003	1.493567
48	1	0	5.807583	-2.577365	1.596942
49	6	0	4.987048	-0.603968	1.306435
50	1	0	5.956704	-0.116433	1.264184
51	6	0	3.826512	0.161992	1.166571
52	1	0	3.915681	1.230960	1.009698
53	6	0	0.121638	0.576350	2.532872
54	6	0	0.045869	-0.537776	3.384983
55	1	0	0.612117	-1.437059	3.173414
56	6	0	-0.763913	-0.501786	4.522155
57	1	0	-0.808440	-1.369446	5.174028
58	6	0	-1.512621	0.639562	4.818325

59	1	0	-2.145698	0.662991	5.700490
60	6	0	-1.443073	1.750956	3.974510
61	1	0	-2.022915	2.642397	4.195022
62	6	0	-0.633060	1.722291	2.838788
63	1	0	-0.598589	2.589645	2.189421
64	7	0	-1.952468	0.629371	0.008384
65	7	0	-0.989580	-1.790568	-0.168067
66	7	0	1.194339	-1.531154	-1.575978
67	7	0	0.575983	1.727377	-1.688063
68	15	0	1.007739	0.479017	0.928188
69	44	0	-0.224804	-0.115984	-0.930259
70	1	0	-0.817301	-0.509864	-2.553869
71	1	0	-1.563135	-0.122982	-2.463850
72	8	0	-3.006613	0.383025	-2.934814
73	6	0	-3.970090	-0.218457	-2.350301
74	8	0	-5.070602	0.219201	-2.013896
75	8	0	-3.741301	-1.574260	-2.054900
76	1	0	-2.874439	-1.808471	-2.418495

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^{1}TS10 E_{opt} = -2232.74401590 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.238528	1.557929	-1.910688
2	1	0	2.570749	0.563541	-2.186973
3	6	0	3.050416	2.673368	-2.087834
4	1	0	4.037865	2.553444	-2.519763
5	6	0	2.573703	3.922930	-1.691297
6	1	0	3.184232	4.812488	-1.805725

7	6	0	1.295922	4.015477	-1.144724
8	1	0	0.900783	4.975548	-0.834318
9	6	0	0.522365	2.862007	-0.998528
10	6	0	-0.849717	2.857932	-0.455097
11	6	0	-1.592026	3.967274	-0.045666
12	1	0	-1.166764	4.962875	-0.087155
13	6	0	-2.895517	3.774248	0.416202
14	1	0	-3.485469	4.625901	0.737696
15	6	0	-3.445399	2.491850	0.459903
16	1	0	-4.459712	2.340624	0.810018
17	6	0	-2.667990	1.409474	0.044029
18	6	0	-3.060341	-0.012435	0.038144
19	6	0	-4.304611	-0.476827	0.468429
20	1	0	-5.056302	0.225811	0.808201
21	6	0	-4.564788	-1.844705	0.471550
22	1	0	-5.525777	-2.217210	0.810523
23	6	0	-3.569659	-2.723650	0.041172
24	1	0	-3.726154	-3.796725	0.033101
25	6	0	-2.352956	-2.203382	-0.386594
26	1	0	-1.550178	-2.843372	-0.735009
27	6	0	0.755633	-2.109959	-2.838841
28	1	0	-0.032370	-1.689039	-3.450821
29	6	0	1.581408	-3.131816	-3.350262
30	1	0	1.413311	-3.483093	-4.362424
31	6	0	2.584001	-3.646163	-2.563785
32	1	0	3.250871	-4.421969	-2.928323
33	6	0	2.745748	-3.150630	-1.245178
34	6	0	3.762614	-3.627840	-0.376677
35	1	0	4.436538	-4.397110	-0.742635
36	6	0	3.894939	-3.122371	0.897971

37	1	0	4.679405	-3.484989	1.554635
38	6	0	2.999505	-2.132246	1.361366
39	1	0	3.106320	-1.747446	2.371358
40	6	0	1.988054	-1.647809	0.548654
41	6	0	1.856090	-2.132812	-0.784069
42	6	0	-0.252568	-1.165153	2.392844
43	6	0	-1.395431	-0.464046	2.821460
44	1	0	-1.618352	0.515753	2.411766
45	6	0	-2.260229	-1.023620	3.761588
46	1	0	-3.138084	-0.469038	4.080211
47	6	0	-2.006204	-2.298383	4.275665
48	1	0	-2.684288	-2.738714	5.000950
49	6	0	-0.882145	-3.007095	3.846031
50	1	0	-0.681865	-4.000884	4.236390
51	6	0	-0.008842	-2.447185	2.909169
52	1	0	0.852657	-3.018383	2.581484
53	6	0	1.738809	0.941138	1.854137
54	6	0	1.203324	1.742713	2.875866
55	1	0	0.244051	1.501994	3.320789
56	6	0	1.902050	2.861975	3.335179
57	1	0	1.477037	3.468118	4.130198
58	6	0	3.137148	3.200782	2.777488
59	1	0	3.675645	4.074477	3.132973
60	6	0	3.677869	2.407300	1.762108
61	1	0	4.638168	2.660907	1.322306
62	6	0	2.986328	1.285802	1.303019
63	1	0	3.418215	0.681698	0.512681
64	7	0	1.007865	1.635158	-1.373810
65	7	0	-1.398908	1.619359	-0.387077
66	7	0	-2.093184	-0.883458	-0.394458

67	7	0	0.876808	-1.602696	-1.611466
68	15	0	0.758739	-0.398617	1.065378
69	44	0	-0.317974	0.066156	-0.957080
70	1	0	-0.881025	0.212659	-2.547742
71	6	0	-2.403795	0.027009	-3.349529
72	8	0	-2.281842	-1.052318	-3.838231
73	8	0	-2.957062	1.056755	-3.131158

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^{1}TS11 E_{opt} = -2497.76204925 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.778610	-2.486956	0.116988
2	1	0	1.080348	-3.001510	-0.532640
3	6	0	2.755458	-3.176378	0.829235
4	1	0	2.824289	-4.254586	0.737018
5	6	0	3.626996	-2.456377	1.644012
6	1	0	4.401331	-2.961587	2.211705
7	6	0	3.493626	-1.071458	1.721589
8	1	0	4.160914	-0.490678	2.346773
9	6	0	2.488381	-0.436885	0.993487
10	6	0	2.274582	1.025769	1.000815
11	6	0	2.996628	1.972723	1.727897
12	1	0	3.790628	1.669056	2.399076
13	6	0	2.680432	3.323296	1.570785
14	1	0	3.231813	4.073213	2.127883
15	6	0	1.661155	3.717752	0.702022
16	1	0	1.418088	4.766177	0.579370
17	6	0	0.959231	2.735115	0.000811

18	6	0	-0.170018	2.942114	-0.931631
19	6	0	-0.668720	4.198056	-1.277890
20	1	0	-0.200446	5.095353	-0.891315
21	6	0	-1.779200	4.285643	-2.115595
22	1	0	-2.181436	5.256045	-2.387171
23	6	0	-2.364738	3.112983	-2.591070
24	1	0	-3.233622	3.135398	-3.239440
25	6	0	-1.812503	1.889567	-2.222157
26	1	0	-2.224922	0.950093	-2.570330
27	6	0	-1.195427	-1.868042	-2.881676
28	1	0	-0.724581	-1.202299	-3.589978
29	6	0	-1.856689	-3.021591	-3.352883
30	1	0	-1.874425	-3.212433	-4.420122
31	6	0	-2.431277	-3.885487	-2.453921
32	1	0	-2.915982	-4.802963	-2.774551
33	6	0	-2.411121	-3.550186	-1.076883
34	6	0	-3.028671	-4.361576	-0.089147
35	1	0	-3.496425	-5.290543	-0.402141
36	6	0	-3.047132	-3.972690	1.232428
37	1	0	-3.522612	-4.596055	1.982833
38	6	0	-2.477388	-2.736858	1.611695
39	1	0	-2.546107	-2.412487	2.645443
40	6	0	-1.846861	-1.931537	0.678304
41	6	0	-1.766761	-2.339276	-0.681579
42	6	0	-2.685555	0.826001	1.090428
43	6	0	-2.510980	2.215600	1.225767
44	1	0	-1.519346	2.636078	1.341739
45	6	0	-3.608686	3.074334	1.195504
46	1	0	-3.453463	4.144235	1.297992
47	6	0	-4.896796	2.561268	1.018252

48	1	0	-5.750802	3.231476	0.986733
49	6	0	-5.079476	1.184588	0.875766
50	1	0	-6.076594	0.777455	0.735364
51	6	0	-3.982531	0.319055	0.909500
52	1	0	-4.146367	-0.746086	0.789390
53	6	0	-0.462689	-0.309236	2.683951
54	6	0	-0.429891	0.827966	3.507816
55	1	0	-0.941771	1.737978	3.218832
56	6	0	0.263647	0.800737	4.719617
57	1	0	0.278093	1.687671	5.346255
58	6	0	0.933339	-0.356585	5.123466
59	1	0	1.474452	-0.373241	6.064927
60	6	0	0.901936	-1.492869	4.311177
61	1	0	1.420882	-2.397575	4.613752
62	6	0	0.212749	-1.470725	3.098833
63	1	0	0.210364	-2.357369	2.475280
64	7	0	1.637824	-1.154463	0.193508
65	7	0	1.281479	1.433870	0.178207
66	7	0	-0.746143	1.798316	-1.414431
67	7	0	-1.093716	-1.539521	-1.594031
68	15	0	-1.206689	-0.261296	1.007141
69	44	0	0.217179	0.055793	-0.772903
70	6	0	1.216457	-0.030103	-2.914026
71	8	0	0.602408	0.605469	-3.765463
72	8	0	1.783638	-1.209100	-3.278591
73	1	0	2.511225	-1.406547	-2.624221
74	6	0	4.138360	0.030363	-1.610027
75	8	0	3.948290	-1.188441	-1.785340
76	8	0	5.347684	0.469942	-1.190627
77	8	0	3.290686	0.983501	-1.775850

78	1	0	2.087014	0.538470	-1.990232
79	1	0	5.915303	-0.315288	-1.103358

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^{1}TS12 E_{opt} = -2923.371276 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034424	-2.724919	1.297908
2	1	0	-0.314660	-3.234784	0.382736
3	6	0	0.243042	-3.425984	2.467314
4	1	0	0.194816	-4.509199	2.465455
5	6	0	0.564709	-2.710709	3.620741
6	1	0	0.776641	-3.225584	4.551789
7	6	0	0.606891	-1.319556	3.564043
8	1	0	0.854988	-0.742386	4.446601
9	6	0	0.332679	-0.669525	2.360231
10	6	0	0.362329	0.797516	2.198602
11	6	0	0.671419	1.740790	3.180864
12	1	0	0.920890	1.428713	4.187588
13	6	0	0.655211	3.094804	2.842983
14	1	0	0.898131	3.840076	3.592471
15	6	0	0.319897	3.496892	1.548313
16	1	0	0.300787	4.547966	1.288560
17	6	0	0.012664	2.522670	0.597984
18	6	0	-0.404164	2.746457	-0.800995
19	6	0	-0.511690	4.008485	-1.386370
20	1	0	-0.259584	4.894976	-0.817423
21	6	0	-0.948811	4.117390	-2.704643
22	1	0	-1.040136	5.093183	-3.169980

23	6	0	-1.269679	2.957669	-3.410218
24	1	0	-1.618008	2.996467	-4.436358
25	6	0	-1.140059	1.726659	-2.774107
26	1	0	-1.377601	0.797268	-3.278220
27	6	0	-0.673141	-2.090920	-2.882628
28	1	0	0.214180	-1.547034	-3.173574
29	6	0	-1.095252	-3.195494	-3.651947
30	1	0	-0.516389	-3.472462	-4.526142
31	6	0	-2.204876	-3.904829	-3.264502
32	1	0	-2.541372	-4.780931	-3.811066
33	6	0	-2.938455	-3.460504	-2.135727
34	6	0	-4.123418	-4.108958	-1.699129
35	1	0	-4.452297	-4.997041	-2.230943
36	6	0	-4.846561	-3.615936	-0.635071
37	1	0	-5.752874	-4.114675	-0.307152
38	6	0	-4.426268	-2.434467	0.014827
39	1	0	-5.028331	-2.024854	0.820106
40	6	0	-3.263924	-1.787508	-0.370790
41	6	0	-2.475311	-2.306164	-1.434223
42	6	0	-3.824982	1.071976	-0.396824
43	6	0	-3.565102	2.432077	-0.146729
44	1	0	-2.744493	2.725121	0.497185
45	6	0	-4.346228	3.423956	-0.738125
46	1	0	-4.128267	4.468375	-0.535425
47	6	0	-5.391459	3.075040	-1.597994
48	1	0	-5.994836	3.848174	-2.064580
49	6	0	-5.651170	1.728513	-1.859942
50	1	0	-6.459364	1.448189	-2.529275
51	6	0	-4.873586	0.730315	-1.266566
52	1	0	-5.087835	-0.308605	-1.490763

53	6	0	-2.986942	-0.263225	2.111730
54	6	0	-3.150568	0.912050	2.864653
55	1	0	-3.224978	1.877102	2.378270
56	6	0	-3.220318	0.854378	4.257996
57	1	0	-3.350185	1.772097	4.824206
58	6	0	-3.122453	-0.372329	4.918907
59	1	0	-3.173259	-0.413870	6.002974
60	6	0	-2.957800	-1.545063	4.177800
61	1	0	-2.875451	-2.503753	4.681283
62	6	0	-2.886284	-1.493508	2.785577
63	1	0	-2.740687	-2.412797	2.230287
64	7	0	0.008297	-1.380300	1.232301
65	7	0	0.056024	1.211923	0.944663
66	7	0	-0.720691	1.614286	-1.503669
67	7	0	-1.294290	-1.666784	-1.782388
68	15	0	-2.693730	-0.196695	0.301108
69	44	0	-0.492323	-0.139243	-0.392100
70	6	0	1.552800	-0.530306	-1.442419
71	8	0	1.631111	-0.029310	-2.570505
72	8	0	1.971501	-1.856946	-1.334595
73	1	0	1.862482	-2.134121	-0.410486
74	6	0	6.052916	-3.527699	-1.057592
75	6	0	5.667147	-2.364223	-1.724627
76	6	0	4.996616	-1.395118	-0.974029
77	6	0	4.720699	-1.591859	0.397433
78	6	0	5.103120	-2.758206	1.062777
79	6	0	5.775780	-3.722541	0.310034
80	1	0	6.574665	-4.304320	-1.608107
81	1	0	5.871394	-2.217846	-2.779196
82	1	0	4.888425	-2.901505	2.115987

83	1	0	6.091306	-4.643799	0.789637
84	6	0	2.919930	2.651208	-0.883563
85	6	0	2.932469	4.041149	-0.761781
86	6	0	3.731928	4.654553	0.204894
87	6	0	4.534796	3.873998	1.041610
88	6	0	4.546579	2.485298	0.907865
89	6	0	3.732635	1.867333	-0.053227
90	1	0	2.281459	2.172808	-1.618978
91	1	0	2.303331	4.639898	-1.412367
92	1	0	3.730501	5.735824	0.306601
93	1	0	5.161738	4.345352	1.792690
94	1	0	5.192539	1.886465	1.541075
95	7	0	4.062250	-0.470665	0.846982
96	7	0	4.507993	-0.157281	-1.317779
97	6	0	3.769333	0.377694	-0.236505
98	6	0	4.618520	0.400933	-2.656257
99	1	0	3.904019	-0.080435	-3.329324
100	1	0	4.418734	1.470547	-2.627262
101	1	0	5.637685	0.240069	-3.015959
102	6	0	3.651900	-0.290787	2.229551
103	1	0	3.041391	0.603314	2.317839
104	1	0	3.079640	-1.160254	2.556854
105	1	0	4.535032	-0.184850	2.866308
106	1	0	2.397501	0.115203	-0.536768

E_{opt}（^{1}TS13）= -2232.70040803 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.710726	2.480175	-1.127072
2	1	0	2.403725	1.750815	-1.530892
3	6	0	2.081112	3.808458	-0.932456
4	1	0	3.082030	4.129961	-1.198349
5	6	0	1.151924	4.690520	-0.383837
6	1	0	1.410658	5.728771	-0.204160
7	6	0	-0.122107	4.221508	-0.066876
8	1	0	-0.861682	4.889700	0.358183
9	6	0	-0.441676	2.884416	-0.302472
10	6	0	-1.773289	2.302303	-0.031480
11	6	0	-2.902894	2.976485	0.437165
12	1	0	-2.860286	4.033816	0.669265
13	6	0	-4.095548	2.266526	0.587881
14	1	0	-4.983140	2.776108	0.947540
15	6	0	-4.158566	0.908361	0.268774
16	1	0	-5.088399	0.362172	0.373131
17	6	0	-3.000657	0.272117	-0.184375
18	6	0	-2.848848	-1.154594	-0.545519
19	6	0	-3.884414	-2.086683	-0.473105
20	1	0	-4.877616	-1.774195	-0.173405
21	6	0	-3.627384	-3.422582	-0.775643
22	1	0	-4.423196	-4.157693	-0.714729
23	6	0	-2.337439	-3.798078	-1.148612
24	1	0	-2.092240	-4.827266	-1.386212
25	6	0	-1.347690	-2.821056	-1.214341
26	1	0	-0.329070	-3.059710	-1.499253
27	6	0	1.783002	-1.133485	-2.965060
28	1	0	0.957768	-0.913054	-3.631684
29	6	0	3.002346	-1.637391	-3.463593
30	1	0	3.096855	-1.820248	-4.528331

31	6	0	4.043925	-1.868238	-2.596769
32	1	0	5.002603	-2.238349	-2.947968
33	6	0	3.857783	-1.616100	-1.213378
34	6	0	4.884308	-1.817375	-0.253396
35	1	0	5.850411	-2.177078	-0.595585
36	6	0	4.661209	-1.557754	1.081570
37	1	0	5.452522	-1.706278	1.809323
38	6	0	3.393138	-1.107828	1.514617
39	1	0	3.224313	-0.922350	2.571232
40	6	0	2.365138	-0.906316	0.609036
41	6	0	2.587699	-1.135227	-0.777160
42	6	0	-0.069092	-1.804958	1.975303
43	6	0	-1.434124	-1.751099	2.311977
44	1	0	-2.023863	-0.873200	2.074401
45	6	0	-2.054322	-2.832772	2.935979
46	1	0	-3.109897	-2.774040	3.184610
47	6	0	-1.324799	-3.989767	3.223799
48	1	0	-1.809824	-4.835256	3.702826
49	6	0	0.027770	-4.056375	2.884880
50	1	0	0.601135	-4.953600	3.099626
51	6	0	0.654504	-2.973019	2.262586
52	1	0	1.702582	-3.052061	1.997320
53	6	0	0.846641	0.992172	2.243234
54	6	0	-0.190579	1.309936	3.136026
55	1	0	-1.059631	0.668741	3.226577
56	6	0	-0.118588	2.462852	3.920607
57	1	0	-0.927213	2.692711	4.608384
58	6	0	0.982643	3.316258	3.819564
59	1	0	1.033887	4.215228	4.426848
60	6	0	2.017651	3.007573	2.933385

61	1	0	2.877181	3.665703	2.845688
62	6	0	1.952128	1.855301	2.149036
63	1	0	2.758829	1.638801	1.458155
64	7	0	0.489634	2.019887	-0.816179
65	7	0	-1.853828	0.978941	-0.300283
66	7	0	-1.587597	-1.533008	-0.922477
67	7	0	1.567846	-0.874869	-1.676452
68	15	0	0.668383	-0.395847	1.051890
69	44	0	-0.231659	0.061026	-0.972555
70	6	0	-1.300594	1.335498	-3.210348
71	8	0	-0.918900	0.136884	-3.261127
72	8	0	-1.929835	1.656121	-4.411683
73	1	0	-2.189906	2.585173	-4.317784

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^{1}TS14 E_{opt} = -189.150387856 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.091098	0.422145	-0.000383
2	8	0	1.176748	-0.168940	0.000148
3	8	0	-1.112128	-0.265634	-0.000012
4	1	0	-1.063544	0.943725	0.001213

E_{opt}（^{1}TS15）= -265.647742675 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.558530	-0.249496	-0.027314

2	8	0	-1.736713	-0.585739	0.019245
3	8	0	-0.290897	1.127518	0.010181
4	1	0	0.693072	1.099962	-0.034471
5	1	0	0.778388	-0.662323	-0.088024
6	8	0	1.986021	-0.357984	-0.098926
7	1	0	2.212436	-0.411025	0.842379

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^{1}TS16 E_{opt} = -342.106136407 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.125556	0.142343	0.027273
2	8	0	2.344010	0.313170	0.081554
3	8	0	0.744702	-1.206544	-0.125739
4	1	0	-0.236265	-1.203887	-0.146694
5	8	0	-2.076480	-0.888595	-0.029267
6	1	0	-2.222453	-1.103882	0.902462
7	1	0	-1.847804	0.091403	-0.010356
8	8	0	-1.148785	1.577868	0.056777
9	1	0	-1.215254	1.912467	-0.850454
10	1	0	-0.139136	1.082655	0.074802

E_{opt}（$^{2}Ru^{III}$-H）= -2043.99195792 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.327471	1.946840	-1.196438
2	1	0	2.854148	1.010139	-1.331308

3	6	0	3.005249	3.154754	-1.081353
4	1	0	4.087658	3.164686	-1.137557
5	6	0	2.272209	4.322988	-0.877105
6	1	0	2.774003	5.278381	-0.767223
7	6	0	0.882308	4.252756	-0.810677
8	1	0	0.293414	5.147673	-0.651429
9	6	0	0.251931	3.017269	-0.951494
10	6	0	-1.204739	2.817630	-0.904621
11	6	0	-2.174604	3.806582	-0.729779
12	1	0	-1.887108	4.844303	-0.612917
13	6	0	-3.518176	3.434311	-0.703932
14	1	0	-4.285063	4.189632	-0.571759
15	6	0	-3.880029	2.093581	-0.836846
16	1	0	-4.921083	1.796519	-0.801710
17	6	0	-2.876113	1.139414	-1.007278
18	6	0	-3.053409	-0.318225	-1.102034
19	6	0	-4.282234	-0.973487	-1.041194
20	1	0	-5.199324	-0.402331	-0.965599
21	6	0	-4.315076	-2.366210	-1.062920
22	1	0	-5.264790	-2.887544	-1.009426
23	6	0	-3.117993	-3.078165	-1.140093
24	1	0	-3.100427	-4.161916	-1.147311
25	6	0	-1.920713	-2.374384	-1.197810
26	1	0	-0.962028	-2.876928	-1.247399
27	6	0	1.710640	-1.628045	-2.935444
28	1	0	1.088882	-1.195520	-3.708463
29	6	0	2.769496	-2.488454	-3.272456
30	1	0	2.947062	-2.720753	-4.316080
31	6	0	3.560577	-2.998126	-2.269629
32	1	0	4.398967	-3.652022	-2.490753

33	6	0	3.281049	-2.663991	-0.921290
34	6	0	4.074483	-3.148751	0.150790
35	1	0	4.917357	-3.793192	-0.080358
36	6	0	3.783771	-2.802441	1.451660
37	1	0	4.396774	-3.167241	2.269279
38	6	0	2.676184	-1.972077	1.728214
39	1	0	2.454147	-1.707678	2.757741
40	6	0	1.868341	-1.487124	0.710522
41	6	0	2.171742	-1.808473	-0.642515
42	6	0	-0.832455	-1.435179	1.894881
43	6	0	-2.132008	-0.906229	2.003610
44	1	0	-2.356119	0.077595	1.603930
45	6	0	-3.148115	-1.647338	2.605335
46	1	0	-4.146717	-1.227336	2.679617
47	6	0	-2.884473	-2.931348	3.090817
48	1	0	-3.678258	-3.513117	3.550009
49	6	0	-1.600244	-3.467546	2.975021
50	1	0	-1.390977	-4.467314	3.344171
51	6	0	-0.576039	-2.726824	2.379235
52	1	0	0.410966	-3.166059	2.286706
53	6	0	0.959188	0.911424	2.107930
54	6	0	0.038029	1.585521	2.927916
55	1	0	-0.988311	1.244119	3.004382
56	6	0	0.435840	2.705566	3.660083
57	1	0	-0.285055	3.211843	4.295466
58	6	0	1.750173	3.172579	3.577245
59	1	0	2.055111	4.046224	4.145682
60	6	0	2.670061	2.508957	2.762283
61	1	0	3.694256	2.863341	2.691980
62	6	0	2.280765	1.385845	2.030544

63	1	0	3.008357	0.885277	1.401196
64	7	0	0.985247	1.877066	-1.134834
65	7	0	-1.579785	1.525955	-1.047718
66	7	0	-1.889460	-1.029574	-1.190433
67	7	0	1.410164	-1.284453	-1.678150
68	15	0	0.407698	-0.435450	0.993785
69	44	0	-0.150729	0.125294	-1.319344
70	1	0	-0.400913	0.373490	-2.915610

E_{opt}（$^{2}Ru^{III}$-CO_2^-）= -2232.13573307 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.726451	1.279386	-1.191962
2	1	0	2.996645	0.268453	-1.475368
3	6	0	3.684132	2.281412	-1.069792
4	1	0	4.725445	2.055033	-1.270562
5	6	0	3.275861	3.555476	-0.677002
6	1	0	3.996717	4.357618	-0.557890
7	6	0	1.923330	3.788343	-0.437381
8	1	0	1.584270	4.771258	-0.132509
9	6	0	1.006142	2.747410	-0.592890
10	6	0	-0.449676	2.903195	-0.394207
11	6	0	-1.132373	4.079665	-0.075360
12	1	0	-0.595745	5.008959	0.072817
13	6	0	-2.522829	4.042538	0.040410
14	1	0	-3.066887	4.948188	0.286645
15	6	0	-3.219882	2.849902	-0.167024
16	1	0	-4.300078	2.823376	-0.086778

17	6	0	-2.498922	1.697140	-0.481552
18	6	0	-3.041170	0.342849	-0.717120
19	6	0	-4.397801	0.026103	-0.637230
20	1	0	-5.124215	0.802146	-0.427568
21	6	0	-4.806306	-1.293773	-0.815884
22	1	0	-5.857614	-1.553379	-0.748241
23	6	0	-3.844925	-2.271440	-1.073359
24	1	0	-4.117206	-3.312045	-1.211138
25	6	0	-2.508029	-1.893787	-1.153558
26	1	0	-1.722589	-2.614172	-1.352363
27	6	0	1.121722	-2.118778	-2.761547
28	1	0	0.525403	-1.611063	-3.509380
29	6	0	1.962846	-3.190380	-3.125881
30	1	0	1.999046	-3.496810	-4.165472
31	6	0	2.724170	-3.808192	-2.163530
32	1	0	3.396585	-4.625163	-2.408103
33	6	0	2.623241	-3.366793	-0.819728
34	6	0	3.380775	-3.951014	0.229294
35	1	0	4.061027	-4.762146	-0.013943
36	6	0	3.258560	-3.497584	1.524512
37	1	0	3.845416	-3.943664	2.321065
38	6	0	2.354144	-2.454563	1.825257
39	1	0	2.252854	-2.115217	2.851839
40	6	0	1.592927	-1.863850	0.830143
41	6	0	1.730376	-2.293719	-0.519931
42	6	0	-1.008422	-1.338171	2.077726
43	6	0	-2.187548	-0.598008	2.284191
44	1	0	-2.261779	0.423276	1.928414
45	6	0	-3.282722	-1.172870	2.927682
46	1	0	-4.185096	-0.587018	3.076199

47	6	0	-3.224030	-2.500236	3.361774
48	1	0	-4.079997	-2.950909	3.855536
49	6	0	-2.063663	-3.247048	3.148644
50	1	0	-2.012030	-4.281189	3.476962
51	6	0	-0.961263	-2.673555	2.508952
52	1	0	-0.074853	-3.275415	2.343611
53	6	0	1.151672	0.678680	2.208070
54	6	0	0.381797	1.542606	3.005614
55	1	0	-0.689438	1.403276	3.095746
56	6	0	0.987626	2.595875	3.693789
57	1	0	0.379422	3.251747	4.310047
58	6	0	2.364405	2.807770	3.587839
59	1	0	2.832558	3.631443	4.118798
60	6	0	3.136453	1.953832	2.795968
61	1	0	4.207340	2.111117	2.705515
62	6	0	2.537391	0.896908	2.109646
63	1	0	3.150666	0.250704	1.492034
64	7	0	1.422350	1.492922	-0.954035
65	7	0	-1.147716	1.756272	-0.570065
66	7	0	-2.105874	-0.623145	-0.983391
67	7	0	1.003477	-1.659831	-1.515978
68	15	0	0.350370	-0.560056	1.118032
69	44	0	-0.147436	0.107912	-1.028277
70	6	0	-0.452254	0.863560	-3.237168
71	8	0	-0.999413	-0.072567	-3.823489
72	8	0	-0.097227	2.012250	-3.454305

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