Supporting Information for:

Insights Into Metal-Ligand Hydrogen Transfer: A Square-Planar Ruthenate Complex Supported by a Tetradentate Amino-amido-diolefin Ligand

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Experimental

General Comments

All reactions were carried out under an argon atmosphere using standard Schlenk and glove box techniques unless otherwise stated. $RuCl_2(PPh_3)_3$[1] was synthesized according to a known literature procedure and stored in an argon-filled glove box. (±)trop$_2$dach was synthesized using the same procedure as for enantionpure (*R,R*)-trop$_2$dach[2] except (±)1,2-diaminocyclohexane (dach) was used. Celite, KHMDS, and 18c6, were stored in an argon-filled glove box prior to use. PPh_3 was used as received. THF-d_8 ampoules were opened in an argon-filled glove box and dried over activated 3 Å molecular sieves prior to use. Anhydrous DMSO-d_6 was purchased and stored in an argon-filled glove box prior to use. Solvents were degassed and dried according to standard procedures.[3]

Solution state NMR spectroscopic data were collected using a Bruker 400 MHz (operating at 400 MHz for ^{1}H, 101 MHz for ^{13}C), Bruker 500 MHz (operating at 500 MHz for ^{1}H, 126 MHz for ^{13}C), Agilent 600 MHz (operating at 500 MHz for ^{1}H) or Agilent 700 MHz equipped with an Agilent HC XSens cryogenically-cooled probe. (operating at 176 MHz for ^{13}C). ^{1}H and ^{13}C NMR samples were referenced to their respective residual solvent peaks[4] and ^{31}P spectra were referenced to an external sample of 85% H_3PO_4 (0 ppm). Data was collected at 298 K. Coupling constant J values are given in Hz. All spectral data was processed using MNova 10.0.

CP/MAS solid-state NMR spectra were collected on a 16.45 T Agilent DD2 700 spectrometer (operating at 283 MHz for ^{31}P, 176 MHz for ^{13}C at MAS rates of 18 kHz) equipped with a 1.6 mm Double Resonance T3-HX MAS Solids Balun Probe. ^{31}P chemical shifts were referenced to an external sample of 85% H_3PO_4 (0 ppm) and ^{13}C chemical shifts were externally referenced to 43.67 ppm using glycine powder. The sample was ground to a fine powder and packed into 1.6 mm OD zirconia rotor. All spectral data was processed using MNova 10.0.

IR data were collected on a Perkin-Elmer Spectrum One FTIR spectrometer, UV-vis data were collected on a Hewlett-Packard Agilent 8453 UV-vis spectrophotometer, and EA data were collected on a Thermo Instruments Flash 2000 CHN analyzer. Although all precautions were taken to exclude air and moisture during EA sample preparation, combustion analysis of **4** consistently produced a lower than expected carbon value.

Single-crystal X-ray diffraction data were collected at 100 K using a Bruker APEX-II CCD or at 147 K using a Bruker APEX-DUO CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å). The structures were solved and refined using ShelXL-2013.[5] Refinement was by full-matrix least-squares on F^2 using all data.

Ru_2Cl_4(trop$_2$dach)$(PPh_3)_2$ (1)

In an argon-filled glove box, $RuCl_2(PPh_3)_3$, (974 mg, 1.02 mmol, 2 equiv.), (±)trop$_2$dach (377 mg, 0.762 mmol, 1.5 equiv.), PPh_3 (400 mg, 1.52 mmol, 3 equiv.), and a Teflon-

coated stir bar were combined in a Schlenk flask. THF (30 mL) was added via syringe and the solution was refluxed under argon with vigorous stirring for 24 h. In air, the precipitate was isolated on a medium-pore glass frit, washed with THF (20 mL), Et_2O (20 mL), and then dried under high vacuum overnight to afford the analytically pure **1** as a pale pink solid (573 mg, 83% based on Ru). Note: without excess PPh_3 present during synthesis, the resulting product was not analytically pure. In ethereal solvents such as THF or DME, there was always PPh_3=O present in the washings during workup, even though all precautions were taken to exclude air and moisture. The addition of excess (±)trop$_2$dach increased product yield without compromising purity. The product is air and moisture stable and insoluble in common organic solvents. X-ray quality crystals were obtained by reacting enantiopure (*S,S*)-trop$_2$dach with $RuCl_2(PPh_3)_2$ in DME in an NMR tube under argon without stirring at 60 °C, after which pink needle-shaped crystals formed. EA Found: C 63.3, H 4.9, N 2.0. Calc. for $C_{72}H_{64}Cl_4N_2P_2Ru_2$: C 63.4, H 4.7, N 2.05%. Solid-state CP/MAS NMR: δC{^{1}H} (18 kHz) 141.4–127.9 (C_{ar}, C_{quat}), 92.4-61.9 (CH_{olef}, CH_{dach}, CH_{benzyl}), 39.9-25.3 (CH_2, overlapping with spinning sideband). δP{^{1}H} (18 kHz) 59.6–48.1 (PPh_3). ^{1}H NMR did not reveal any resolved signals. mp 275-277 °C (dec). IR (KBr): ν_{max} (cm^{-1}) 3214w (NH), 3055m, 2988s, 2932m, 2849w, 1484s, 1435s, 1090s, 742s, 697s.

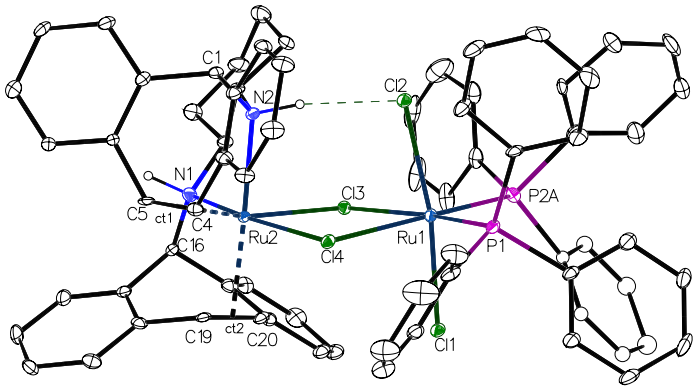


Figure S1. Molecular Structure of (*S,S*)-**1** with 30% probablility ellipsoids. Most hydrogen atoms have been omitted for clarity. Distances (Å), angles (°), and torsions (°): Ru1–P1 2.282(2), Ru1–P2A 2.23(1), Ru1–Cl1 2.421(1), Ru1–Cl2 2.434(1), Ru1–Cl3 2.504(1), Ru1–Cl4 2.477(1), Ru2–Cl3 2.460(1), Ru2–Cl4 2.432(1), Cl2···H2 2.213, Ru2–N1 2.123(5), Ru2–N2 2.135(5), Ru2–ct1 2.127(4), Ru2–ct2 2.136(6), C4–C5 1.412(7), C19–C20 1.373(6); P1-Ru1-P2A 95.5(4), Cl1-Ru1-Cl2 168.96(5), N1-Ru2-N2 80.1(2), ct1-Ru2-ct2 99.0(2); C4-C5-C19-C20 -74.8(5).

The ruthenium atoms are bridged by two chloride ligands and both metals conform to a distorted octahedral geometry. The bridging chlorine atoms, Cl1 and Cl2, respectively, are slightly closer to Ru2 (2.460(1) and 2.432(1) Å) versus Ru1 (2.504(1) and 2.477(1) Å). Atom Cl2 is canted towards the H atom connected to N2 (Cl2···H2 = 2.213 Å) making the Cl1-Ru1-Cl2 angle acute (168.96(5)°). The trop$_2$dach ligand is bonded in a tetradentate fashion to the metal and possesses long Ru-centroid bonds (Ru2–ct1 = 2.127(4), Ru2–ct2 = 2.136(6) Å), which may be due to the strained non-planar coordination geometry of the trop$_2$dach ligand. In fact, this is the first instance of a

structurally characterized trop$_2$(diamine) complex where its tetradentate binding mode is not planar; otherwise trop$_2$(diamine) ligands typically bind κ^3, leaving one trop unit uncoordinated.[2, 6] The dihedral angle generated between the olefin ligands (C4-C5 and C19-C20) are approaching orthogonality (-74.8(5)°).

Ru^0(trop2dach) (2)

Complex **1** (250 mg, 0.183 mmol) and KHMDS (146 mg, 0.734 mmol), THF (10 mL), and a Teflon-coated stir bar were combined in a 100 mL Schlenk tube fitted with a Teflon screw valve. The argon atmosphere was removed via two freeze-pump-thaw cycles and replaced with H_2 (1 atm, ultra high purity). The flask was sealed and vigorously stirred at 60 °C for 1 h. The H_2 atmosphere was replaced with argon via two freeze-pump-thaw cycles and taken into an argon-filled glove box. The deep brown-orange solution was then filtered through a pad of Celite on a medium-pore glass frit to remove any salts. The Celite pad was washed with 20 mL THF and the filtrate was dried under high vacuum. About 50 mL hexanes was added to the brown residue and the solution was stirred vigorously until the residue became a fine powder (about 2 h). The solid was isolated on a medium-pore glass frit, washed with 20 mL hexanes, and dried under vacuum. The dark reddish-pink filtrate contains $RuH_6(PPh_3)_2$[7-9] (sample spectra provided below; hydride and phosphorus chemical shifts may vary during different reactions due to the highly reactive nature of these species in solution) and other aromatic products while the brown powder is predominantly complex **2** (108 mg, see spectra). The product could not be made analytically pure due to the persistence of soluble aromatic- and/or polyhydride-containing byproducts. Complex **2** is soluble in ethereal and aromatic hydrocarbon solvents, but decomposes in acetonitrile, DMSO, chlorinated solvents, and alcohols. Attempts at large scale crystallizations failed due to the highly sensitive nature of **2**, which slowly decomposes over the course of several weeks in solution or the solid state. Mass spectral analysis was unsuccessful after several attempts due to the air and moisture sensitivity of **2**. X-ray quality crystals were grown by slow evaporation of **2** from a concentrated THF solution. NMR: δH (500 MHz; THF-d_8) 7.44 (2 H, m; CH_{ar}), 7.35 (2 H, m; CH_{ar}), 7.06 (m, 2H; CH_{ar}), 7.02 (m, 2H; CH_{ar}), 6.93 (m, 4H; CH_{ar}), 6.85 (m, 4H; CH_{ar}), 4.83 (s, 2H; CH_{benzyl}), 4.70 (d, ^{3}J(H,H) = 11.2 Hz, 2H; NH), 2.59 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 2.51 (m, 2H; CH_2), 1.99 (m, 2H; CH_{dach}), 1.69 (m, 2H; CH_2), 1.60 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 1.10-1.00 (m, 4H; CH_2). δH (500 MHz; C_6D_6) 7.83 (m, 2H; CH_{ar}), 7.64 (m, 2H; CH_{ar}), 7.21 (m, 2H; CH_{ar}), 7.04-6.83 (m, 8H; CH_{ar}), 6.72 (m, 2H; CH_{ar}), 4.46 (s, 2H; CH_{benzyl}), 3.18 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 2.49 (d, ^{3}J(H,H) = 11.9 Hz, 2H; NH), 2.21 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 1.74 (m, 2H; CH_2), 1.24 (m, 2H; CH_{dach}), 1.13 (m, 2H; CH_2), 0.42 (m, 2H; CH_2), -0.55 (m, 2H; CH_2). δC{^{1}H} (126 MHz; THF-d_8) 150.64 (C_{quat}), 148.49 (C_{quat}), 136.85 (C_{quat}), 136.62 (C_{quat}), 130.05 (C_{ar}), 128.97 (C_{ar}), 128.63 (C_{ar}), 128.27 (C_{ar}), 128.22 (C_{ar}), 127.18 (C_{ar}), 122.84 (C_{ar}), 121.70 (C_{ar}), 65.26 (CH_{benzyl}), 61.92 (CH_{dach}), 60.17 (C_{olef}), 50.09 (C_{olef}), 30.24 (CH_2), 25.63 (CH_2). δC{^{1}H} (126 MHz; C_6D_6) 150.27 (C_{quat}), 148.04 (C_{quat}), 135.70 (C_{quat}), 135.38 (C_{quat}), 129.94 (C_{ar}), 129.69 (C_{ar}), 129.16 (C_{ar}), 129.04 (C_{ar}), 128.47 (C_{ar}), 127.79 (C_{ar}), 123.13 (C_{ar}), 121.91 (C_{ar}), 65.48 (CH_{benzyl}), 60.81 CH_{dach}), 60.40 (C_{olef}), 50.27 (C_{olef}), 29.74 (CH_2), 24.36 (CH_2). IR (KBr): ν_{max} (cm^{-1}) 3194w (NH), 3053w, 3012w, 2931s, 2857m, 1891br, 1595m, 1482s, 1457s, 1434s, 1090m, 751s 696m. UV-vis: λ_{max}(THF)/nm 401 (ε/dm^3 mol^{-1} cm^{-1} 5600) and 806 (1800).

$[K]_2$[Ru(trop$_2$dach-2H)] (3)

In an argon-filled glove box, compound **2** (0.017 mmol, 10 mg) and KHMDS (0.034 mmol, 6 mg) were combined in a J. Young NMR tube. The mixture was dissolved in THF-d_8, heated to 65 °C for 30 min and the deep orange solution was then investigated by NMR spectroscopy. The major product **3** was not isolated. NMR: δH (400 MHz; THF-d_8) 7.27 (d, ^{3}J(H,H) = 7.0 Hz, 2H; CH_{ar}), 7.12 (d, ^{3}J(H,H) = 7.3 Hz, 2H; CH_{ar}), 6.93 (d, ^{3}J(H,H) = 7.2 Hz, 4H; CH_{ar}), 6.75 (d, ^{3}J(H,H) = 7.1 Hz, 2H; CH_{ar}), 6.63 (m, 4H; CH_{ar}), 6.56 (d, 2H; CH_{ar}), 4.83 (s, 2H; CH_{benzyl}), 2.49 (m, 2H; CH_2), 2.25 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 2.09 (m, 2H; CH_{dach}), 1.59 (m, 2H; CH_2), 1.32 (d, ^{3}J(H,H) = 8.0 Hz, 2H; CH_{olef}), 1.12 (m, 2H; CH_2), 0.65 (m, 2H; CH_2), 0.00 (br, HMDS). δC{^{1}H} (101 MHz; THF-d_8) 152.74 (C_{quat}), 152.32 (C_{quat}), 148.17 (C_{quat}), 144.47 (C_{quat}), 127.40 (C_{ar}), 127.29 (C_{ar}), 126.35 (C_{ar}), 126.02 (C_{ar}), 125.94 (C_{ar}), 123.68 (C_{ar}), 119.47 (C_{ar}), 118.86 (C_{ar}), 74.14 CH_{dach}), 70.32 (CH_{benzyl}), 55.85 (C_{olef}), 51.47 (C_{olef}), 32.35 ($CH_{2(dach)}$), 27.07 ($CH_{2(dach)}$).

[K(18c6·THF)][Ru(trop$_2$dach-H)]·THF (4)

In an argon-filled glove box, compound **2** (50 mg, 0.084 mmol) and KHMDS (33mg, 0.17 mmol), THF (4mL), and a Teflon-coated stir bar were combined in a Schlenk tube fitted with a Teflon screw valve. The flask was sealed, removed from the glove box, and heated at 65 °C for 30 min and then the deep orange solution was cooled to -78 °C. Under a dynamic flow of argon, a solution of 18-crown-6 (44 mg, 0.17 mmol) dissolved in 4 mL Et_2O was slowly layered onto the solution via syringe. The flask was sealed, removed from the cold bath, and left undisturbed overnight at room temperature, after which large black needles formed (which were also suitable for X-ray diffraction). The deep orange solution was decanted, and the remaining crystals were washed with Et_2O (about 3 mL), and dried under high vacuum to afford **4** (25 mg, 29 %). The complex is insoluble in THF and hydrocarbon solvents and decomposes in pure DMSO, however **4** is soluble and stable when DMSO is added to a THF solution containing the crystals. Mass spectral analysis was unsuccessful after several attempts due to the air and moisture sensitivity of **4**. EA attempts on independent batches of crystals resulted in consistently low carbon percentages during combustion analysis. EA Found: C 62.85, H 6.9, N 2.5. Calc. for $C_{48}H_{57}N_2O_6KRu{\cdot}2C_4H_8O$: C 64.5, H 7.1, N 2.7%. NMR: δH (600 MHz; 4:1 THF-d_8:DMSO-d_6) 7.22 (d, ^{3}J(H,H) = 7.0 Hz, 1H; CH_{ar}), 7.17 (m, 2H; CH_{ar}), 7.11 (d, ^{3}J(H,H) = 7.7 Hz, 1H; CH_{ar}), 6.90 (d, ^{3}J(H,H) = 7.0 Hz, 1H; CH_{ar}), 6.82 (m, 1H; CH_{ar}), 6.78-6.75 (m, 4H; CH_{ar}), 6.71 (m, 1H; CH_{ar}), 6.65-6.59 (m, 3H; CH_{ar}), 6.56-6.53 (m, 2H; CH_{ar}), 4.92 (s, 1H; CH_{benzyl}), 4.66 (s, 1H; CH_{benzyl}), 3.62 (m, 8H; $CH_{2(THF)}$), 3.56 (m, 24H; $CH_{2(18c6)}$), 3.08 (m, 1H; CH_{dach}), 2.57 (d, ^{3}J(H,H) = 8 Hz, 1H; CH_{olef}, *coupled to CH_{olef} @ 1.32*), 2.44 (br, partly buried under residual DMSO signal, 1H; $CH_{2(dach)}$), 2.22 (d, ^{3}J(H,H) = 8 Hz, 1H; CH_{olef}, *coupled to CH_{olef} @ 0.93*), 2.18 (m, 1H; $CH_{2(dach)}$), 1.78 (m, 8H; $CH_{2(THF)}$); 1.59 (br m, 1H; $CH_{2(dach)}$), 1.55 (br m, 1H; $CH_{2(dach)}$), 1.45 (m, 1H; CH_{dach}), 1.32 (d, ^{3}J(H,H) = 8 Hz, 1H; CH_{olef}, *coupled to CH_{olef} @ 2.57*), 1.15-1.09 (m, 2H; CH_{dach}), 0.93 (d, ^{3}J(H,H) = 8 Hz, 1H; CH_{olef}, *coupled to CH_{olef} @ 2.22*), 0.91 (m, 1H; CH_{dach}), 0.57 (m, 1H; CH_{dach}). δC{^{1}H}(176 MHz; 4:1 THF-d_8:DMSO-d_6) 155.75 (C_{quat}),

152.93 (C_{quat}), 152.46 (C_{quat}), 151.77 (C_{quat}), 150.04 (C_{quat}), 145.81 (C_{quat}), 137.51 (C_{quat}), 135.34 (C_{quat}), 129.69 (C_{ar}), 128.55 (C_{ar}), 128.28 (C_{ar}), 127.59 (C_{ar}), 127.06 (C_{ar}), 126.92 (C_{ar}), 126.12 (C_{ar}), 126.11 (C_{ar}), 126.08 (C_{ar}), 125.96 (C_{ar}), 125.34 (C_{ar}), 125.09 (C_{ar}), 120.19 (C_{ar}), 119.02 (C_{ar}), 118.94 (C_{ar}), 118.50 (C_{ar}), 71.89 (CH_{dach}), 70.78 ($C_{(18c6)}$), 69.34 (C_{benzyl}), 68.03 (C_{THF}) 65.55 (C_{benzyl}), 64.69 (CH_{dach}), 58.55 (C_{olef}), 54.80 (C_{olef}), 54.35 (C_{olef}), 48.95 (C_{olef}), 32.95 ($CH_{2(dach)}$), 29.47 ($CH_{2(dach)}$), 26.57 ($CH_{2(dach)}$), 26.17 (C_{THF}), 25.99 ($CH_{2(dach)}$). IR (KBr): ν_{max} (cm^{-1}) 3054w, 3053w, 2911br, 1591w, 1476m, 1452m, 1351m, 1285w, 1250w, 1108s, 961m, 749m. UV-vis: λ_{max}(4:1 THF:DMSO)/nm 400 (ε/dm^3 mol^{-1} cm^{-1} 5700) and 570 (900).

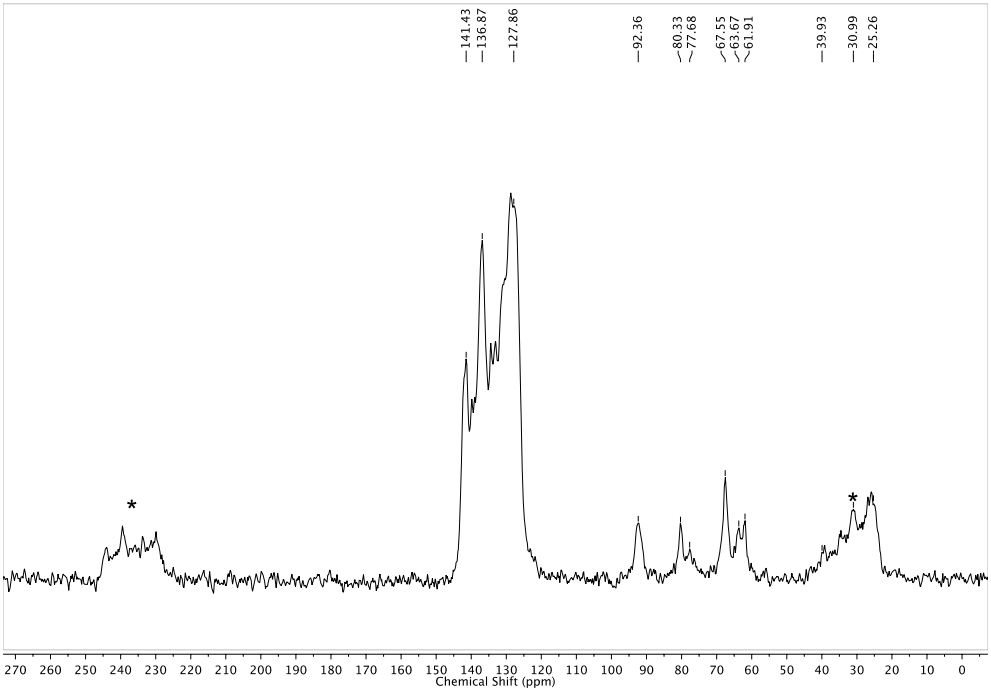


Figure S2. CP/MAS ^{13}C NMR (176 MHz, MAS rate = 18 kHz) of **1**. * = spinning sidebands.

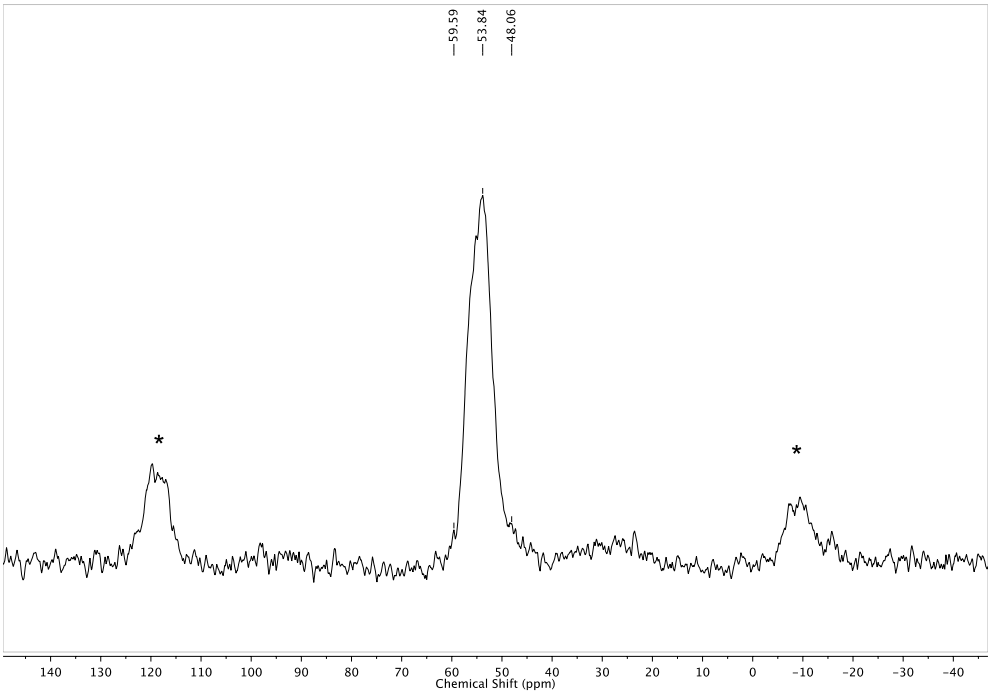


Figure S3. CP/MAS ^{31}P NMR (283 MHz, MAS rate = 18 kHz) of **1**. * = spinning sidebands.

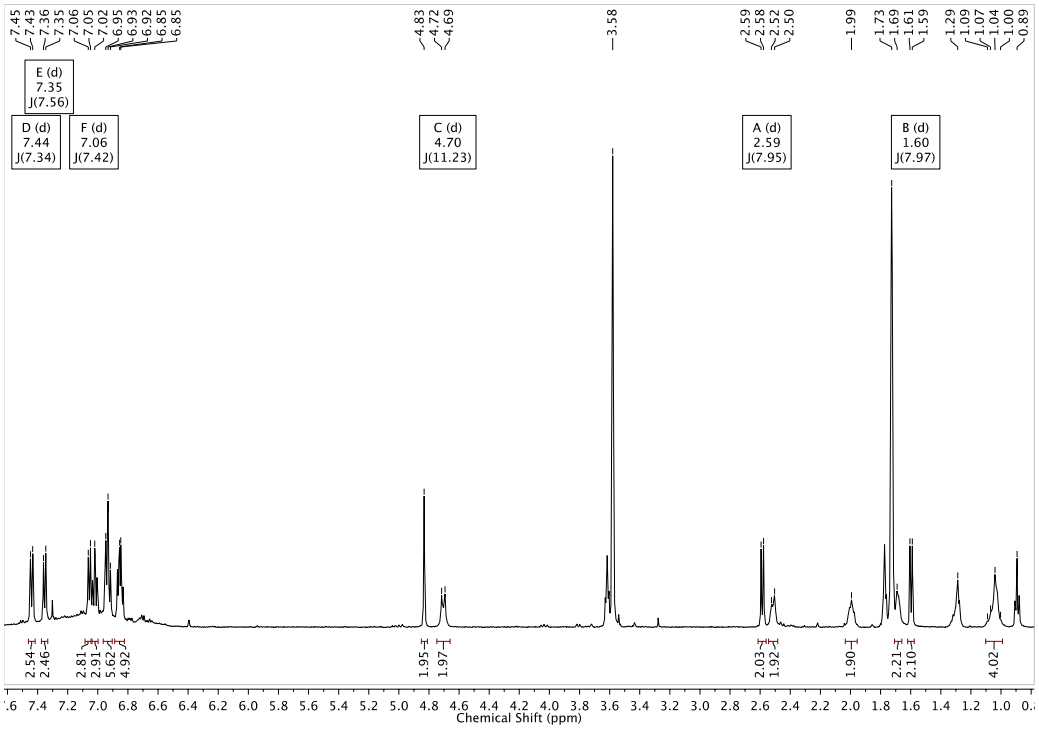


Figure S4. ^{1}H NMR (500 MHz; THF-d_8) of **2**.

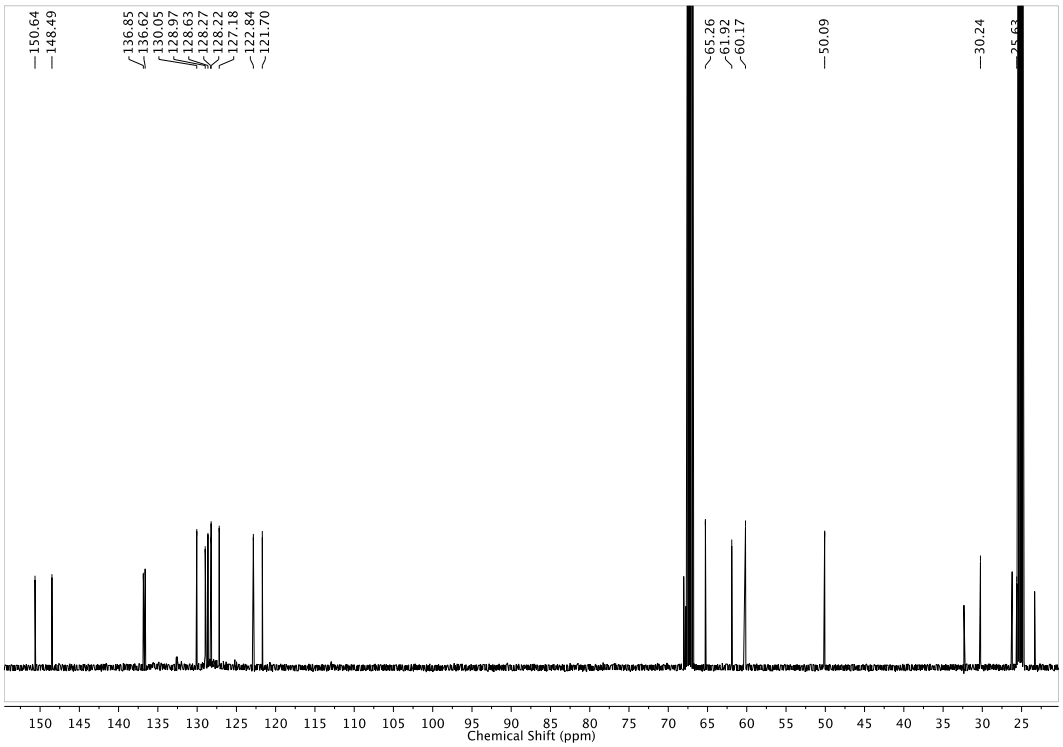


Figure S5. ^{13}C NMR (126 MHz; THF-d_8) of **2**.

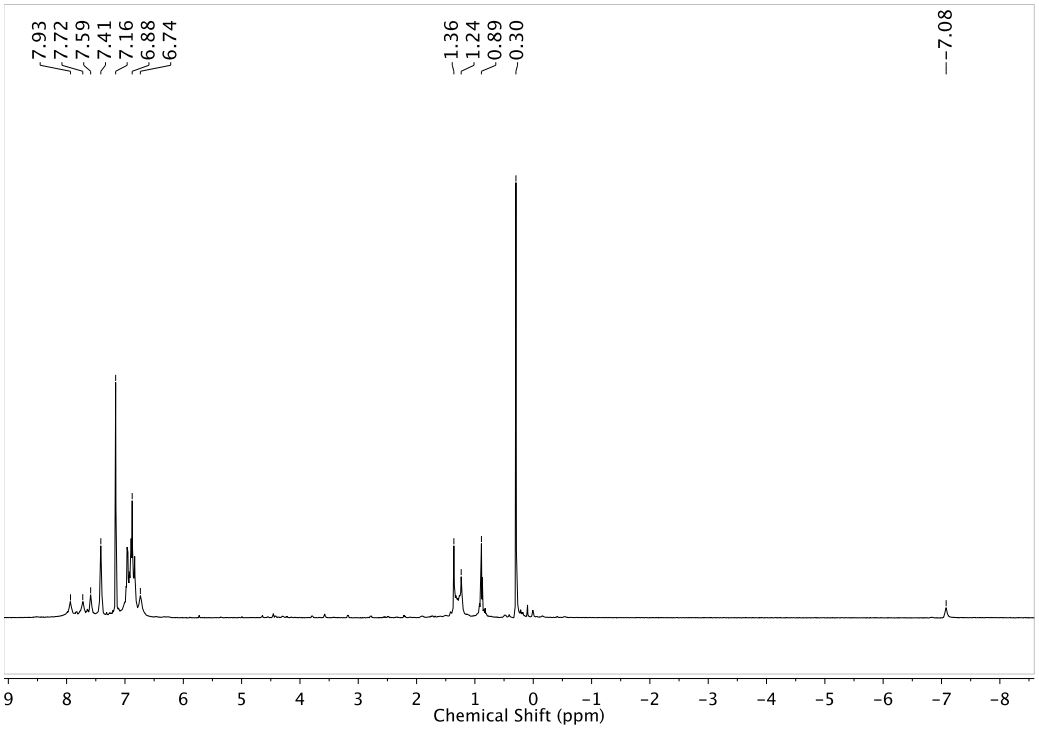


Figure S6. ^{1}H NMR (500 MHz; C_6D_6) of filtrate during workup of **2**.

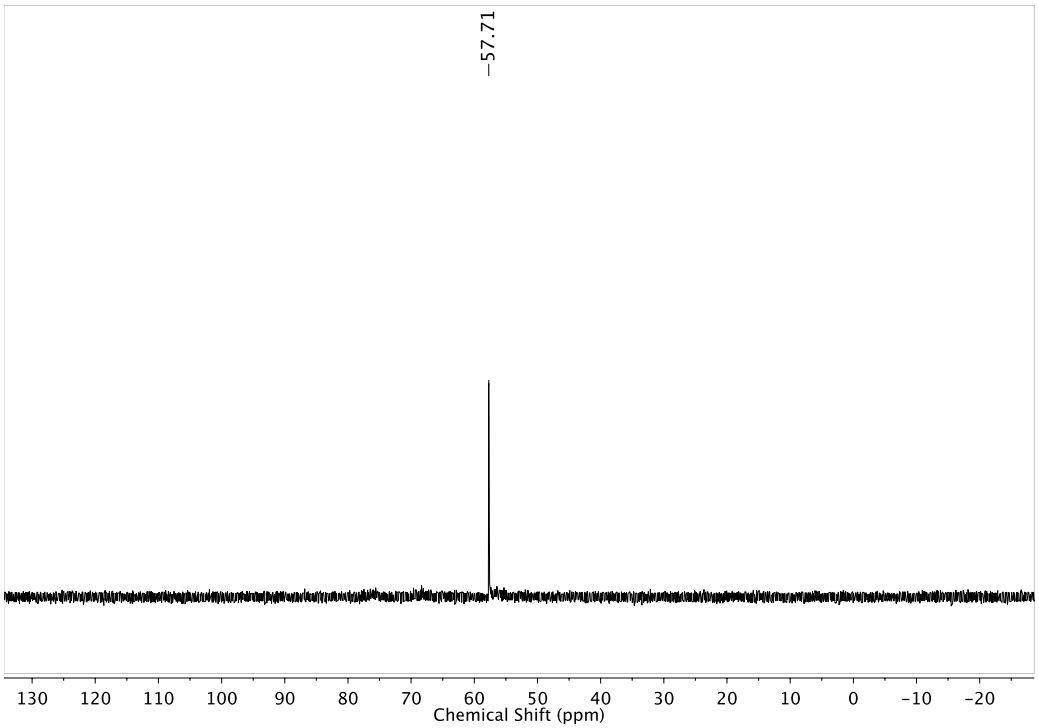


Figure S7. ^{31}P NMR (203 MHz; C_6D_6) of filtrate during workup of **2**.

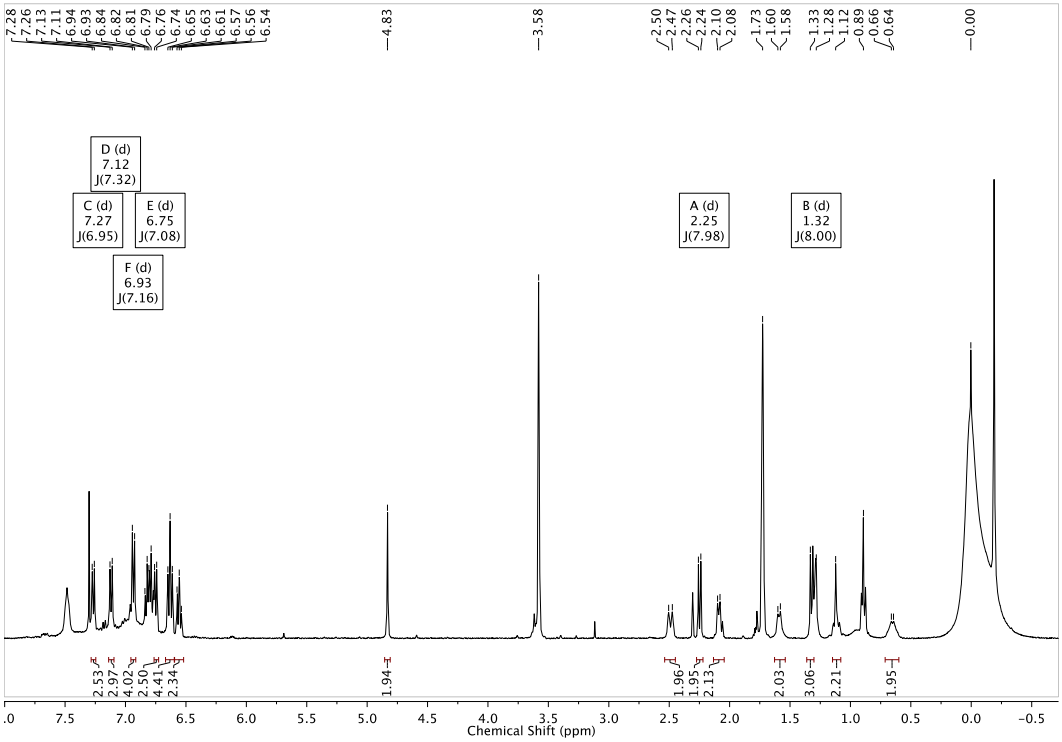


Figure S8. ^{1}H NMR (400 MHz; THF-d_8) of **3**.

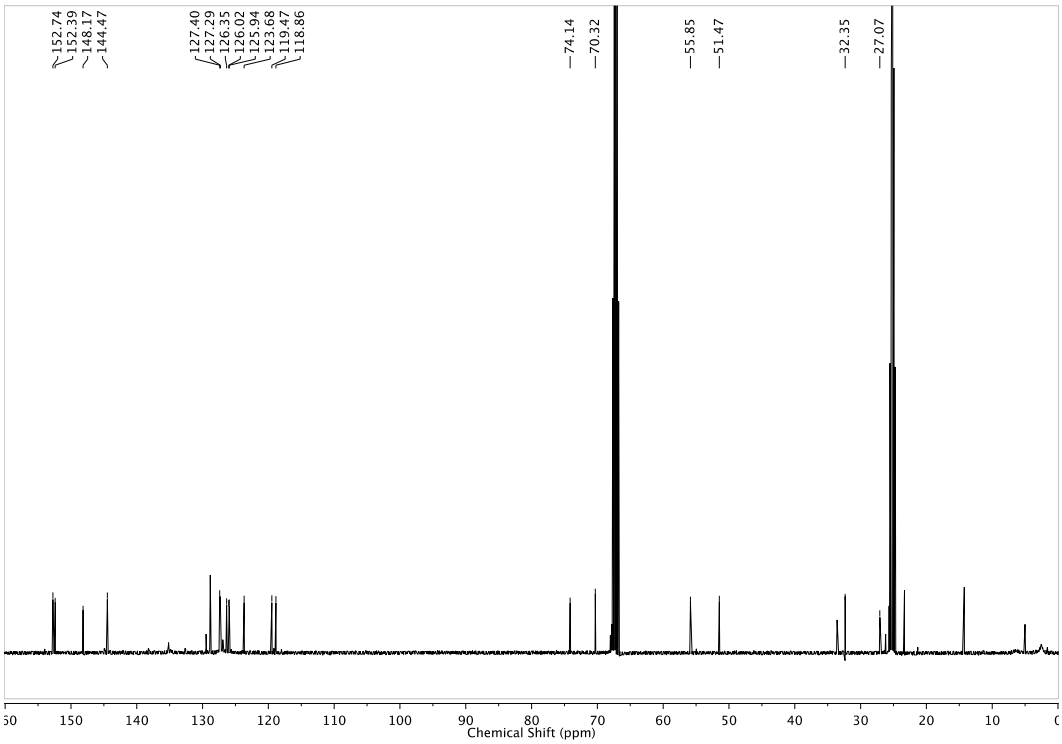


Figure S9. ^{13}C NMR (101 MHz; THF-d_8) of **3**.

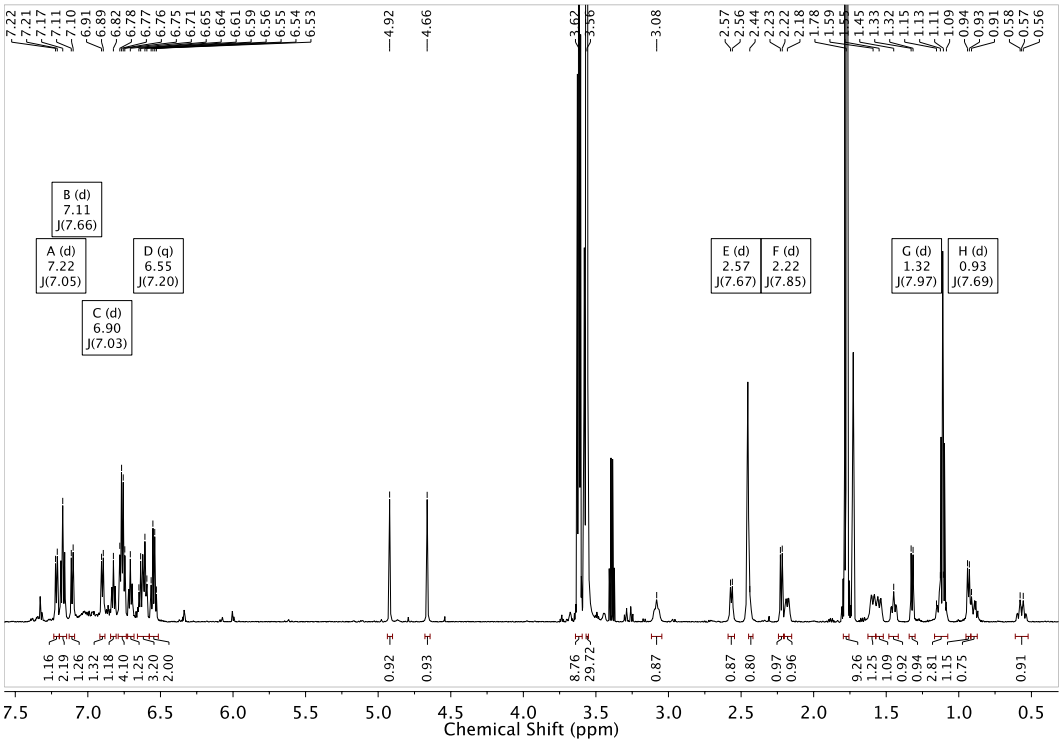


Figure S10. ^{1}H NMR (600 MHz; 4:1 THF-d_8:DMSO-d_6) of **4**.

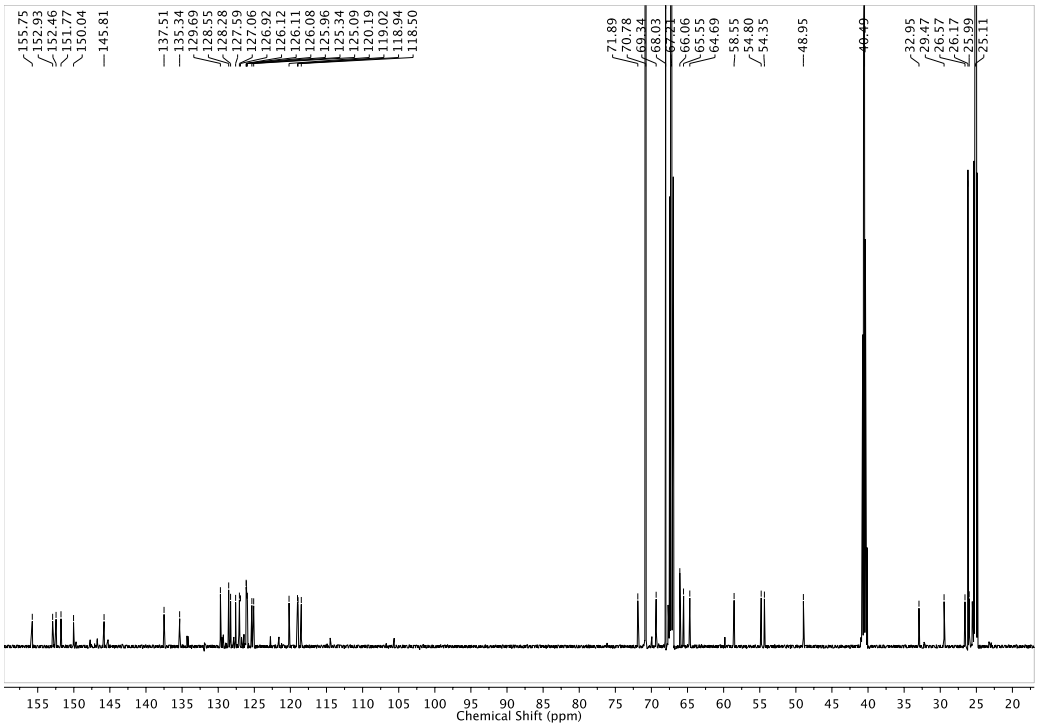


Figure S11. ^{13}C NMR (176 MHz; 4:1 THF-d_8:DMSO-d_6) of **4**.

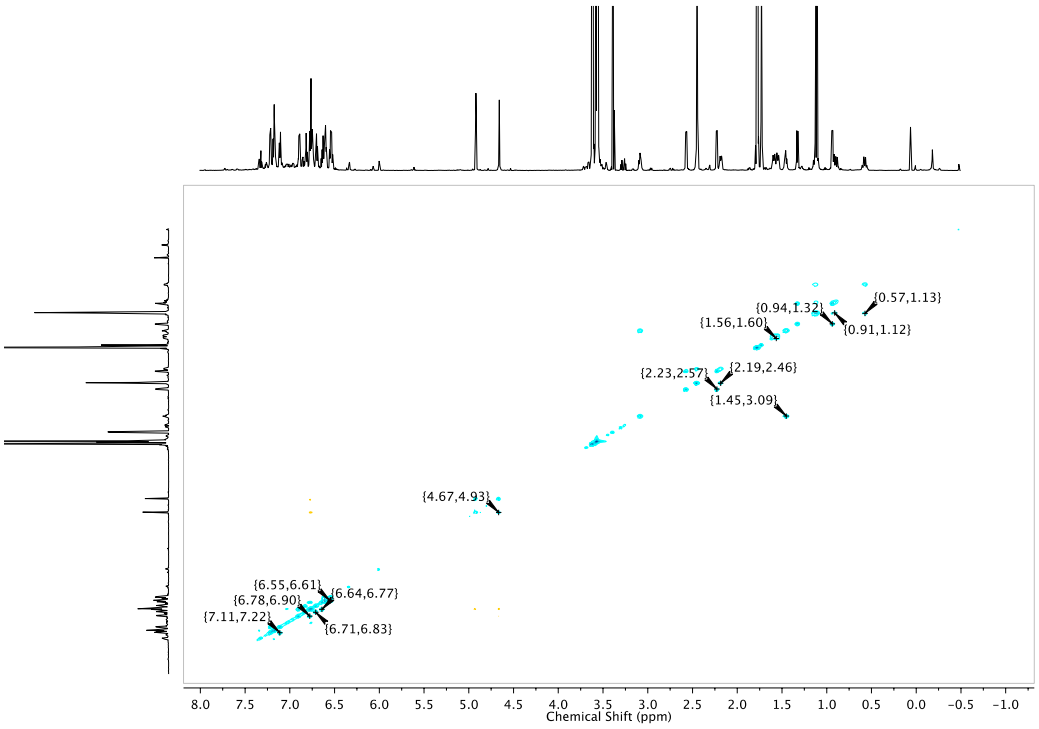


Figure S12. ^{1}H-^{1}H EXSY (600 MHz; 4:1 THF-d_8:DMSO-d_6) of **4** (600 ms mixing time, 1 s relaxation delay).

Table S1. Calculation of rate constants[10, 11] on going from **4**-**5** measured from ^{1}H-^{1}H EXSY peak intensities of **4**.

Proton Assignment	Chemical Shifts (ppm)	Diagonal Peak to Cross Peak Intensity Ratio (r)	Rate constant k (s^{-1})	Free Energy (kcal·mol^{-1})
CH_{ar}	6.71, 6.83	1.83	2.0	17.0
CH_{benzyl}	4.67, 4.93	1.43	2.9	16.8
CH_{dach}	1.45, 3.09	1.58	2.5	16.9
CH_{olef}	2.23, 2.57	1.41	3.0	16.8
CH_{olef}	0.94, 1.32	1.43	2.9	16.8

From the above data, $\boldsymbol{k_{avg}}$ **= 2.7 ± 0.4 s^{-1};** $\boldsymbol{\Delta G^{\ddagger}}$ **= 16.9 ± 0.1 kcal/mol**

$k = (1/t_m)\ln((r + 1)/(r - 1))$, where t_m = mixing time (600 ms)

$\Delta G^{\ddagger} = -RT\ln(hk/k_BT)$, where R = gas constant, T = temperature (298 K), h = Planck's constant, k_B = Boltzmann's constant.

Table S2. Comparison of NMR η^2-olefin chemical shift data for complexes **A** (Rh/Ir),[2, 12] **B** (Rh/Ir),[2, 12] **2**, and **4**.

Complex	η^2-olefin ^{1}H (ppm)	η^2-olefin ^{13}C (ppm)
A (Rh)	5.4, 4.2	83, 70
A (Ir)	4.8, 4.0	60, 53
2	**2.6, 1.6**	**60, 50**
B (Rh)	4.8, 4.3, 3.5, 3.0	81, 71, 67, 67
B (Ir)	4.1, 3.5, 3.3, 2.7	63, 55, 51, 48
4	**2.6, 2.2, 1.3, 0.9**	**64, 58, 54, 48**

DFT Calculations

Closed-shell DFT calculations were performed using Gaussian 09 (Rev. D.01)[13] at the M06[14]/TZVP[15]/TZVPfit level of theory with QZVP[16] on ruthenium. Either normal (opt) or tight (opt = tight) convergence criteria were used for all optimizations, and a pruned (99,590) integration grid was used throughout (grid = ultrafine). Optimizations were performed in a tetrahydrofuran solvent continuum using the integral equation formalism polarizable continuum model (IEF-PCM)[17] with radii and non-electrostatic terms from the SMD solvation model (scrf = smd).[18] Full vibrational and thermochemical analyses (1 atm, 298 K) were performed on optimized structures to obtain solvent-corrected free energies ($G°$) and enthalpies ($H°$). Optimized ground states have zero imaginary frequencies while transition states have one imaginary frequency. Transition states $\mathbf{TS_{4,5}}$ and $\mathbf{TS_{5,6}}$ were connected to their ground state geometries by performing intrinsic reaction coordinate (IRC) calculations in the forward and reverse directions.[19] Calculations were performed by the facilities of the Shared Hierarchical Academic Research Computing Network (SHARCNET) and Compute/Calcul Canada.[20]

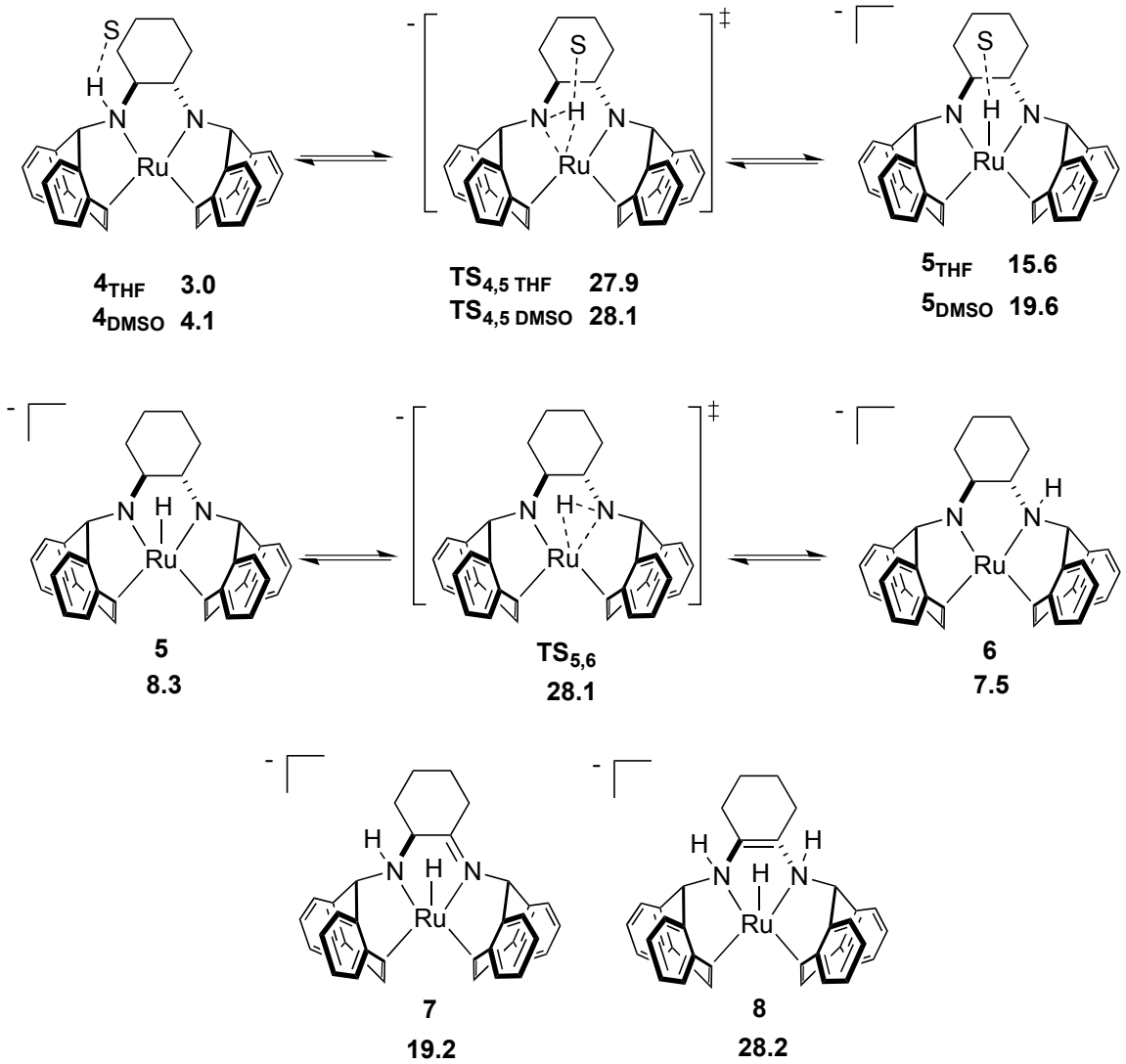
Table S2**.** Selected experimental and calculated metrical parameters for complex **2**.

Parameter	Experimental	Calculated
	Length (Å) or Angle (°)	
Ru1–N1	2.131(4)	2.170
Ru1–N2	2.129(3)	2.165
Ru1–ct1	1.980(4)	1.979
Ru1–ct2	1.973(5)	1.982
C4–C5	1.423(7)	1.436
C19–C20	1.435(7)	1.434
N1–Ru1-N2	82.0(2)	80.74
ct1-Ru1-ct2	98.30(2)	98.37
N1-Ru1-ct2	91.38(2)	92.62
N2-Ru1-ct1	92.18(2)	89.54
N1-Ru1-ct1	163.51(2)	161.28
N2-Ru1-ct2	162.37(2)	162.78

Table S3**.** Selected experimental and calculated metrical parameters for complex **4**.

Parameter	Experimental	Calculated
	Length (Å) or Angle (°)	
Ru1–N1	2.091(5)	2.181
Ru1–N2	1.995(4)	1.993
Ru1–ct1	1.992(4)	1.973

Ru1–ct2	1.997(3)	1.995
C7–C8	1.445(5)	1.449
C22–C23	1.435(5)	1.448
N1–Ru1-N2	80.2(2)	80.64
ct1-Ru1-ct2	98.73(2)	98.90
N1-Ru1-ct2	90.90(2)	91.69
N2-Ru1-ct1	90.98(2)	92.16
N1-Ru1-ct1	167.65(2)	156.73
N2-Ru1-ct2	169.07(2)	166.84



Scheme S1. Additional calculated structures with free energies relative to **4** (see main text). Energies are presented in kcal/mol.

Solvent-Corrected Free Energies (*G°*, Hartree), Solvent-Corrected Enthalpies (*H°*, Hartree), TS imaginary Frequencies (cm^{-1}), and Cartesian Coordinates (Å) of Optimized Structures

THF

H° = -232.248922

G° = -232.282908

C	-4.76876	1.11385	-0.17567
O	-3.58072	1.89170	-0.05298
C	-2.46290	1.02554	0.11148
C	-4.38608	-0.30899	0.18241
H	-5.13554	1.17212	-1.21027
H	-5.54071	1.53306	0.47681
C	-2.94043	-0.35496	-0.28814
H	-5.02853	-1.05042	-0.29391
H	-4.43375	-0.45762	1.26574
H	-2.89940	-0.47283	-1.37561
H	-2.35412	-1.15361	0.16775
H	-2.13909	1.03482	1.16271
H	-1.63393	1.39668	-0.49782

DMSO

H° = -553.055537

G° = -553.091188

S	0.00000	0.23039	-0.45464
O	0.00000	1.49414	0.39383
C	1.34852	-0.80559	0.18858
C	-1.34852	-0.80559	0.18858
H	1.22232	-0.91451	1.26725
H	-2.28554	-0.29399	-0.02990
H	1.33484	-1.77766	-0.30705
H	2.28554	-0.29399	-0.02990
H	-1.33484	-1.77766	-0.30705
H	-1.22232	-0.91451	1.26725

2

H° = -1595.494218

G° = -1595.58409

Ru	-0.00881	0.09351	-0.64424
N	1.35398	0.19871	1.03495
H	1.32652	1.19061	1.28404
N	-1.36415	-0.49921	0.94312
H	-1.36665	-1.51948	0.87703
C	-1.40416	1.15537	-1.74480
H	-0.98305	1.76668	-2.54525
C	0.74511	-0.54346	2.16693
H	0.80407	-1.61598	1.92506
C	-1.58842	-0.23217	-2.05685
H	-1.24050	-0.51250	-3.05407
C	-2.73982	-1.03506	-1.63345
C	-2.18868	1.95098	-0.79182
C	-4.46123	-1.69700	-0.05973
H	-4.91220	-1.59600	0.92357
C	-3.28273	-1.96443	-2.52904
H	-2.82147	-2.06618	-3.50707
C	-4.99374	-2.59397	-0.97086
H	-5.86252	-3.18773	-0.71041
C	1.38689	-0.65757	-1.97424
H	0.95995	-1.05087	-2.89916
C	-2.80241	1.42643	0.36541
C	1.55935	0.76722	-1.93700
H	1.20686	1.28121	-2.83457
C	4.39534	1.73890	0.38531
H	4.85047	1.39706	1.31065
C	3.20705	2.60540	-1.93610
H	2.74274	2.94577	-2.85714
C	-2.27773	3.33202	-1.00276
H	-1.80868	3.74697	-1.89003
C	-0.73648	-0.15449	2.24125
H	-0.79780	0.93886	2.35535
C	3.30572	1.04033	-0.12034
C	-3.46925	2.27797	1.23667
H	-3.93322	1.85497	2.12395
C	2.20998	-1.65730	-1.28023
C	-0.70450	-0.53866	4.72914
H	-0.75550	0.53760	4.94023
H	-1.21452	-1.04468	5.55316
C	-2.75803	-0.04316	0.70184
H	-3.35782	-0.18851	1.60853
C	-4.38709	-2.73245	-2.21000
H	-4.78066	-3.43753	-2.93456
C	2.76111	-0.11742	0.67454
H	3.36891	-0.19653	1.58381
C	-1.41999	-0.82811	3.42109
H	-1.43023	-1.91229	3.23669
H	-2.46339	-0.50570	3.47989
C	-3.34627	-0.92661	-0.36673
C	0.74843	-0.96715	4.65027
H	0.79915	-2.05523	4.51358
H	1.27100	-0.74389	5.58434
C	2.69252	1.45878	-1.31765
C	1.44954	-0.28295	3.48956
H	1.47181	0.80369	3.65819
H	2.48909	-0.61738	3.42782
C	3.04098	-3.94591	-1.24505
H	3.10653	-4.91833	-1.72127
C	2.32460	-2.93010	-1.85138
H	1.83403	-3.11225	-2.80296
C	-3.54645	3.64255	1.00585
H	-4.06595	4.28690	1.70592
C	2.84808	-1.43929	-0.04242
C	-2.94292	4.16822	-0.12504
H	-2.98990	5.23321	-0.32556
C	4.28725	3.29675	-1.41998
H	4.65838	4.17736	-1.93359

C	3.56882	-2.46587	0.55336
H	4.05243	-2.27629	1.50816
C	4.89843	2.85928	-0.25474
H	5.74793	3.39074	0.15879
C	3.67372	-3.71707	-0.03397
H	4.23496	-4.50534	0.45473

4

H° = -1594.998594

G° = -1595.08752

Ru	-0.01066	0.17945	-0.59251
N	-1.24524	-0.59711	0.76628
C	0.80873	-1.07930	1.92847
H	0.88825	-2.01729	1.35859
C	-0.68416	-0.77674	2.09346
H	-0.76000	0.15731	2.70146
C	-1.32248	-1.89423	2.91869
H	-2.38505	-1.68826	3.07554
H	-1.26339	-2.82461	2.33567
C	-0.63436	-2.07067	4.26332
H	-0.77054	-1.15846	4.86019
H	-1.10640	-2.88243	4.82557
C	0.85067	-2.33750	4.09214
H	0.98754	-3.30034	3.58182
H	1.34401	-2.42628	5.06497
C	1.51023	-1.24425	3.26638
H	2.56820	-1.47978	3.11206
H	1.47117	-0.28795	3.80801
C	1.46114	-0.10629	-2.06526
H	1.09300	-0.27788	-3.07975
C	1.49388	1.28117	-1.65005
H	1.10517	1.96876	-2.40832
C	2.57683	1.89033	-0.88051
C	2.99042	3.19455	-1.18871
H	2.49121	3.71069	-2.00413
C	4.01014	3.82835	-0.50266
H	4.29821	4.83766	-0.77907
C	4.66741	3.17257	0.52731
H	5.47109	3.65656	1.07085
C	4.26550	1.88899	0.86296
H	4.75463	1.36915	1.68255
C	3.23589	1.24588	0.18825
C	2.99360	-1.20465	-0.35565
C	3.79779	-2.28421	-0.01390
H	4.26095	-2.29374	0.96985
C	4.01174	-3.34409	-0.88203
H	4.63787	-4.17864	-0.58713
C	3.39842	-3.31935	-2.12524
H	3.54311	-4.13826	-2.82249
C	2.60109	-2.24829	-2.48235
H	2.12672	-2.23604	-3.45966
C	2.37338	-1.16048	-1.62521
C	-1.58565	0.33365	-2.01363
H	-1.26726	0.41846	-3.05789
C	-1.43055	1.54813	-1.24004
H	-1.01396	2.38742	-1.80307
C	-2.35758	2.02122	-0.19657
C	-2.62921	3.38742	-0.09283
H	-2.16667	4.06360	-0.80701
C	-3.46404	3.89684	0.89085
H	-3.64469	4.96557	0.94529
C	-4.06367	3.04007	1.79796
H	-4.71050	3.42622	2.57847
C	-3.81421	1.67582	1.70406
H	-4.27453	0.99144	2.41297
C	-2.97115	1.15881	0.73273
C	-2.68824	-0.61335	-1.84153
C	-3.22395	-1.26198	-2.96073
H	-2.80609	-1.03179	-3.93738
C	-4.26395	-2.17032	-2.85896
H	-4.65067	-2.65095	-3.75207
C	-4.81239	-2.45503	-1.61854
H	-5.62694	-3.16474	-1.52229
C	-4.29116	-1.82850	-0.49470
H	-4.70050	-2.05734	0.48626
C	-3.23897	-0.92800	-0.58085
C	2.79625	-0.11387	0.66603
H	3.42116	-0.36506	1.53350
C	-2.67055	-0.32438	0.68207
H	-3.21829	-0.78424	1.51706
N	1.37691	-0.01199	1.07913
H	1.26949	0.86927	1.58378

4_{THF}

H° = -1827.261289

G° = -1827.365678

Ru	-0.23618	-0.41847	-0.67169
N	-1.46048	-0.28601	0.89358
C	0.53092	-0.82778	2.13023
H	0.32406	-1.89725	1.97156
C	-0.82583	-0.11559	2.18620
H	-0.62415	0.96009	2.40862
C	-1.61347	-0.66702	3.37529
H	-2.58218	-0.16517	3.45343
H	-1.82228	-1.72984	3.18459
C	-0.85060	-0.50501	4.68092
H	-0.71889	0.56543	4.88990
H	-1.43278	-0.91398	5.51290
C	0.51256	-1.17063	4.61022
H	0.37804	-2.25579	4.50606
H	1.06958	-1.01276	5.53910
C	1.31310	-0.65751	3.42313
H	2.26787	-1.19009	3.36195
H	1.54905	0.40761	3.55755
C	0.94124	-1.58999	-1.95093
H	0.43106	-1.99414	-2.82895
C	1.37655	-0.21036	-2.07107
H	1.10002	0.25038	-3.02544
C	2.68227	0.26026	-1.60954
C	3.41379	1.15966	-2.39899
H	2.96886	1.50411	-3.32887
C	4.68199	1.58858	-2.04921

H	5.21626	2.27482	-2.69867
C	5.27359	1.12803	-0.88230
H	6.27148	1.44595	-0.60155
C	4.55276	0.27168	-0.06338
H	4.98630	-0.06932	0.87318
C	3.27179	-0.14974	-0.39502
C	2.28840	-2.41212	0.04471
C	2.78785	-3.48610	0.76883
H	3.32660	-3.28260	1.69130
C	2.60575	-4.79772	0.35619
H	2.99725	-5.61915	0.94578
C	1.90445	-5.03440	-0.81628
H	1.74329	-6.05100	-1.16066
C	1.40767	-3.97472	-1.55184
H	0.86069	-4.16939	-2.47010
C	1.57857	-2.63862	-1.15687
C	-1.89509	-0.56466	-1.99438
H	-1.66603	-1.01607	-2.96453
C	-1.44790	0.80076	-1.84972
H	-0.94253	1.20785	-2.73036
C	-2.16597	1.85328	-1.11110
C	-2.16188	3.15779	-1.60849
H	-1.66547	3.34880	-2.55659
C	-2.75378	4.20801	-0.92158
H	-2.71779	5.21150	-1.33381
C	-3.38659	3.97078	0.28656
H	-3.84463	4.78370	0.83975
C	-3.41858	2.67427	0.78823
H	-3.90977	2.47487	1.73771
C	-2.81696	1.62095	0.11694
C	-3.13130	-1.09505	-1.41433
C	-3.87818	-2.03767	-2.12975
H	-3.52032	-2.34157	-3.11009
C	-5.05059	-2.58081	-1.63117
H	-5.60053	-3.30987	-2.21781
C	-5.51961	-2.18619	-0.38854
H	-6.43535	-2.60353	0.01626
C	-4.79029	-1.25683	0.34093
H	-5.13769	-0.95336	1.32563
C	-3.60708	-0.71647	-0.14156
C	2.51857	-1.02069	0.57687
H	3.14786	-1.11537	1.47193
C	-2.80737	0.23217	0.72044
H	-3.33766	0.30495	1.68028
N	1.24579	-0.34680	0.92729
H	1.45393	0.64992	1.07173
C	0.52822	3.17793	0.66260
O	1.62582	2.64877	1.41194
C	2.83081	3.32008	1.03190
C	2.43328	4.40155	0.04273
C	1.15021	3.83614	-0.54731
H	-0.13727	2.34893	0.40179
H	-0.02396	3.90474	1.27701
H	3.31885	3.71714	1.92806
H	3.50615	2.58858	0.57106
H	2.22314	5.34193	0.56230
H	3.21215	4.58848	-0.69846
H	0.50447	4.59310	-0.99443
H	1.37066	3.07226	-1.30381

4_{DMSO}

$H°$ = -2148.068468

$G°$ = -2148.172203

Ru	-0.17464	-0.47435	-0.66557
N	-1.40551	-0.43220	0.89411
C	0.60736	-0.89884	2.12571
H	0.45202	-1.97479	1.95089
C	-0.78206	-0.25070	2.19204
H	-0.62695	0.82940	2.42577
C	-1.54448	-0.85456	3.37132
H	-2.53389	-0.39668	3.45936
H	-1.70788	-1.92226	3.16322
C	-0.78837	-0.68115	4.67970
H	-0.70417	0.39054	4.90638
H	-1.35161	-1.12955	5.50443
C	0.60331	-1.28355	4.59888
H	0.51736	-2.37164	4.47516
H	1.15181	-1.11789	5.53155
C	1.38035	-0.71427	3.42202
H	2.35779	-1.20290	3.35226
H	1.56932	0.35790	3.57357
C	1.08561	-1.56985	-1.94328
H	0.60173	-2.00647	-2.82068
C	1.41954	-0.16434	-2.06867
H	1.10683	0.27494	-3.02190
C	2.65806	0.43628	-1.58011
C	3.27088	1.45533	-2.32531
H	2.79816	1.76567	-3.25348
C	4.45510	2.05129	-1.92978
H	4.89744	2.82986	-2.54378
C	5.07970	1.64531	-0.75923
H	6.01242	2.09732	-0.44046
C	4.47488	0.66358	0.01120
H	4.92925	0.36309	0.95163
C	3.27854	0.07003	-0.36702
C	2.52337	-2.29738	0.02303
C	3.14121	-3.32945	0.71617
H	3.67196	-3.09105	1.63490
C	3.08878	-4.64394	0.27604
H	3.57349	-5.43272	0.84045
C	2.39508	-4.92705	-0.89037
H	2.33445	-5.94709	-1.25625
C	1.77946	-3.90844	-1.59414
H	1.24144	-4.13901	-2.50946
C	1.82109	-2.57091	-1.17237
C	-1.81028	-0.67657	-2.00687
H	-1.55035	-1.08062	-2.99044
C	-1.44668	0.70941	-1.81292
H	-0.95908	1.17210	-2.67611
C	-2.26082	1.68796	-1.07265
C	-2.40438	2.98261	-1.57760
H	-1.91218	3.23058	-2.51467

C	-3.15886	3.94609	-0.92451
H	-3.24530	4.94227	-1.34696
C	-3.79614	3.63390	0.26419
H	-4.38175	4.37997	0.79066
C	-3.66854	2.34932	0.78078
H	-4.16445	2.09014	1.71319
C	-2.91221	1.38018	0.13841
C	-3.00547	-1.30846	-1.44440
C	-3.67896	-2.28840	-2.18282
H	-3.29928	-2.54136	-3.16939
C	-4.80558	-2.93217	-1.69860
H	-5.29756	-3.68761	-2.30310
C	-5.30390	-2.60387	-0.44801
H	-6.18459	-3.09991	-0.05437
C	-4.64739	-1.63877	0.30424
H	-5.01677	-1.38563	1.29516
C	-3.50884	-0.99851	-0.16266
C	2.61835	-0.90042	0.58002
H	3.25297	-0.95007	1.47525
C	-2.78441	-0.01111	0.72486
H	-3.32343	0.00294	1.68258
N	1.28961	-0.35348	0.93508
H	1.41321	0.65904	1.09132
S	1.19227	3.30611	0.14028
O	1.66349	2.50820	1.36202
C	-0.15376	4.34292	0.77384
C	2.41000	4.64124	-0.03272
H	0.19397	4.82772	1.68820
H	3.35280	4.17382	-0.31941
H	-0.44178	5.07785	0.02115
H	-0.99432	3.68073	0.98862
H	2.08698	5.33267	-0.81290
H	2.51392	5.14992	0.92741

$TS_{4,5}$

$H°$= -1594.963195

$G°$= -1595.051496

ν = 1225*i*

Ru	-0.00497	-0.07915	-0.57072
N	-1.26739	-0.33385	0.94412
C	0.75452	-0.14153	2.22347
H	0.83302	-1.25133	2.27169
C	-0.74446	0.17215	2.20776
H	-0.84566	1.28106	2.25662
C	-1.40591	-0.39039	3.46130
H	-2.47166	-0.14094	3.47551
H	-1.33682	-1.48730	3.43121
C	-0.74806	0.14628	4.72402
H	-0.91319	1.23102	4.77899
H	-1.22412	-0.28517	5.61056
C	0.74530	-0.12924	4.73359
H	0.91148	-1.21385	4.78506
H	1.20937	0.29884	5.62800
C	1.41199	0.41622	3.48016
H	2.47857	0.16770	3.49251
H	1.34095	1.51287	3.45659
C	1.49718	-0.95478	-1.77700
H	1.08075	-1.54749	-2.59317
C	1.51786	0.46435	-2.00846
H	1.10826	0.76810	-2.97528
C	2.58318	1.35732	-1.54824
C	3.01220	2.40085	-2.37561
H	2.54271	2.51384	-3.34905
C	4.01429	3.27537	-1.99236
H	4.32166	4.07177	-2.66242
C	4.62542	3.12590	-0.75750
H	5.41333	3.80229	-0.44460
C	4.20374	2.10644	0.08345
H	4.66176	1.99353	1.06257
C	3.19116	1.23048	-0.28294
C	3.06216	-1.21141	0.20126
C	3.93070	-2.01238	0.92859
H	4.37780	-1.60665	1.83325
C	4.22220	-3.31230	0.53835
H	4.89360	-3.92458	1.13054
C	3.63212	-3.81834	-0.60828
H	3.84239	-4.83312	-0.92990
C	2.76723	-3.02694	-1.34592
H	2.30821	-3.42859	-2.24524
C	2.46107	-1.71517	-0.97026
C	-1.54316	-0.45732	-2.02443
H	-1.16678	-0.73964	-3.01108
C	-1.43974	0.94477	-1.71446
H	-0.99282	1.54919	-2.50476
C	-2.42213	1.72017	-0.93439
C	-2.73858	3.01693	-1.34079
H	-2.26477	3.41198	-2.23532
C	-3.63349	3.80555	-0.63350
H	-3.85134	4.81285	-0.97290
C	-4.24226	3.30523	0.50482
H	-4.93401	3.91667	1.07413
C	-3.94404	2.01385	0.92038
H	-4.40875	1.61155	1.81744
C	-3.04409	1.22145	0.22409
C	-2.61075	-1.33415	-1.54360
C	-3.07165	-2.36749	-2.36754
H	-2.62304	-2.48251	-3.35059
C	-4.07986	-3.22839	-1.97024
H	-4.41063	-4.01773	-2.63754
C	-4.66723	-3.07345	-0.72458
H	-5.45861	-3.73979	-0.39909
C	-4.21552	-2.06244	0.11156
H	-4.65508	-1.94581	1.09879
C	-3.19231	-1.20399	-0.26601
C	2.72633	0.17987	0.69759
H	3.30817	0.33900	1.61657
C	-2.69497	-0.16712	0.71477
H	-3.26036	-0.32798	1.64297
N	1.31378	0.35086	0.97896
H	0.55697	1.27577	0.08392

$TS_{4,5\ THF}$

$H°$ = -1827.223305

$G°$ = -1827.325945

ν = 1157i

Ru	-0.13674	-0.71830	-0.54985
N	-1.36403	-0.43210	0.98402
C	0.71066	-0.19053	2.16332
H	0.65926	-1.26034	2.46876
C	-0.74267	0.28861	2.08828
H	-0.71384	1.38274	1.87714
C	-1.41877	0.11619	3.44396
H	-2.44682	0.49077	3.40775
H	-1.47980	-0.95819	3.66971
C	-0.65615	0.84418	4.54102
H	-0.68971	1.92462	4.34347
H	-1.14736	0.69155	5.50755
C	0.79323	0.39473	4.60294
H	0.83005	-0.66160	4.90203
H	1.33701	0.95400	5.37116
C	1.47573	0.55155	3.25284
H	2.50377	0.17874	3.31440
H	1.53931	1.61481	2.97935
C	1.21958	-2.03644	-1.49998
H	0.71220	-2.76699	-2.13257
C	1.38288	-0.73405	-2.08856
H	0.97482	-0.64304	-3.09854
C	2.55565	0.11854	-1.88152
C	3.06871	0.85670	-2.95403
H	2.57637	0.77383	-3.91923
C	4.18276	1.66677	-2.82076
H	4.55358	2.22094	-3.67681
C	4.82183	1.76400	-1.59452
H	5.69568	2.39486	-1.47428
C	4.31504	1.05724	-0.51373
H	4.79276	1.14633	0.45872
C	3.19281	0.24771	-0.63156
C	2.82267	-1.95702	0.46365
C	3.63057	-2.63836	1.36239
H	4.15220	-2.06799	2.12765
C	3.77068	-4.01857	1.31425
H	4.39755	-4.53161	2.03547
C	3.08662	-4.72947	0.34167
H	3.17750	-5.80938	0.28730
C	2.28068	-4.06000	-0.56437
H	1.74777	-4.62278	-1.32593
C	2.12697	-2.67035	-0.53374
C	-1.75563	-1.26364	-1.85265
H	-1.44803	-1.82167	-2.74076
C	-1.49302	0.15207	-1.90122
H	-1.00852	0.49221	-2.81797
C	-2.37927	1.19086	-1.34354
C	-2.60341	2.35842	-2.07459
H	-2.12126	2.46694	-3.04262
C	-3.42100	3.37286	-1.59864
H	-3.56952	4.26953	-2.19157
C	-4.03983	3.23942	-0.36686
H	-4.67181	4.03077	0.02164
C	-3.82915	2.08372	0.37403
H	-4.30364	1.96786	1.34563
C	-3.00885	1.06710	-0.09225
C	-2.89464	-1.86773	-1.15975
C	-3.49598	-3.01129	-1.69840
H	-3.10061	-3.41315	-2.62749
C	-4.57574	-3.62843	-1.09125
H	-5.01480	-4.51347	-1.54032
C	-5.09518	-3.10930	0.08383
H	-5.94087	-3.58178	0.57151
C	-4.50628	-1.98284	0.63980
H	-4.89383	-1.57910	1.57163
C	-3.41161	-1.36464	0.05174
C	2.65269	-0.45742	0.59079
H	3.28268	-0.13441	1.43255
C	-2.77376	-0.17684	0.73645
H	-3.31681	-0.03788	1.68127
N	1.27713	-0.06766	0.83326
H	0.59024	0.68427	-0.26060
C	1.91179	3.69850	0.65704
O	1.71160	4.10607	-0.68395
C	0.36952	3.75108	-0.97371
C	-0.42805	3.99581	0.31273
C	0.65829	4.14879	1.38722
H	2.00822	2.60043	0.71030
H	2.83839	4.14787	1.02091
H	0.03485	4.34891	-1.82452
H	0.31889	2.68694	-1.25920
H	-1.04966	4.89032	0.24135
H	-1.09193	3.15152	0.51885
H	0.75574	5.19217	1.69774
H	0.45968	3.54788	2.27866

$TS_{4,5\ DMSO}$

$H°$ = -2148.029522

$G°$ = -2148.133927

ν = 1166i

Ru	0.00230	-0.90617	-0.49562
N	-1.23624	-0.57585	1.02684
C	0.79967	0.05781	2.12650
H	0.86095	-0.94831	2.60099
C	-0.69487	0.36858	1.99728
H	-0.77621	1.41002	1.61170
C	-1.35189	0.35635	3.37190
H	-2.41310	0.61298	3.28930
H	-1.30122	-0.66368	3.77937
C	-0.66954	1.33859	4.31314
H	-0.81207	2.35851	3.92903
H	-1.14385	1.30912	5.29953
C	0.81809	1.05595	4.42944
H	0.96186	0.07717	4.90728
H	1.29955	1.79297	5.07996
C	1.48604	1.04374	3.06317
H	2.54451	0.78531	3.17409
H	1.45121	2.04636	2.61146

C	1.51902	-2.11905	-1.36275
H	1.10493	-2.96470	-1.91444
C	1.48696	-0.86744	-2.06643
H	1.05035	-0.92295	-3.06685
C	2.49875	0.18521	-1.95801
C	2.80931	0.95414	-3.08529
H	2.30800	0.72369	-4.02157
C	3.73157	1.98587	-3.03819
H	3.94606	2.55952	-3.93403
C	4.38201	2.27655	-1.84941
H	5.10782	3.08059	-1.79753
C	4.07538	1.53653	-0.71610
H	4.55499	1.77716	0.22904
C	3.14225	0.50917	-0.74601
C	3.13863	-1.64433	0.52766
C	4.05848	-2.12331	1.44917
H	4.50937	-1.42133	2.14684
C	4.39755	-3.46821	1.50748
H	5.11007	-3.82215	2.24459
C	3.80174	-4.35066	0.62118
H	4.04894	-5.40679	0.65078
C	2.88427	-3.88384	-0.30562
H	2.42094	-4.58026	-0.99928
C	2.53048	-2.53314	-0.38140
C	-1.55493	-1.77904	-1.68970
H	-1.19479	-2.39823	-2.51524
C	-1.45929	-0.35781	-1.90606
H	-1.02787	-0.07571	-2.86829
C	-2.45633	0.63085	-1.45753
C	-2.83974	1.65337	-2.32805
H	-2.39020	1.69068	-3.31690
C	-3.78587	2.60185	-1.96793
H	-4.06496	3.38032	-2.67056
C	-4.36475	2.55556	-0.71019
H	-5.09359	3.30107	-0.41092
C	-3.98903	1.55008	0.17124
H	-4.43384	1.50334	1.16239
C	-3.05123	0.59124	-0.18404
C	-2.60662	-2.42276	-0.90113
C	-3.07222	-3.68656	-1.28190
H	-2.64112	-4.15045	-2.16498
C	-4.06389	-4.34650	-0.57716
H	-4.39818	-5.32582	-0.90407
C	-4.62999	-3.75025	0.53836
H	-5.40780	-4.25507	1.10086
C	-4.17432	-2.50242	0.93838
H	-4.59650	-2.03516	1.82428
C	-3.16707	-1.83767	0.25296
C	2.75341	-0.18108	0.54051
H	3.33982	0.29770	1.33694
C	-2.66626	-0.51112	0.77873
H	-3.21565	-0.32506	1.71181
N	1.33854	0.02266	0.78207
H	0.54371	0.59256	-0.36103
S	-0.04082	4.07346	0.51711
O	0.92812	5.16207	0.96703
C	-1.36381	4.91829	-0.39423
C	0.71696	3.29478	-0.93804
H	-0.91578	5.54493	-1.16796
H	1.59829	2.75117	-0.59169
H	-2.02838	4.16730	-0.83049
H	-1.91673	5.53047	0.31805
H	0.00311	2.59866	-1.38860
H	1.00447	4.08003	-1.64072

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H° = -1594.985342

G° = -1595.074372

Ru	-0.01567	0.58235	-0.30786
N	-1.24995	-0.49789	0.76248
C	0.76645	-1.24537	1.76956
H	0.79729	-2.12797	1.08513
C	-0.71468	-0.98180	2.02873
H	-0.77566	-0.18454	2.80142
C	-1.38216	-2.22395	2.60568
H	-2.43706	-2.03254	2.82514
H	-1.35417	-3.02470	1.85210
C	-0.68215	-2.67207	3.88083
H	-0.81443	-1.89743	4.64852
H	-1.15437	-3.57952	4.27124
C	0.80266	-2.89793	3.65625
H	0.93862	-3.74582	2.97113
H	1.29274	-3.17654	4.59492
C	1.46687	-1.66719	3.05676
H	2.52311	-1.88167	2.86550
H	1.43579	-0.83025	3.76911
C	1.38962	0.14831	-1.84857
H	0.88963	0.01856	-2.80825
C	1.58913	1.51346	-1.46012
H	1.23566	2.25544	-2.17861
C	2.71970	1.98125	-0.65463
C	3.26767	3.24107	-0.91318
H	2.84877	3.83049	-1.72443
C	4.31977	3.74864	-0.17040
H	4.71867	4.73155	-0.39928
C	4.85933	2.99645	0.86045
H	5.68214	3.38034	1.45375
C	4.32371	1.74623	1.13409
H	4.73143	1.15496	1.94981
C	3.26106	1.22778	0.40566
C	2.98182	-1.11777	-0.34749
C	3.83126	-2.19753	-0.15822
H	4.34255	-2.29813	0.79632
C	4.02319	-3.14979	-1.15062
H	4.68073	-3.99503	-0.97777
C	3.35025	-3.01743	-2.35400
H	3.48049	-3.75540	-3.13863
C	2.50390	-1.93837	-2.55499
H	1.98039	-1.83414	-3.50154
C	2.30479	-0.96977	-1.56912
C	-1.48238	0.66486	-1.89973
H	-1.02483	0.87758	-2.86758

C	-1.63691	1.80197	-1.05917
H	-1.27959	2.73880	-1.48455
C	-2.70470	2.00399	-0.07045
C	-3.19910	3.29280	0.13886
H	-2.78738	4.10871	-0.44880
C	-4.19352	3.55025	1.06870
H	-4.55216	4.56456	1.20893
C	-4.72328	2.51178	1.81665
H	-5.49634	2.70101	2.55343
C	-4.24001	1.22472	1.62507
H	-4.63783	0.40396	2.21637
C	-3.23677	0.95797	0.70490
C	-2.39473	-0.48220	-1.94831
C	-2.65251	-1.09635	-3.17595
H	-2.16716	-0.70331	-4.06518
C	-3.51577	-2.17483	-3.28395
H	-3.69500	-2.62883	-4.25290
C	-4.14758	-2.66702	-2.15397
H	-4.82256	-3.51299	-2.22427
C	-3.89225	-2.07726	-0.92333
H	-4.36381	-2.47174	-0.02694
C	-3.02025	-1.00616	-0.80247
C	2.71084	-0.13195	0.76886
H	3.30064	-0.47076	1.63424
C	-2.69085	-0.44447	0.56001
H	-3.21593	-1.06656	1.29393
N	1.30213	-0.06294	1.11522
H	0.24938	2.04042	0.21538

5_{THF}

$H°$ = -1827.240128

$G°$ = -1827.345580

Ru	0.31173	-0.37068	-0.67403
N	-0.80907	-0.96269	0.82945
C	0.84708	0.15174	2.11397
H	1.35995	-0.82108	2.31439
C	-0.64297	-0.17070	2.04072
H	-1.17144	0.80235	1.93557
C	-1.13150	-0.80114	3.33773
H	-2.20946	-0.98918	3.29412
H	-0.64180	-1.77713	3.47041
C	-0.83347	0.10853	4.52099
H	-1.41207	1.03667	4.40813
H	-1.17298	-0.35719	5.45185
C	0.64368	0.45065	4.60234
H	1.21284	-0.46548	4.81086
H	0.83389	1.13055	5.43937
C	1.14431	1.06107	3.30179
H	2.22016	1.24972	3.37861
H	0.66421	2.03528	3.12733
C	2.20004	-0.94576	-1.47116
H	2.10775	-1.84084	-2.08650
C	1.81664	0.26982	-2.12261
H	1.49477	0.15845	-3.15968
C	2.40278	1.58187	-1.83735
C	2.55639	2.50148	-2.87906
H	2.25986	2.20221	-3.88074
C	3.06908	3.76963	-2.66639
H	3.17169	4.45805	-3.49898
C	3.44944	4.15257	-1.39044
H	3.84872	5.14410	-1.20631
C	3.29954	3.25356	-0.34424
H	3.58081	3.55047	0.66270
C	2.77802	1.98151	-0.53969
C	3.51738	-0.13646	0.53060
C	4.54395	-0.34293	1.44002
H	4.71166	0.40211	2.21429
C	5.34007	-1.47959	1.38764
H	6.12885	-1.62863	2.11715
C	5.10115	-2.42710	0.40605
H	5.70746	-3.32520	0.35236
C	4.07973	-2.22806	-0.50995
H	3.89604	-2.97197	-1.28038
C	3.27251	-1.08959	-0.47247
C	-0.54292	-1.93043	-1.91914
H	0.10650	-2.19117	-2.75684
C	-1.27499	-0.72243	-2.09376
H	-1.09873	-0.21200	-3.03967
C	-2.59881	-0.41923	-1.53228
C	-3.47569	0.38241	-2.26611
H	-3.16354	0.73089	-3.24673
C	-4.71944	0.74411	-1.77323
H	-5.37413	1.37185	-2.36876
C	-5.11904	0.30734	-0.52048
H	-6.08569	0.59275	-0.11956
C	-4.25946	-0.49038	0.22326
H	-4.55562	-0.82860	1.21337
C	-3.01000	-0.85321	-0.25825
C	-1.01902	-3.10631	-1.18560
C	-0.69913	-4.38175	-1.65786
H	-0.10019	-4.46592	-2.56062
C	-1.13446	-5.52820	-1.01339
H	-0.86694	-6.50364	-1.40602
C	-1.91273	-5.42327	0.12763
H	-2.25841	-6.31243	0.64349
C	-2.22927	-4.16377	0.61769
H	-2.81768	-4.07060	1.52675
C	-1.78534	-3.00953	-0.00995
C	2.60381	1.06421	0.64876
H	2.95193	1.63641	1.52192
C	-2.06712	-1.66017	0.60445
H	-2.58643	-1.85179	1.55086
N	1.21320	0.68605	0.81475
H	-0.08142	1.01860	-1.28163
C	-1.85635	2.93781	0.26056
O	-2.28361	3.89540	-0.70220
C	-3.61496	4.21562	-0.36051
C	-3.59419	4.35461	1.14820
C	-2.63626	3.23056	1.55328
H	-2.07864	1.92309	-0.10188
H	-0.77081	3.01802	0.36507
H	-3.90421	5.12231	-0.89619

H	-4.29692	3.40097	-0.66170
H	-3.18448	5.33138	1.41963
H	-4.58316	4.26224	1.59997
H	-1.98100	3.52142	2.37656
H	-3.18808	2.34154	1.87245

5_{DMSO}

$H°$ = -2148.042652

$G°$ = -2148.147546

Ru	-0.09725	-0.27690	-0.55056
N	-1.42176	-0.61558	0.86381
C	0.50231	-1.35305	2.04881
H	0.28644	-2.41315	1.76566
C	-0.86067	-0.68217	2.20752
H	-0.67192	0.34384	2.59545
C	-1.70028	-1.42097	3.24185
H	-2.66567	-0.92575	3.38504
H	-1.91506	-2.43204	2.86488
C	-0.97411	-1.49479	4.57771
H	-0.86347	-0.47768	4.97754
H	-1.57589	-2.05036	5.30456
C	0.40140	-2.12236	4.43424
H	0.28757	-3.17428	4.13804
H	0.92194	-2.12644	5.39767
C	1.23432	-1.40090	3.38513
H	2.19813	-1.90900	3.27522
H	1.45206	-0.37178	3.70514
C	1.14933	-1.33954	-1.92687
H	0.59467	-1.64311	-2.81453
C	1.56773	0.02798	-1.92547
H	1.28967	0.59550	-2.81626
C	2.79452	0.51967	-1.29337
C	3.50394	1.56219	-1.89735
H	3.13273	1.96467	-2.83671
C	4.65638	2.08502	-1.33384
H	5.18473	2.89147	-1.83275
C	5.13059	1.57242	-0.13718
H	6.02836	1.97497	0.31917
C	4.43366	0.54261	0.47873
H	4.78783	0.14722	1.42685
C	3.27582	0.01063	-0.07177
C	2.56510	-2.37686	-0.10607
C	3.20542	-3.49553	0.40640
H	3.73078	-3.40678	1.35450
C	3.17267	-4.71699	-0.25415
H	3.66754	-5.58298	0.17226
C	2.48581	-4.81883	-1.45253
H	2.44284	-5.76542	-1.98115
C	1.84678	-3.70610	-1.97640
H	1.30981	-3.78800	-2.91768
C	1.87061	-2.47084	-1.32519
C	-1.67155	-0.42179	-2.03052
H	-1.29477	-0.69314	-3.01849
C	-1.46829	0.94387	-1.67035
H	-0.95990	1.54945	-2.42154
C	-2.36331	1.74222	-0.82200
C	-2.58081	3.08451	-1.13791
H	-2.09236	3.49697	-2.01738
C	-3.40198	3.89256	-0.36717
H	-3.54674	4.93311	-0.63997
C	-4.02167	3.37204	0.75646
H	-4.65503	3.99677	1.37691
C	-3.81795	2.03816	1.08516
H	-4.29842	1.61885	1.96543
C	-3.00190	1.21901	0.31877
C	-2.84411	-1.21303	-1.63766
C	-3.40675	-2.10237	-2.55622
H	-2.95013	-2.19213	-3.53813
C	-4.52998	-2.85373	-2.25082
H	-4.94202	-3.53416	-2.98868
C	-5.12511	-2.72844	-1.00616
H	-6.00355	-3.31224	-0.75344
C	-4.57243	-1.85898	-0.07602
H	-5.01835	-1.76902	0.91122
C	-3.43988	-1.11326	-0.36671
C	2.53381	-1.07688	0.67022
H	3.10464	-1.25026	1.59424
C	-2.81480	-0.23588	0.69297
H	-3.38366	-0.40040	1.61627
N	1.18547	-0.64953	0.98136
H	0.41495	1.19170	-0.44755
S	1.08657	3.82026	0.13537
O	1.56822	3.36786	1.50415
C	-0.17826	5.08148	0.47201
C	2.35374	4.97545	-0.47105
H	0.23856	5.80638	1.17437
H	3.26585	4.39272	-0.60632
H	-0.48773	5.56552	-0.45606
H	-1.02614	4.56379	0.92284
H	2.04031	5.40458	-1.42437
H	2.51316	5.75379	0.27789

$TS_{5,6}$

$H°$ = -1594.95291

$G°$ = -1595.04267

ν = 1166i

Ru	0.03549	0.36874	-0.40935
N	-1.25589	-0.27344	0.96320
C	0.73160	-1.37032	1.74606
H	0.56076	-2.28010	1.12390
C	-0.65901	-0.87078	2.15561
H	-0.49919	-0.08954	2.92804
C	-1.45097	-1.99631	2.79849
H	-2.44872	-1.65715	3.09294
H	-1.59147	-2.80260	2.06534
C	-0.71007	-2.51221	4.02587
H	-0.67956	-1.71405	4.77980
H	-1.26170	-3.34347	4.47633
C	0.71148	-2.93865	3.69534
H	0.67770	-3.82269	3.04473
H	1.23528	-3.24556	4.60628

C	1.48676	-1.83648	2.98521
H	2.47831	-2.21078	2.71107
H	1.64372	-0.97838	3.65469
C	1.48473	0.53529	-1.95324
H	1.05819	0.70491	-2.94475
C	1.55943	1.69996	-1.11386
H	1.15918	2.60600	-1.57185
C	2.68791	1.98995	-0.22062
C	3.18510	3.29369	-0.14963
H	2.70383	4.06513	-0.74478
C	4.27294	3.61835	0.64395
H	4.63452	4.64105	0.67370
C	4.89739	2.63289	1.39182
H	5.75009	2.87273	2.01795
C	4.40728	1.33543	1.34521
H	4.87582	0.56011	1.94591
C	3.31037	1.00204	0.56320
C	2.96854	-1.10717	-0.71678
C	3.74059	-2.25901	-0.75214
H	4.19141	-2.60945	0.17368
C	3.93224	-2.97728	-1.92560
H	4.52630	-3.88480	-1.92203
C	3.34328	-2.52325	-3.09395
H	3.47801	-3.06816	-4.02273
C	2.57757	-1.36885	-3.07721
H	2.12182	-1.01421	-3.99794
C	2.36777	-0.63321	-1.90519
C	-1.47954	0.15511	-1.89790
H	-1.06353	0.03171	-2.89916
C	-1.49443	1.50996	-1.41625
H	-1.08623	2.25081	-2.10758
C	-2.52215	2.06432	-0.53342
C	-2.92694	3.39295	-0.69963
H	-2.48068	3.97050	-1.50436
C	-3.87339	3.98007	0.12184
H	-4.16119	5.01378	-0.03978
C	-4.45220	3.24549	1.14464
H	-5.19421	3.69349	1.79634
C	-4.05852	1.92874	1.33370
H	-4.49505	1.34782	2.14187
C	-3.10225	1.33073	0.52491
C	-2.52515	-0.84167	-1.61393
C	-2.92452	-1.71435	-2.62895
H	-2.44817	-1.63043	-3.60191
C	-3.90704	-2.67104	-2.42822
H	-4.18873	-3.33324	-3.24028
C	-4.52688	-2.77700	-1.19383
H	-5.29392	-3.52467	-1.02389
C	-4.13954	-1.92500	-0.16879
H	-4.60282	-2.00915	0.81131
C	-3.14861	-0.97410	-0.35844
C	2.73833	-0.39347	0.60217
H	3.31294	-0.94362	1.36102
C	-2.69564	-0.10197	0.78972
H	-3.23019	-0.42416	1.69001
N	1.34079	-0.30384	0.97227
H	-0.67715	1.10764	0.86821

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$H°$ = -1594.98652

$G°$ = -1595.075554

Ru	-0.01568	0.66185	-0.28932
N	-1.42005	-0.07941	1.20062
C	0.68320	-1.36802	1.55031
H	0.55620	-2.09509	0.71719
C	-0.71325	-1.05528	2.09857
H	-0.54467	-0.50614	3.03668
C	-1.46727	-2.32404	2.44572
H	-2.46566	-2.09302	2.82937
H	-1.59949	-2.93663	1.54513
C	-0.68754	-3.10501	3.49586
H	-0.66948	-2.52329	4.42734
H	-1.20422	-4.04225	3.72435
C	0.73937	-3.37931	3.05139
H	0.72313	-4.06691	2.19530
H	1.29149	-3.88932	3.84740
C	1.46086	-2.10384	2.64017
H	2.46535	-2.35324	2.28658
H	1.58326	-1.43404	3.50456
C	1.43990	0.43694	-1.79628
H	1.01794	0.41282	-2.80321
C	1.52267	1.75731	-1.23009
H	1.17858	2.56399	-1.88488
C	2.56671	2.19184	-0.29841
C	3.00761	3.51955	-0.33719
H	2.56183	4.18891	-1.06822
C	3.98921	3.99370	0.51591
H	4.30254	5.03110	0.45659
C	4.57097	3.13818	1.43762
H	5.34076	3.49387	2.11397
C	4.14178	1.81970	1.49698
H	4.57855	1.14621	2.22993
C	3.14679	1.33380	0.65992
C	3.05491	-0.91283	-0.39661
C	3.97008	-1.95119	-0.30619
H	4.45377	-2.13873	0.64973
C	4.26519	-2.75553	-1.39934
H	4.97418	-3.57100	-1.30381
C	3.62720	-2.51357	-2.60498
H	3.83641	-3.13508	-3.46970
C	2.72045	-1.47030	-2.70814
H	2.22949	-1.27736	-3.65849
C	2.41550	-0.64734	-1.62030
C	-1.39295	0.54759	-1.86389
H	-0.97755	0.69849	-2.86399
C	-1.66663	1.77218	-1.14807
H	-1.38080	2.67503	-1.69415
C	-2.86347	1.98897	-0.33813
C	-3.48731	3.24548	-0.35695
H	-3.04505	4.02728	-0.96831
C	-4.64275	3.50696	0.35472
H	-5.09483	4.49235	0.30415

C	-5.22750	2.50995	1.12236
H	-6.13679	2.70047	1.68140
C	-4.61634	1.26766	1.17913
H	-5.04630	0.48432	1.79779
C	-3.44976	0.99506	0.47525
C	-2.11911	-0.71481	-1.76715
C	-2.12235	-1.57188	-2.87759
H	-1.62073	-1.23899	-3.78244
C	-2.74327	-2.80752	-2.85479
H	-2.71837	-3.43950	-3.73668
C	-3.40249	-3.23007	-1.71114
H	-3.89985	-4.19302	-1.68021
C	-3.40197	-2.40400	-0.59656
H	-3.90097	-2.73059	0.31229
C	-2.76120	-1.17264	-0.59597
C	2.67867	-0.09424	0.81893
H	3.24655	-0.50814	1.66768
C	-2.78279	-0.34473	0.66386
H	-3.37649	-0.89249	1.40470
N	1.25108	-0.11230	1.08146
H	-1.50501	0.77848	1.74390

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H° = -1594.966695

G° = -1595.056914

Ru	-0.01279	-0.84614	-0.24814
N	1.36439	-0.02129	1.20316
H	1.35492	-0.76071	1.90392
N	-1.26376	0.45383	0.83440
C	-2.68493	0.51266	0.46611
H	-3.23710	1.20251	1.11045
C	-3.33128	-0.84172	0.62470
C	-2.83672	-1.97935	-0.04019
C	-1.68104	-1.95234	-0.94297
H	-1.44149	-2.94346	-1.33102
C	-1.37798	-0.86712	-1.84442
H	-0.92538	-1.18810	-2.78614
C	-2.13291	0.37777	-2.00398
C	-2.77066	1.04931	-0.94096
C	-4.43438	-0.95126	1.45929
H	-4.79739	-0.05935	1.96350
C	-5.07119	-2.16577	1.67133
H	-5.92800	-2.22801	2.33290
C	-4.58256	-3.29499	1.03429
H	-5.05771	-4.25844	1.18863
C	-3.48839	-3.19555	0.19284
H	-3.11072	-4.08419	-0.30512
C	-2.18648	0.98291	-3.26617
H	-1.69482	0.48474	-4.09748
C	-2.84048	2.18512	-3.47825
H	-2.85474	2.62121	-4.47201
C	-3.47570	2.82607	-2.42714
H	-3.99014	3.76815	-2.58047
C	-3.42861	2.24858	-1.16495
H	-3.90267	2.74923	-0.32431
C	2.79644	0.13113	0.78319
H	3.38544	0.45324	1.65280
C	2.90633	1.19752	-0.25867
C	2.16194	1.08416	-1.45205
C	1.32496	-0.05712	-1.77195
H	0.84645	0.08522	-2.74186
C	1.60439	-1.47855	-1.47807
H	1.38196	-2.14894	-2.31517
C	2.76800	-1.93184	-0.72218
C	3.33695	-1.21019	0.35410
C	3.64729	2.34070	0.00773
H	4.19276	2.39845	0.94729
C	3.68536	3.40676	-0.87865
H	4.27280	4.29032	-0.65574
C	2.94088	3.32080	-2.04915
H	2.94303	4.14458	-2.75640
C	2.20090	2.18790	-2.32499
H	1.62481	2.13363	-3.24527
C	3.34569	-3.17540	-1.02249
H	2.92693	-3.74670	-1.84665
C	4.40951	-3.69320	-0.30715
H	4.81622	-4.66299	-0.57696
C	4.95792	-2.97520	0.74469
H	5.79257	-3.36822	1.31428
C	4.40859	-1.74001	1.05920
H	4.81987	-1.16597	1.88593
C	0.78067	1.19539	1.82681
H	1.16587	2.05928	1.26195
C	1.20969	1.33851	3.28334
H	0.89360	0.43563	3.82446
H	2.30219	1.37915	3.33759
C	0.59474	2.56203	3.93701
H	0.96532	3.46748	3.43804
H	0.90962	2.62602	4.98234
C	-0.91745	2.51345	3.83664
H	-1.36635	3.39827	4.29673
H	-1.29065	1.64278	4.38993
C	-1.36660	2.41603	2.38226
H	-2.45375	2.36931	2.32365
H	-1.06729	3.33860	1.86095
C	-0.72193	1.27016	1.66246
H	-0.12370	-2.05460	0.96474

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H° = -1594.953575

G° = -1595.042644

Ru	-0.15380	-0.84625	-0.84123
N	-1.34168	1.05479	-0.85962
H	-1.57141	1.27548	-1.82753
N	0.97818	0.45130	0.58563
H	0.60064	0.16482	1.49206
C	2.44743	0.15792	0.66742
H	2.88929	0.75787	1.47289
C	3.14531	0.52854	-0.60750
C	2.72899	-0.02511	-1.83386
C	1.67874	-1.02720	-1.94571
H	1.54780	-1.31437	-2.98845

C	1.48451	-2.16847	-1.02589	H	-3.30023	2.58052	1.86548
H	1.33116	-3.12507	-1.53301	C	-2.45190	1.61857	3.58329
C	2.16992	-2.34672	0.24705	H	-2.74160	2.40621	4.26963
C	2.60933	-1.28438	1.07367	C	-1.72754	0.51987	4.02503
C	4.18530	1.44936	-0.57160	H	-1.44093	0.43856	5.06865
H	4.49981	1.84451	0.39153	C	-1.37556	-0.48103	3.13838
C	4.81775	1.88227	-1.72648	H	-0.81713	-1.34390	3.49352
H	5.62614	2.60300	-1.67491	C	-4.02664	-2.30672	-1.51980
C	4.38135	1.38506	-2.94786	H	-3.74519	-3.35400	-1.58677
H	4.84821	1.71758	-3.86991	C	-5.21366	-1.87946	-2.08554
C	3.36358	0.45265	-2.99379	H	-5.85689	-2.59174	-2.59216
H	3.04505	0.05296	-3.95283	C	-5.57935	-0.54428	-2.00232
C	2.33115	-3.64688	0.75855	H	-6.50616	-0.19404	-2.44285
H	2.00370	-4.48004	0.14236	C	-4.73237	0.34145	-1.35563
C	2.87291	-3.89572	2.00571	H	-4.99999	1.39299	-1.29296
H	2.96981	-4.91969	2.35341	C	-0.50913	2.11427	-0.33119
C	3.29486	-2.84435	2.80619	C	-0.98100	3.51754	-0.58175
H	3.72185	-3.02392	3.78644	H	-0.71914	3.78790	-1.61505
C	3.15237	-1.55077	2.32368	H	-2.07468	3.55185	-0.53729
H	3.46916	-0.71241	2.93945	C	-0.39066	4.52481	0.38776
C	-2.65981	0.95308	-0.12805	H	-0.86862	4.40493	1.36937
H	-3.18758	1.91222	-0.21100	H	-0.60411	5.54324	0.05147
C	-2.41217	0.71614	1.33125	C	1.09873	4.29505	0.53209
C	-1.72981	-0.43683	1.77761	H	1.55283	5.04607	1.18444
C	-1.27782	-1.50252	0.90136	H	1.57969	4.39290	-0.45043
H	-0.73689	-2.28230	1.44308	C	1.37357	2.90580	1.07738
C	-1.90122	-1.95140	-0.31553	H	2.44407	2.70348	1.01781
H	-1.80239	-3.02299	-0.49037	H	1.11961	2.85738	2.14842
C	-3.16099	-1.43080	-0.85382	C	0.59264	1.83564	0.37126
C	-3.53366	-0.07542	-0.78824	H	-0.71447	-1.40570	-2.27339
C	-2.77343	1.70475	2.23703				

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