

Supporting Information

For

Mechanistic Studies of Styrene Production from Benzene and Ethylene using $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ as Catalyst Precursor: Identification of a Bis-Rh^I Mono-Cu^{II} Complex as Catalyst

Charles B. Musgrave III^{†,‡}, Weihao Zhu^{§,‡}, Nathan Coutard[§], Jeffrey F. Ellena[§], Diane A. Dickie[§], T. Brent Gunnoe^{*,§} and William A. Goddard III^{*,†}

[†] Materials and Process Simulation Center, Department of Chemistry, California Institute of Technology, Pasadena, California 91125, United States

[§] Department of Chemistry, University of Virginia, Charlottesville, Virginia 22904, United States

[§] Biomolecular Magnetic Resonance Facility, School of Medicine, University of Virginia, Charlottesville, Virginia 22908, United States

[‡] These authors contributed equally

Corresponding Authors:

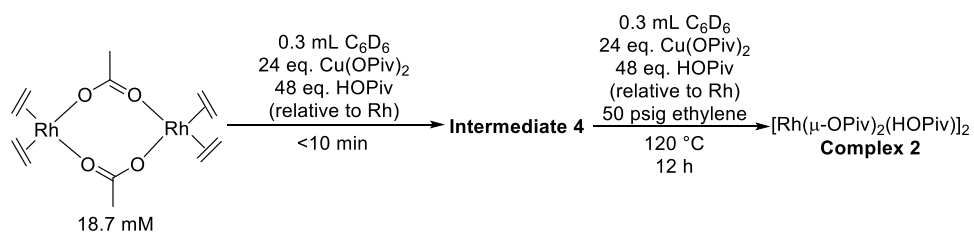
*tbg7h@virginia.edu

*wag@caltech.edu

Content:

^1H NMR spectra for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ to $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4) at room temperature and $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) at 120 °C under 50 psig ethylene.	S4
^1H NMR spectra for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ to $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4) at room temperature and $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) at 120 °C in the absence of ethylene.	S5
ORTEP of $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2).	S6
^1H NMR spectra for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ at 120 °C after 12 hours.	S7
Kinetic plots for conversion of intermediate 5 to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) at 21, 45, 50, and 60 °C under 50 psig ethylene.	S8
Kinetic plots for conversion of intermediate 5 to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) using 48 (A), 72 (B), 96 (C) or 120 (D) eq. HOPiv (relative to Rh).	S10
Log–log plots of observed rate constants (k_{obs}) for conversion of intermediate 5 to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) versus concentration of HOPiv.	S12
^{13}C NMR spectrum of obtained $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4) solid.	S12
^1H NMR spectrum of obtained $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4) solid.	S13
Dependence of R1 on concentration for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4).	S13
Experimental determination of the average $\text{C}_2\text{H}_4\text{--Cu}$ distance of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4) using R ₁	S14
Average $\text{C}_2\text{H}_4\text{--Cu}$ distance of complex 4 from the crystal structure and DFT	S15
Computational methods.	S16
DFT structure energies.	S16
X-ray crystallography data and structure determination.	S19
Crystallographic data for $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2) and $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4)	S20
Bond lengths (Å) for $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2).	S21
Bond angles (°) for $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (2)	S21

ORTEP of complex $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4).....	S24
Bond lengths (Å) for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4).	S24
Bond angles (°) for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4).....	S25
Additional calculations	S27
DFT Structures	S29
References	S83



Formation of complex 2 after heating

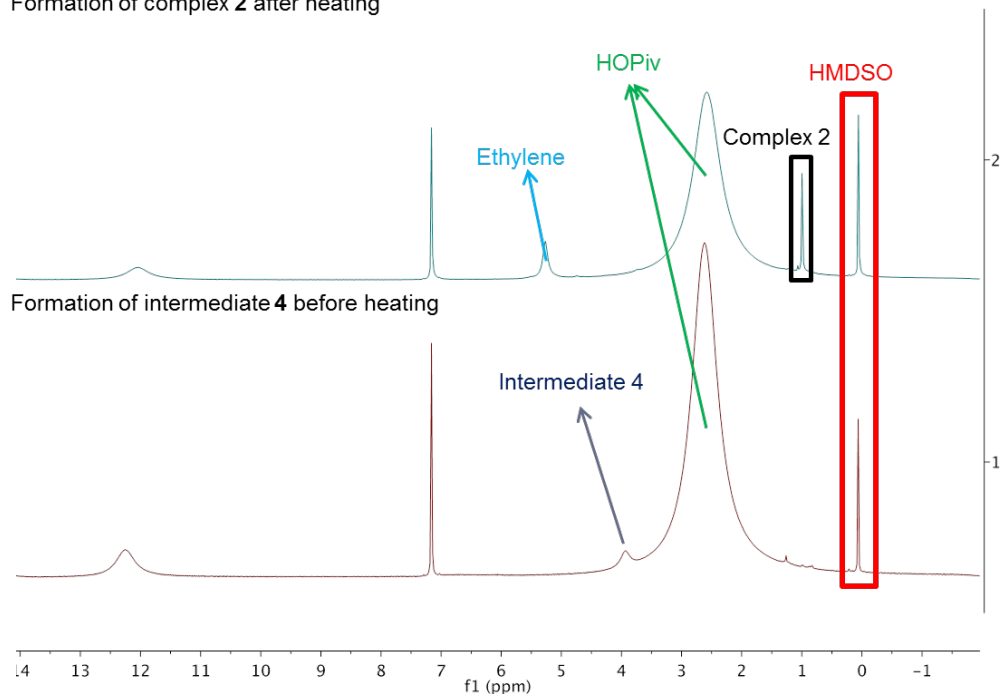


Figure S1. ¹H NMR spectra for conversion of [(η²-C₂H₄)₂Rh(μ-OAc)]₂ (**1**) to [(η²-C₂H₄)₂Rh^I(μ-OPiv)₂]₂(μ-Cu) (**4**) at room temperature and [(HOPIv)Rh(μ-OPiv)₂]₂ (**2**) at 120 °C under 50 psig ethylene.

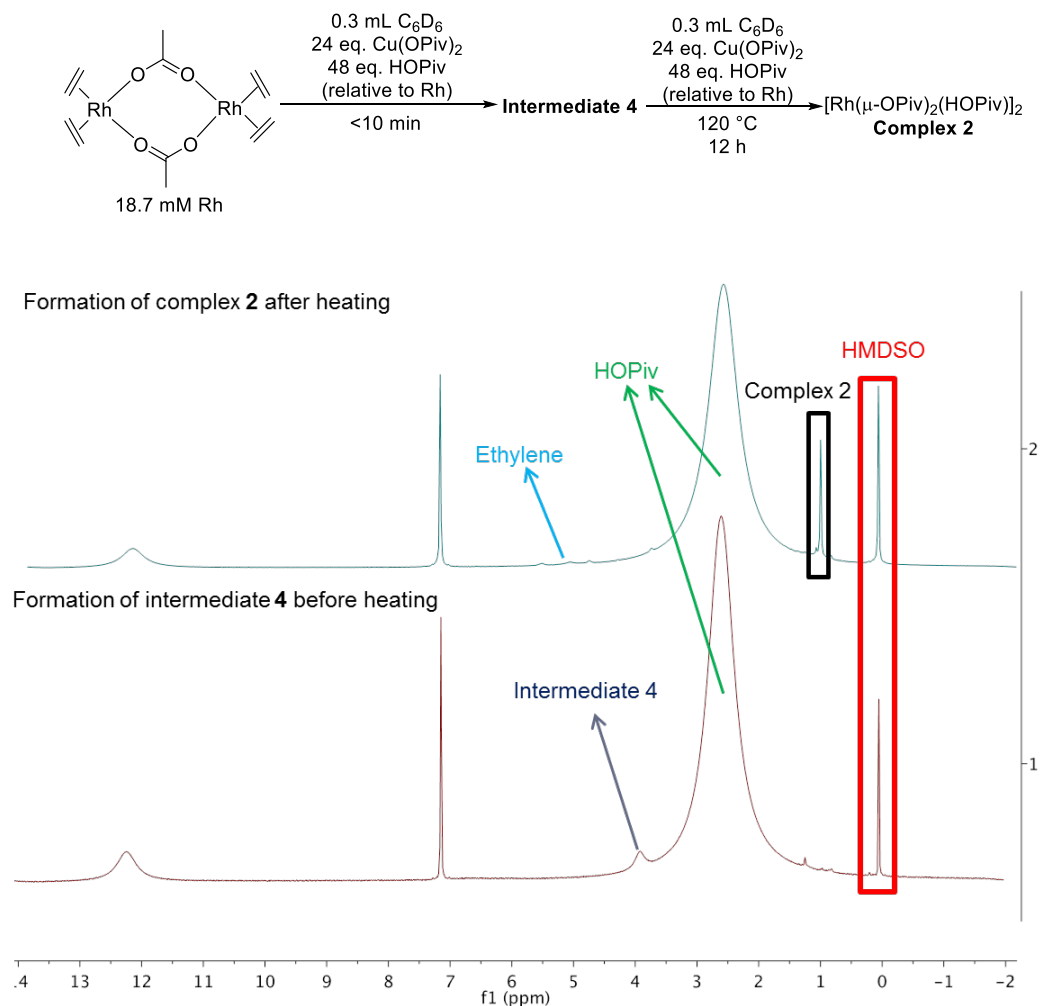


Figure S2. ^1H NMR spectra for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ (**1**) to $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) at room temperature and $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**) at 120°C in the absence of ethylene.

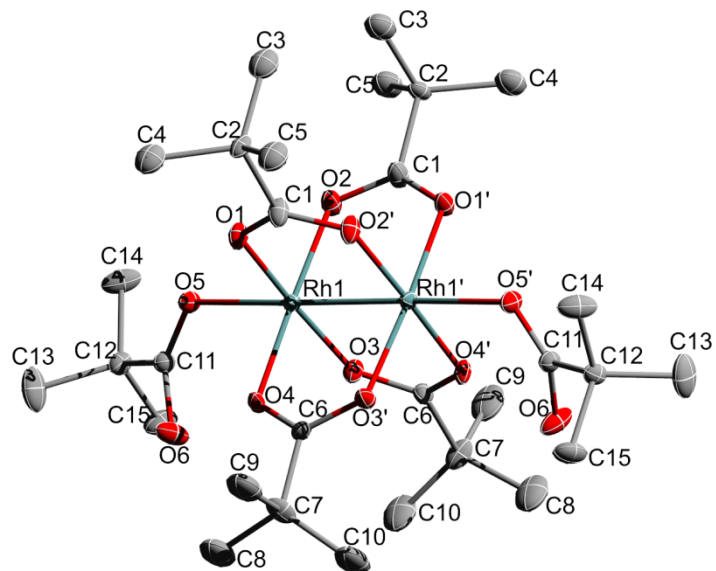


Figure S3. ORTEP of $[(\text{HOPIV})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**) (50% probability). H atoms are omitted for clarity. Only the major position for the disordered atoms is shown. For the structure of complex **2**, only the major position for the disordered pivalate ligands is shown.

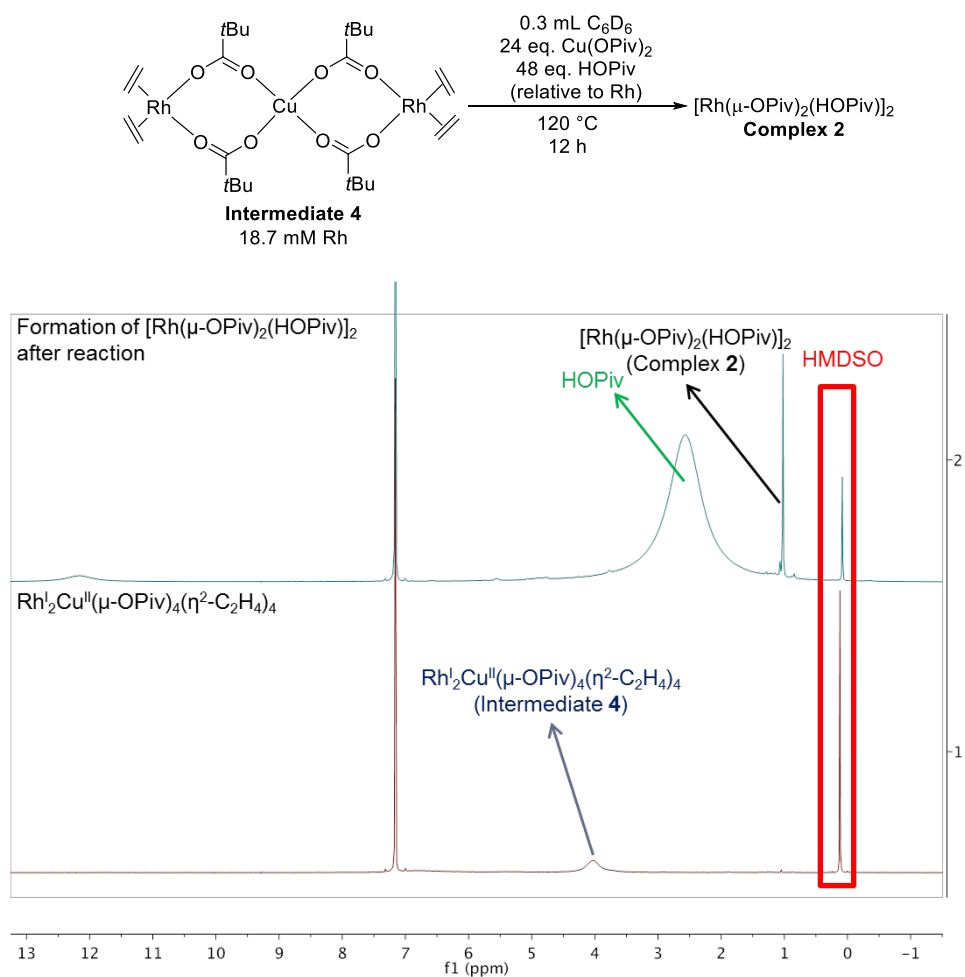


Figure S4. ¹H NMR spectra for conversion of [(η²-C₂H₄)₂Rh^I(μ-OPiv)₂]₂(μ-Cu) (**4**) to [(HOPiv)Rh(μ-OPiv)₂]₂ (**2**) at 120 °C after 12 hours.

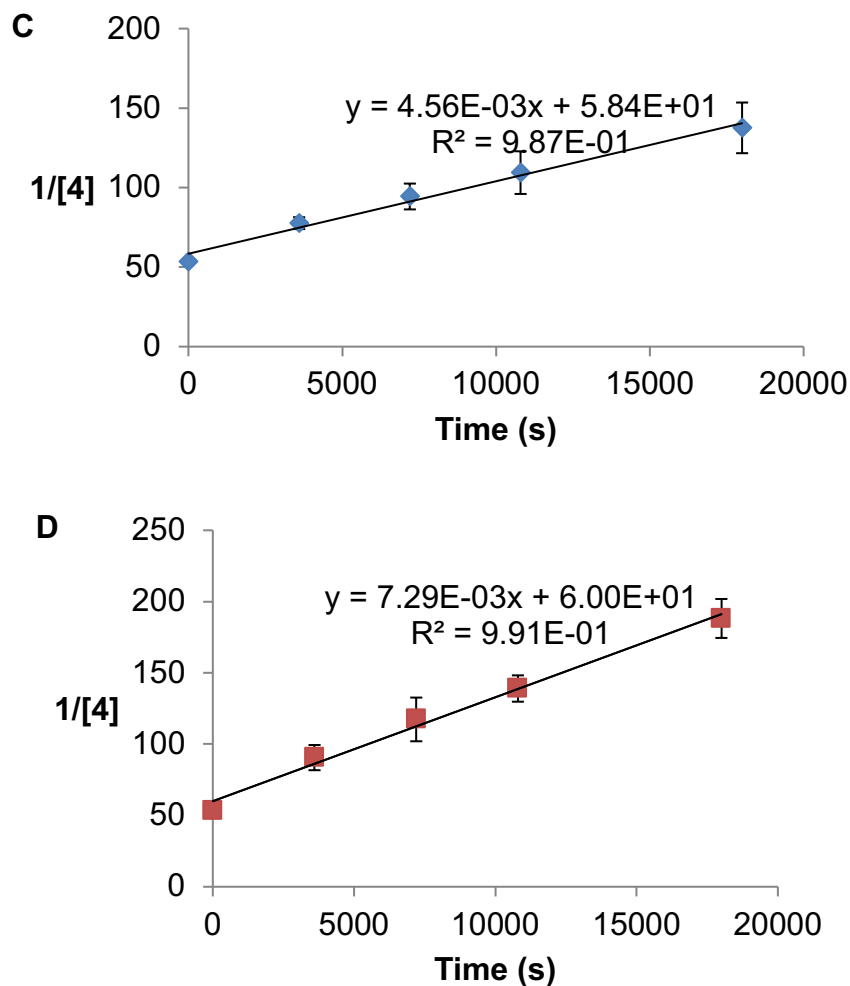
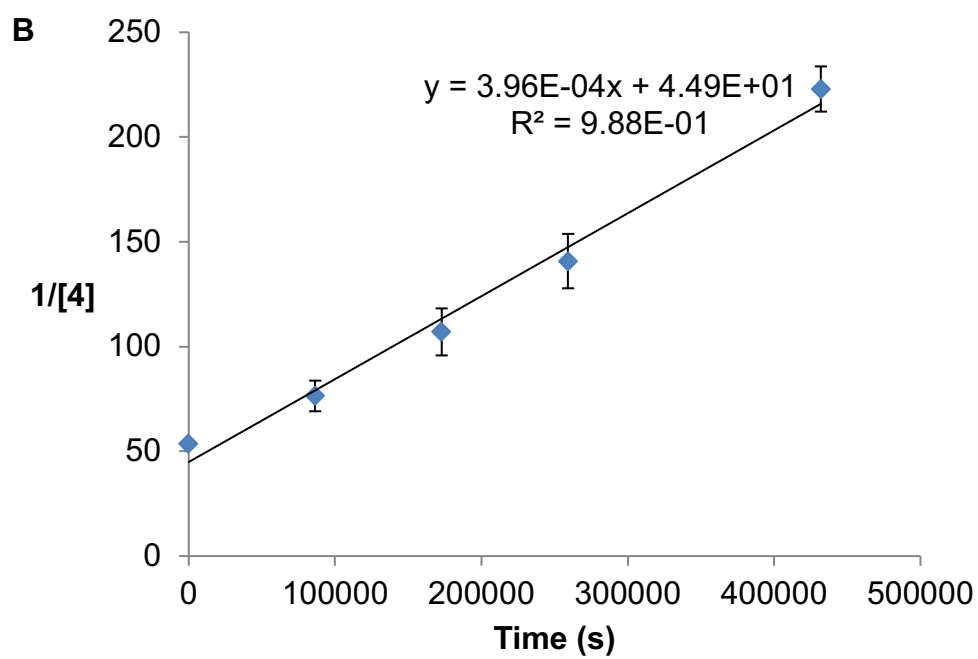
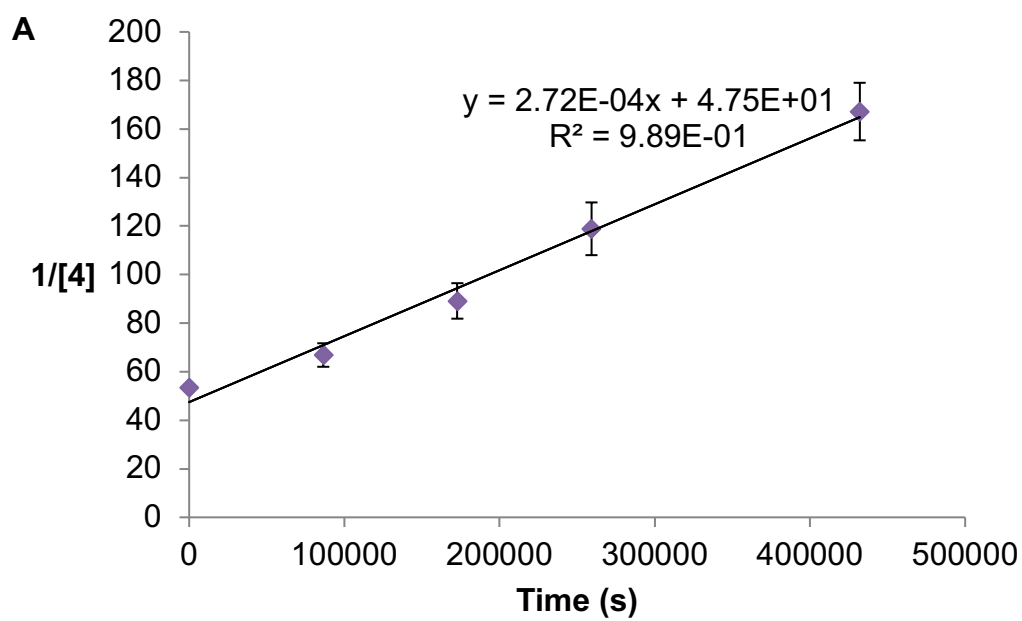


Figure S5. Kinetic plots for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**) at 21 (A), 45 (B), 50 (C), and 60 (D) °C under 50 psig ethylene. Decay of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) is calculated based on the amount of formed $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**). Each data point is the average of three separate experiments. Error bars represent the standard deviations based on a minimum of three independent experiments.



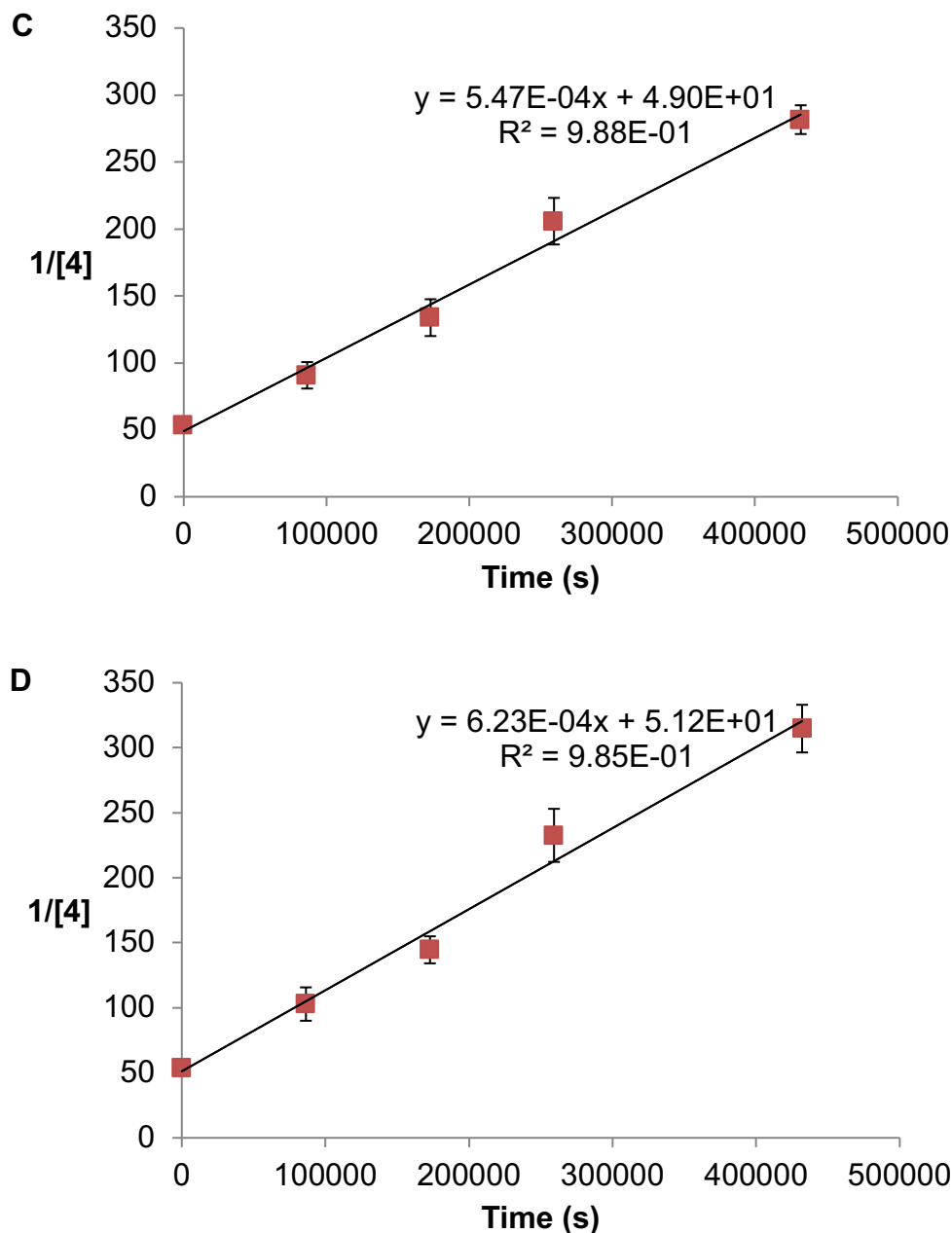


Figure S6. Kinetic plots for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**) using 48 (A), 72 (B), 96 (C) or 120 (D) eq. of HOPiv (relative to Rh). Reaction conditions: 9.35 mM of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ as starting material, 0.3 mL benzene- d_6 , 24 eq. $\text{Cu}(\text{OPiv})_2$ (relative to Rh), 50 psig ethylene, 21 °C. Decay of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) is calculated based on the amount of formed $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**). Each data point is the average of three separate experiments. Error bars represent the standard deviations based on a minimum of three independent experiments.

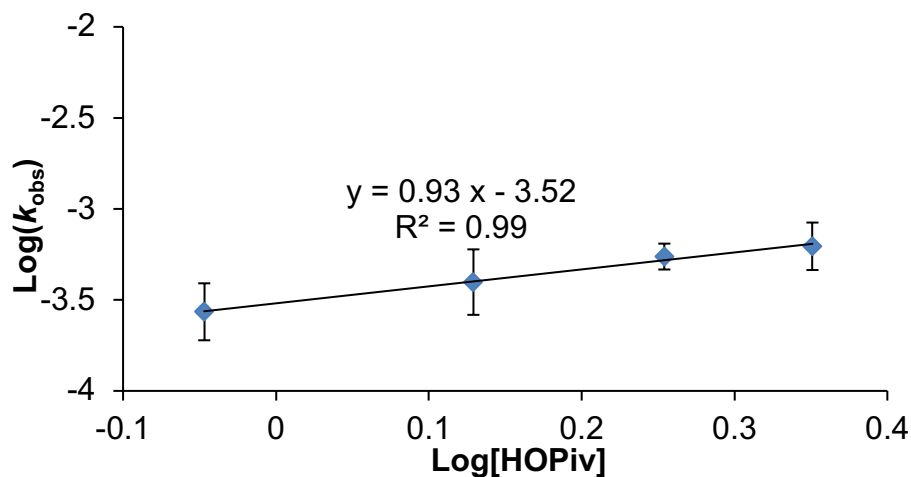


Figure S7. Log–log plot of observed rate constants (k_{obs}) for conversion of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) to $[(\text{HOPiv})\text{Rh}(\mu\text{-OPiv})_2]_2$ (**2**) versus concentration of HOPiv. Reaction conditions: 9.35 mM of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})]_2$ as starting material, 0.3 mL benzene- d_6 , 24 eq. $\text{Cu}(\text{OPiv})_2$ (relative to Rh), 48 (A), 72 (B), 96 (C) or 120 (D) eq. HOPiv (relative to Rh), 50 psig ethylene, 21 °C. Each data point is the average of three separate experiments. Error bars represent the standard deviations based on a minimum of three independent experiments.

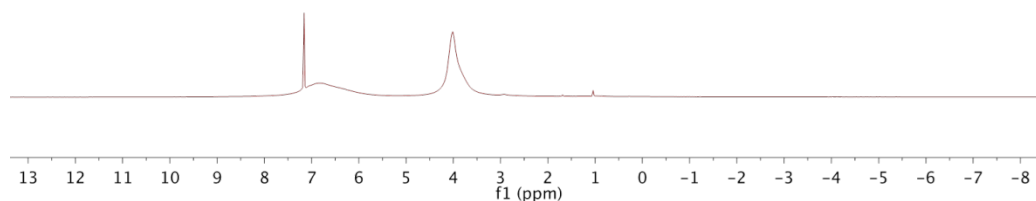


Figure S8. Paramagnetic ^1H NMR spectrum of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) (800 MHz, benzene- d_6).

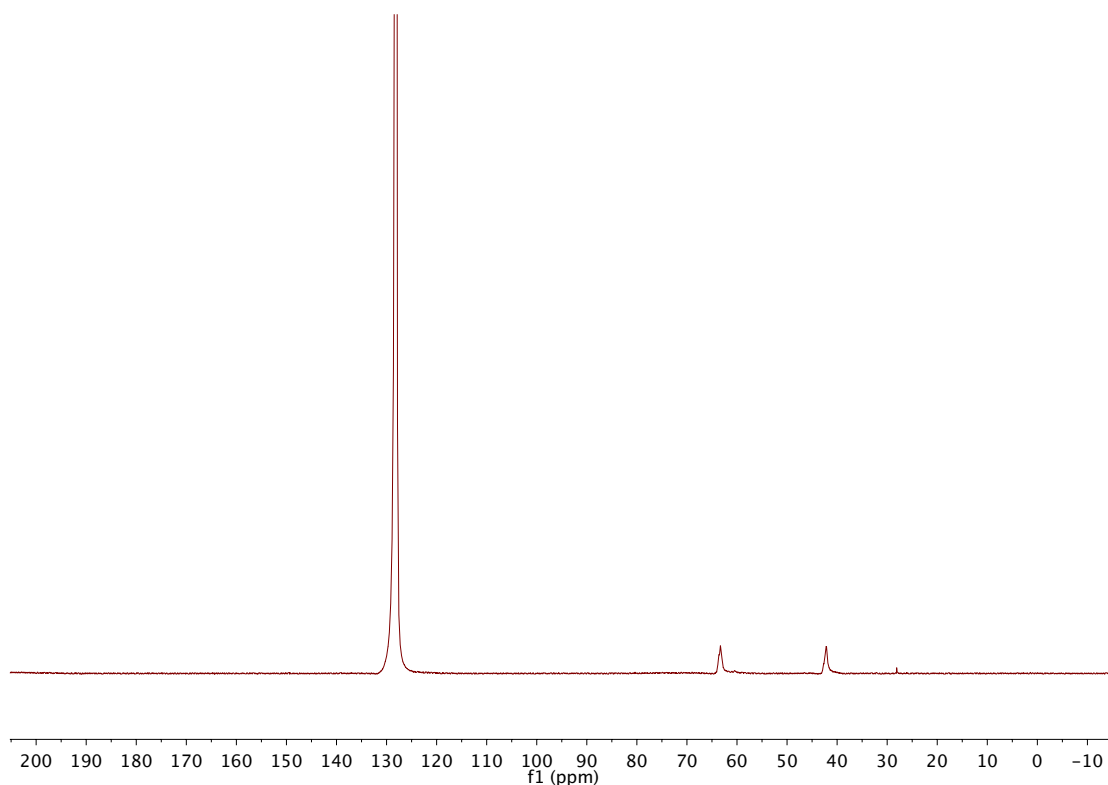


Figure S9. Paramagnetic ^{13}C NMR spectrum of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) (201 MHz, benzene- d_6).

Dependence of R_1 on concentration for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (4**)**

In Figure S10, the spin-lattice relaxation rate of the ethylene protons (~ 4.0 ppm in the ^1H NMR spectrum) of a solution $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) in benzene- d_6 is plotted as a function of relative concentration, obtained by dilution of an initial solution with further benzene- d_6 . The intercept of this plot at 0 concentration (141 ± 7 s $^{-1}$) gives us the purely intramolecular spin lattice relaxation rate for these protons. Since the slope is small, meaning a weak dependence on concentration, we conclude that most or all of the spin lattice relaxation observed occurs from an intramolecular phenomenon, indicative that the paramagnetic center (Cu^{II}) and ethylene protons belong to the same molecule, supporting the persistence of **4** in solution.

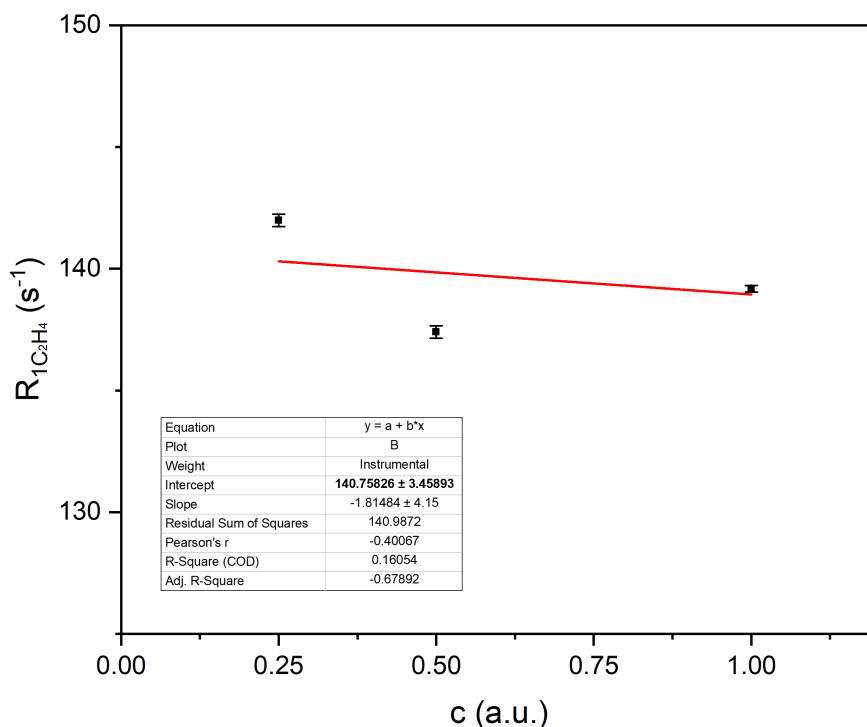


Figure S10. Plot of the spin-lattice relaxation rate (R_1) of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) as a function of concentration.

Experimental determination of the average $\text{C}_2\text{H}_4\text{-Cu}$ distance of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) using R_1

Although not essential to prove the existence of complex **4** in solution, equation (2) is a simplified Solomon-Bloembergen equation,¹ which allows us to estimate the distance between the unpaired electron on Cu and the ethylene protons of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) in dilute solution by measuring the ethylene proton spin-lattice relaxation rate (R_1). Although there are uncertainties that limit this method, we believe the assessment provides additional evidence for the existence of **4** in solution. We first needed to obtain the rotational correlation time of **4**. This was done by using the molecular volume of **4** (828 \AA^3) which was obtained from the crystal structure, then using the equation that relates the volume of a sphere to its radius. The radius of **4** is 5.83 \AA from the solid-state X-ray structure. We used equation (1)² to obtain the rotational correlation time (τ_R) of **4** ($1.22 \times 10^{-10} \text{ s}$).

$$\tau_R = \frac{4\pi\eta r^3}{3k_B T} \quad (1)$$

η is the viscosity of benzene at 25°C (0.604 cP), $r = 5.83 \text{ \AA}$ (see above), k_B is Boltzmann's constant and T is the temperature.

R_1 of the ethylene protons was measured at three dilute concentrations. The dependence of R_1 on concentration was linear and the R_1 value at 0 concentration (141 s^{-1}) is due to intramolecular dipolar spin-lattice relaxation.³ We then used equation (2) to calculate r , the average distance between the unpaired electron on Cu and the ethylene protons of **4** (6.05 \AA).

$$r = 540 \left(\left(\frac{3\tau_c}{1 + \omega_I^2 \tau_c^2} + \frac{7\tau_c}{1 + \omega_S^2 \tau_c^2} \right) / R_1 \right)^{\frac{1}{6}} \quad (2)$$

where $\tau_c^{-1} = \tau_R^{-1} + \tau_{el}^{-1}$, τ_R (see above), τ_{el} is the electron spin-lattice relaxation time (1×10^{-9} s),^{4, 5} ω_I is the proton Larmor frequency (3.77×10^9 rad/s), ω_S is the electron Larmor frequency (2.48×10^{12} rad/s) and the constant value (540) contains contributions from the electron spin quantum number, the proton magnetogyric ratio, the Bohr magneton, and the Lande g factor.

Average C₂H₄-Cu distance of complex 4 from the crystal structure and DFT

We compare the average distance between Cu and the ethylene protons (C₂H₄-Cu) derived from spin-lattice relaxation in dilute solution with the average distance found in the original crystal structure and the structure predicted by DFT. Amongst the 16 ethylene protons, we find an average C₂H₄-Cu distance of 4.33 Å in the crystal structure. This average is composed of two separate averages consisting of short and long C₂H₄-Cu distances. The short and long C₂H₄-Cu averages are 3.58 and 5.08 Å, respectively. We concurrently evaluated the average C₂H₄-Cu distance using DFT. Similar to the crystal structure, we arrive at an average C₂H₄-Cu distance of 4.32 Å. The short and long C₂H₄-Cu averages predicted by DFT are 3.48 and 5.16 Å, respectively (Figure S11). The crystal structure and DFT structure are nearly identical based on the average C₂H₄-Cu distance. The DFT structure predicts the average ethylene C=C bond to be 1.39 Å and the average Rh-Cu distance to be 3.09 Å.

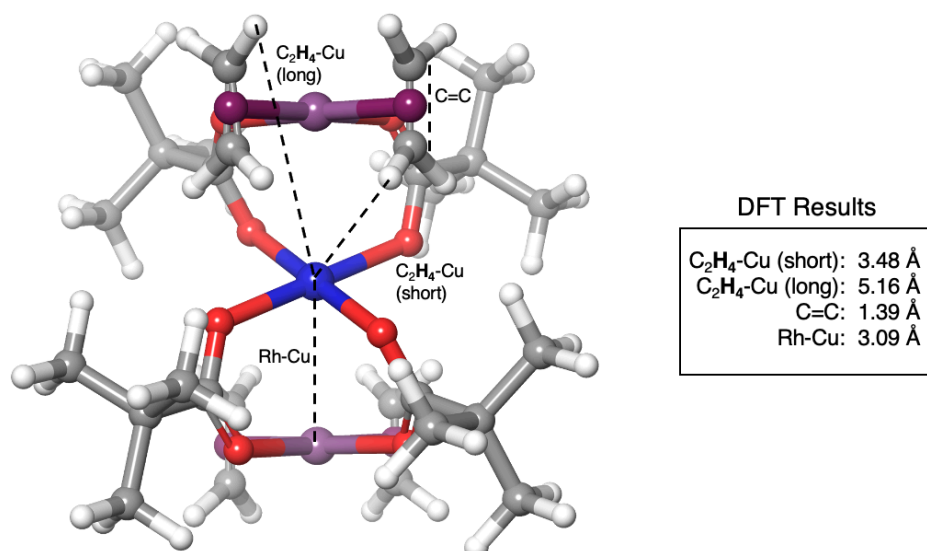


Figure S11. DFT average pair distances for the Rh-Cu-Rh trimer. The total C₂H₄-Cu average of 4.32 Å is composed of the long and short averages.

We also calculated Mulliken spin populations to determine if the unpaired spin on Cu(II) in complex 4 is delocalized. Spin populations reveal that with a net spin of +1.00, Cu(II) contains +0.64 unpaired spin density. The remaining +0.36 unpaired spin resides on the 4 oxygens bound to the Cu, such that each oxygen atom has a net unpaired spin of +0.09. This result indicates 36% spin delocalization in complex 4.

Limitations to the Experimental determination of the average C₂H₄–Cu distance of [(η^2 -C₂H₄)₂Rh^I(μ -OPiv)₂](μ -Cu) (**4**) using R₁

The limitations of this method, which likely prevent a highly accurate determination of the ethylene H and Cu distances include: 1) Uncertainty of the electron relaxation time. We have used previous estimates of electron relaxation time for Cu(II), but the 36% spin delocalization predicted by theory (see above) indicates that these previous estimates are likely not be reliable. 2) We have use the solid-state X-ray structure to measure complex **4**'s radius, but this value in solution is likely to be changed. 3) We have modeled solution structure using implicit solvent.

Computational Methods

All Density Functional Theory (DFT) calculations were performed using the Jaguar software version 10.9 by Schrodinger Inc.⁶ Structure optimizations were performed using the B3LYP⁷ flavor of DFT including the Grimme-Becke-Johnson D3 correction for London dispersion.⁸ Non-metal atoms were described by the triple-zeta 6-311G**++ basis set⁹ while Rh and Cu were treated with the Los Alamos small-core (18 explicit electrons) effective core potential (LACV3P**++).^{10, 11} Ultra-fine DFT grids were used for all calculations.

Vibrational frequency calculations at 423 K were performed at the B3LYP-D3 level and used to predict thermochemical properties including zero point energies, enthalpies as a function of temperature, and entropies as a function of temperature. These frequency calculations were also used to confirm local minima (no negative eigenvalues in Hessian) and transition states (1 negative eigenvalue in Hessian).

In such calculations there are 3 translational degrees of freedom (dof) and 3 rotational dof leading to large entropies, but in solvent these dof become hindered librational dof, reducing the entropy by 40 to 60 %. This becomes an issue for reactions that change the number of molecules. To account for this entropy loss, a correction is often applied to translational and rotational modes.¹² We assume in this paper a factor of 50%. This entropy correction is implemented via the following formula: $G = H - T^*(0.5*(S_{tran}+S_{rot})+S_{vib}+S_{elec}))$

All calculations included implicit solvent treatment. Solvent effects were implemented via the Poisson-Boltzmann finite element method (PBF).^{13, 14} A dielectric constant of 2.284 and a probe radius of 2.6 Å were used to represent benzene.

DFT Structure Energies

Energies for the various structures at 423 K are listed in the following tables. The labels used here (1, 2, etc) for structures are defined in the manuscript. H is enthalpy, G is free energy, and S is total entropy.

Table S1. Energies at 423 K for the various structures from Scheme 5 in the manuscript. C₂H₄ is ethylene, HOAc is acetic acid, and C₆H₆ is benzene.

Structure	H (Hartree)	G (Hartree)	S (cal/mol/K)
2	-2298.798	-2298.925	376.559
4	-1643.7452	-1643.8312	255.328
1	-990.46403	-990.53251	203.193
5	-495.20742	-495.25016	126.812
6	-566.54466	-566.57988	104.518
7	-795.06909	-795.11385	132.804
Cu(OAc) ₂	-653.21842	-653.25471	107.656
Cu(OAc)	-424.68808	-424.71598	82.798
C ₂ H ₄	-78.560925	-78.580826	59.043
HOAc	-229.10325	-229.1287	75.502
C ₆ H ₆	-232.20689	-232.23121	72.16

Table S2. Energies at 423 K for the various structures from Scheme 6 in the manuscript.

Structure	H (Hartree)	G (Hartree)	S (cal/mol/K)
4	-1643.7452	-1643.8312	255.328
4b	-1797.3616	-1797.4553	278.049
TS4.1	-1797.369	-1797.4436	221.214
4c	-1797.3817	-1797.4563	221.591
TS4.1'	-1797.361	-1797.4363	223.462
TS4.2	-1797.3653	-1797.4378	214.89
4d	-1797.3842	-1797.4606	226.759
4d'	-576.85585	-576.90543	147.095
TS4.3	-1797.3674	-1797.4426	223.313
4e	-1797.3828	-1797.459	226.098
TS4.4	-1797.38	-1797.4556	224.086
4f	-1566.3568	-1566.4268	207.757

Table S3. Energies at 423 K for the various structures from Scheme 7 in the manuscript.

Structure	H (Hartree)	G (Hartree)	S (cal/mol/K)
1	-990.46403	-990.53251	203.193
1b	-1144.0796	-1144.1506	210.596
TS1.1	-1144.0859	-1144.1418	166.05
1c	-1144.0942	-1144.1518	170.96
TS1.2	-1144.0745	-1144.1309	167.405
TS1.1'	-1144.0629	-1144.1205	170.74
1d	-1144.0935	-1144.1503	168.481
TS1.3	-1144.0825	-1144.1401	171.1
1e	-1144.0891	-1144.1458	168.142
TS1.4	-1144.0889	-1144.1435	162.032
1f	-913.06087	-913.11139	149.888

Table S4. Energies at 423 K for the various structures from Scheme 8 in the manuscript.

Structure	H (Hartree)	G (Hartree)	S (cal/mol/K)
5	-495.20742	-495.25016	126.812
5b	-648.83352	-648.8804	139.097
TS5.1	-648.81047	-648.85912	144.343
TS5.1'	-648.78023	-648.82745	140.094
5c	-648.8146	-648.86142	138.904
TS5.2	-648.80351	-648.8487	134.078
5d	-576.85585	-576.90543	147.095
TS5.3	-576.82864	-576.87603	140.589
5e	-576.8621	-576.912	148.038
TS5.4	-576.8561	-576.90483	144.592
5f	-345.82902	-345.86762	114.527

Table S5. Energies at 423 K for various structures from Scheme S1-S4 in the SI.

Scheme	Structure	H	G	S
S1	[Cu(OAc) ₂] ₂	-1306.4713	-1306.5301	174.4
	[Cu(OAc) ₂] ₃	-1959.7393	-1959.8025	187.611
	Cu(OAc) ₂	-653.21842	-653.25471	107.656
	Cu(OAc)	-424.68808	-424.71598	82.798
	Cu(OAc)(HOAc) ₂	-882.96988	-883.01784	142.293
	Cu(OAc)(HOAc)(C ₂ H ₄)	-732.42592	-732.47349	141.118
	Cu(OAc)(C ₂ H ₄)	-581.86914	-581.91317	130.657
S2	Rh(II)Cu(II)Rh(II)	-1715.6454	-1715.7326	258.675
	Rh(III)Cu(II)Rh(1)	-1794.2502	-1794.3435	276.943
	Rh(III)Rh(I)	-1140.9777	-1141.0483	209.54
	Rh(II)Rh(II)	-1062.3641	-1062.4311	198.632
S3	TS: Premature C ₂ H ₄ Insertion	-1797.3463	-1797.4174	210.938
S4	TS: External OAc Deprotonation	-2025.9667	-2026.0687	302.357

X-ray crystallography data and structure determination

A suitable single crystal of [(HOPIv)Rh(μ -OPiv)₂]₂ (**2**) or [(η^2 -C₂H₄)₂Rh^I(μ -OPiv)₂]₂(μ -Cu) (**4**) was coated with Paratone oil and mounted on a MiTeGen MicroLoop. The X-ray intensity data were measured on a Bruker Kappa APEXII Duo system equipped with a fine-focus sealed tube (Mo K α , λ = 0.71073 Å) and a graphite monochromator.

Complex **4** was identified as a two-component twin using CELL_NOW.¹⁵ Starting with 1163 reflections, 963 reflections were fit to the first domain, 716 to the second

domain (112 exclusively), with 88 unindexed reflection remaining. The twin domain was oriented at a 179.6° rotation about the real axis -0.002 1.000 0.000. The twin law was -1.000 0.255 -0.007 / -0.003 1.000 0.000 / 0.005 1.000 -1.000. The frames of **2** or **4** were integrated with the Bruker SAINT software package¹⁶ using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method SADABS (**2**) or TWINABS (**4**).¹⁶

The structures were solved and refined using the Bruker SHELXTL Software Package¹⁷ within APEX3¹⁵ and OLEX2.¹⁸ Non-hydrogen atoms were refined anisotropically. The O-H hydrogen atoms in **2** were located in the diffraction map and refined isotropically. All other hydrogen atoms in both structures were placed in geometrically calculated positions with $U_{iso} = 1.2U_{equiv}$ of the parent atom ($1.5U_{equiv}$ for methyl). Complex **4** was refined on HKLF5 data, with the BASF for the twin domains refining to 0.24640. In **2**, each ligand was disordered over multiple positions. The relative occupancies were freely refined, with the sum of each ligand set to one. Constraints and restraints were used on the bonds and anisotropic displacement parameters of the disordered atoms as needed.

Table S6. Crystallographic data for [(HOPiv)Rh(μ -OPiv)₂]₂ (**2**) and [(η^2 -C₂H₄)₂Rh^I(μ -OPiv)₂]₂(μ -Cu) (**4**).

	2	4
CCDC number	2046179	2046180
Formula	C ₃₀ H ₅₆ O ₁₂ Rh ₂	C ₂₈ H ₅₂ CuO ₈ Rh ₂
FW (g/mol)	817.69	786.05
Temp (K)	100(2)	100(2)
Size (mm)	0.320 x 0.452 x 0.690	0.130 x 0.176 x 0.331
Crystal habit	green block	yellow rod
Crystal system	monoclinic	triclinic
Space group	C 2/c	P -1
a (Å)	19.0942(19)	9.3325(14)
b (Å)	16.8025(16)	9.9290(14)
c (Å)	11.7586(12)	10.2933(15)
α (°)	90	61.195(3)
β (°)	90.409(2)	86.071(3)
γ (°)	90	82.255(3)
Volume (Å ³)	3772.4(6)	828.2(2)
Z	4	1
Density (g/cm ³)	1.440	1.576
μ (mm ⁻¹)	0.928	1.663
F(000)	1695	403
θ range (°)	1.61 to 33.17	2.20 to 28.32

Index ranges	-29 ≤ h ≤ 29 -25 ≤ k ≤ 25 -18 ≤ l ≤ 14	-12 ≤ h ≤ 12 -11 ≤ k ≤ 13 0 ≤ l ≤ 113
Data / restraints / parameters	7212 / 156 / 376	4111 / 0 / 185
GOF on F ²	1.037	1.106
R ₁ (I>2σ(I))	0.0223	0.0367
wR ₂ (all data)	0.0543	0.0945

Table S7. Bond lengths (Å) for [(HOPiv)Rh(μ-OPiv)₂]₂ (**2**).

Rh1-O3'	2.026(16)	Rh1-O4	2.027(15)
Rh1-O1	2.0294(9)	Rh1-O2'	2.0321(9)
C12-C15	1.536(3)	Rh1-O5	2.2988(19)
O1-C1	1.2780(14)	O2-C1	1.2660(14)
C1-C2	1.562(3)	C2-C5	1.526(5)
C2-C4	1.550(5)	C2-C3	1.561(4)
C7-C9	1.558(9)	O3-C6	1.273(9)
O4-C6	1.274(9)	C6-C7	1.532(8)
C7-C10	1.488(8)	C7-C8	1.528(9)
C12-C13	1.545(4)	O5-C11	1.223(3)
O6-C11	1.334(3)	O6-H6	0.83(5)
C11-C12	1.520(3)	C12-C14	1.525(4)
C3-H3A	0.98	C3-H3B	0.98
C3-H3C	0.98	C4-H4A	0.98
C4-H4B	0.98	C4-H4C	0.98
C5-H5A	0.98	C5-H5B	0.98
C5-H5C	0.98	C8-H8A	0.98
C8-H8B	0.98	C8-H8C	0.98
C9-H9A	0.98	C9-H9B	0.98
C9-H9C	0.98	C10-H10A	0.98
C10-H10B	0.98	C10-H10C	0.98

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1

Table S8. Bond angles (°) for [(HOPiv)Rh(μ-OPiv)₂]₂ (**2**).

O3'-Rh1-O4	88.4(8)	O3'-Rh1-O1	174.8(4)
O4-Rh1-O1	90.4(5)	O3'-Rh1-O2'	91.2(6)

O4-Rh1-O2'	177.8(3)	O1-Rh1-O2'	89.81(4)
O3'-Rh1-O5	88.4(4)	O4-Rh1-O5	95.0(3)
O1-Rh1-O5	96.68(6)	O2'-Rh1-O5	87.16(6)
C1-O1-Rh1	118.84(7)	C1-O2-Rh1'	119.45(8)
O2-C1-O1	125.06(11)	O2-C1-C2	117.44(13)
O1-C1-C2	116.62(13)	C5-C2-C4	108.9(3)
C5-C2-C3	110.1(2)	C4-C2-C3	112.1(2)
C5-C2-C1	107.5(2)	C4-C2-C1	108.7(2)
C3-C2-C1	109.4(2)	C2-C3-H3A	109.5
C2-C3-H3B	109.5	H3A-C3-H3B	109.5
C2-C3-H3C	109.5	H3A-C3-H3C	109.5
H3B-C3-H3C	109.5	C2-C4-H4A	109.5
C2-C4-H4B	109.5	H4A-C4-H4B	109.5
C2-C4-H4C	109.5	H4A-C4-H4C	109.5
H4B-C4-H4C	109.5	C2-C5-H5A	109.5
C2-C5-H5B	109.5	H5A-C5-H5B	109.5
C2-C5-H5C	109.5	H5A-C5-H5C	109.5
C6-O3-Rh1'	121.5(11)	C5A-C2A-C1	115.3(8)
C6-O4-Rh1	118.0(10)	O3-C6-O4	124.0(11)
O3-C6-C7	116.2(9)	O4-C6-C7	119.7(9)
C10-C7-C8	112.1(6)	C10-C7-C6	111.8(5)
C8-C7-C6	110.2(6)	C10-C7-C9	110.5(5)
C8-C7-C9	108.0(5)	C6-C7-C9	103.8(6)
C7-C8-H8A	109.5	C7-C8-H8B	109.5
H8A-C8-H8B	109.5	C7-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
C7-C9-H9A	109.5	C7-C9-H9B	109.5
H9A-C9-H9B	109.5	C7-C9-H9C	109.5
H9A-C9-H9C	109.5	H9B-C9-H9C	109.5
C7-C10-H10A	109.5	C7-C10-H10B	109.5
H10A-C10-H10B	109.5	C7-C10-H10C	109.5
H10A-C10-H10C	109.5	H10B-C10-H10C	109.5
C11-O5-Rh1	122.42(16)	C11-O6-H6	111.(3)
O5-C11-O6	123.1(2)	O5-C11-C12	123.2(2)
O6-C11-C12	113.75(19)	C11-C12-C14	109.72(19)

C11-C12-C15	109.04(19)	C14-C12-C15	109.8(2)
C11-C12-C13	108.7(2)	C14-C12-C13	109.8(2)
C15-C12-C13	109.7(2)	C12-C13-H13A	109.5
C12-C13-H13B	109.5	H13A-C13-H13B	109.5
C12-C13-H13C	109.5	H13A-C13-H13C	109.5
H13B-C13- H13C	109.5	C12-C14-H14A	109.5
C12-C14-H14B	109.5	H14A-C14-H14B	109.5
C12-C14-H14C	109.5	H14A-C14-H14C	109.5
H14B-C14- H14C	109.5	C12-C15-H15A	109.5
C12-C15-H15B	109.5	H15A-C15-H15B	109.5
C12-C15-H15C	109.5	H15A-C15-H15C	109.5
H15B-C15- H15C	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1

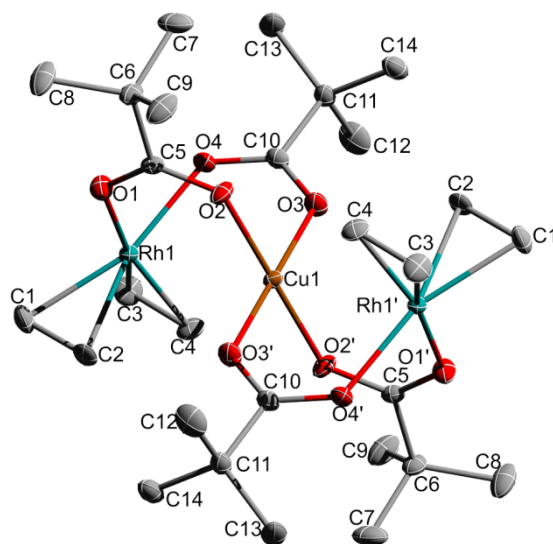


Figure S12. ORTEP of $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**) (50% probability). H atoms are omitted for clarity.

Table S9. Bond lengths (Å) for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**).

Rh1-O4'	2.078(3)	Rh1-O1	2.079(3)
Rh1-C1	2.112(4)	Rh1-C3	2.112(4)
Rh1-C2	2.118(3)	Rh1-C4	2.122(4)
Rh1-Cu1	3.0095(5)	Cu1-O2'	1.948(3)
Cu1-O2	1.948(3)	Cu1-O3'	1.949(3)
Cu1-O3	1.949(3)	O1-C5	1.261(5)
O2-C5	1.262(4)	O3-C10	1.263(5)
O4-C10	1.264(5)	C1-C2	1.393(6)
C1-H1A	0.99	C1-H1B	0.99
C2-H2A	0.99	C2-H2B	0.99
C3-C4	1.402(6)	C3-H3A	0.99
C3-H3B	0.99	C4-H4A	0.99
C4-H4B	0.99	C5-C6	1.541(5)
C6-C9	1.523(5)	C6-C8	1.525(6)
C6-C7	1.546(5)	C7-H7A	0.98
C7-H7B	0.98	C7-H7C	0.98
C8-H8A	0.98	C8-H8B	0.98
C8-H8C	0.98	C9-H9A	0.98
C9-H9B	0.98	C9-H9C	0.98

C10-C11	1.532(5)	C11-C14	1.523(5)
C11-C13	1.539(5)	C11-C12	1.549(5)
C12-H12A	0.98	C12-H12B	0.98
C12-H12C	0.98	C13-H13A	0.98
C13-H13B	0.98	C13-H13C	0.98
C14-H14A	0.98	C14-H14B	0.98
C14-H14C	0.98		

Symmetry transformations used to generate equivalent atoms:

'-x+1, -y+1, -z+1

Table S10. Bond angles (°) for $[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})$ (**4**).

O4'-Rh1-O1	87.78(11)	O4'-Rh1-C1	160.42(14)
O1-Rh1-C1	88.93(15)	O4'-Rh1-C3	87.99(14)
O1-Rh1-C3	159.70(14)	C1-Rh1-C3	88.43(18)
O4'-Rh1-C2	160.41(13)	O1-Rh1-C2	88.04(14)
C1-Rh1-C2	38.45(16)	C3-Rh1-C2	102.16(17)
O4'-Rh1-C4	88.44(13)	O1-Rh1-C4	160.80(13)
C1-Rh1-C4	100.63(17)	C3-Rh1-C4	38.66(16)
C2-Rh1-C4	89.24(16)	O4'-Rh1-Cu1	76.48(8)
O1-Rh1-Cu1	77.99(8)	C1-Rh1-Cu1	121.59(11)
C3-Rh1-Cu1	120.14(12)	C2-Rh1-Cu1	83.93(11)
C4-Rh1-Cu1	82.83(11)	O2'-Cu1-O2	180.0
O2'-Cu1-O3'	90.05(12)	O2-Cu1-O3'	89.95(12)
O2'-Cu1-O3	89.95(12)	O2-Cu1-O3	90.05(12)
O3'-Cu1-O3	180.0	O2'-Cu1-Rh1	101.06(8)
O2-Cu1-Rh1	78.94(8)	O3'-Cu1-Rh1	80.31(8)
O3-Cu1-Rh1	99.69(8)	O2'-Cu1-Rh1'	78.94(8)
O2-Cu1-Rh1'	101.06(8)	O3'-Cu1-Rh1'	99.69(8)
O3-Cu1-Rh1'	80.31(8)	Rh1-Cu1-Rh1'	180.0
C5-O1-Rh1	123.5(2)	C5-O2-Cu1	129.7(2)
C10-O3-Cu1	127.1(2)	C10-O4-Rh1'	126.2(2)
C2-C1-Rh1	71.0(2)	C2-C1-H1A	116.5
Rh1-C1-H1A	116.5	C2-C1-H1B	116.5
Rh1-C1-H1B	116.5	H1A-C1-H1B	113.5
C1-C2-Rh1	70.5(2)	C1-C2-H2A	116.6
Rh1-C2-H2A	116.6	C1-C2-H2B	116.6

Rh1-C2-H2B	116.6	H2A-C2-H2B	113.6
C4-C3-Rh1	71.1(2)	C4-C3-H3A	116.5
Rh1-C3-H3A	116.5	C4-C3-H3B	116.5
Rh1-C3-H3B	116.5	H3A-C3-H3B	113.5
C3-C4-Rh1	70.3(2)	C3-C4-H4A	116.6
Rh1-C4-H4A	116.6	C3-C4-H4B	116.6
Rh1-C4-H4B	116.6	H4A-C4-H4B	113.6
O1-C5-O2	125.9(3)	O1-C5-C6	117.7(3)
O2-C5-C6	116.3(3)	C9-C6-C8	110.6(3)
C9-C6-C5	109.6(3)	C8-C6-C5	112.0(3)
C9-C6-C7	109.3(4)	C8-C6-C7	110.2(4)
C5-C6-C7	105.0(3)	C6-C7-H7A	109.5
C6-C7-H7B	109.5	H7A-C7-H7B	109.5
C6-C7-H7C	109.5	H7A-C7-H7C	109.5
H7B-C7-H7C	109.5	C6-C8-H8A	109.5
C6-C8-H8B	109.5	H8A-C8-H8B	109.5
C6-C8-H8C	109.5	H8A-C8-H8C	109.5
H8B-C8-H8C	109.5	C6-C9-H9A	109.5
C6-C9-H9B	109.5	H9A-C9-H9B	109.5
C6-C9-H9C	109.5	H9A-C9-H9C	109.5
H9B-C9-H9C	109.5	O3-C10-O4	125.7(3)
O3-C10-C11	117.2(3)	O4-C10-C11	117.0(3)
C14-C11-C10	110.3(3)	C14-C11-C13	110.7(3)
C10-C11-C13	111.3(3)	C14-C11-C12	109.7(3)
C10-C11-C12	104.9(3)	C13-C11-C12	109.8(3)
C11-C12-H12A	109.5	C11-C12-H12B	109.5
H12A-C12-H12B	109.5	C11-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
C11-C13-H13A	109.5	C11-C13-H13B	109.5
H13A-C13-H13B	109.5	C11-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
C11-C14-H14A	109.5	C11-C14-H14B	109.5
H14A-C14-H14B	109.5	C11-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5

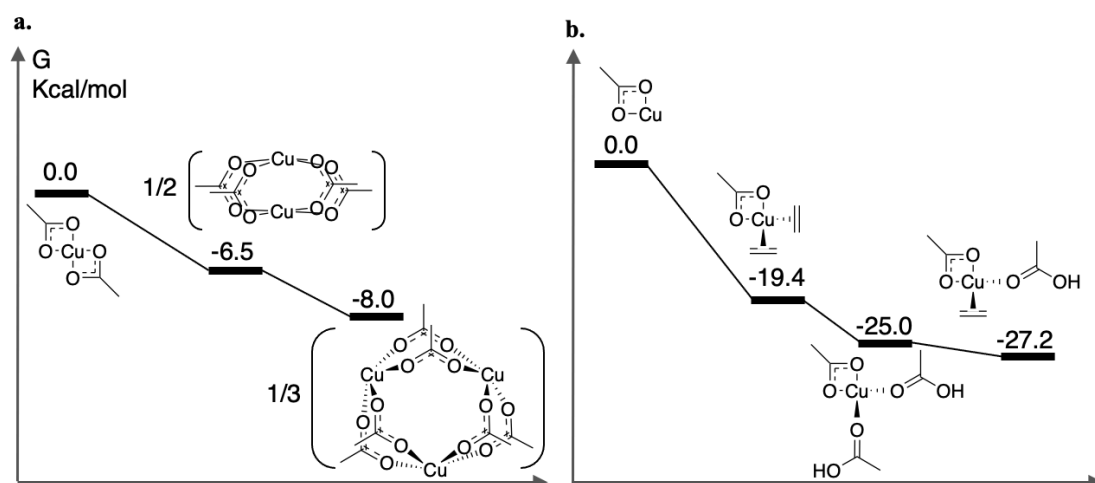
Symmetry transformations used to generate equivalent atoms:

'-x+1, -y+1, -z+1

Additional Calculations

Copper modeling

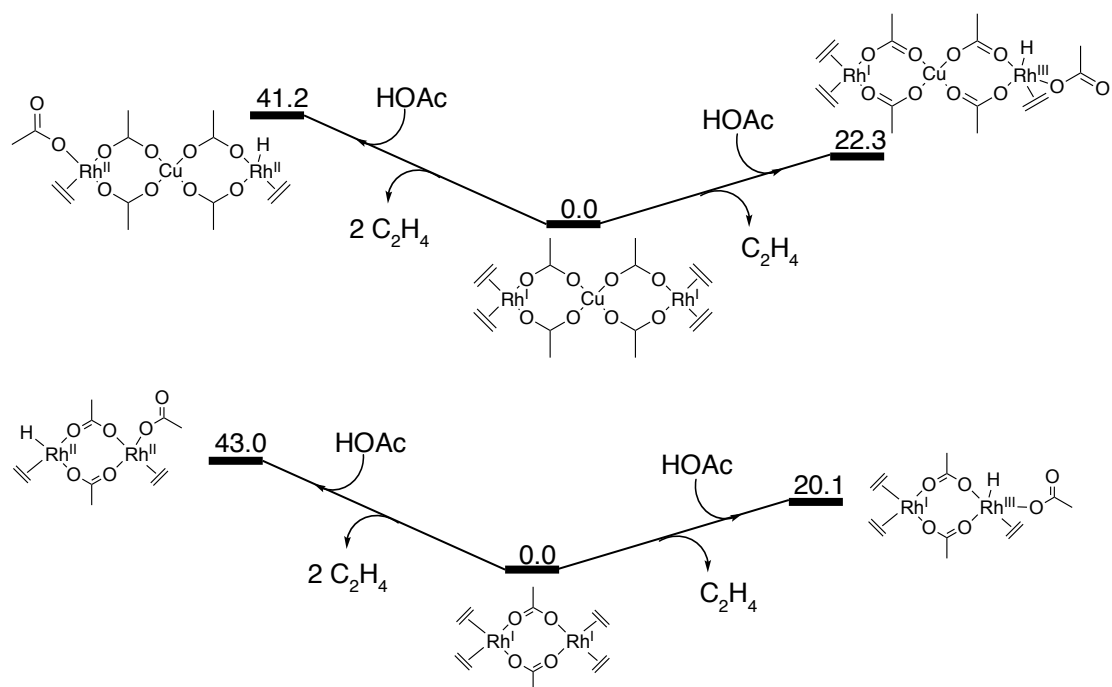
The modeling of Cu significantly impacts the energetic for Rh oxidation and reduction. For $\text{Cu}(\text{OAc})_2$ we examined the monomeric, dimer, and trimeric forms (Scheme S1a). We found the trimeric $[\text{Cu}(\text{OAc})_2]_3$ to be the most stable, the monomeric $\text{Cu}(\text{OAc})_2$ to be the least stable, and the $[\text{Cu}(\text{OAc})_2]_2$ dimer was moderately stable. Under catalytic conditions, Cu carboxylate oxidizes Rh to regenerate the active catalyst. This is observed to be a 1-electron oxidation, meaning $\text{Cu}(\text{OAc})_2$ is reduced to some form of $\text{Cu}(\text{OAc})$. We examined different ligand configurations of $\text{Cu}(\text{OAc})$ with HOAc and C_2H_4 (Scheme S1b). We find $\text{Cu}(\text{OAc})(\text{HOAc})(\text{C}_2\text{H}_4)$ to be the most stable $\text{Cu}(\text{OAc})$ configuration. Based on these results, we predict Rh oxidation occurs by reduction of a trimeric $[\text{Cu}(\text{OAc})_2]_3$ to form the $[\text{Cu}(\text{OAc})_2]_2$ dimer and liberate a $\text{Cu}(\text{OAc})$, which coordinates an HOAc and C_2H_4 to form $\text{Cu}(\text{OAc})(\text{HOAc})(\text{C}_2\text{H}_4)$.



Scheme S1. B3LYP-D3 free energies at 423 K for (a) different configurations of $\text{Cu}(\text{OAc})_2$ and (b) different ligand arrangements of $\text{Cu}(\text{OAc})$.

Rh oxidation by HOAc

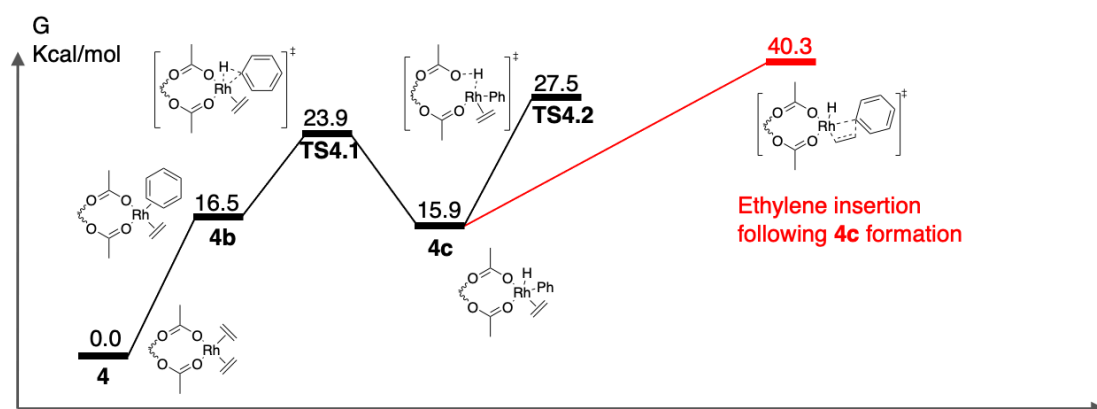
In addition to Rh oxidation by Cu carboxylate, HOAc could also potentially oxidize Rh. (Scheme S2). **4** could be oxidized in a single step to a Rh(I)/Cu(II)/Rh(III) trimer or through multiple steps to form a Rh(II)/Cu(II)/Rh(II) trimer. **1** could be oxidized in a single step to a Rh(I)/Rh(III) dimer or to a Rh(II)/Rh(II) dimer through multiples steps. However, DFT predicts this 2-electron oxidation to be uphill in energy and therefore not feasible.



Scheme S2. B3LYP-D3 free energies at 423 K for oxidation of the Rh(I)/Cu(II)/Rh(I) trimer (top) and the Rh(I)/Rh(I) dimer (bottom) by HOAc.

Premature ethylene insertion of **4c**

Following oxidative addition to yield the Rh-Ph bond, ethylene insertion into the Rh-Ph can occur. We calculate ethylene insertion following intermediate **4c**, finding a free energy barrier of 40.3 kcal/mol (s). This pathway is consequently not competitive.

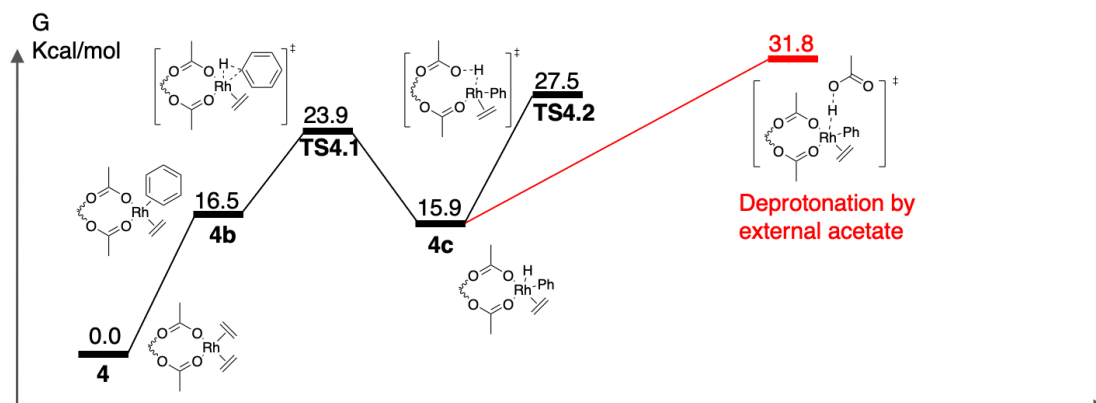


Scheme S3. B3LYP-D3 free energies at 423 K for premature ethylene insertion following the formation of intermediate **4c**.

Deprotonation of **4c** by an external acetate

Previous studies have proposed the deprotonation of the transition metal by an external acetate ligand to yield HOAc. In our case this is highly unlikely due to excess HOAc and Cu, effectively suppressing any free acetate ligands in solution. We calculate the transition state for deprotonation of **4c** by an external acetate, finding a free energy

barrier of 31.8 kcal/mol relative to the starting state **4** (Scheme S4). Thus, this pathway is not favorable due to the high barrier and lack of free acetates.



Scheme S4. B3LYP-D3 free energies at 423 K for deprotonation of intermediate **4c** by an external acetate.

DFT Structures

Scheme 5 Structures

$[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}(\mu\text{-OAc})_2]$ **1**

Rh1 -0.1670662842000 0.0123614243000 -0.7435728695000
 Rh2 -0.0427973372000 0.3776538613000 2.5640254836000
 O3 1.8497700268000 0.4824734391000 -0.2450034969000
 C4 2.4770362330000 0.1704443223000 0.8098972024000
 O5 1.9600800299000 -0.0054125906000 1.9478124575000
 C6 3.9761769349000 0.0166163553000 0.6863756916000
 H7 4.4272200904000 -0.2261347346000 1.6471900456000
 H8 4.1953730062000 -0.7705828041000 -0.0394194988000
 H9 4.4006078277000 0.9458172406000 0.2975374400000
 O10 0.1047663928000 -1.9485313047000 0.0462043344000
 C11 -0.1748409587000 -2.3735962643000 1.2022686399000
 O12 -0.5354636948000 -1.6596931595000 2.1827939214000
 C13 -0.0831742556000 -3.8684881571000 1.4150333433000
 H14 -0.3228839226000 -4.1321664251000 2.4438132400000
 H15 -0.7663382309000 -4.3768576974000 0.7297296188000
 H16 0.9298042184000 -4.1994497907000 1.1724500784000
 C17 -1.7600938129000 0.3477142676000 3.8673945627000
 C18 -2.1385095653000 0.8526329568000 2.6256078064000
 H19 -1.9034101606000 -0.7018557083000 4.1010311096000
 H20 -2.6012327409000 0.2084248142000 1.8889393114000
 H21 -2.3206607156000 1.9131631681000 2.4885989701000
 H22 -1.6397035610000 1.0026745716000 4.7231536766000
 X23 -1.0283733292000 -0.4820451926000 5.1864400580000
 X24 -0.6131896850000 -0.0369930264000 4.3929974887000

C25 -0.5649648395000 2.1097044702000 -0.9892788147000
 C26 0.0113412171000 1.6256977552000 -2.1614748065000
 H27 -1.6254440359000 2.3324729880000 -0.9410700034000
 H28 -0.5866354657000 1.4613959332000 -3.0509476463000
 H29 1.0790342071000 1.7194823290000 -2.3284498056000
 H30 0.0427339298000 2.6056871208000 -0.2433664347000
 X31 0.8918582063000 0.6551213942000 -3.1657750527000
 X32 0.4458410726000 0.2307995261000 -2.3777270409000
 C33 -1.7073768416000 -0.8662598276000 -1.9558027233000
 C34 -2.2725944991000 -0.4141198866000 -0.7629673775000
 H35 -1.8613269574000 -0.3275752786000 -2.8845629784000
 H36 -2.8791019764000 0.4848719944000 -0.7404458039000
 H37 -2.4464560361000 -1.1054845684000 0.0543489436000
 H38 -1.4168422692000 -1.9058650437000 -2.0662482153000
 X39 -1.2457508015000 -1.4135889392000 -2.9595553417000
 X40 -0.7964888223000 -0.8130891715000 -2.2980693607000
 C41 0.7953440787000 1.9778941813000 3.7279563665000
 C42 0.4514685574000 2.4677918050000 2.4677745824000
 H43 0.1945774732000 2.2128747974000 4.5998053952000
 H44 -0.4226838341000 3.0961363191000 2.3349350466000
 H45 1.2071378492000 2.5635214492000 1.6955955896000
 H46 1.8137506070000 1.6673269812000 3.9370424890000
 X47 1.6015211733000 1.7127503857000 4.3100335750000
 X48 1.0387020585000 1.1677262820000 3.6885970374000
 X49 -0.2768118112000 1.8677011127000 -1.5753768106000
 X50 -1.9899856703500 -0.6401898571000 -1.3593850504000
 X51 -1.9493016891000 0.6001736122000 3.2465011845500
 X52 0.6234063180500 2.2228429931500 3.0978654744500

$[(\eta^2\text{-C}_2\text{H}_4)\text{Rh}(\mu\text{-OAc})_2(\eta^2\text{-C}_2\text{H}_4)(\eta^2\text{-C}_6\text{H}_6)]$ **1b**

Rh1 -0.4317567058000 9.0896701831000 4.7041434711000
 C3 -0.1215229324000 7.7114660155000 6.3223500937000
 C4 -0.0820395642000 10.7522087991000 6.0153223772000
 C5 0.9563629488000 7.6162805386000 5.4442299991000
 C6 1.0012651090000 10.6212053699000 5.1441462341000
 Rh7 -3.8009485144000 8.9026513764000 4.8915906558000
 O8 -3.3532423108000 10.7310057944000 3.9144719555000
 O9 -3.2830516707000 7.9672602936000 3.0834694001000
 O10 -1.1992024552000 10.4947497722000 3.3017055033000
 O11 -1.1167431993000 7.4901619053000 3.4602234544000
 C12 -3.6030166013000 6.9710823746000 5.7899765293000
 C13 -2.1765553562000 7.4375532009000 2.7764545184000
 C14 -2.3455534295000 11.0209455891000 3.2157259679000
 C15 -4.9152653813000 7.1232304130000 5.3335052265000

C16 -2.1333857340000 6.6335787201000 1.4963974887000
 C17 -2.5255290863000 12.0936661960000 2.1629355895000
 H18 -1.1988241916000 6.8273847359000 0.9684153912000
 H19 -3.3010033696000 12.7976555362000 2.4647851434000
 H20 -1.5852308320000 12.6096845276000 1.9684672180000
 H21 -2.1567680164000 5.5703652009000 1.7543148422000
 H22 -2.9890690906000 6.8617392284000 0.8625488676000
 H23 -2.8493743349000 11.6087536664000 1.2364374636000
 H24 -0.9407081790000 7.0064258095000 6.2638044053000
 H25 -0.0155667153000 8.2155599355000 7.2771578889000
 H26 0.0094029878000 10.4594040392000 7.0559902138000
 H27 -0.8712001199000 11.4627143335000 5.8039584711000
 H28 1.9196495361000 8.0451227719000 5.6969796999000
 H29 0.9746138041000 6.8531930838000 4.6739472423000
 H30 1.0531854215000 11.2168754662000 4.2391438071000
 H31 1.9477237445000 10.2198840273000 5.4892650709000
 H32 -3.3720210563000 7.0226134773000 6.8486771328000
 H33 -2.8747413847000 6.4306183843000 5.1964402527000
 H34 -5.2188189561000 6.7096439337000 4.3777252677000
 H35 -5.7235644463000 7.2982444843000 6.0373148561000
 X36 0.4174200082000 7.6638732770500 5.8832900464000
 X37 0.4596127724000 10.6867070845000 5.5797343056500
 X38 -4.2591409913000 7.0471563938000 5.5617408779000
 C39 -3.2156396432000 10.7740319908000 7.2914219931000
 C40 -3.4041362755000 12.0584865123000 6.8371543997000
 C41 -4.5617555127000 12.3911756764000 6.0993407393000
 C42 -5.5085929273000 11.4338597119000 5.8163861037000
 C43 -5.3242835105000 10.0991519400000 6.2550662741000
 C44 -4.1735968954000 9.7639796560000 7.0072085892000
 H45 -2.3452174446000 10.5202697695000 7.8832758308000
 H46 -2.6687678114000 12.8253329369000 7.0534171600000
 H47 -4.7021112506000 13.4112758239000 5.7591726997000
 H48 -6.4002475928000 11.6890953250000 5.2562076726000
 H49 -6.1629885581000 9.4188925388000 6.1987998302000
 H50 -4.1484615464000 8.8535983572000 7.5918121093000

[(HOPiv)Rh(μ -OPiv)₂]₂ **2**

Rh1 0.2077201347000 0.0335649276000 -0.2569158428000
 Rh2 -0.0317881265000 0.0168429255000 2.1625237867000
 O3 1.8091697324000 1.3303742199000 0.0129880641000
 C4 2.1543760483000 1.7023158127000 1.1641700663000
 O5 1.5815350732000 1.3266028021000 2.2447236403000
 C6 3.3370733842000 2.6676333678000 1.2576621869000
 C7 3.6476703115000 3.0367841955000 2.7135221291000

C8 4.5552349974000 1.9736309281000 0.6133222247000
C9 2.9678093421000 3.9329556892000 0.4554899184000
O10 -1.0973952775000 1.6443449552000 -0.2848795156000
C11 -1.5673706972000 2.0921825876000 0.8051166427000
O12 -1.3131898255000 1.6346636584000 1.9583005067000
C13 -2.5103372883000 3.2938397113000 0.6944070410000
C14 -3.0557453671000 3.6918340656000 2.0717706408000
C15 -1.7036388284000 4.4582429841000 0.0830849317000
C16 -3.6688057082000 2.9076628580000 -0.2462242073000
O17 1.4769517213000 -1.5924295567000 -0.0509736887000
C18 1.7406697545000 -2.0429600604000 1.1052052251000
O19 1.2817325707000 -1.5871572773000 2.1941657652000
C20 2.7042633189000 -3.2316808662000 1.1666171055000
C21 2.8857827488000 -3.7160155271000 2.6107132294000
C22 2.1238430780000 -4.3618340056000 0.2934567117000
C23 4.0551516070000 -2.7623940464000 0.5881669914000
O24 -1.4144518372000 -1.2601521244000 -0.3333939988000
C25 -1.9852246928000 -1.6453053121000 0.7471671545000
O26 -1.6290916069000 -1.2895582253000 1.8974353110000
C27 -3.1706713276000 -2.5957220836000 0.5896470239000
C28 -3.7419640797000 -2.9746479596000 1.9619071623000
C29 -4.2446793496000 -1.8775501028000 -0.2544371377000
C30 -2.6760497289000 -3.8574268519000 -0.1482044658000
H31 -4.5878434355000 -3.6547508054000 1.8295718997000
H32 -2.9903126708000 -3.4690787179000 2.5796175142000
H33 -4.0853416741000 -2.0917712955000 2.5036735122000
H34 -5.1059103614000 -2.5374164490000 -0.3879653253000
H35 -4.5891569168000 -0.9666177903000 0.2422849047000
H36 -3.8631624168000 -1.6068282275000 -1.2399914783000
H37 -3.5085783790000 -4.5534102582000 -0.2805223059000
H38 -2.2730558942000 -3.6127950387000 -1.1319801883000
H39 -1.8963929971000 -4.3664185677000 0.4247310301000
H40 2.8051285067000 -5.2172023314000 0.2950788644000
H41 1.1575257068000 -4.6981900919000 0.6799292987000
H42 1.9832292935000 -4.0246721690000 -0.7341111497000
H43 3.5755567237000 -4.5647378801000 2.6280265260000
H44 3.2910557760000 -2.9250125683000 3.2441922122000
H45 1.9348301441000 -4.0309333529000 3.0445784644000
H46 4.7677288901000 -3.5919130725000 0.5932791506000
H47 3.9360562078000 -2.4056633416000 -0.4356727585000
H48 4.4767027164000 -1.9506511226000 1.1878091743000
H49 -2.3484480983000 5.3338415914000 -0.0327151094000
H50 -0.8673250622000 4.7371424229000 0.7303746705000
H51 -1.3037698028000 4.1826410071000 -0.8935928378000

H52 -3.7269216932000 4.5489760074000 1.9656968079000
H53 -3.6096599340000 2.8703399532000 2.5301168779000
H54 -2.2474792551000 3.9643774278000 2.7526463784000
H55 -4.3447585974000 3.7584468084000 -0.3687617245000
H56 -3.2909325715000 2.6132464887000 -1.2259268145000
H57 -4.2453979672000 2.0738596270000 0.1642791465000
H58 3.8045629186000 4.6363916226000 0.4738089821000
H59 2.7399880382000 3.6821152665000 -0.5809498316000
H60 2.0960765736000 4.4319330618000 0.8881791322000
H61 4.4936451131000 3.7283678681000 2.7406259716000
H62 2.7971963574000 3.5249099585000 3.1943028318000
H63 3.9127442154000 2.1565368843000 3.3031317143000
H64 5.4158481408000 2.6475571920000 0.6355573084000
H65 4.8229728838000 1.0641261754000 1.1584388568000
H66 4.3445885783000 1.7036530402000 -0.4219712683000
O67 -0.1969737179000 0.0427451011000 4.4850886497000
C68 0.4994602475000 0.6546036186000 5.2836547855000
O69 1.5027031503000 1.4447157977000 4.9271373723000
C70 0.2594763708000 0.5417106949000 6.7864181419000
C5 1.2158729395000 1.4268213630000 7.5967261899000
C72 -1.2043284165000 0.9535061072000 7.0489269209000
C73 0.4583754383000 -0.9425130297000 7.1629781307000
H74 0.9995633488000 1.3117541992000 8.6621533872000
H75 2.2577799391000 1.1495175882000 7.4260466398000
H76 1.1022342612000 2.4807851316000 7.3354295227000
H77 0.2518221638000 -1.0793240520000 8.2276160175000
H78 -0.2142708973000 -1.5808968117000 6.5885184322000
H79 1.4855881317000 -1.2644047965000 6.9712898295000
H80 -1.4332169517000 0.8325289256000 8.1109203734000
H81 -1.3735407556000 2.0000386880000 6.7811246055000
H82 -1.8903305899000 0.3355616378000 6.4682495352000
H17 1.6108036354000 1.4682692403000 3.9441211383000
O84 0.3469933135000 -0.0182019634000 -2.5908721032000
C85 -0.3807670938000 -0.6214321928000 -3.3694301307000
O86 -1.3949275241000 -1.3812595471000 -2.9841909868000
C87 -0.1599645418000 -0.5427685952000 -4.8774944633000
C88 -1.2195953116000 -1.3289725435000 -5.6607910180000
C89 -0.1988236886000 0.9485140429000 -5.2711211513000
C90 1.2461771354000 -1.1167174569000 -5.1562140349000
H91 -1.0192275460000 -1.2385270259000 -6.7317281359000
H92 -1.2061971292000 -2.3879851648000 -5.3966136249000
H93 -2.2239417548000 -0.9477668723000 -5.4657893621000
H94 1.4674839424000 -1.0375352596000 -6.2237381736000
H95 2.0055682243000 -0.5672367029000 -4.5979529912000

H96 1.3052845232000 -2.1715355364000 -4.8744117257000
H97 0.0101012881000 1.0502119562000 -6.3391334683000
H98 -1.1829910852000 1.3826765330000 -5.0748688113000
H99 0.5453869770000 1.5163124642000 -4.7111854310000
H100 -1.4787601319000 -1.3938809923000 -1.9963055614000

$[(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\mu\text{-OAc})_2]_2(\mu\text{-Cu})$ **4**

Rh1 2.4022802886000 9.0894057833000 4.2454355954000
Cu2 -0.6230520352000 9.0660703219000 4.6289195349000
O3 2.0829473287000 7.2598856013000 5.2627102109000
O4 2.0970669245000 10.1254602596000 6.0783008854000
O5 -0.0787690311000 7.5695001380000 5.8040176198000
O6 -0.1374247027000 10.3722437512000 6.0370218861000
C7 1.9514842818000 10.9388740445000 3.2289780931000
C8 1.0082964330000 10.5829836812000 6.5273058195000
C9 1.9522874960000 7.9941275854000 2.4401277290000
C10 1.0244432851000 6.9615661807000 5.8867024503000
C11 3.3144992029000 10.9026299452000 3.5101354085000
C12 1.0811410954000 11.4917744058000 7.7329968335000
C13 3.3239428153000 7.9404394344000 2.6676246795000
C14 1.0843559349000 5.7843014002000 6.8327447576000
H15 0.1860653241000 11.3849866269000 8.3455274359000
H16 1.9229144279000 5.1331734617000 6.5879235077000
H17 0.1437701507000 5.2326747670000 6.8095881842000
H18 1.1298414275000 12.5266736217000 7.3795016880000
H19 1.9776511308000 11.2855941236000 8.3167502457000
H20 1.2244580674000 6.1705440418000 7.8476305138000
Rh21 -3.6510902872000 8.9680075563000 4.9940611024000
O22 -3.3459448850000 10.8262976011000 4.0240497663000
O23 -3.3306718583000 7.9826018334000 3.1367891261000
O24 -1.1820888995000 10.5666809071000 3.4650994277000
O25 -1.0912510406000 7.7772347836000 3.2000725398000
C26 -3.1828160829000 7.0807649508000 5.9327173825000
C27 -2.2258460105000 7.5693459575000 2.6826108759000
C28 -3.2101684328000 9.9875603846000 6.8457388138000
C29 -2.2941443314000 11.1617159533000 3.4078683922000
C30 -4.5541666506000 7.1392821571000 5.7046720726000
C31 -2.2603619267000 6.7118770476000 1.4382035723000
C32 -4.5718569304000 10.0974305613000 6.5845335323000
C33 -2.3735176725000 12.3662944894000 2.4990840283000
H34 -1.3734226243000 6.8891073504000 0.8317614068000
H35 -3.2281402390000 12.9894489911000 2.7553527331000
H36 -1.4492216798000 12.9381583108000 2.5514289604000
H37 -2.2545936553000 5.6622278702000 1.7448730255000

H38 -3.1667511829000 6.8988650902000 0.8648382395000
 H39 -2.4923827355000 12.0125526598000 1.4729548548000
 H40 1.2488592786000 11.4556318914000 3.8708436180000
 H41 1.5795093535000 10.7577775720000 2.2280623551000
 H42 1.5369391065000 8.6409308597000 1.6759414161000
 H43 1.2907460676000 7.2000900938000 2.7620657547000
 H44 4.0393846118000 10.7007155613000 2.7282906939000
 H45 3.7092839677000 11.3950668383000 4.3933431923000
 H46 3.7655212470000 7.0872970064000 3.1741955641000
 H47 4.0108281122000 8.5385240673000 2.0774563619000
 H48 -2.7688338853000 7.2246568199000 6.9224738743000
 H49 -2.5107454560000 6.5823759154000 5.2458590962000
 H50 -2.5124146240000 10.7685899647000 6.5703235901000
 H51 -2.8423271679000 9.3000178507000 7.5988601868000
 H52 -4.9905433156000 6.6816955074000 4.8221902751000
 H53 -5.2433988006000 7.3214426477000 6.5223580016000
 H54 -5.2963512907000 9.5053851642000 7.1350690453000
 H55 -4.9671669017000 10.9819150487000 6.0947071393000

$(\eta^2\text{-C}_2\text{H}_4)_2\text{Rh}^{\text{I}}(\kappa^2\text{-OAc})$ **5**

Rh1 -0.0158701429000 0.2392801228000 0.1837707636000
 C9 -2.1282890399000 0.5444560270000 0.4718784596000
 C10 -1.9258608353000 -0.2809052778000 -0.6339150906000
 H11 -2.3578985799000 0.1266851487000 1.4478461225000
 H5 -1.9730644932000 -1.3619892250000 -0.5341054630000
 H13 -2.0589929751000 0.0945791310000 -1.6425354480000
 H14 -2.4214156700000 1.5809475169000 0.3354287267000
 X15 -2.0270749376000 0.1317753746000 -0.0810183155000
 C22 0.1997619329000 1.7907105351000 -1.2934838006000
 C23 0.2717207986000 2.3502815247000 -0.0178312034000
 H24 1.1005895663000 1.5492965414000 -1.8503450730000
 H15 1.2342244916000 2.5338578003000 0.4518913813000
 H26 -0.5554301112000 2.9197773240000 0.3914622935000
 H27 -0.6927947457000 1.9179163033000 -1.8984880253000
 X28 0.2357413657500 2.0704960299000 -0.6556575020000
 O32 0.3891282052000 -1.6527680020000 1.1809583149000
 C33 1.6298842359000 -1.3582964771000 1.2368208428000
 O34 2.0258441793000 -0.2505780213000 0.7434967118000
 C35 2.5984174059000 -2.3012925075000 1.8853126096000
 H20 3.6219338911000 -1.9503114893000 1.7586911575000
 H21 2.3646912325000 -2.3720409630000 2.9515967278000
 H22 2.4824005471000 -3.2996481091000 1.4570635502000

$\text{Rh}^{\text{II}}(\kappa^2\text{-OAc})_2$ **6**

Rh1 -0.0501942200000 -0.1358693697000 0.8266162137000
 O3 0.2817058649000 1.4974267339000 -0.4836903838000
 C4 0.2606727810000 2.3177335696000 0.4935384690000
 O5 0.0597008077000 1.8175408914000 1.6488006924000
 C6 0.4743267483000 3.7805547278000 0.2871968225000
 H7 0.2919340198000 4.3296041986000 1.2098600418000
 H8 1.5047533642000 3.9463308068000 -0.0407688002000
 H9 -0.1862434396000 4.1385416638000 -0.5056565289000
 O10 -0.1504484724000 -2.0877803266000 0.0036290170000
 C11 -0.3250434135000 -2.5934228589000 1.1620051882000
 O12 -0.3646293002000 -1.7739491124000 2.1379164325000
 C13 -0.4568201076000 -4.0673345011000 1.3582857891000
 H14 -0.8059761523000 -4.2900089186000 2.3656636197000
 H15 -1.1419577976000 -4.4790428224000 0.6144702778000
 H16 0.5212164909000 -4.5332651921000 1.2034250207000

Rh^{III}(κ^2 -OAc)₃ 7

C1 -2.1755648458000 -5.1461774448000 1.5174111546000
 O2 -2.3713396792000 -5.0176178100000 0.2624200131000
 O3 -1.9335145938000 -4.0705599560000 2.1593159356000
 C4 -2.2210598077000 -6.4766804141000 2.1849226230000
 H5 -2.1234475882000 -6.3636472905000 3.2636874758000
 H6 -3.1616273018000 -6.9749318541000 1.9389384718000
 H7 -1.4036777610000 -7.0935894723000 1.8011164452000
 C8 -0.1826558426000 -1.4286755246000 0.7764781763000
 O9 -0.0194533544000 -2.6550570674000 0.4616817755000
 O10 -1.3914519458000 -1.0374544575000 0.8934177926000
 C11 0.9731138088000 -0.5128874560000 0.9835489356000
 H12 0.6290344651000 0.4597767834000 1.3320627564000
 H13 1.6610295659000 -0.9544543386000 1.7082037261000
 H14 1.5092641885000 -0.3998050017000 0.0371061943000
 Rh15 -2.0923167389000 -2.9463202839000 0.4008669131000
 C16 -3.9233106940000 -2.2672246134000 -1.1082245668000
 O17 -2.6961128608000 -2.1807355412000 -1.4502350852000
 O18 -4.1469997927000 -2.7181850548000 0.0639094431000
 C19 -5.0211270321000 -1.8683698834000 -2.0318006736000
 H20 -5.9881606771000 -1.9800416000000 -1.5437258443000
 H21 -4.8724090386000 -0.8308522043000 -2.3414855681000
 H22 -4.9782619425000 -2.4964889565000 -2.9259031438000

Scheme 6 structures

$[(\eta^2\text{-C}_2\text{H}_4)\text{Rh}^{\text{I}}(\mu\text{-OPiv})_2]_2(\mu\text{-Cu})(\eta^2\text{-C}_2\text{H}_4)(\eta^2\text{-C}_6\text{H}_6)$ **4b**

Rh1 2.4584831173000 9.0064804058000 4.3188301725000
 Cu2 -0.5267339071000 9.2025277350000 4.4461211560000

O3 2.0246595570000 7.2106485459000 5.3651764888000
O4 2.1768068622000 10.1759514042000 6.0667267535000
O5 -0.1879448571000 7.5490391062000 5.5106734611000
O6 -0.0670831648000 10.2017029837000 6.1023934401000
C7 2.1261901327000 10.8346204584000 3.2120167639000
C8 1.0649421334000 10.4830693796000 6.5811250248000
C9 2.0307257566000 7.8680647727000 2.5290811653000
C10 0.8655973114000 6.9082151397000 5.7683249434000
C11 3.4760855728000 10.7434446184000 3.5352378389000
C12 1.0789332398000 11.2823896183000 7.8647697391000
C13 3.3756067912000 7.7182405115000 2.8487386797000
C14 0.7121910985000 5.6794022845000 6.6365148442000
H15 0.2607034395000 10.9641676972000 8.5117975514000
H16 1.6589293286000 5.1538171159000 6.7490126184000
H17 -0.0401008064000 5.0173230274000 6.2021314130000
H18 0.9187491549000 12.3362147882000 7.6178806598000
H19 2.0345190333000 11.1843160275000 8.3776457332000
H20 0.3453701696000 5.9883972659000 7.6191401811000
Rh21 -3.5744458700000 8.9649510045000 5.0413677325000
O22 -3.3339918732000 10.6049740104000 3.7160145235000
O23 -3.3045427870000 7.7826114349000 3.3369513523000
O24 -1.0994815803000 10.8560772115000 3.5674279398000
O25 -1.1022220861000 8.0846839358000 2.9337130894000
C26 -3.1654162567000 7.2562580692000 6.2772036065000
C27 -2.2435981075000 7.6084250805000 2.6745545857000
C28 -2.2960717334000 11.1589320298000 3.2730211173000
C29 -4.4884401365000 7.1856647720000 5.8413267951000
C30 -2.3390677464000 6.7233293857000 1.4525690482000
C31 -2.4735606364000 12.3108328043000 2.3122444976000
H32 -1.9555056206000 7.2628471831000 0.5841379556000
H33 -3.5250469683000 12.5733753303000 2.2131186642000
H34 -1.8999264771000 13.1690797829000 2.6683413483000
H35 -1.7053470158000 5.8456469974000 1.6031714790000
H36 -3.3672729469000 6.4104955910000 1.2765476949000
H37 -2.0691974483000 12.0261031658000 1.3378910278000
H38 1.4353076561000 11.4142334723000 3.8124839521000
H39 1.7750949176000 10.6301630031000 2.2077843152000
H40 1.7159569212000 8.5093885260000 1.7147663261000
H41 1.2891162420000 7.1398523113000 2.8327502894000
H42 4.2111136170000 10.4708557463000 2.7854237134000
H43 3.8667181352000 11.2491777571000 4.4125596098000
H44 3.7115689978000 6.8588218727000 3.4207260221000
H45 4.1436864444000 8.2377902786000 2.2861537981000
H46 -2.9346321650000 7.5563493815000 7.2952498038000

H47 -2.3727186480000 6.7128296508000 5.7824174985000
 H48 -4.7493984301000 6.5925561345000 4.9712579825000
 H49 -5.3168948373000 7.4134242738000 6.5042833879000
 X50 2.8011378527500 10.7890325384000 3.3736273014000
 X51 2.7031662739000 7.7931526421000 2.6889099225000
 X52 -3.8269281966000 7.2209614206000 6.0592652008000
 C53 -2.7565651715000 11.7227958378000 6.4189914689000
 C54 -3.7383586622000 12.5935410226000 6.0051143612000
 C55 -5.0953534272000 12.1994829052000 6.0006092198000
 C56 -5.4524822951000 10.9490467854000 6.4496200429000
 C57 -4.4562639718000 10.0383703231000 6.8967128057000
 C58 -3.0960670133000 10.4164965112000 6.8539374332000
 H59 -1.7126285544000 12.0006402568000 6.3993123050000
 H60 -3.4731674470000 13.5909253324000 5.6714568655000
 H61 -5.8550354718000 12.8909410231000 5.6540291995000
 H62 -6.4944619450000 10.6517446243000 6.4868706753000
 H63 -4.7660689141000 9.1896730311000 7.4917262888000
 H64 -2.3247021576000 9.8171430005000 7.3166294363000

TS4.1

Rh1	2.3810747606	9.6226821080	3.9937022468
Cu2	-0.6270584470	9.5167403394	4.2012647964
O3	2.0447266973	9.0201512331	6.0192467153
O4	1.9243805455	11.6008932743	4.5716570435
O5	-0.1156488069	8.4556080705	5.7738845018
O6	-0.2162516387	11.2156787674	5.1385368278
C7	1.8079460461	10.2059469708	2.0017440224
C8	0.8238585117	11.9298160513	5.0997314978
C9	2.1646026307	7.5416798118	3.4271690718
C10	0.9452853028	8.5762847967	6.4541358530
C11	3.1724647622	10.4403006919	2.1605227387
C12	0.7368080973	13.2856801901	5.7606206756
C13	3.4970992545	7.7922366205	3.7324067868
C14	0.8651344640	8.1406715114	7.8975251498
H15	0.6670531962	13.1370176680	6.8416945969
H16	1.8185109936	8.2756997818	8.4055224093
H17	0.5644362323	7.0908618412	7.9394804396
H18	-0.1714146688	13.7974636066	5.4378093469
H19	1.6154643726	13.8879162257	5.5361251139
H20	0.0844934647	8.7240233473	8.3921882457
O21	-3.6366388128	10.6283940247	3.6325874987
O22	-3.1058497131	7.8423265837	2.8722328757
O23	-1.5383034069	10.6070016845	2.8162988193
O24	-0.8699847405	7.9277615992	3.0513087760

C25	-1.9387965771	7.5764453490	2.4712827805
C26	-2.7321266405	11.0228530316	2.8398712988
C27	-1.7956356120	6.7804254105	1.1957932905
C28	-3.0952770694	12.1109103298	1.8566223781
H29	-1.5637943581	7.4756972475	0.3828323435
H30	-2.7739504544	13.0723696212	2.2693825315
H31	-2.5647462133	11.9578449664	0.9163926641
H32	-0.9634726999	6.0807036815	1.2839132905
H33	-2.7185989716	6.2537646823	0.9572117841
H34	-4.1714750244	12.1417812399	1.6928544861
H35	1.0806089695	10.9990395213	2.1372550488
H36	1.4454759441	9.3580096711	1.4330305240
H37	1.8316814285	7.4484653552	2.4011670162
H38	1.4793978819	7.1229775707	4.1533313100
H39	3.9037557257	9.7817721126	1.7031825535
H40	3.5349181136	11.4300875568	2.4212171898
H41	3.8898921103	7.5754018837	4.7214146029
H42	4.2393311966	7.8911428234	2.9475990329
X43	2.6383999999#	10.9009500001#	3.4390500000#
X44	2.5943000000#	8.1144000000#	2.5217500000#
X45	2.8556636123#	10.3222815147#	2.1974555665#
X46	2.6584660414#	7.5284850813#	3.4905297092#
Rh47	-3.6310176896	8.8014337144	4.7159557209
C48	-2.4790438954	10.9281668767	8.9507924726
C49	-2.3607403872	11.5911459701	7.7313937059
C50	-2.8557996900	11.0219945768	6.5599673072
C51	-3.4313725621	9.7451577420	6.5813046062
C52	-3.6035570720	9.1098505700	7.8223694093
C53	-3.1153275498	9.6877028566	8.9922203323
H54	-2.0950511490	11.3777097681	9.8602089404
H55	-1.8757139521	12.5598422333	7.6813178857
H56	-2.7469490995	11.5557165810	5.6299045626
H57	-4.1136969642	8.1568684902	7.8897081049
H58	-3.2415963030	9.1692608471	9.9372808671
H59	-4.7973976101	9.4467063788	5.7052893218
C60	-4.3506493268	6.8679169907	5.4059555557
C61	-2.9855834478	6.9407829739	5.6456470547
H62	-4.7309693137	6.3927085343	4.5073108372
H63	-2.2717860149	6.5366069202	4.9386952852
H64	-2.5801755795	7.1289369862	6.6291910822
H65	-5.0692076396	6.9841474204	6.2096267807
X66	-2.9534332716#	6.8658886657#	6.0249908487#

4c

Rh1	2.0647758368000	9.3131386819000	4.5130919657000
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Cu2	-0.5287510426000	9.8399674806000	3.1052134441000
O3	0.8590906872000	9.8717846875000	6.1903052799000
O4	2.1290170742950	11.3867856204626	4.2364983564370
O5	-1.0993033745000	9.3442446346000	5.2760340811000
O6	0.0837379948000	11.6773447886000	3.3441631666000
C7	2.6913733008000	8.9731123620000	2.4798071995000
C8	1.1907703728975	12.1023148927610	3.7812981293483
C9	1.3328395896000	7.2860068666000	4.6192253557000
C10	-0.4046558605000	9.8455230402000	6.2095527350000
C11	3.8191060100000	9.0433218998000	3.2959278699000
C12	1.4018081658349	13.6003103718914	3.7668452019887
C13	2.4037564774000	7.4237741499000	5.4987329215000
C14	-1.0973925768000	10.4540711074000	7.4080500841000
H15	0.7644478791369	14.0486624758188	4.5347806813324
H16	-0.4036792767000	11.0629631443000	7.9855872751000
H17	-1.4824779165000	9.6581416989000	8.0513550639000
H18	1.0968739726595	14.0084326654386	2.8012933875828
H19	2.4400467079587	13.8536149493637	3.9751687112894
H20	-1.9443251949000	11.0543237283000	7.0705053924000
O21	-3.3922736961000	11.3801683393000	4.6451441505000
O22	-3.4413972769000	8.8377892060000	2.7513428214000
O23	-3.2956311159000	11.4813504510000	2.4042212584000
O24	-1.3363671306000	8.3170485264000	2.1820934842000
C25	-2.5669265615000	8.0995821618000	2.1553556001000
C26	-3.2283457499000	12.0212853567000	3.6096048963000
C27	-3.0928523977000	6.9175286729000	1.3836385151000
C28	-2.8846026082000	13.4759224059000	3.5985181594000
H29	-2.2910873855000	6.4074582496000	0.8522186465000
H30	-1.8058550226000	13.5357771260000	3.4238635657000
H31	-3.3930713480000	13.9924297310000	2.7835245972000
H32	-3.5731711083000	6.2264321726000	2.0821376487000
H33	-3.8612551710000	7.2520885134000	0.6824465108000
H34	-3.1247034859000	13.9291492447000	4.5582005197000
H35	2.3542067625000	9.8435265249000	1.9276814866000
H36	2.3348291629000	8.0241284067000	2.0964017009000
H37	1.4543467115000	6.7650610317000	3.6761023521000
H38	0.3078331632000	7.3891230124000	4.9536812102000
H39	4.3672260855000	8.1449006622000	3.5599887109000
H40	4.3726808729000	9.9721370627000	3.3927670860000
H41	2.2354109263000	7.6306907317000	6.5510184293000
H42	3.3763990226000	7.0078685611000	5.2582287902000
X44	2.5943000000000	8.1144000000000	2.5217500000000
X45	2.8770410000000	10.2574380000000	2.5011240000000
X46	2.0974430000000	7.6045910000000	3.6964660000000

Rh47	-3.3450565823000	9.0932030405000	4.9242687132000
H48	-3.3969996560000	10.4918574274000	2.4707726475000
X67	3.2552396554000	9.0082171309000	2.8878675347000
X68	1.8682980335000	7.3548905082500	5.0589791386000
C48	-3.3826578610687	9.1793857851495	9.9232465334431
C49	-3.9416296218452	10.1764770562219	9.1229635918432
C50	-3.8818787306899	10.0869373015975	7.7319181504953
C51	-3.2500640000000	8.9994590000000	7.1050020000000
C52	-2.7042110342392	7.9992770047287	7.9198384234945
C53	-2.7679319101191	8.0874111250842	9.3130451965129
H54	-3.4321118049714	9.2486574601281	11.0048564100562
H55	-4.4338350898294	11.0288662218556	9.5823693507815
H56	-4.3354672042969	10.8691645095747	7.1353046628192
H57	-2.2243288938711	7.1309467086601	7.4825217807433
H58	-2.3383803167013	7.2954892504920	9.9195741036958
C60	-4.3316910000000	7.0016750000000	4.8331110000000
C61	-2.9995000000000	6.7508720000000	5.1248480000000
H62	-4.6750690000000	7.0327230000000	3.8051360000000
H63	-2.2892610000000	6.5701710000000	4.3251790000000
H64	-2.7006830000000	6.4285050000000	6.1149700000000
H65	-5.1039950000000	6.8576480000000	5.5781740000000
X66	-3.6655950000000	6.8762730000000	4.9789790000000

TS4.2

Rh1	2.0373898481	9.7065887541	4.0627034479
Cu2	-0.6216495041	10.0818820789	3.5231868902
O3	1.4137774153	9.0530038915	5.9760902607
O4	1.8699354029	11.6889312591	4.7160363399
O5	-0.7093118465	8.8775323377	5.3486321882
O6	-0.3198617475	11.8427755765	4.2699777499
C7	1.9599752585	10.5095751803	2.0165616930
C8	0.7623153754	12.3009990111	4.7420078247
C9	1.6562116558	7.6627409229	3.3080620518
C10	0.2001446860	8.7482869954	6.2085299860
C11	3.2857602808	10.4166847569	2.4088848655
C12	0.7187949980	13.6544007775	5.3957624334
C13	2.9165237122	7.7015246400	3.8711911061
C14	-0.1514268035	8.1862417592	7.5600733150
H15	0.4724302702	13.5120886101	6.4527591273
H16	0.6570464066	8.3376998004	8.2742648163
H17	-0.3402689885	7.1128609452	7.4479940737
H18	-0.0602676637	14.2685488658	4.9438962694
H19	1.6902449359	14.1437090174	5.3326636493
H20	-1.0770845941	8.6471562085	7.9077439799
O21	-2.6473017850	10.2565817310	3.8483128034

O22	-2.2961454595	7.3352895271	3.2605275149
O23	-4.8305318769	10.1353139612	3.5655343412
O24	-0.8672031360	8.7200634131	2.2037968411
C25	-1.5947260297	7.6609301981	2.2937757979
C26	-3.7263125500	10.6843057951	3.3182945657
C27	-1.5251979811	6.7342855867	1.0996951609
C28	-3.6500855675	11.8417692571	2.3664570735
H29	-1.3701099595	7.2946099386	0.1826812459
H30	-3.3317589906	11.4616170878	1.3915403537
H31	-4.6212504908	12.3207863831	2.2549337318
H32	-0.6742599709	6.0661137674	1.2356607246
H33	-2.4264794231	6.1294060545	1.0343819132
H34	-2.9017439747	12.5534375033	2.7128715172
H35	1.4357188939	11.4563193218	2.0881965246
H36	1.5053120781	9.7813922896	1.3566934499
H37	1.5192024533	7.6887469485	2.2353040885
H38	0.7936722571	7.3318473783	3.8716978832
H39	3.9166060979	9.6161655876	2.0400934429
H40	3.8076807240	11.2801620801	2.8089895633
H41	3.0746056207	7.4102222691	4.9040168072
H42	3.8047887074	7.7441419863	3.2514538526
X43	2.6383999998#	10.9009500002#	3.4390499999#
X44	2.5943000001#	8.1144000001#	2.5217500000#
X45	2.8770408244#	10.2574380178#	2.5011237168#
X46	2.0974428772#	7.6045906335#	3.6964658939#
Rh47	-3.0105720308	8.4393012563	5.1280464808
C48	-3.9503682743	11.2700648995	8.9404328805
C49	-2.9849319420	11.5816043723	7.9834212712
C50	-2.7738784310	10.7402165958	6.8922132677
C51	-3.5128482074	9.5516232684	6.7236269107
C52	-4.4843894485	9.2621327416	7.6949425308
C53	-4.7013977491	10.1057047351	8.7853106642
H54	-4.1177080572	11.9245896070	9.7881991304
H55	-2.3942403862	12.4870611479	8.0837125441
H56	-2.0245894603	11.0161224490	6.1610458144
H57	-5.0930377825	8.3690937337	7.6177352442
H58	-5.4632847928	9.8495852122	9.5144053474
H59	-4.4378539674	9.1046361526	4.4115978957
C60	-4.6110548849	7.0600682047	5.2693757291
C61	-3.5128968437	6.6250022028	6.0496393335
H62	-4.7710969508	6.6226210795	4.2918764189
H63	-2.8516406862	5.8595202553	5.6571054129
H64	-3.5494172648	6.6866957829	7.1308227127
H65	-5.5094497417	7.4432505018	5.7369353307

X66	-3.4463413410#	6.6898271182#	5.7518292191#
TS4.1'			
Rh1	-0.5117062237	11.0218986886	9.2498158700
Cu2	-1.3544405124	11.2075806344	6.4420409193
O3	-1.7999108564	9.3251659401	9.3619215697
O4	-2.2127578899	12.3088664966	9.3843567353
O5	-2.2988959853	9.1684065050	7.2047513955
O6	-2.6393628225	12.4910376655	7.1862648661
C7	0.6088847845	12.7254875579	8.5606059839
C8	-2.8855721408	12.7314632158	8.4020141852
C9	0.9786403799	9.6968434111	8.4475792111
C10	-2.3982135127	8.7655683092	8.4010741885
C11	0.6403967286	12.6950569765	9.9539598755
C12	-4.0861494004	13.6052079833	8.6953794548
C13	1.0639776164	9.6696906716	9.8377287861
C14	-3.2402279657	7.5553506233	8.7324727446
H15	-4.9528610528	13.2285370150	8.1477361983
H16	-3.4214379374	7.5035265827	9.8043605237
H17	-2.7025489057	6.6559304686	8.4219804991
H18	-3.8853272788	14.6166052972	8.3321770041
H19	-4.2997679092	13.6402959431	9.7620246617
H20	-4.1835207483	7.5916046014	8.1900725636
O21	-2.9129429336	10.8361520209	4.7193797395
O22	-1.0438390982	8.4491280763	4.5314476256
O23	-5.0597902891	11.0780271821	4.1796374519
O24	0.0235997136	10.2180992828	5.4590710963
C25	-0.0178563351	9.1523639703	4.7953930055
C26	-3.8704253682	11.5438933426	4.3223004753
C27	1.3050831783	8.6349397089	4.2629819666
C28	-3.6307019107	12.9943252195	4.0435558744
H29	1.8340315336	9.4419673971	3.7525249441
H30	-2.7426761252	13.1050020799	3.4200189097
H31	-4.4939957021	13.4633656795	3.5762135599
H32	1.9229493936	8.3227044986	5.1096310287
H33	1.1630752264	7.7919392213	3.5888719926
H34	-3.4182517766	13.4608993834	5.0099571635
H35	-0.1022207183	13.3510935336	8.0334394387
H36	1.4726052967	12.4305201593	7.9764139019
H37	1.7038622170	10.2308110965	7.8458887744
H38	0.4119860272	8.9515670453	7.9026375372
H39	1.5344777113	12.3825650679	10.4820495109
H40	-0.0576582415	13.2904076494	10.5336717863
H41	0.5648717570	8.8923042101	10.4073230773

H42	1.8716668701	10.1779632444	10.3536077184
X43	2.6383999998#	10.9009500002#	3.4390499999#
X44	2.5943000001#	8.1144000001#	2.5217500000#
X45	2.5825683226#	10.4512856260#	2.1173739141#
X46	2.6635270613#	7.6605020685#	3.4769305490#
Rh47	-3.0961782104	8.7165681613	5.1359229832
C48	-7.3893126587	8.8429294387	7.4709016904
C49	-6.3672990272	9.7518037009	7.7528350581
C50	-5.2337959594	9.7935119090	6.9504721653
C51	-5.0757449229	8.9289615963	5.8394488073
C52	-6.1371788585	8.0412624956	5.5672864719
C53	-7.2758555736	7.9950924762	6.3698362350
H54	-8.2729112715	8.8047366550	8.0986809407
H55	-6.4555691432	10.4252884319	8.5986385360
H56	-4.4531651044	10.5141971821	7.1689915920
H57	-6.0857933196	7.3804055053	4.7095981894
H58	-8.0747269841	7.2996907632	6.1339518861
H59	-5.0567414375	9.9715341315	4.7611653704
C60	-3.3493914278	6.7728926168	4.1944189807
C61	-3.1359168703	6.5628576508	5.5480555091
H62	-2.5218868311	6.7213426065	3.4957970258
H63	-2.1424480883	6.3326928525	5.9138930846
H64	-3.9632372849	6.3241297523	6.2033448146
H65	-4.3431309030	6.7046088586	3.7668464785
X66	-3.4074037590#	6.8390054744#	5.8798962600#
X67	0.6099777664#	12.6311081989#	9.1971362772#
X68	0.8557633633#	9.6303641676#	9.1046284193#
X69	-3.1565336914#	6.5833954627#	4.9389526294#
4d			
Rh1	2.1339590711	9.3090184226	4.3122841625
Cu2	-0.5160577983	9.8521879708	3.1307105207
O3	1.0419732925	10.0151534139	6.0082810248
O4	2.2890261226	11.3511003625	3.7363631501
O5	-0.9784368558	9.4130964843	5.3068970520
O6	0.0921134586	11.7042313410	3.4181196003
C7	2.5918833494	8.8332145386	2.2617449297
C8	1.2808513661	12.1009074292	3.5754408137
C9	1.3860275490	7.3059122792	4.6076725228
C10	-0.2168122555	10.0212506714	6.1255242753
C11	3.7816202509	8.9111750134	2.9830606116
C12	1.5188411250	13.5944783760	3.5941672911
C13	2.5149633175	7.4882997259	5.4024259114
C14	-0.7925161562	10.8092478007	7.2748975695
H15	1.2366745991	13.9752734196	4.5808064465

H16	-0.0953634034	11.5936515079	7.5673660816
H17	-0.9504608679	10.1454480419	8.1274155452
H18	0.8917239219	14.0873330273	2.8498649307
H19	2.5692904024	13.8247649490	3.4220795260
H20	-1.7600211672	11.2246176773	6.9995630491
O21	-3.3405615817	11.1810597679	5.0447368044
O22	-3.3896734952	8.8636106884	2.7952421817
O23	-3.2993943447	11.4826564387	2.8178644716
O24	-1.3227043813	8.4370752860	2.0519447079
C25	-2.5622035235	8.2464554983	2.0343692901
C26	-3.1986073745	11.9085021849	4.0555631364
C27	-3.1256005212	7.2114737749	1.0927145231
C28	-2.8417736598	13.3524646447	4.1826184810
H29	-2.3631625243	6.8520270563	0.4038861348
H30	-1.7635524027	13.4112682591	3.9995517609
H31	-3.3502405653	13.9505840165	3.4257641494
H32	-3.5078049663	6.3704573387	1.6801035541
H33	-3.9704581145	7.6319437001	0.5434143022
H34	-3.0636841840	13.7131966101	5.1847637979
H35	2.2363117115	9.6835501853	1.6900865351
H36	2.1763056068	7.8775577843	1.9639835823
H37	1.4395233139	6.7187353642	3.6974878744
H38	0.3891462587	7.4469091870	5.0060214948
H39	4.3221859485	8.0114589158	3.2580305740
H40	4.3679803712	9.8247199111	2.9825807967
H41	2.4183656183	7.7703103091	6.4463588433
H42	3.4661304086	7.0439146992	5.1294374513
X44	2.5942999997#	8.1143999987#	2.5217500003#
X45	2.8770410004#	10.2574379986#	2.5011240003#
X46	2.0974429994#	7.6045909989#	3.6964660003#
Rh47	-3.2216238569	8.9679146368	5.1540857461
H48	-3.3839748189	10.4819070021	2.7782329171
X67	3.2552396553#	9.0082171294#	2.8878675351#
X68	1.8682980328#	7.3548905072#	5.0589791389#
C48	-4.2055292348	9.3045157769	9.8617176219
C49	-4.8768349464	10.0686791259	8.9076669913
C50	-4.5614053344	9.9434173408	7.5531088374
C51	-3.5706085018	9.0496571540	7.1269465350
C52	-2.9062727343	8.2836253046	8.0913003627
C53	-3.2178087189	8.4129070905	9.4468512835
H54	-4.4485280022	9.4042698802	10.9140906087
H55	-5.6462600841	10.7700550768	9.2151335104
H56	-5.0808920639	10.5660513019	6.8331082914
H57	-2.1185025136	7.5963279288	7.8071706358

H58	-2.6822533718	7.8145540138	10.1775783290
C60	-4.0290557111	6.9401642363	5.1433881549
C61	-2.6439958962	6.8677908393	5.1083113364
H62	-4.6087092708	6.8958675954	4.2267190802
H63	-2.1050692048	6.7476113722	4.1755917018
H64	-2.0797241007	6.6188711679	5.9973331120
H65	-4.5678412358	6.7517876230	6.0649350040
X66	-3.6655950010#	6.8762730008#	4.9789789999#

TS4.3

Rh1	2.1750900746	9.5123749142	4.0517863486
Cu2	-0.6127680815	10.0161434872	3.3724784062
O3	1.3997251088	8.9069340967	5.9389303777
O4	1.9370440631	11.5592787083	4.6140956026
O5	-0.7723540997	9.0111969064	5.4427430623
O6	-0.2021541115	11.8391564596	3.9818696559
C7	2.3160053151	10.2050004510	2.0193409250
C8	0.8754125684	12.2386067894	4.5041833124
C9	1.6959807923	7.5374999546	3.3585274761
C10	0.1774119521	8.7779293777	6.2396681746
C11	3.5905521726	10.1970341646	2.5832700730
C12	0.8860624129	13.6413313540	5.0720761019
C13	2.9728950189	7.5122493425	3.9155918787
C14	-0.1234720515	8.2981573331	7.6448989880
H15	0.3532658297	13.6290926588	6.0277741789
H16	0.7632295086	8.3613550831	8.2727957273
H17	-0.4448758846	7.2541289997	7.6041137746
H18	0.3531343512	14.3201953846	4.4049590670
H19	1.9033791261	13.9907917566	5.2411601461
H20	-0.9358563337	8.8827655245	8.0771852283
O21	-3.0550623069	10.3076970069	3.7949425815
O22	-2.5924774916	7.4078751570	3.3191598903
O23	-4.4993974075	11.9084299855	4.4343390262
O24	-1.0412321580	8.5582095495	2.1481119002
C25	-1.8579988138	7.6133040324	2.3083587400
C26	-3.5525911084	11.4240189601	3.6491864468
C27	-1.9439398074	6.5859277949	1.1941463825
C28	-3.0953985962	12.3442385339	2.5683660593
H29	-1.6549400666	7.0261684573	0.2403079572
H30	-3.0460790618	11.7959861357	1.6272417848
H31	-3.7404913318	13.2156670923	2.4784364100
H32	-1.2463608626	5.7736541793	1.4215398907
H33	-2.9464494776	6.1623734834	1.1333239566
H34	-2.0756533935	12.6456662509	2.8275264075

H35	1.7324820558	11.1175297710	1.9817212449
H36	2.0071102562	9.4414035828	1.3157011594
H37	1.5432537161	7.5211794384	2.2866542895
H38	0.8244328282	7.2495154854	3.9348408206
H39	4.3089605871	9.4292084440	2.3175128527
H40	4.0126389618	11.1053685332	3.0014670858
H41	3.1217193691	7.2003966964	4.9442629683
H42	3.8522051776	7.4622472302	3.2824299228
X43	2.6384000003#	10.9009500000#	3.4390500012#
X44	2.5943000005#	8.1144000001#	2.5217500007#
X45	2.8770408251#	10.2574380179#	2.5011237181#
X46	2.0974428773#	7.6045906334#	3.6964658945#
Rh47	-3.0776516771	8.5657059198	5.1405087616
H59	-4.6737767566	11.2916387537	5.1764211883
C2	-2.8375485176	6.5180403651	5.9084117868
H3	-3.4329085391	5.9069191559	5.2409701303
C4	-3.4169514599	7.2364106875	6.9286450597
H5	-2.8375994062	7.6279091140	7.7526636489
H6	-4.4864069398	7.1869365244	7.0984997054
H7	-1.7688055205	6.3452062382	5.8704257151
C55	-4.6879757450	11.9085286387	8.2596074714
C56	-3.3280617617	11.7912629968	7.9670786207
C57	-2.8666184807	10.7707050307	7.1356036768
C58	-3.7555207256	9.8391077658	6.5767326483
C59	-5.1197250019	9.9622818356	6.8860036178
C60	-5.5837103787	10.9919944183	7.7143577365
H14	-5.0444699513	12.7059335071	8.9018788865
H62	-2.6220840960	12.5055831199	8.3788861765
H63	-1.8154233048	10.7238467546	6.8815422772
H64	-5.8372730980	9.2527740064	6.4854763840
H65	-6.6446225280	11.0707676133	7.9288231051
X	-3.2856520008#	7.2160449999#	6.5682499989#
4e			
Rh1	2.0923837488	9.3169682522	4.4222116542
Cu2	-0.5244306853	9.7877506442	3.1696315787
O3	0.9551232232	9.8028557051	6.1699650614
O4	2.1746242523	11.3994702983	4.0150686878
O5	-1.0482745524	9.3471572178	5.3105802941
O6	0.0367511626	11.6727206915	3.3660396600
C7	2.6071794709	9.0389429266	2.3390338530
C8	1.1704806862	12.1078043067	3.7109787244
C9	1.3778543263	7.2823954084	4.5123083516
C10	-0.3073316203	9.7957742859	6.2373676082
C11	3.7791839818	9.0895574882	3.0912437574

C12	1.3427403412	13.6110665542	3.7655413134
C13	2.4905030267	7.3944527444	5.3419150926
C14	-0.9444305558	10.3613068428	7.4854039437
H15	0.7900712553	13.9920803066	4.6294100542
H16	-0.1985283850	10.8309718093	8.1240357950
H17	-1.4406317948	9.5606096993	8.0393386732
H18	0.9168635198	14.0665227478	2.8698061076
H19	2.3914115729	13.8847242398	3.8689273754
H20	-1.7126175880	11.0813842544	7.1968088501
O21	-3.4272228889	11.3244893502	4.7693141890
O22	-3.3941342941	8.9030256561	2.8333065096
O23	-3.2575405730	11.4960641103	2.5358032459
O24	-1.3419444695	8.2783496490	2.1969019470
C25	-2.5822266161	8.1158416358	2.2180502487
C26	-3.2319462777	11.9951831255	3.7524747115
C27	-3.1882623369	6.9503807984	1.4783220501
C28	-2.9117049173	13.4542966543	3.8078526007
H29	-2.4211082994	6.3495290489	0.9934986914
H30	-1.8343385356	13.5380799793	3.6361834217
H31	-3.4262694677	13.9955415139	3.0129098433
H32	-3.7535108451	6.3342393000	2.1821329308
H33	-3.8985551895	7.3255491337	0.7371058629
H34	-3.1625031178	13.8629215156	4.7843440149
H35	2.2378870407	9.9230465996	1.8317049370
H36	2.2312582949	8.0989576825	1.9524473423
H37	1.4522375465	6.7911598715	3.5487782390
H38	0.3715740969	7.3624060140	4.9046937458
H39	4.3396581177	8.1828541331	3.2936915090
H40	4.3367578057	10.0166703604	3.1793409604
H41	2.3726449615	7.5672828637	6.4069996817
H42	3.4516490211	6.9928692990	5.0390288971
X44	2.5943000000#	8.1144000000#	2.5217500000#
X45	2.8770410000#	10.2574380000#	2.5011240000#
X46	2.0974430000#	7.6045910000#	3.6964660000#
Rh47	-3.3478466429	9.1218215753	5.0905089206
H48	-3.3381500268	10.4964184936	2.5699845898
H49	-3.8920734085	6.4957386343	4.7426707390
C50	-7.4944543319	6.8662320293	8.2793016049
C51	-7.3581037633	7.1041628098	6.9095915042
C52	-6.1021418584	7.3397159057	6.3600569536
C53	-4.9555726887	7.3334952316	7.1675197535
C54	-5.1051739338	7.1082677084	8.5412489876
C55	-6.3634507109	6.8709275889	9.0936558673
H56	-8.4749598402	6.6854517804	8.7058108662

H57	-8.2349647002	7.1137718181	6.2707766760
H58	-6.0127971092	7.5447405363	5.2981302577
H59	-4.2293143501	7.1126916873	9.1828797761
H60	-6.4579033376	6.6930540683	10.1596094114
C61	-3.5877290864	7.5432738353	6.6157080063
H62	-2.8187923146	7.6275070921	7.3780502878
H63	-3.5739982312	9.3622238461	6.5959771413
C64	-3.1819853212	7.0416211830	5.3574388849
H65	-2.1409293106	6.7770216118	5.2031903256
X66	-3.4310660286#	7.3657532165#	6.0458595796#
X67	3.2552396554#	9.0082171309#	2.8878675347#
X68	1.8682980335#	7.3548905082#	5.0589791386#

TS4.4

Rh1	2.0647758368000	9.3131386819000	4.5130919657000
Cu2	-0.5287510426000	9.8399674806000	3.1052134441000
O3	0.8590906872000	9.8717846875000	6.1903052799000
O4	2.1290170742950	11.3867856204626	4.2364983564370
O5	-1.0993033745000	9.3442446346000	5.2760340811000
O6	0.0837379948000	11.6773447886000	3.3441631666000
C7	2.6913733008000	8.9731123620000	2.4798071995000
C8	1.1907703728975	12.1023148927610	3.7812981293483
C9	1.3328395896000	7.2860068666000	4.6192253557000
C10	-0.4046558605000	9.8455230402000	6.2095527350000
C11	3.8191060100000	9.0433218998000	3.2959278699000
C12	1.4018081658349	13.6003103718914	3.7668452019887
C13	2.4037564774000	7.4237741499000	5.4987329215000
C14	-1.0973925768000	10.4540711074000	7.4080500841000
H15	0.7644478791369	14.0486624758188	4.5347806813324
H16	-0.4036792767000	11.0629631443000	7.9855872751000
H17	-1.4824779165000	9.6581416989000	8.0513550639000
H18	1.0968739726595	14.0084326654386	2.8012933875828
H19	2.4400467079587	13.8536149493637	3.9751687112894
H20	-1.9443251949000	11.0543237283000	7.0705053924000
O21	-3.3922736961000	11.3801683393000	4.6451441505000
O22	-3.4413972769000	8.8377892060000	2.7513428214000
O23	-3.2956311159000	11.4813504510000	2.4042212584000
O24	-1.3363671306000	8.3170485264000	2.1820934842000
C25	-2.5669265615000	8.0995821618000	2.1553556001000
C26	-3.2283457499000	12.0212853567000	3.6096048963000
C27	-3.0928523977000	6.9175286729000	1.3836385151000
C28	-2.8846026082000	13.4759224059000	3.5985181594000
H29	-2.2910873855000	6.4074582496000	0.8522186465000
H30	-1.8058550226000	13.5357771260000	3.4238635657000
H31	-3.3930713480000	13.9924297310000	2.7835245972000

H32	-3.5731711083000	6.2264321726000	2.0821376487000
H33	-3.8612551710000	7.2520885134000	0.6824465108000
H34	-3.1247034859000	13.9291492447000	4.5582005197000
H35	2.3542067625000	9.8435265249000	1.9276814866000
H36	2.3348291629000	8.0241284067000	2.0964017009000
H37	1.4543467115000	6.7650610317000	3.6761023521000
H38	0.3078331632000	7.3891230124000	4.9536812102000
H39	4.3672260855000	8.1449006622000	3.5599887109000
H40	4.3726808729000	9.9721370627000	3.3927670860000
H41	2.2354109263000	7.6306907317000	6.5510184293000
H42	3.3763990226000	7.0078685611000	5.2582287902000
X44	2.5943000000000	8.1144000000000	2.5217500000000
X45	2.8770410000000	10.2574380000000	2.5011240000000
X46	2.0974430000000	7.6045910000000	3.6964660000000
Rh47	-3.3450565823000	9.0932030405000	4.9242687132000
H48	-3.3969996560000	10.4918574274000	2.4707726475000
H49	-4.1002640437000	6.3993009555000	5.0079482374000
C50	-7.3562445508000	6.7217300536000	8.4608883703000
C51	-7.3093210859000	7.5990226313000	7.3773672018000
C52	-6.0840151905000	7.9375658751000	6.8067669772000
C53	-4.8920259815000	7.4043789964000	7.3055177542000
C54	-4.9467158346000	6.5286318735000	8.3941195800000
C55	-6.1712986136000	6.1883470127000	8.9679454505000
H56	-8.3080483181000	6.4602100117000	8.9100722528000
H57	-8.2248760542000	8.0252586110000	6.9807859521000
H58	-6.0503088342000	8.6306461774000	5.9706353479000
H59	-4.0284865109000	6.1091989814000	8.7939988464000
H60	-6.1988068047000	5.5088216855000	9.8130994857000
C61	-3.5640044826000	7.7256347068000	6.6626830852000
H62	-2.7350940070000	7.6051154324000	7.3635266658000
H63	-3.5579446361000	9.4027865560000	6.4887888937000
C64	-3.2981275747000	7.0058717262000	5.4290360739000
H65	-2.3166370439000	6.5499250226000	5.3073860505000
X66	-3.4310660286500	7.3657532165000	6.0458595795500
X67	3.2552396554000	9.0082171309000	2.8878675347000
X68	1.8682980335000	7.3548905082500	5.0589791386000

4f

Rh1	2.0432947677	9.3050678188	4.4872837005
Cu2	-0.4712288285	9.8647407297	3.1150180703
O3	0.8145794890	9.6919901669	6.1916097947
O4	2.1749511746	11.4050332653	4.1852246372
O5	-1.1645682540	9.3939968067	5.2196403111
O6	0.1097928420	11.7219798865	3.3512568186
C7	2.6760862729	9.1015717716	2.4371800152

C8	1.2201134222	12.1356466723	3.7895411982
C9	1.3019084830	7.2803961034	4.4611419426
C10	-0.4473903213	9.6740513813	6.2308229705
C11	3.8026534828	9.1271646298	3.2569070957
C12	1.4189564306	13.6338332409	3.8575021947
C13	2.3907686429	7.3457524503	5.3267396087
C14	-1.1080217183	10.0060739743	7.5470579939
H15	0.8191992205	14.0263078390	4.6840871868
H16	-0.3623878559	10.2664096676	8.2961973056
H17	-1.6928119213	9.1488376721	7.8887456063
H18	1.0627067820	14.0983949420	2.9363812376
H19	2.4645193243	13.8842164671	4.0293644293
H20	-1.8046430216	10.8341840006	7.4014623555
O21	-3.3685794349	11.3526016495	4.5538622546
O22	-3.3046910645	8.7287028383	2.6242544521
O23	-3.2018096002	11.3335115877	2.3118897245
O24	-1.1580121202	8.3181590000	2.1325165782
C25	-2.3773606409	8.0298337510	2.0809160123
C26	-3.1909887921	11.9361607446	3.4780642807
C27	-2.7976655797	6.7769662650	1.3510833357
C28	-2.8954524470	13.3982952623	3.4147332565
H29	-1.9550209378	6.3211323995	0.8336136206
H30	-1.8098816209	13.4821491188	3.3004409450
H31	-3.3694818817	13.8562166311	2.5460408518
H32	-3.2090512781	6.0658530485	2.0743520073
H33	-3.5954885101	7.0149875127	0.6441837829
H34	-3.2037749275	13.8885966219	4.3358401396
H35	2.3327169292	10.0022948171	1.9405057074
H36	2.3242051504	8.1768050435	1.9951366895
H37	1.3969707183	6.8320093488	3.4790570683
H38	0.2845540966	7.3587376626	4.8250078891
H39	4.3567537780	8.2178150860	3.4641605042
H40	4.3493056741	10.0520790031	3.4127377294
H41	2.2436613710	7.4734534861	6.3947802632
H42	3.3552616008	6.9427791488	5.0360196793
X44	2.5943000000#	8.1144000000#	2.5217500000#
X45	2.8770410000#	10.2574380000#	2.5011240000#
X46	2.0974430000#	7.6045910000#	3.6964660000#
Rh47	-3.4099077018	9.1856415321	4.9456070941
H48	-3.2648572283	10.3320329756	2.4072615620
X67	3.2552396554#	9.0082171309#	2.8878675347#
X68	1.8682980335#	7.3548905082#	5.0589791386#
C60	-4.4856925096	7.3283481510	5.1986174853
C61	-3.1315881875	7.1010331259	5.4300741876

H62	-4.9198920796	7.1184681551	4.2255939126
H63	-2.4921074294	6.6932095831	4.6545633552
H64	-2.7512692219	7.0060183581	6.4406777993
H65	-5.1825877108	7.4102837229	6.0258271401
X66	-3.6655950000#	6.8762730000#	4.9789790000#
H57	-3.7111413930	9.4743174565	6.4185134534

Scheme 7 Structures

1b

Rh1	-0.4317567058	9.0896701831	4.7041434711
C3	-0.1215229324	7.7114660155	6.3223500937
C4	-0.0820395642	10.7522087991	6.0153223772
C5	0.9563629488	7.6162805386	5.4442299991
C6	1.0012651090	10.6212053699	5.1441462341
Rh7	-3.8009485144	8.9026513764	4.8915906558
O8	-3.3532423108	10.7310057944	3.9144719555
O9	-3.2830516707	7.9672602936	3.0834694001
O10	-1.1992024552	10.4947497722	3.3017055033
O11	-1.1167431993	7.4901619053	3.4602234544
C12	-3.6030166013	6.9710823746	5.7899765293
C13	-2.1765553562	7.4375532009	2.7764545184
C14	-2.3455534295	11.0209455891	3.2157259679
C15	-4.9152653813	7.1232304130	5.3335052265
C16	-2.1333857340	6.6335787201	1.4963974887
C17	-2.5255290863	12.0936661960	2.1629355895
H18	-1.1988241916	6.8273847359	0.9684153912
H19	-3.3010033696	12.7976555362	2.4647851434
H20	-1.5852308320	12.6096845276	1.9684672180
H21	-2.1567680164	5.5703652009	1.7543148422
H22	-2.9890690906	6.8617392284	0.8625488676
H23	-2.8493743349	11.6087536664	1.2364374636
H24	-0.9407081790	7.0064258095	6.2638044053
H25	-0.0155667153	8.2155599355	7.2771578889
H26	0.0094029878	10.4594040392	7.0559902138
H27	-0.8712001199	11.4627143335	5.8039584711
H28	1.9196495361	8.0451227719	5.6969796999
H29	0.9746138041	6.8531930838	4.6739472423
H30	1.0531854215	11.2168754662	4.2391438071
H31	1.9477237445	10.2198840273	5.4892650709
H32	-3.3720210563	7.0226134773	6.8486771328
H33	-2.8747413847	6.4306183843	5.1964402527
H34	-5.2188189561	6.7096439337	4.3777252677
H35	-5.7235644463	7.2982444843	6.0373148561
X36	-0.0390639581#	7.4856943008#	5.7251781396#
X37	0.1848845976#	10.4074529351#	5.8642810549#

X38	-3.8753000000#	7.1838000000#	5.8009500000#
C39	-3.2156396432	10.7740319908	7.2914219931
C40	-3.4041362755	12.0584865123	6.8371543997
C41	-4.5617555127	12.3911756764	6.0993407393
C42	-5.5085929273	11.4338597119	5.8163861037
C43	-5.3242835105	10.0991519400	6.2550662741
C44	-4.1735968954	9.7639796560	7.0072085892
H45	-2.3452174446	10.5202697695	7.8832758308
H46	-2.6687678114	12.8253329369	7.0534171600
H47	-4.7021112506	13.4112758239	5.7591726997
H48	-6.4002475928	11.6890953250	5.2562076726
H49	-6.1629885581	9.4188925388	6.1987998302
H50	-4.1484615464	8.8535983572	7.5918121093
TS1.1			
Rh1	-0.3469371945	8.9938635532	4.4851860952
C3	-0.0496477928	7.4659733430	5.9827469364
C4	-0.1371244243	10.5210332754	5.9962929191
C5	1.0679480579	7.4992939824	5.1465193679
C6	0.9873635133	10.5453686233	5.1780345507
Rh7	-3.6206986982	8.9329143397	5.0135594481
O8	-3.2885129208	10.7408905917	3.9585330630
O9	-3.2622002302	7.9181874161	3.1475226623
O10	-1.1847179510	10.4815236148	3.2237602683
O11	-1.0648161799	7.4810922002	3.1896376336
C12	-3.5301201368	6.9469413852	5.8705607215
C13	-2.2203720590	7.3876048354	2.6826979393
C14	-2.3186466642	11.0288839212	3.2071699798
C15	-4.8602637013	7.2379035940	5.5712855455
C16	-2.3397019465	6.5580568001	1.4208128142
C17	-2.5420877520	12.1321699862	2.1962291844
H18	-1.6153263354	6.9181212958	0.6807157892
H19	-3.0830555312	12.9595795118	2.6540892276
H20	-1.5949122630	12.4799255080	1.7833016888
H21	-2.0760976464	5.5257148389	1.6508973851
H22	-3.3459519827	6.6085785790	1.0069328122
H23	-3.1580261519	11.7347546450	1.3965288236
H24	-0.8317246846	6.7378486731	5.8154378609
H25	-0.0171986714	7.8805322433	6.9887781686
H26	-0.1013936544	10.1076087154	6.9978960980
H27	-0.9549886612	11.2086338884	5.8244853771
H28	2.0110256796	7.9338463648	5.4720900163
H29	1.1463844221	6.8153392827	4.3051674647
H30	1.0404714791	11.2481628452	4.3526474025
H31	1.9410863851	10.1463082072	5.5116905711

H32	-3.1515217686	6.9668344627	6.8835925906
H33	-2.9325151596	6.3637806749	5.1748035968
H34	-5.3034637044	6.9124270466	4.6445751283
H35	-5.5591893214	7.4979874750	6.3457460499
X36	0.4174200082#	7.6638732771#	5.8832900464#
X37	0.4596127724#	10.6867070845#	5.5797343056#
X38	-4.2591409913#	7.0471563938#	5.5617408779#
C39	-3.0982574338	11.9173208492	8.1387763082
C40	-3.2074942060	11.2118744954	9.3394354374
C41	-3.6045782716	9.8759549086	9.3074216359
C42	-3.8586882099	9.2434185865	8.0886035159
C43	-3.6747426314	9.9210479504	6.8657612875
C44	-3.3496261363	11.2901458966	6.9232380297
H45	-2.8183796202	12.9683412911	8.1440949430
H46	-3.0066385682	11.7034639876	10.2844492331
H47	-3.7304912577	9.3158514007	10.2358544089
H48	-4.1969307850	8.2087173404	8.1168508030
H49	-4.8927265527	9.6742513862	5.7803464902
H50	-3.2762543738	11.8609806714	6.0051816544
1c			
Rh1	-0.6129778625	8.9885933354	4.7706575955
C3	-0.5690070117	7.3922483557	6.2510173069
C4	-0.8619355558	10.4754634802	6.3512864720
C5	0.6990480549	7.5458328742	5.7097334588
C6	0.4167295585	10.5886070065	5.8250703120
Rh7	-3.6786704988	8.9010462670	4.8021061478
O8	-3.2969970794	10.7762035766	3.9022820868
O9	-3.1556839747	7.9358821693	2.8383409930
O10	-1.1378614983	10.4732640809	3.3705499623
O11	-1.0012912614	7.5126467750	3.3251506349
C12	-3.8117156879	6.8336907940	5.5522640360
C13	-2.0373415852	7.4289249812	2.5833001869
C14	-2.2493673027	11.0662766400	3.2601388419
C15	-5.0990883380	7.2523031681	5.2815841920
C16	-1.8692868963	6.6232456180	1.3135591933
C17	-2.3435055689	12.2062322798	2.2747572975
H18	-1.0605832802	7.0526562000	0.7171699184
H19	-2.9988234408	12.9853999750	2.6656345752
H20	-1.3571850973	12.6087072476	2.0476611413
H21	-1.5765863687	5.6021957490	1.5720814278
H22	-2.7925756262	6.6086873207	0.7365802571
H23	-2.7911551670	11.8243695822	1.3520264182
H24	-1.2184800343	6.6162689510	5.8704983764
H25	-0.8055566696	7.7619369250	7.2425748101

H26	-1.0375764612	10.0014531689	7.3091163589
H27	-1.6664282443	11.1199771164	6.0196799062
H28	1.4900894519	8.0423485765	6.2601424493
H29	1.0230309737	6.9158889562	4.8874638747
H30	0.6342163772	11.3198819998	5.0535962957
H31	1.2782216630	10.2126446321	6.3661780102
H32	-3.4450469937	6.7966225912	6.5693814326
H33	-3.2706380845	6.2350862461	4.8291397090
H34	-5.5794392904	6.9855434819	4.3468245256
H35	-5.7554003619	7.5856029572	6.0765280346
X36	0.4174200082#	7.6638732770#	5.8832900464#
X37	0.4596127724#	10.6867070845#	5.5797343056#
X38	-4.2591409913#	7.0471563938#	5.5617408779#
C39	-4.8847804870	11.8609110486	7.6809500651
C40	-4.5973430520	11.2935669797	8.9232036821
C41	-4.0854081492	9.9991128640	8.9722876565
C42	-3.8631736441	9.2824704613	7.7929643170
C43	-4.1321769687	9.8422423064	6.5351712212
C44	-4.6570109000	11.1449914883	6.5055086952
H45	-5.2871475150	12.8680774168	7.6238714250
H46	-4.7724613322	11.8513012909	9.8371266526
H47	-3.8566032314	9.5395655545	9.9293443778
H48	-3.4533603882	8.2832555361	7.8791181299
H49	-5.1015761485	9.2088453670	4.3698874070
H50	-4.8690547358	11.6145154180	5.5531073785
TS1.2			
Rh1	-0.9784252629	10.6315538512	3.3004137076
C7	-1.0737752426	12.6310799530	4.1168270244
C9	0.8902965660	11.0690121711	2.3614611092
C11	-0.7547819904	11.7496546770	5.1423223590
C13	1.0957549142	10.1003702149	3.3440685919
O21	-3.0508285580	10.3407096386	3.8157892110
O22	-2.1478780007	7.4594045955	3.0987357669
O23	-5.0862875886	9.5327440175	3.5117032329
O24	-1.1645554427	9.0851466020	1.8835423360
C25	-1.6486014041	7.9153715585	2.0485009190
C26	-4.2026107949	10.3914461067	3.2613026875
C27	-1.5620448305	6.9953002020	0.8486906713
C28	-4.4796254941	11.5065850168	2.3024329763
H29	-1.4284611045	7.5591736325	-0.0760452104
H30	-3.8132901294	11.3897393322	1.4290092895
H31	-5.5226689983	11.4910749470	1.9782608112
H32	-0.6982985139	6.3367495916	0.9794255053
H33	-2.4516114081	6.3740572549	0.7982318121

H34	-4.2501225051	12.4649223868	2.7889163654
H35	-2.1007888476	12.9449534576	3.9648197149
H36	-0.3254539026	13.2830421799	3.6823056451
H37	1.2012149603	12.0954693046	2.5183902199
H38	0.7625093968	10.7742737636	1.3285136024
H39	0.2562736823	11.6924156253	5.5267161401
H40	-1.5223896285	11.3669213886	5.8055441392
H41	1.1259334779	9.0464488498	3.0833438343
H42	1.5635328930	10.3578749689	4.2874612082
X44	0.5608621907#	12.2126559719#	3.2444564800#
X45	-0.3866764112#	11.4475189637#	5.0304340049#
X46	0.5837926996#	11.3441204343#	2.1805719779#
Rh47	-2.8028884822	8.4412942816	4.9960696779
C48	-3.7395593451	10.9241721176	9.0174759857
C49	-4.7364554912	10.8123501633	8.0417377630
C50	-4.5234545527	10.0424041806	6.8970318743
C51	-3.3051003385	9.3643616668	6.6965987696
C52	-2.3235048852	9.4688663844	7.7038156123
C53	-2.5309379476	10.2458776259	8.8438375778
H54	-3.9052867368	11.5251960365	9.9048950727
H55	-5.6844705991	11.3281366879	8.1703429655
H56	-5.3142455106	9.9789629550	6.1506871138
H57	-1.3719490999	8.9486377517	7.5991948637
H58	-1.7492846981	10.3150453555	9.5984388910
H59	-4.3853599440	8.6548355606	4.3303504306
C60	-3.8250433847	6.6267660794	5.5284043728
C61	-2.5013418061	6.5609513296	5.9625737615
H62	-4.1116788032	6.1489996438	4.5977818005
H63	-1.7611354907	6.0271444723	5.3745681442
H64	-2.2682867173	6.7062552602	7.0111171453
H65	-4.6336437394	6.8311644061	6.2217519763
X66	-3.4463413410#	6.6898271181#	5.7518292190#
TS1.1'			
Rh1	-1.3925915759	11.4789302729	6.0229290682
C7	-2.3789871012	13.2470001936	6.7960193512
C9	0.4490305904	12.1867207264	6.8540951493
C11	-2.8666934811	12.1217640968	7.4548175301
C13	-0.0051959899	11.0995072266	7.6058959907
O21	-3.0601619742	11.0152230020	4.6710998774
O22	-1.3955149298	8.4913019435	4.3920413167
O23	-5.1202064674	11.1546975529	3.9044233618
O24	-0.1211851895	10.3036515473	4.8329974240
C25	-0.3351775133	9.1532701067	4.3256148776
C26	-3.9658382236	11.6575742338	4.0457501079

C27	0.8387731355	8.5209975451	3.6057814059
C28	-3.6798905667	12.9909145409	3.4273447883
H29	1.5355799354	9.2812503691	3.2539352571
H30	-3.7806210552	12.8904129254	2.3432335778
H31	-4.4222961262	13.7207591078	3.7563508721
H32	1.3654990622	7.8679398939	4.3092737535
H33	0.4856538789	7.9064682654	2.7773786664
H34	-2.6737896298	13.3259733244	3.6673519102
H35	-2.9364148796	13.6952722450	5.9807415847
H36	-1.6818010126	13.9196062874	7.2829628323
H37	0.3797032489	13.1966080480	7.2422878011
H38	1.1800310265	12.0384633688	6.0667138691
H39	-2.5692034729	11.8897956879	8.4712804125
H40	-3.7982080985	11.6684232222	7.1363502173
H41	0.3771455669	10.1020395226	7.4169364042
H42	-0.4413781932	11.2475896985	8.5878571683
X44	-1.1841958763#	13.0627030664#	7.3225030005#
X45	-3.0745101570#	12.4488349240#	6.9417652587#
X46	-0.1057876543#	12.6144728079#	6.5994159990#
Rh47	-3.4450683467	8.8985917938	4.9550435986
C48	-7.9056263442	8.5294998251	6.9300482301
C49	-7.7475435891	8.1484094510	5.5984392845
C50	-6.5459963195	8.3992970761	4.9365659602
C51	-5.4584472090	9.0364076635	5.5710075141
C52	-5.6662279532	9.4377127988	6.9098229298
C53	-6.8563043958	9.1788222730	7.5844045107
H54	-8.8359443820	8.3301485930	7.4513929755
H55	-8.5604308381	7.6566767124	5.0727845691
H56	-6.4553135626	8.1104542337	3.8944403655
H57	-4.8653947994	9.9337169874	7.4464189402
H58	-6.9674897640	9.4810523453	8.6215795115
H59	-5.1071193072	10.0964178205	4.5695338382
C60	-3.7234867774	6.8512810543	4.4200688224
C61	-3.4724379866	6.9372838068	5.7945628537
H62	-2.9185067077	6.6121095211	3.7332346330
H63	-2.4714967959	6.7661390315	6.1786161175
H64	-4.2757644334	6.8136545651	6.5128589065
H65	-4.7244848533	6.6476900833	4.0575288180
X66	-3.4355194990#	6.6442066478#	4.9924763564#
X	-0.1162853042#	11.7072082566#	7.2099966538#
1d			
Rh1	-0.7188189814	9.9647360755	3.8516186538
C7	-1.1563044396	11.8366465135	4.8268490220
C9	0.4631061927	11.0167594937	2.3887191919

C11	-0.2598564411	11.1214687447	5.6164245457
C13	1.3108580788	10.2204738996	3.1661155655
O21	-4.0203141433	10.5360548152	3.7405163328
O22	-2.8990409439	7.8199865178	2.7276571246
O23	-4.5405323690	9.6072753557	1.7607014423
O24	-0.7669285847	8.3984639492	2.3705056474
C25	-1.7932961597	7.7237502491	2.0968111256
C26	-4.5332075264	10.6023857567	2.6223936175
C27	-1.7117197234	6.7210274087	0.9719871737
C28	-5.1929763686	11.8519410425	2.1250720744
H29	-0.8184537926	6.8807707829	0.3700697209
H30	-4.5383631517	12.3190161635	1.3824574743
H31	-6.1354185543	11.6137897886	1.6281537013
H32	-1.6798375200	5.7156352676	1.4037977082
H33	-2.6081253524	6.7799089124	0.3513172652
H34	-5.3549390211	12.5453154372	2.9478622723
H35	-2.2169602517	11.8198561964	5.0480169162
H36	-0.8198804373	12.6755419896	4.2272587808
H37	0.4422451925	12.0934953650	2.5211769303
H38	0.1134864259	10.6625116384	1.4244098660
H39	0.7899897436	11.3937819514	5.6491299379
H40	-0.6212857626	10.5548264619	6.4660179918
H41	1.6129988629	9.2388905667	2.8157329478
H42	1.9555467745	10.6642389460	3.9168831144
X44	0.5608621907#	12.2126559719#	3.2444564800#
X45	-0.3866764112#	11.4475189637#	5.0304340049#
X46	0.5837926996#	11.3441204343#	2.1805719779#
Rh47	-3.0242353221	8.8555046837	4.7811299821
C48	-3.9388480452	11.0495159459	9.0270940910
C49	-4.6436846428	11.3519914164	7.8633787126
C50	-4.3345176855	10.7144020973	6.6603613170
C51	-3.3138154575	9.7458524656	6.5687333342
C52	-2.6310453064	9.4496691493	7.7643732889
C53	-2.9291637804	10.0905283581	8.9676988640
H54	-4.1736330738	11.5481365906	9.9614464578
H55	-5.4382428683	12.0923641526	7.8864963642
H56	-4.8940079833	10.9930281387	5.7766699714
H57	-1.8419236636	8.7073488591	7.7842977309
H58	-2.3690389588	9.8335760398	9.8621116252
H59	-4.0022859612	8.8348377015	2.1054994083
C60	-2.6900428599	6.9702167935	5.6965999284
C61	-1.4328054466	7.5285207343	5.4563365646
H62	-3.0950265412	6.2298514763	5.0122879186
H63	-0.8473622577	7.1957162474	4.6073839909

H64	-0.8479415633	7.9604412320	6.2578113822
H65	-3.1151980523	6.9678432836	6.6941437965
X66	-3.4463413410#	6.6898271181#	5.7518292190#
TS1.3			
Rh1	-0.4930867698	9.4195456027	4.1443084635
C7	-0.3007824723	11.2439509892	5.2443128120
C9	1.0978115011	10.0743303342	2.8327867641
C11	0.1268362821	10.1737669334	6.0367208460
C13	1.5841176493	9.0166804085	3.6026734355
O21	-3.6117499584	10.4864919674	3.2515920515
O22	-3.0211479196	7.6812053567	3.0659136668
O23	-3.6211558909	12.4406539470	4.3763073724
O24	-0.8529366967	7.9949069437	2.6019589299
C25	-1.9865204843	7.4750621212	2.3782713288
C26	-3.6718545344	11.7155113360	3.2694083174
C27	-2.0793942832	6.5256271329	1.2065048890
C28	-3.7830850595	12.5376667199	2.0240059873
H29	-1.8861427435	7.0753301475	0.2818307661
H30	-3.9606459770	11.8886911729	1.1702685015
H31	-4.5713340074	13.2868052831	2.1226360174
H32	-1.3045848153	5.7599929714	1.2998424581
H33	-3.0640970219	6.0623409055	1.1647824295
H34	-2.8405501339	13.0756985454	1.8816173976
H35	-1.2901572969	11.6617076837	5.3532067161
H36	0.4224672135	11.9192128227	4.7982946383
H37	1.4024137037	11.0946297061	3.0404653004
H38	0.7102606243	9.8966289073	1.8347916999
H39	1.1829633000	10.0090327594	6.2206665150
H40	-0.5300226387	9.7349198738	6.7819472247
H41	1.5714020023	8.0052906054	3.2116740161
H42	2.2755299151	9.1946130548	4.4194546279
X44	-0.0295973610#	8.5932244802#	1.9552233203#
X45	-0.1711377772#	11.7421048249#	4.7624923726#
X46	1.2243541586#	9.4255721060#	3.3417257520#
Rh47	-3.1043091316	8.9800075386	4.7610038292
H59	-3.5775557470	11.8531743645	5.1669412922
C2	-2.5142405772	7.2070142945	5.9410133705
H3	-3.1535841442	6.4098178940	5.5767388701
C4	-3.0237480591	8.2156599378	6.7900100690
H5	-2.3379658633	8.6727492957	7.4905982509
H6	-4.0076646542	8.0449170836	7.2079752163
H7	-1.4446582594	7.0530033254	5.8428098778
C55	-5.2220453860	11.8775405151	8.2696946600
C56	-3.8317697625	11.9082523752	8.2231922991

C57	-3.1293494307	11.0741934032	7.3444994938
C58	-3.7982379587	10.1959869070	6.4722556074
C59	-5.2123964554	10.1922087019	6.5299856996
C60	-5.9120543020	11.0094067552	7.4206218015
H14	-5.7607312469	12.5276465983	8.9500958881
H62	-3.2819882048	12.5905557431	8.8643658023
H63	-2.0486888444	11.1185145142	7.3507099149
H64	-5.7763985594	9.5541666400	5.8561723064
H65	-6.9976062647	10.9813726650	7.4355179264
X	-3.2081879894#	7.1743973157#	6.6442487454#
Ie			
Rh1	-0.6727082648	9.9064796350	4.1676164249
C7	-0.9691308319	11.8110074438	5.0899237474
C9	0.5848070535	10.8118427210	2.6438740190
C11	0.0326186285	11.1240782446	5.7820014099
C13	1.3557287415	9.8984777776	3.3636006588
O21	-4.3136645592	10.7775212711	4.3876935016
O22	-3.1343048698	8.1759263333	3.1890722568
O23	-5.0153756535	9.9114778900	2.4337147732
O24	-0.9539318149	8.3128931915	2.7277986638
C25	-2.1041258202	7.8852837958	2.4824597542
C26	-4.9773763815	10.8608442793	3.3650584160
C27	-2.3206317769	6.9656020004	1.3079815738
C28	-5.8293019417	12.0492854243	3.0292266757
H29	-1.4468771854	6.9574925970	0.6580781354
H30	-5.4331354466	12.5353048998	2.1330874934
H31	-6.8482321011	11.7257761051	2.8030371195
H32	-2.5011630110	5.9539559154	1.6843696632
H33	-3.2082690238	7.2699771589	0.7487983745
H34	-5.8308284566	12.7524572315	3.8593181007
H35	-1.9954400886	11.8196149586	5.4373642589
H36	-0.7098105374	12.6222979616	4.4174127912
H37	0.7079118637	11.8797026171	2.7966384928
H38	0.1373074990	10.5287006521	1.6966990114
H39	1.0725589142	11.4105167938	5.6588557341
H40	-0.1703203605	10.5970273703	6.7076172469
H41	1.4934222539	8.8876156961	2.9947409467
H42	2.0897968624	10.2344908708	4.0870284596
X44	0.5608621907#	12.2126559719#	3.2444564801#
X45	-0.7080804403#	11.4790576291#	5.2216367839#
X46	0.8869821358#	10.6186166966#	2.7774173787#
Rh47	-3.0044456009	8.9937971734	5.1361773699
C48	-5.3143867469	10.5956614445	7.5585504117
C49	-4.0035646576	10.9852817783	7.4072340553

C50	-2.9744582132	10.0166159369	7.2898163886
C51	-3.2832239921	8.6376700966	7.3648373633
C52	-4.6486558655	8.2646522885	7.5228878960
C53	-5.6370600757	9.2214492483	7.6181095248
H54	-6.0999909955	11.3382201941	7.6414456065
H55	-3.7446474587	12.0374780080	7.3770084119
H56	-1.9462030013	10.3357247024	7.3717571358
H57	-4.8977772647	7.2106577490	7.5899522760
H58	-6.6703461199	8.9179520283	7.7499701230
H59	-4.3915926528	9.1747993914	2.6709001024
C60	-2.1721142261	7.5929732188	7.3462519491
C61	-1.9345888888	7.3881001711	5.8484819148
H62	-2.4736691281	6.6882918245	7.8848990740
H63	-2.4190055468	6.4874349051	5.4563979336
H64	-0.8810194545	7.3831848451	5.5595801225
H65	-1.2858241082	7.9925257846	7.8470297409
X	-2.7438221452#	7.9354791313#	7.0769327177#
TS1.4			
Rh1	-0.7590750895	9.8898414961	4.0095758927
C7	-1.3160927978	11.7753748492	4.8560516794
C9	0.6977287478	10.8865038407	2.7276072434
C11	-0.5529958625	11.0722731891	5.7910318013
C13	1.3774620513	10.0630422367	3.6235761763
O21	-4.2328586293	10.4546396028	3.6860613742
O22	-2.9007953914	7.9647426944	2.5610820544
O23	-4.5467087232	9.7274579086	1.5698838759
O24	-0.6823931329	8.2826630946	2.5534824855
C25	-1.7271766050	7.7706301190	2.0795964899
C26	-4.6986226236	10.6078201746	2.5535258484
C27	-1.6152619480	6.8658405577	0.8832273634
C28	-5.4810585572	11.8247141390	2.1674439659
H29	-0.5792881675	6.7841326160	0.5627895245
H30	-4.9067403859	12.3951910340	1.4328230204
H31	-6.4163154369	11.5240227326	1.6920593142
H32	-2.0018667133	5.8796355307	1.1431254751
H33	-2.2210651967	7.2532578799	0.0670013293
H34	-5.6882473529	12.4427732178	3.0408919652
H35	-2.3999175668	11.7739907963	4.9105113433
H36	-0.8848394934	12.6035396779	4.3018846062
H37	0.6935353783	11.9647745837	2.8567594187
H38	0.4765095254	10.5424103095	1.7224755092
H39	0.4818907671	11.3441181067	5.9777888848
H40	-1.0339328924	10.5414266117	6.6048954195
H41	1.6828229432	9.0628059444	3.3311185461

H42	1.9146086967	10.4813457362	4.4689752641
X44	0.5608621907#	12.2126559719#	3.2444564800#
X45	-0.7080804404#	11.4790576291#	5.2216367839#
X46	0.8869821357#	10.6186166966#	2.7774173787#
Rh47	-3.0843288428	8.8042090339	4.6172033402
H59	-3.9706114994	8.9687816769	1.8738136196
H49	-2.5136167571	6.2279957934	5.2613959833
C50	-6.0514937134	6.8020126112	8.9116506861
C51	-5.9373699832	6.3675885165	7.5881467596
C52	-4.8398028191	6.7417793937	6.8194516825
C53	-3.8339614279	7.5607485188	7.3559169671
C54	-3.9619678228	7.9954481728	8.6829029764
C55	-5.0582861002	7.6168750471	9.4561561556
H56	-6.9093065989	6.5100906305	9.5095714047
H57	-6.7085940351	5.7379828094	7.1540652605
H58	-4.7696712836	6.4032244652	5.7917219642
H43	-3.1937683470	8.6322690632	9.1159681032
H60	-5.1367943153	7.9620607366	10.4824980796
C61	-2.6314516320	7.9811126639	6.5704814404
H62	-1.9283332740	8.5585295172	7.1660846512
H63	-3.2020923053	9.5003522291	6.0641319075
C64	-2.0519145571	7.1677678559	5.5545467351
H65	-0.9797069868	7.2193173528	5.3986835703
X66	-2.4278299913#	7.6024378231#	6.3213597125#
If			
Rh1	-0.7216242612	9.9316605558	3.8365998264
C9	-1.4621891039	7.6777658379	5.6491307862
C13	-2.7075228356	7.0484167735	5.7039519601
O21	-4.1128389241	10.5646801016	3.8434132286
O22	-2.9382773093	7.8253477592	2.6916213838
O23	-4.4955853390	9.7247973841	1.7923603313
O24	-0.7670238248	8.3069772766	2.4202328543
C25	-1.8062254554	7.6602828077	2.1258644952
C26	-4.5866314801	10.6631453743	2.7085958670
C27	-1.7096766278	6.6073542443	1.0481547407
C28	-5.3116628482	11.8930150719	2.2559237869
H29	-0.7482442944	6.6536693074	0.5391555450
H30	-4.6886885363	12.4153970173	1.5235296103
H31	-6.2430319356	11.6185199387	1.7567195245
H32	-1.8317503774	5.6220413770	1.5078200001
H33	-2.5259662497	6.7341750493	0.3334439531
H34	-5.5069117266	12.5486699484	3.1015762516
H37	-1.0474611763	8.1564629375	6.5275391823
H38	-0.7296744977	7.3681441134	4.9110974663

H41	-2.9611331904	6.2704439552	4.9885965415
H42	-3.0841481286	9.6373983209	6.1189405157
X44	0.5608621907#	12.2126559719#	3.2444564800#
X46	-2.2017113242#	7.2760660822#	5.7662110593#
Rh47	-3.0247039893	8.9086010544	4.7545518323
H59	-3.9457025289	8.9475633981	2.1120328160
C7	-1.1487541133	11.8352843252	4.7458518331
C29	0.5012124534	10.9205840616	2.3558631953
C11	-0.3170955480	11.1078831311	5.5964638516
C30	1.3306517691	10.1622699877	3.1867586182
H35	-2.2203479694	11.8587020297	4.9104951090
H36	-0.7542121035	12.6546986394	4.1542491695
H39	0.4741711384	12.0021807639	2.4379687367
H40	0.1719032939	10.5207022150	1.4021976997
H43	0.7378254476	11.3482925461	5.6811212945
H44	-0.7367511094	10.5675284381	6.4379691844
H45	1.6417207677	9.1663533547	2.8885154891
H46	1.9547181831	10.6401284240	3.9342301103
X45	-0.7080800000#	11.4790580000#	5.2216370000#
X39	0.8869820000#	10.6186170000#	2.7774170000#
H47	-3.2808876697	7.0393457176	6.6265504624

Scheme 8 Structures

5b

Rh1	-0.0519851853	0.1975598115	0.2166274076
C22	0.2926185840	1.7612291580	-1.1950400888
C23	0.2300734559	2.3031737451	0.0952480427
H24	1.2499623018	1.5409814506	-1.6583867129
H15	1.1391868586	2.5019935429	0.6553010366
H26	-0.6359017790	2.8748265344	0.4142725542
H27	-0.5263709965	1.9084816581	-1.8925161049
X28	0.2357413658#	2.0704960299#	-0.6556575020#
O32	0.4866898063	-1.7237434002	1.1995859970
C33	1.6985470103	-1.3519474768	1.1752101444
O34	1.9821656380	-0.2157111495	0.6579426968
C35	2.7792580516	-2.2168275407	1.7515106262
H20	3.7626384059	-1.7871614976	1.5629327158
H21	2.6205855824	-2.3121035642	2.8297270627
H22	2.7148595194	-3.2186939416	1.3196320627
C16	-2.1162023772	-0.1572474085	-0.6600093769
C17	-2.2715847291	0.4795056537	0.5980103672
C18	-2.5645873555	-0.3106351123	1.7470934796
C19	-2.6598503687	-1.6785039410	1.6410325433
C20	-2.5045805284	-2.3139738273	0.3843087638
C21	-2.2562406537	-1.5723711916	-0.7469209242

H23	-2.1393622882	0.4234877368	-1.5735313634
H25	-2.4189734350	1.5511624143	0.6528036232
H28	-2.7113751240	0.1807178742	2.7020330769
H29	-2.8594950839	-2.2793680961	2.5210244440
H30	-2.5872302033	-3.3930079784	0.3189827544
H31	-2.1649957502	-2.0536639279	-1.7137585843

TS5.1

Rh1 -3.2665174098735 8.6486494812802 5.0288381628814
 C2 -2.8025491792229 9.5526205997829 2.6952127462521
 O3 -3.3835308989599 10.2456001783524 3.6022869945633
 O4 -2.4526472153706 8.3609232793021 2.9598668117780
 C5 -2.5348686289747 10.1688810182822 1.3558950091008
 H6 -3.4285756899150 10.6871089339557 1.0021436433764
 H7 -1.7414077668806 10.9149480095862 1.4636098594418
 C9 -3.3383839623327 11.3731196139088 9.0232615340018
 C10 -3.2280752743291 11.9099706007659 7.7408956676901
 C11 -3.3082162084968 11.0857270116476 6.6187008309440
 C12 -3.4646907003854 9.6988360247878 6.7665624397398
 C13 -3.6147751887906 9.1719809743200 8.0567300885647
 C14 -3.5410631955687 10.0029180904641 9.1750408465548
 H15 -3.2785988138037 12.0177474838630 9.8934604079317
 H16 -3.0848258256816 12.9775496945289 7.6077102497799
 H17 -3.2389771677461 11.5219459024853 5.6294432028513
 H18 -3.7920316773229 8.1138222533881 8.2086505604499
 H19 -3.6474621784657 9.5737839359692 10.1661833820723
 H29 -4.6024619819208 8.8543065895180 5.7428147782868
 C30 -3.6129222050211 6.6222674797682 5.7738423751398
 C31 -2.3079157275230 6.9924401054595 6.0615959068825
 H32 -3.8480157101222 6.0528028487396 4.8795797408001
 H33 -1.4980552861251 6.7302335040472 5.3859195173880
 H34 -2.0079045093352 7.2741641450542 7.0628005732216
 H35 -4.3698479202033 6.5974154348588 6.5495474282471
 X -2.9604189662720 6.8073537926138 5.9177191410111
 H30 -2.2211138130323 9.4107528743344 0.6392537240987

5c (2-olefin variant)

Rh1	-0.4422230347	1.8655555442	1.4991053708
C8	0.5013260940	6.5715027452	1.8356828917
C9	-0.2633625328	6.0919977857	0.7714325535
C10	-0.6387328763	4.7468844546	0.7249071855
C11	-0.2362255766	3.8458403417	1.7254620094
C12	0.5076643905	4.3536210592	2.8048286631
C13	0.8837084030	5.6977960697	2.8547672376
H14	0.7859603706	7.6180003159	1.8769034439
H15	-0.5766368301	6.7672943495	-0.0195466634

H16	-1.2463348710	4.3982760418	-0.1045153623
H17	0.8022657260	3.6954654254	3.6171503706
H18	1.4666579365	6.0642182165	3.6949630838
C23	-0.4927115170	-0.1949370642	0.4614535437
C24	-0.0278815526	-0.3960188679	1.7336809447
H25	-1.5219591537	-0.4051158530	0.1930574644
H26	-0.6718922227	-0.7755216286	2.5195661349
H27	1.0378326193	-0.4263038732	1.9474124783
H28	0.1906767617	-0.0594985995	-0.3736790503
X29	-0.1009084412#	0.0544147331#	0.9333886367#
C31	-1.9810164910	1.8837915001	2.9594954459
C32	-2.5451717290	2.0367796950	1.6720403528
H33	-2.0327501547	0.9278508767	3.4730916030
H34	-3.0406997654	1.2003935835	1.1857303177
H35	-2.8851221120	3.0154415533	1.3442583884
H36	-1.8870275326	2.7444560332	3.6154248354
X37	-2.6068471678#	1.2368394136#	2.4585888672#

TS5.2

Rh1 -1.5271798362000 1.8870821536000 2.0572070167000
 C2 2.7639684210000 1.7017110521000 2.1600473010000
 C3 3.1146859271000 2.6243845640000 1.1747275791000
 C4 2.1138003928000 3.3246114511000 0.5023472301000
 C5 0.7685162887000 3.1045327931000 0.8098929071000
 C6 0.4192043624000 2.1613861561000 1.7824701860000
 C7 1.4214651222000 1.4664185960000 2.4647713447000
 O8 -1.8472872311000 3.9250908105000 2.2235455114000
 C9 -1.6117502981000 4.4224565626000 3.3973690270000
 C10 -1.7026591891000 5.9309596339000 3.4848735268000
 H11 -1.8448801373000 6.2457744250000 4.5173861142000
 C12 -1.3036058365000 -0.2064546858000 1.4184480129000
 C13 -1.5953140194000 -0.1897461059000 2.7697851571000
 O16 -1.3117312079000 3.7417145988000 4.3906887447000
 H17 -0.7632154074000 6.3518215226000 3.1144898391000
 H18 -2.5087852964000 6.3057322355000 2.8536896730000
 H19 -0.8298434844000 -0.3648229435000 3.5160990488000
 C18 4.5963869569887 2.8779736945219 0.8402808555284
 H20 2.3737127331258 4.0510022594917 -0.2534318175260
 H21 0.0074119920989 3.6797985105292 0.3037411472038
 H23 1.1722895362000 0.7525563004000 3.2402765611000
 H24 3.5349744932000 1.1600423831000 2.6987462958000
 H25 -1.2273382406000 2.0914368766000 3.5531169826000
 H30 -2.0901318845000 -0.3423462784000 0.6796077311000
 H31 -0.2916271889000 -0.3733828521000 1.0686717754000
 H32 -2.6161964456000 -0.3110216566000 3.1233920584000

X -1.4494599279500 -0.1981003958500 2.0941165850000
H28 4.6683255886884 3.6262440655819 0.0509670490718
H29 5.1137019968762 3.2378685811213 1.7296406365539
H33 5.0573595402404 1.9495518246605 0.5031798186665

TS5.1'

Rh1 -1.6545656514000 2.0654850658000 1.9415832864000
C9 2.5460985722000 0.2181637560000 2.8631609174000
C10 2.4229548158000 1.0691412342000 1.7632879161000
C11 1.3429136521000 1.9473403748000 1.6801300203000
C12 0.3466814679000 1.9786372614000 2.6786297218000
C13 0.5175767899000 1.1383228461000 3.7988707061000
C14 1.5955857334000 0.2578210692000 3.8848197232000
H15 3.3896804139000 -0.4610366994000 2.9324477593000
H16 3.1739127941000 1.0551407278000 0.9795062955000
H10 1.2718392819000 2.6234610242000 0.8336209470000
H18 -0.1991025546000 1.1814401865000 4.6133144073000
H19 1.7026113311000 -0.3878669395000 4.7508500308000
H29 -0.1434173986000 3.3175536752000 2.9949187465000
C41 -1.5599259191000 4.7378556260000 3.0476522543000
O42 -2.3390224789000 3.9324270983000 2.4647728970000
O43 -0.3539608966000 4.4502772811000 3.3518270595000
C44 -2.0643310277000 6.1107265353000 3.3892697435000
H45 -3.1399628697000 6.1779124472000 3.2380207807000
H46 -1.8046644771000 6.3487013416000 4.4223071131000
H47 -1.5586617470000 6.8365646202000 2.7460471899000
C30 -3.2661911824000 1.9808471074000 0.4773409235000
C31 -3.7339183285000 1.4623437071000 1.6785460542000
H32 -3.4858558681000 3.0043449080000 0.1921849406000
H24 -4.3265790250000 2.0720749289000 2.3522828826000
H34 -3.8064477295000 0.3886189973000 1.8315690859000
H35 -2.9628357961000 1.3234819370000 -0.3334622911000
X36 -3.5000547554500 1.7215954072500 1.0779434888500

5d

Rh1 -1.0546770834351 0.4205711569621 2.5224753422208
H2 0.3008874184698 2.2092253997774 1.3681971444169
C14 1.3918845046070 0.3823979656545 1.4453445963544
H15 1.9680821380948 -0.2806310506208 2.0743226202590
C17 0.8823904007163 1.5111816174050 1.9583684180737
H18 1.0497546834563 1.7493870216696 3.0021107542830
X19 0.7888724890685 0.6711033453026 1.9290897123405
C23 -2.2799513442826 1.5602618064836 0.5797631940853
C24 -1.8626859808301 0.4040903570030 0.0452742508814
H25 -3.2445930914389 1.6436518946611 1.0604108529206
H26 -2.4802747595689 -0.4846067463280 0.0765817634155

H27 -0.9035694088503 0.3320401625172 -0.4549880249374
H28 -1.6749230954640 2.4542458620022 0.5308623339139
X29 -1.9941239395349 0.9436833269737 0.4913857755644
X30 -1.6101112124889 0.8277869486158 1.0000302267432
C31 -2.8695980062514 -1.3096408186767 2.8160386901189
C32 -3.2459954198026 -0.1172261451233 3.3036928538371
H33 -3.0498364003106 -1.6037938028729 1.7937888727127
H34 -3.7547680855172 0.6180283469204 2.6902252790843
H35 -3.0554885240674 0.1257907467180 4.3388537031040
H36 -2.3642799356467 -2.0245690177787 3.4574735791138
X37 -2.6112765697242 -0.6405167655506 3.0006141589879
X38 -2.2998077302126 -0.4856542965429 2.5588841515965
H29 1.2461258094993 0.0990440677268 0.4097392893863
C26 0.9293416845941 -0.9789084608471 6.6450950953399
C27 0.6502268714219 0.3809645631548 6.4313344971080
C28 0.0742856984358 0.7976938366497 5.2200329498744
C29 -0.2225406613781 -0.1454499138574 4.2224920008727
C30 0.0565331449467 -1.5052932668537 4.4361663547794
C33 0.6325153247803 -1.9220522113541 5.6475541463382
H32 1.3818112397902 -1.3062983365140 7.5967149794393
H37 0.8834758308568 1.1218496534722 7.2151322447591
H38 -0.1449759041728 1.8659984736396 5.0521245691009
H39 -0.1766740779238 -2.2461133641228 3.6524870722113
H40 0.8517769273889 -2.9903568483441 5.8154625271117

TS5.3

Rh1 -0.7055489072000 1.9577753733000 1.6556172925000
C2 1.1441074565000 2.8127825660000 1.0425523666000
H3 1.9437792889000 2.1329707364000 1.3247667094000
C4 0.8313650887000 3.8677811103000 1.9456082930000
H5 0.6627392072000 4.8439876577000 1.5084799414000
H6 1.3129496587515 3.9064794821211 2.9115165380765
H7 1.1003076298000 3.0300214929000 -0.0238161383000
C8 -3.3497949941000 5.7610747855000 2.8161600956000
C9 -2.9367762351000 5.5260366325000 1.5030021293000
C10 -1.8777801480000 4.6576286889000 1.2486078118000
C11 -1.2385549431000 3.9623387200000 2.2916536526000
C12 -1.6424803311000 4.2381965970000 3.6053999360000
C13 -2.6882180607000 5.1233150031000 3.8663829507000
H14 -4.1671731887000 6.4446934961000 3.0186598378000
H15 -3.4321210681000 6.0293250098000 0.6783799362000
H16 -1.5498402515000 4.5093009463000 0.2232702337000
H17 -1.1508542389000 3.7430188688000 4.4362174106000
H18 -2.9911984129000 5.3095150574000 4.8922006882000
C23 -0.4048764553753 0.1293426292056 0.3526981157385

C24 0.2074085635318 -0.1247806411069 1.5714646031019
H25 -1.3694273872996 -0.3089388966815 0.1177924014557
H26 -0.2714914520544 -0.7487215740997 2.3174595418148
H27 1.2816981431191 -0.0338752780018 1.6851099888975
H28 0.1805686174890 0.4410233903268 -0.5068329054108
X29 -0.0987339459217 0.0022809940494 0.9620813594202
C31 -2.3803220214025 1.1339494229790 3.0866937489750
C32 -2.9758173974186 1.3681514951295 1.8707460840069
H33 -2.1014498635576 0.1286947888132 3.3826674722255
H34 -3.1672006892010 0.5572752586946 1.1771645098379
H35 -3.5186423899464 2.2857768549509 1.6808093240765
H36 -2.4449220539533 1.8570475347521 3.8907915547479
X37 -2.6780697094105 1.2510504590542 2.4787199164910

5e

Rh1 -3.0322901822065 8.6598527442865 4.8743489248049
H2 -4.2197892250295 6.5381285674028 6.0404216369775
C3 -7.9101203121752 8.6733281054245 8.2991069901385
C4 -7.5329094833718 8.8199611409170 6.9636334293260
C5 -6.1901574684989 8.7364466541275 6.6046288206527
C6 -5.2040910965103 8.5026120505920 7.5690050613641
C7 -5.5902474519240 8.3619060529025 8.9045968269261
C8 -6.9345352015937 8.4452136825337 9.2681374939248
H9 -8.9550176757741 8.7404776224794 8.5816516991122
H10 -8.2842798605153 9.0037973267229 6.2027395697851
H11 -5.8946158611045 8.8534749709903 5.5654285130165
H12 -4.8368303688056 8.1836236237064 9.6655898561637
H13 -7.2180714382405 8.3334703483397 10.3094076683552
C14 -3.7537860815007 8.3721419348145 7.1683188037102
H15 -3.0888583771350 8.4763449234511 8.0287758839551
H16 -3.5266298607001 9.2944536807067 6.6259384642866
C17 -3.3960300396615 7.2064578184953 6.2915215699389
H18 -2.5059047821088 6.6554050048849 6.5939211855387
X19 -3.5749080605811 7.7892998766549 6.7299201868246
C23 -1.9701194458813 7.2450373280988 3.6140344177643
C24 -3.1834579730798 7.5839545168728 3.0126835308355
H25 -1.0410470006728 7.6962388309361 3.2791518261310
H26 -3.2125320898437 8.2808492760446 2.1795309680409
H27 -4.0354308757905 6.9129320318658 3.0730545626422
H28 -1.8600463102308 6.3030407554042 4.1404769841566
X29 -2.5767887094805 7.4144959224858 3.3133589742999
X30 -2.8011524485927 7.9411930310600 4.1982907719654
C31 -3.4430693794141 10.6427907049506 3.8607426637391
C32 -2.0836739626912 10.4285366118619 3.8034544743792
H33 -4.0808612584470 10.4403473813483 3.0068742560590

H34 -1.6139497363376 10.0576127067770 2.8977128375586
H35 -1.4101544904600 10.8850133456203 4.5221525786970
H36 -3.8743247218894 11.2845084197916 4.6235711144457
X37 -2.7633716710527 10.5356636584062 3.8320985690591
X38 -3.0668993954326 9.7342759078590 4.3582531310630

TS5.4

Rh1	-1.1388112077	0.4484087067	2.0890389424
H2	0.9721384396	0.6455741508	0.4582525233
C3	3.5824591137	-2.5515924156	3.4488562093
C4	2.6943955999	-2.6049570204	2.3722376467
C5	1.8458664502	-1.5343513970	2.1075743389
C6	1.8744559859	-0.3813733580	2.9055328785
C7	2.7624289977	-0.3432227223	3.9879429998
C8	3.6101135720	-1.4171141271	4.2578772077
H9	4.2388952045	-3.3893449295	3.6575423814
H10	2.6563543697	-3.4886087341	1.7437463316
H11	1.1374976158	-1.5986974245	1.2892682608
H12	2.7922324086	0.5362071491	4.6241370729
H13	4.2909784247	-1.3658464109	5.1010693349
C14	1.0019378752	0.7997922827	2.6369543971
H15	1.1319602958	1.5964051400	3.3666237294
H16	-0.3716833418	0.3026742646	3.4417972888
C17	0.6270778631	1.2104096472	1.3210606339
H18	0.4830984548	2.2721325653	1.1336203719
X19	0.8458716948#	1.0570021884#	2.0886629523#
C31	-2.8242033271	-0.5425775540	1.0623144919
C32	-3.2265561729	0.7403777963	1.3961004901
H33	-2.4883303698	-0.7906544117	0.0600017817
H34	-3.2153962098	1.5471581173	0.6692971733
H35	-3.8179279674	0.9294489493	2.2881103530
H36	-3.088218182	-1.3937137151	1.6840362140
X37	-3.0255816536#	0.0730434129#	1.1365478106#

5f

Rh1 -1.0546770834351 0.4205711569621 2.5224753422208
H2 0.3008874184698 2.2092253997774 1.3681971444169
C14 1.3918845046070 0.3823979656545 1.4453445963544
H15 1.9680821380948 -0.2806310506208 2.0743226202590
H16 -0.3587984862754 -0.0133487176495 3.8912800555721
C17 0.8823904007163 1.5111816174050 1.9583684180737
H18 1.0497546834563 1.7493870216696 3.0021107542830
X19 0.7888724890685 0.6711033453026 1.9290897123405
C23 -2.2799513442826 1.5602618064836 0.5797631940853
C24 -1.8626859808301 0.4040903570030 0.0452742508814
H25 -3.2445930914389 1.6436518946611 1.0604108529206

H26 -2.4802747595689 -0.4846067463280 0.0765817634155
H27 -0.9035694088503 0.3320401625172 -0.4549880249374
H28 -1.6749230954640 2.4542458620022 0.5308623339139
X29 -1.9941239395349 0.9436833269737 0.4913857755644
X30 -1.6101112124889 0.8277869486158 1.0000302267432
C31 -2.8695980062514 -1.3096408186767 2.8160386901189
C32 -3.2459954198026 -0.1172261451233 3.3036928538371
H33 -3.0498364003106 -1.6037938028729 1.7937888727127
H34 -3.7547680855172 0.6180283469204 2.6902252790843
H35 -3.0554885240674 0.1257907467180 4.3388537031040
H36 -2.3642799356467 -2.0245690177787 3.4574735791138
X37 -2.6112765697242 -0.6405167655506 3.0006141589879
X38 -2.2998077302126 -0.4856542965429 2.5588841515965
H29 1.2461258094993 0.0990440677268 0.4097392893863

Additional Structures

[Cu^{II}(μ-OAc)₂]₃

Cu1 1.7001041201000 0.9749080867000 -0.0270682404000
C2 0.0148657465000 2.5834155618000 -1.8453255785000
O3 1.0958587124000 2.4970675478000 -1.1872886530000
O4 -1.0231687139000 1.8793150367000 -1.6586403441000
C5 -2.2210138567000 -1.3212284027000 1.8746320854000
O6 -1.6018982501000 -2.2000913425000 1.2018518605000
O7 -2.1566597143000 -0.0670707743000 1.6951555506000
C8 -3.1335200970000 -1.8089368121000 2.9824909596000
H9 -3.0687895991000 -1.1347841787000 3.8412448870000
H10 -4.1664552254000 -1.7860660157000 2.6138215754000
H11 -2.8802878305000 -2.8296534720000 3.2750406277000
C12 -0.0520298176000 3.6276692034000 -2.9404034563000
H13 0.9474211437000 3.9639840925000 -3.2216938914000
H14 -0.5786604537000 3.2206769476000 -3.8080717972000
H15 -0.6298659816000 4.4820176745000 -2.5681924041000
Cu16 -0.0107473109000 -1.9584497118000 -0.0019311117000
C17 -2.2945957407000 -1.2603681438000 -1.8242964303000
O18 -2.7367018480000 -0.2931434432000 -1.1310365354000
O19 -1.1904791451000 -1.8550728759000 -1.6459376975000
C20 -0.0139403919000 2.5896904114000 1.8380639438000
O21 1.0315817432000 1.8986633163000 1.6470924789000
O22 -1.0927135630000 2.5006297919000 1.1758258346000
C23 0.0304926884000 3.6302124418000 2.9376428430000
H24 -0.9459604009000 3.7183034506000 3.4194964405000
H25 0.8023143501000 3.3797563443000 3.6686717956000
H26 0.2799709199000 4.5975446330000 2.4846287103000
C27 -3.1624721599000 -1.7136550082000 -2.9801944632000
H28 -3.0904612328000 -0.9668464598000 -3.7795234938000

H29 -2.8324309233000 -2.6824575710000 -3.3587326309000
 H30 -4.2080428855000 -1.7618957065000 -2.6630702199000
 Cu31 -1.7045457930000 0.9776178337000 0.0223858570000
 C32 2.2751363052000 -1.2777947068000 1.8210625357000
 O33 2.7151611782000 -0.3039893001000 1.1365337192000
 O34 1.1696858895000 -1.8707096460000 1.6421790219000
 C35 3.1485425753000 -1.7458785034000 2.9674645329000
 H36 3.0892426618000 -1.0048146752000 3.7729458051000
 H37 2.8147763225000 -2.7153743551000 3.3410265106000
 H38 4.1908899373000 -1.7990498132000 2.6405288052000
 C39 2.2202033847000 -1.3291066212000 -1.8694461336000
 O40 2.1725558033000 -0.0736471337000 -1.6919431025000
 O41 1.5830937664000 -2.1988439095000 -1.2017217893000
 C42 3.1403964909000 -1.8351714478000 -2.9625090429000
 H43 4.1528243235000 -1.9157669507000 -2.5464393675000
 H44 2.8219470593000 -2.8197299665000 -3.3115019466000
 H45 3.1695135524000 -1.1225951820000 -3.7913717684000

[Cu^{II}(μ-OAc)₂]

Cu1 1.4492955659000 0.7079322153000 0.0170462470000
 Cu16 0.1737136361000 -1.5204259287000 0.2444761440000
 C32 -1.0420316958000 0.4514194989000 -1.4784229391000
 O33 -0.1062864876000 1.2797063811000 -1.2179680784000
 O34 -1.1398783806000 -0.7242285548000 -1.0276793545000
 C35 -2.1080198512000 0.9400733643000 -2.4263031397000
 H36 -1.6800486294000 1.0029415638000 -3.4308750918000
 H37 -2.9546002582000 0.2558791762000 -2.4361150464000
 H38 -2.4272518322000 1.9432370514000 -2.1395290486000
 C39 -0.5242101169000 0.5360773647000 2.1544498420000
 O40 0.3518759372000 1.3193861281000 1.6564637482000
 O41 -0.7819544573000 -0.6358404160000 1.7604582473000
 C42 -1.3379661066000 1.0825520091000 3.3001218999000
 H43 -2.2699181424000 1.4865715815000 2.8918866950000
 H44 -1.5911708192000 0.2812408933000 3.9946323194000
 H45 -0.8038259900000 1.8840905577000 3.8081765588000
 C17 2.6260235064000 -1.3181515415000 1.7544831215000
 O18 2.8384969774000 -0.1509129208000 1.2834852951000
 O19 1.6334482418000 -2.0544797004000 1.4944172272000
 C20 3.6599991505000 -1.8350762750000 2.7226991470000
 H21 3.5596240153000 -1.2860154494000 3.6634305252000
 H22 3.5136901772000 -2.8977101197000 2.9082301255000
 H23 4.6619830542000 -1.6456331767000 2.3345548753000
 C24 2.1161575908000 -1.3878492359000 -1.8937613061000
 O25 2.3870415102000 -0.1769321895000 -1.5960137239000

O26 1.2838460391000 -2.1299921129000 -1.3004960182000
 C27 2.8840285983000 -1.9836315260000 -3.0465234797000
 H28 3.7243950035000 -2.5536823514000 -2.6383550031000
 H29 2.2466719302000 -2.6726073793000 -3.6014552951000
 H30 3.2736695405000 -1.2035604553000 -3.6986341894000

Cu(OAc)(HOAc)(η^2 -C₂H₄)

C1 -1.2930207909000 -4.2269949930000 -3.0021980958000
 O2 -1.1921039639000 -5.5069149500000 -2.7926055193000
 C3 -2.2244157510000 -3.8560115736000 -4.1195009798000
 O4 -0.6883037161000 -3.3624115352000 -2.3527030971000
 H5 -2.2214989637000 -2.7798278209000 -4.2765006186000
 H6 -1.9231901625000 -4.3736811041000 -5.0333949728000
 H7 -3.2336018813000 -4.1962234074000 -3.8716041403000
 C8 -0.0700816133000 -5.8309325265000 0.3924213085000
 O9 0.1237427636000 -4.5871493656000 0.5637417033000
 C10 -0.3303252376000 -6.6676133203000 1.6267578797000
 O11 -0.0836837862000 -6.4045604723000 -0.7309844978000
 H12 -0.0047637094000 -7.6954570564000 1.4676336458000
 H13 0.1569747731000 -6.2378440368000 2.5014020647000
 H14 -1.4100175957000 -6.6806073905000 1.8077483552000
 Cu15 0.7217207698000 -3.3802559041000 -0.8849047457000
 H16 -0.6401479104000 -5.7706839132000 -1.9503454861000
 C17 2.1566685552000 -2.0172772350000 -1.5523542748000
 C18 2.5393152333000 -2.5190589917000 -0.3336856265000
 H19 2.5443466399000 -2.4301746905000 -2.4796312660000
 H20 3.2374576594000 -3.3481786925000 -0.2578746143000
 H21 2.3252351893000 -1.9905123864000 0.5913064670000
 H22 1.6270827005000 -1.0720592121000 -1.6342313606000
 X23 2.3479918942500 -2.2681681133500 -0.9430199506500
 X24 1.6700102992000 -3.1025739138000 -1.0013159852000

Cu(OAc)₂

Cu1	0.9114831144	2.2610617653	1.1129480789
C2	-1.1406208290	3.4121655465	1.2570453536
O3	-0.0270416689	4.0312105114	1.2046906747
O4	-1.0905133727	2.1404784781	1.2311078169
C5	-2.4346391264	4.1531236993	1.3464603229
H6	-3.2764259691	3.4631724775	1.3509072694
H7	-2.4388289525	4.7545548876	2.2595527231
H8	-2.5139439917	4.8404064423	0.5003529605
C18	2.9571115878	1.1023184568	0.9416983410
O19	2.9099030962	2.3761560291	0.9678000455
O20	1.8454494109	0.4863997363	1.0167201425

C21	4.2586585395	0.3775250978	0.8310273449
H22	4.0992754346	-0.6979796176	0.7800631807
H23	4.7883487535	0.7237941087	-0.0599505427
H24	4.8785880579	0.6234186395	1.6976226439
Cu(OAc)			
C1	-0.0388561666	-0.0727142122	-0.0280071665
O2	-0.0652925359	1.1973619901	-0.0289641869
C3	-1.3437766334	-0.8343746981	-0.0095887169
O4	1.0647114811	-0.7000781654	-0.0431096261
H5	-1.1728157371	-1.9091153530	-0.0013485742
H6	-1.9180341029	-0.5428206216	0.8728822328
H7	-1.9319553950	-0.5594499655	-0.8884188455
Cu8	2.0611066502	1.1730264497	-0.0603911484
Cu(OAc)(HOAc)2			
C8	-1.0918645074	-3.7666564868	-3.0651495534
O9	-1.5860636949	-4.9158724657	-2.7438486427
C10	-1.6704649191	-3.1536977517	-4.3085095585
O11	-0.2068090258	-3.1991675829	-2.3978713357
H5	-1.1683913618	-2.2200767663	-4.5538640750
H6	-1.5802476070	-3.8578217168	-5.1384434995
H7	-2.7362419552	-2.9690246685	-4.1517964580
C9	-0.2566796112	-6.0822304566	0.3180909266
O10	0.5014100527	-5.0999155580	0.5969661082
C11	-0.3862553281	-7.1641520613	1.3687141215
O12	-0.9032250742	-6.2288697568	-0.7490676072
H12	-1.4343782538	-7.2489997633	1.6658449366
H13	-0.0938217353	-8.1226016629	0.9335763377
H14	0.2283577997	-6.9476405581	2.2407139899
Cu15	1.0189894823	-3.6084668384	-0.4648979092
H16	-1.1892297952	-5.3471993795	-1.8736025059
C17	2.0986282050	-1.1116579180	-1.7208801893
O18	1.2296665266	-1.0632628200	-2.7046432063
C19	3.0925689970	0.0068146921	-1.7180711951
O20	2.1058841395	-2.0044754661	-0.8669173573
H21	3.7587622088	-0.0819939279	-0.8631845165
H22	3.6688941855	-0.0206497171	-2.6470226226
H23	2.5647554675	0.9635817919	-1.6906841366
H24	0.6068015347	-1.8523955121	-2.6604056232
Cu(OAc)(HOAc)(C₂H₄)			
C1	-1.2930207909	-4.2269949930	-3.0021980958
O2	-1.1921039639	-5.5069149500	-2.7926055193
C3	-2.2244157510	-3.8560115736	-4.1195009798
O4	-0.6883037161	-3.3624115352	-2.3527030971
H5	-2.2214989637	-2.7798278209	-4.2765006186

H6	-1.9231901625	-4.3736811041	-5.0333949728
H7	-3.2336018813	-4.1962234074	-3.8716041403
C8	-0.0700816133	-5.8309325265	0.3924213085
O9	0.1237427636	-4.5871493656	0.5637417033
C10	-0.3303252376	-6.6676133203	1.6267578797
O11	-0.0836837862	-6.4045604723	-0.7309844978
H12	-0.0047637094	-7.6954570564	1.4676336458
H13	0.1569747731	-6.2378440368	2.5014020647
H14	-1.4100175957	-6.6806073905	1.8077483552
Cu15	0.7217207698	-3.3802559041	-0.8849047457
H16	-0.6401479104	-5.7706839132	-1.9503454861
C17	2.1566685552	-2.0172772350	-1.5523542748
C18	2.5393152333	-2.5190589917	-0.3336856265
H19	2.5443466399	-2.4301746905	-2.4796312660
H20	3.2374576594	-3.3481786925	-0.2578746143
H21	2.3252351893	-1.9905123864	0.5913064670
H22	1.6270827005	-1.0720592121	-1.6342313606
X23	2.3408592770#	-2.3688048844#	-1.1087559829#
X24	1.6700102992#	-3.1025739138#	-1.0013159852#
Cu(OAc)(C₂H₄)			
C1	0.3983993014	-5.8101691841	0.4560660363
O2	-0.0643191103	-4.8090347564	1.0488348551
C3	0.4098861308	-7.1603512057	1.1454422226
O4	0.8727755597	-5.7381232320	-0.7316906996
H5	0.8353253878	-7.9334712970	0.5070944188
H6	0.9886109331	-7.0869901705	2.0695434018
H7	-0.6115245403	-7.4320889703	1.4231352026
Cu8	0.5904345359	-3.7445515504	-1.0733358838
C9	-1.3546134881	-3.9216595581	-2.0154560703
C10	-1.0159907304	-2.6066565552	-2.0795828189
H11	-1.1632402057	-4.5995408031	-2.8419183071
H12	-0.5519683393	-2.1838397242	-2.9648561161
H13	-1.3363240922	-1.9049556491	-1.3156183044
H14	-1.9447189254	-4.3126720619	-1.1925948853
X15	-0.8909886349#	-3.0838337865#	-2.5633758190#
X16	-0.2832955649#	-3.4623718193#	-1.8652217805#
C17	2.5254341222	-3.0820930262	-0.3601794979
C18	1.8871260221	-1.9742567054	-0.8219886857
H19	2.4665122300	-3.3735515492	0.6836423182
H20	1.3085355205	-1.3395581378	-0.1577847778
H21	2.0574707549	-1.5989777787	-1.8258908250
H22	3.2213481891	-3.6384043528	-0.9809533570
X23	2.3408590000#	-2.3688050000#	-1.1087560000#
X24	1.6700100000#	-3.1025740000#	-1.0013160000#

Rh(II)Cu(II)Rh(II)

Rh1	1.8235533455	9.8820023157	4.0847015907
Cu2	-0.5663164359	7.9251948854	4.6438070300
O3	2.2711580917	7.7012716374	4.7143029690
O4	1.1356584021	10.4459440023	6.0218275416
O5	0.5089168372	6.3823751259	5.1496198909
O6	-0.3654113096	8.8062252781	6.3733364225
C8	0.2685580533	9.8534870093	6.7172749992
C9	2.0482014977	9.2609517685	2.0099205112
C10	1.7641322219	6.6226885107	5.1049545653
C12	-0.0811762858	10.4148841505	8.0710627128
C13	3.2996681126	9.5894817259	2.5066335060
C14	2.6678136210	5.5080700670	5.5785478642
H15	0.0400723837	9.6351648367	8.8263001971
H16	3.6862220306	5.6609154118	5.2240925204
H17	2.2841579393	4.5423468176	5.2466197983
H18	-1.1361283713	10.6995762354	8.0508903784
H19	0.5422553632	11.2740073688	8.3120566178
H20	2.6681298330	5.5085482686	6.6730485150
Rh21	-3.3763003090	9.0073979754	5.3871059016
O22	-5.2260938460	10.5916968642	5.7828099229
O23	-3.7072115431	7.6150228118	3.8627671184
O24	-3.3067409702	10.4722988799	6.8474487704
O25	-1.6259305757	6.9262608357	3.3306874350
C26	-3.2317663644	7.4073288352	6.8720485038
C27	-2.8798898216	6.9469413387	3.1735861073
C28	-4.4360844228	11.0580443453	6.6316209055
C29	-4.5703640862	7.7031214643	6.7100194520
C30	-3.4419332096	6.0814707735	2.0724689749
C31	-4.7596562758	12.3018542083	7.4131917542
H32	-2.9399461742	6.3262083586	1.1340876856
H33	-5.7360033534	12.1911905785	7.8901228035
H34	-3.9967031411	12.5070869637	8.1629864313
H35	-3.2191838108	5.0358298826	2.2997770825
H36	-4.5167623089	6.2193753175	1.9723741886
H37	-4.8262936225	13.1435396259	6.7185542132
H40	1.5024163519	9.9524090290	1.3782349279
H41	1.7144023665	8.2292062734	1.9853157696
H44	3.9571656077	8.8157456505	2.8909499658
H45	3.7609145818	10.5409340772	2.2658591111
H46	-2.6516353930	7.8320122862	7.6825288689
H47	-2.7811245760	6.5666629131	6.3528896363
H48	1.7593811687	11.3629513664	3.6674960424
H49	-5.0834783504	8.3590337674	7.4031339127

X51	2.5841728011#	8.3838904319#	2.4084324805#
X52	-3.6260456412#	6.9915058172#	6.2665450057#
O53	-2.7311427317	10.4605729507	3.9916576618
O54	-0.6649896628	9.6562975507	3.6833595136
C55	-1.5800889429	10.5282444984	3.4963362743
C56	-1.2400806134	11.7080202342	2.6270070828
H57	-2.1143073663	12.3386230085	2.4783404063
H58	-0.4429403244	12.2809757314	3.1067302927
H59	-0.8594203164	11.3546696725	1.6665882462
H60	-5.1980885354	7.1187427548	6.0469517360
Rh(III)Cu(II)Rh(I)			
Rh1	2.2275755219	9.4695189635	4.4086412277
Cu2	-0.4946787757	8.5315598993	3.8691772001
O3	2.3243870838	7.4775517670	5.0874192859
O4	1.2559763264	10.0366454932	6.2206874454
O5	0.2040109955	6.8795909413	4.6609474090
O6	-0.8010347093	9.3250235015	5.7127403085
C7	1.5461491444	11.3866533091	3.6245131404
C8	0.0401739600	9.8628249622	6.5041078694
C9	2.3599450561	8.6760453218	2.4005404560
C10	1.3606440755	6.6613211920	5.1240772767
C11	2.7996865597	11.5508849381	4.1931070999
C12	-0.4478190623	10.3110910302	7.8548038957
C13	3.6483357131	8.8988332681	2.8790715063
C14	1.5907744499	5.3170121921	5.7692250026
H15	-0.7383798708	9.4312710848	8.4355232365
H16	2.6433139509	5.1694788723	6.0043634577
H17	1.2327037396	4.5284172060	5.1047463524
H18	-1.3475788364	10.9124116237	7.7252515760
H19	0.3315363906	10.8540549474	8.3856933748
H20	1.0015156266	5.2649362815	6.6887662755
Rh21	-3.2248488966	9.0360987237	5.4126634832
O22	-5.6954025893	10.4758113577	6.8533332254
O23	-3.2349739041	7.5010583684	3.9146434852
O24	-3.4370436767	10.4347006162	6.8620471357
O25	-1.4524906958	7.4221695808	2.5362733484
C26	-2.9220027850	7.4817610070	6.9187056774
C27	-2.6170739063	7.0817905739	2.8937925263
C28	-4.6023231624	10.8816250385	7.2410190344
C29	-4.2721461689	7.4974053566	6.6359787674
C30	-3.3232245414	6.0525427133	2.0409644373
C31	-4.5030103002	12.0177097826	8.2476651676
H32	-3.1066661964	6.2296511155	0.9868422872
H33	-5.2659847031	11.8908732315	9.0172766983

H34	-3.5138829642	12.0790832434	8.7007110992
H35	-2.9328347976	5.0637892257	2.3012318319
H36	-4.3968047631	6.0703684456	2.2217788958
H37	-4.7090160895	12.9557055017	7.7238013686
H38	0.6469755526	11.6088122331	4.1838309073
H39	1.4114072582	11.3423496790	2.5509658235
H40	1.9034078066	9.3462938066	1.6813264079
H41	1.9210757274	7.6838869425	2.4385126482
H42	3.6866947445	11.6485944022	3.5770334567
H43	2.8997919964	11.8969299316	5.2177501993
H44	4.2245813059	8.0867562596	3.3112860358
H45	4.2277506177	9.7468921114	2.5301606536
H46	-2.5396661389	7.9963890144	7.7918742694
H47	-2.2535924855	6.7779332691	6.4350617065
H48	-4.7108683862	9.0745766220	5.1543179016
H49	-4.9735634952	8.0211442499	7.2733419021
X50	2.4069459912#	11.2246795476#	3.5524968176#
X51	2.5841728012#	8.3838904319#	2.4084324805#
X52	-3.6260456411#	6.9915058172#	6.2665450057#
O53	-3.0692847754	10.6008894423	4.0192443295
O54	-1.1127584741	10.1447907994	2.9818844313
C55	-2.1604639932	10.8325939991	3.1777061118
C56	-2.3226547404	12.0557090252	2.3052218403
H57	-3.2279234115	12.6018891235	2.5634596707
H58	-1.4480788283	12.6993370179	2.4242420871
H59	-2.3612780655	11.7423218588	1.2589898940
H60	-4.6948689498	6.8037541260	5.9190664192
Rh(III)Rh(I)			
Rh1	-0.5052927297	9.0519787598	4.5969607240
C3	-0.2216794231	7.5433141704	6.1511206568
C4	-0.6556008597	10.5958305771	6.1244572990
C5	0.9446510699	7.6651888720	5.4116213582
C6	0.5781707355	10.7074393182	5.4971170309
Rh7	-3.5407124806	8.9535668636	4.9217337611
O8	-5.9281015429	10.2186750079	6.6998350512
O9	-3.3229948001	7.8687209030	3.1356658780
O10	-3.6835071579	9.9984989310	6.6544322659
O11	-1.1069693241	7.4955279118	3.2969371676
C12	-3.5394585090	7.0749982644	6.0518826135
C13	-2.2352876960	7.3527775330	2.7411063307
C14	-4.8040369435	10.4419823850	7.1475369310
C15	-4.8491801963	7.3234906551	5.6956661175
C16	-2.2908364141	6.4669225927	1.5201335125
C17	-4.6003988856	11.3211106477	8.3712802586

H18	-1.5098164757	6.7649973892	0.8177779833
H19	-5.4805724889	11.2775187956	9.0128637561
H20	-3.7063423145	11.0326821600	8.9246430194
H21	-2.0841170798	5.4365779607	1.8240910403
H22	-3.2694636429	6.5161213383	1.0454125547
H23	-4.4735036833	12.3536210797	8.0313875547
H24	-0.9109664640	6.7407232176	5.9299453617
H25	-0.3079679839	7.9747883089	7.1419389236
H26	-0.7502080138	10.1539677187	7.1085831827
H27	-1.5010253145	11.2063345431	5.8328501338
H28	1.8050842830	8.2006376756	5.7961352601
H29	1.1452465848	6.9861094783	4.5886354360
H30	0.7243782452	11.4116948764	4.6847746601
H31	1.4845655426	10.3677983437	5.9871025039
H32	-3.1730636844	7.3327559382	7.0390081495
H33	-2.9472323396	6.3712159811	5.4790175603
H34	-5.0083357367	9.1990693091	4.6448005795
H35	-5.5436362011	7.7920517146	6.3813089804
X36	0.4174200082#	7.6638732771#	5.8832900464#
X37	0.4596127724#	10.6867070845#	5.5797343056#
X38	-4.2591409913#	7.0471563938#	5.5617408779#
O38	-3.3062425146	10.7632817669	3.8745804686
O39	-1.1909682963	10.4610859194	3.1917888310
C40	-2.3123983401	11.0469967956	3.1502022871
C41	-2.4874211856	12.1645814922	2.1516029056
H42	-3.1338886930	12.9378395939	2.5677472986
H43	-1.5236922623	12.5799083436	1.8596741919
H44	-2.9807703588	11.7579727818	1.2633398923
H45	-5.2835678801	6.8415313209	4.8268735107
Rh(II)Rh(II)			
Rh1	-0.2807690738	8.9856176439	4.5422717436
C3	0.3495901226	7.4983060545	6.0196672454
C5	1.2654990082	7.5182917249	4.9815819561
Rh7	-3.7099040269	8.9543903302	5.0922559030
O8	-5.7441199988	10.1615726502	5.7302724984
O9	-3.6575964548	7.9579677106	3.2600378347
O10	-3.8873596594	9.9985451744	6.8898498505
O11	-1.5066265093	7.3921693991	3.5173815828
C12	-3.5180791425	7.0882795199	6.2172557913
C13	-2.5895220660	7.3906401660	2.8711243660
C14	-5.0684147603	10.4868999809	6.7319840788
C15	-4.8495241276	7.2441296719	5.8843646671
C16	-2.6454466640	6.6392690913	1.5629172053
C17	-5.5836107349	11.4583025530	7.7575052799

H18	-1.7984641017	6.9344450856	0.9404446594
H19	-6.6723288306	11.4204929634	7.7982607495
H20	-5.1534830006	11.2510152344	8.7379373921
H21	-2.5438562944	5.5699927651	1.7693296401
H22	-3.5834107193	6.8217438689	1.0411693810
H23	-5.2850022782	12.4671054094	7.4556913246
H24	-0.4450733255	6.7592265507	6.0251237730
H25	0.5579230637	7.9816188339	6.9670334785
H28	2.2091698047	8.0453692201	5.0853936380
H29	1.2023491190	6.7997384926	4.1709771854
H32	-3.1577103022	7.3666918841	7.2020142175
H33	-2.8689479360	6.4560914165	5.6213957124
H34	0.2135801309	9.9896184947	5.5992470037
H35	-5.5586506449	7.6517189345	6.5942549644
X36	0.4174200082#	7.6638732770#	5.8832900464#
X38	-4.2591409913#	7.0471563938#	5.5617408779#
O31	-3.2731388387	10.7676072414	4.1252550895
O32	-1.1347391698	10.5528705309	3.4475365213
C33	-2.2592457028	11.1367267968	3.4734280567
C34	-2.4092292907	12.3779522853	2.6253654024
H36	-3.1506313487	13.0459694992	3.0627443371
H37	-1.4509915119	12.8834520936	2.5095903035
H38	-2.7650916260	12.0759817400	1.6353987699
H39	-5.2725775221	6.7560728469	5.0139363793

TS: Premature C₂H₄ Insertion

Rh1	2.2922741187	9.4770310146	3.7912845595
Cu2	-0.5923303090	9.8184247435	3.6706030475
O3	1.7210137432	8.6131137976	5.6543344075
O4	2.0963823340	11.3893905190	4.6421278002
O5	-0.5034758084	8.6549341620	5.3880432141
O6	-0.1460343937	11.4252558336	4.7000667407
C7	1.9261226157	10.4234996197	1.8812948906
C8	0.9872268912	11.9031499646	4.9760923832
C9	1.9191797300	7.5205028814	2.8984722529
C10	0.5438545752	8.3717144578	6.0422691835
C11	3.2991681504	10.3942446325	2.1103099631
C12	1.0214026271	13.1751815757	5.7864076125
C13	3.2290027212	7.5711285009	3.3476899684
C14	0.4191261972	7.6910044177	7.3858917142
H15	0.9772480590	12.9071794811	6.8466155527
H16	0.9657447600	8.2707138756	8.1327440867
H17	0.8892808184	6.7057615085	7.3304364529
H18	0.1530298928	13.7916369234	5.5555430771
H19	1.9473779791	13.7205163470	5.6081605862

H20	-0.6168871508	7.5822080670	7.6905417747
O21	-3.4064045957	10.4730286852	4.1385677134
O22	-2.8749645787	7.5743123895	3.3452571316
O23	-1.8425894090	10.9083850798	2.5819465832
O24	-0.9030114462	8.2926358634	2.5250076115
C25	-1.9513765535	7.5753711464	2.4959589662
C26	-2.9803610613	11.0802283040	3.1273223736
C27	-2.0746604573	6.6462818540	1.3084946291
C28	-3.8803225232	12.1350088557	2.5203386660
H29	-2.2021173311	7.2480935164	0.4047716360
H30	-3.8397563136	13.0238451117	3.1561710996
H31	-3.5532161650	12.4031461805	1.5168316951
H32	-1.1519694267	6.0738288266	1.1937988968
H33	-2.9244094037	5.9758659340	1.4250727771
H34	-4.9109499507	11.7800071474	2.5091057443
H35	1.3506207762	11.3181415007	2.0971812331
H36	1.4490844343	9.7329653335	1.1958774901
H37	1.6777900238	7.6171372625	1.8475153876
H38	1.1298156246	7.0894115330	3.4998175327
H39	3.9299764152	9.6835903965	1.5866249827
H40	3.8083648323	11.2655954794	2.5101673137
H41	3.4933283350	7.1851512465	4.3277590955
H42	4.0545647273	7.7010128611	2.6568415921
X43	2.6383999998#	10.9009500003#	3.4390499999#
X44	2.5943000001#	8.1144000002#	2.5217500000#
X45	2.7922575448#	10.0919381090#	2.0484747992#
X46	2.4395227059#	7.4687465692#	3.6438921038#
Rh47	-3.0851198346	8.5879461245	5.2496535194
C48	-3.7990787322	11.9895689497	8.6426011992
C49	-2.5151180043	11.5674281713	8.2964978773
C50	-2.3346993308	10.4615951914	7.4693539897
C51	-3.4364225242	9.7493025446	6.9759006799
C52	-4.7223682005	10.1912951412	7.3127749042
C53	-4.9010467094	11.2989466572	8.1397904196
H54	-3.9390844207	12.8488135464	9.2890915027
H55	-1.6475882537	12.1076602113	8.6617726801
H56	-1.3326477814	10.1677452497	7.1853722977
H57	-5.5922961403	9.6693475568	6.9298195596
H58	-5.9069082514	11.6241847983	8.3862054251
H59	-4.5772984421	8.4320712706	5.0711683815
C60	-3.3428041934	7.7183368996	7.2384506990
C61	-3.0133827338	6.7373172679	6.2606474117
H62	-4.3562946986	7.7167547328	7.6145596329
H63	-3.7830369852	6.0853447272	5.8635514901

H64	-2.0014492921	6.3524626587	6.1965915356
H65	-2.6124908186	7.9380894608	8.0038737521
X66	-3.3125013660#	7.2712294752#	6.9662537869#
TS: External OAc Deprotonation			
Rh1	2.4178624187	9.6475826676	3.4566895442
Cu2	-0.4965392496	9.2094380371	4.2716205220
O3	2.5813016451	8.1402146324	4.9660863131
O4	2.2146399065	11.1068346384	4.9909391521
O5	0.4061554738	7.5689390478	5.1239534405
O6	0.2637709817	10.3350975279	5.8132218835
C7	1.5291295932	11.0761352761	2.1763967722
C8	1.2737384821	11.0939109229	5.8463687774
C9	1.9282900630	8.1055150145	2.0863792929
C10	1.6241596586	7.4597999896	5.4522391958
C11	2.9039105022	11.2557212177	2.1705365401
C12	1.3499498907	12.0767315958	6.9997885098
C13	3.3046502144	8.2515771994	2.1363167569
C14	1.9493718631	6.4261626748	6.5134540541
H15	1.1190711854	11.5664349986	7.9396965060
H16	1.6049940810	6.8018146704	7.4845457922
H17	3.0228776255	6.2320901710	6.5647265668
H18	0.5956306303	12.8558426898	6.8439260647
H19	2.3351693305	12.5432448127	7.0575736227
H20	1.4061208766	5.5001089857	6.3043941574
O21	-6.4540725429	8.3601909283	4.7564287620
O22	-2.7500652853	7.0978310181	4.0762238009
O23	-6.6471990251	6.4059218248	5.9083173765
O24	-1.1978082464	8.0985972341	2.7626745096
C25	-2.1318297532	7.2430596648	2.9885637235
C26	-7.1039383322	7.3133679994	5.1794837697
C27	-2.4995368052	6.3842170675	1.7865083552
C28	-8.5488631229	7.2962899929	4.6948277366
H29	-3.0637261396	7.0085710093	1.0727312783
H30	-8.5766161971	7.3240787155	3.5914285800
H31	-9.0639193644	6.3997445146	5.0568611424
H32	-1.5927897025	6.0247124813	1.2757515327
H33	-3.1227045920	5.5396486560	2.0996991235
H34	-9.0685570660	8.1978255719	5.0603380738
H35	0.8808960667	11.6412261553	2.8404187353
H36	1.0175275058	10.6076907477	1.3387570021
H37	1.3493242988	8.4822385006	1.2469044423
H38	1.4055222645	7.3757848377	2.6972635019
H39	3.5066399026	10.9425143677	1.3194829860
H40	3.3743285319	11.9809692658	2.8329905452

H41	3.9089994203	7.6293412980	2.7947039462
H42	3.8462005681	8.7389940241	1.3285252690
X43	2.6383999998#	10.9009500003#	3.4390499999#
X44	2.5943000001#	8.1144000002#	2.5217500000#
X45	2.7922575448#	10.0919381090#	2.0484747992#
X46	2.4395227059#	7.4687465692#	3.6438921038#
Rh47	-3.4792578868	8.9774152992	5.2805366000
C48	-4.4650098059	13.0201106772	7.5693898231
C49	-3.1511388610	12.6564370313	7.2440213518
C50	-2.8865541760	11.4374909954	6.6073402586
C51	-3.9298477346	10.5537582639	6.2733863914
C52	-5.2422414096	10.9232065918	6.6091874276
C53	-5.5092430887	12.1447225199	7.2467785982
H54	-4.6716708285	13.9674620850	8.0656672568
H55	-2.3252944761	13.3236071909	7.4873232018
H56	-1.8590634159	11.1783876529	6.3609686660
H57	-6.0686637919	10.2637665425	6.3556762605
H58	-6.5369804462	12.4115113094	7.4907652938
H59	-5.1218565747	8.4187614737	5.1486880452
C60	-3.9299639421	7.6939896154	6.9114394759
C61	-2.5927257111	8.0635272660	6.9253445427
H62	-4.2504762390	6.7467423450	6.4892187486
H63	-1.8258761172	7.4203794223	6.4987914613
H64	-2.2251376181	8.8382302353	7.5952289633
H65	-4.6485092100	8.1645018879	7.5795879945
X66	-3.3125013660#	7.2712294752#	6.9662537869#
O67	-3.5291686035	10.2070299232	3.4852342156
O68	-1.3580454844	10.8583237403	3.4788417012
C69	-2.5799580026	10.9496316955	3.1154003069
C70	-2.8869803439	12.0964137908	2.1683836242
H71	-2.7152223211	13.0425083742	2.6970158970
H72	-2.2059052005	12.0649191229	1.3108555085
H73	-3.9256713519	12.0554136652	1.8313383672

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