

Supporting Information

Rhodium-Catalyzed Double Hydroboration of Pyridine: The Origin of the Chemo- and Regioselectivities

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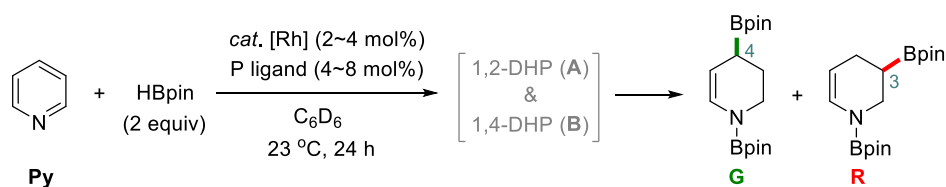
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I. General Considerations

Unless otherwise stated, all catalytic reactions were carried out in J-Young NMR tubes in a nitrogen-filled 'Mbraun' glovebox with a medium capacity recirculator (0.1–1 ppm of O₂). Benzene-d₆ and chloroform-d₁ purchased from Cambridge Isotope Laboratories, Inc. and benzene-d₆ were predried by 4 Å molecular sieves for the catalytic double hydroboration and mechanistic studies. All other commercial reagents from standard suppliers (Sigma Aldrich, Acros, Alfa Aesar, Macklin) were directly used as received without further purification unless otherwise stated. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by the use of UV light (254 nm), exposure to treatment with acidic anisaldehyde, phosphomolybdic acid, ninhydrin or ceric ammonium molybdate stain followed by heating. Column chromatography was undertaken on silica gel (300–400 mesh) using a proper eluent. ¹H NMR was recorded on Bruker Ascend-400 (400 MHz) for routine characterization of compounds and mechanistic studies. ¹H Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak (CHCl₃ in CDCl₃: 7.26 ppm; C₆H₆ in C₆D₆: 7.16 ppm). The following abbreviations were used to describe peak splitting patterns when appropriate in ¹H NMR: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, dd = doublet of doublet, td = triplet of doublet, ddd = doublet of doublet of doublet, m = multiplet. Coupling constants, J, were reported in hertz unit (Hz). ¹³C{¹H} NMR was recorded on Bruker Ascend-400 (101 MHz) and fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center of a multiplet at 77.16 ppm of CDCl₃. ³¹P{¹H} NMR was recorded on Bruker Ascend-400 (162 MHz), while the chemical shifts were reported in ppm referenced to external H₃PO₄ at 0 ppm. ¹¹B{¹H} NMR was recorded on Bruker Ascend-400 (128 MHz), and its chemical shifts were reported in ppm referenced to external BF₃-OEt₂ at 0 ppm. Mass spectra were obtained by using Bruker MALDI-TOF and/or Shimadzu GC mass spectrometers.

II. General Procedure: Rh-Catalyzed Double Hydroboration of Pyridine (Table 1)



General procedure for double hydroboration of pyridine:

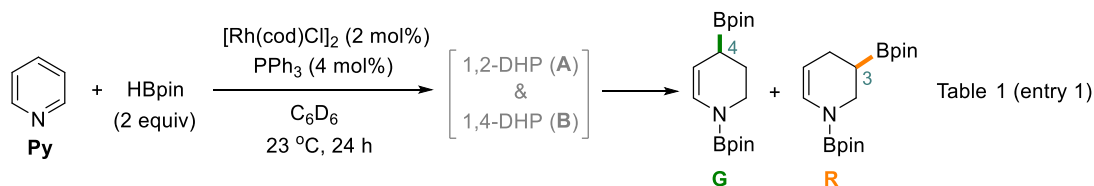
In glove box, HBpin (0.8 mmol, 2 equiv) was added to a solution of a Rh precatalyst (0.008–0.016 mmol, 2–4 mol%) and phosphine ligand (0.016–0.032 mmol, 4–8 mol%) in deuterated benzene (0.5 mL) in a 5 mL screw-cap vial. After shaking briefly, pyridine (0.4 mmol) was added to the above solution, and the whole mixture solution was carefully then transferred to a medium-walled J. Young NMR tube to conduct the catalytic reaction at 23 °C for 24 h. At the end of the catalytic reaction, an internal standard 1,3,5-trimethoxybenzene (0.1 mmol) was added in order to calculate the crude ¹H NMR yields.

Table S1. Variable reaction conditions for the Rh-catalyzed double hydroboration of pyridine.^a

entry	cat. [Rh] (mol%)	P ligand (mol%)	conv. (%)	yield (%) ^b			
				A	B	G	R
1	[Rh(cod)Cl] ₂ (2)	PPh ₃ (4)	quant.	<1	21	50	11
				<1 ^c	20 ^c	51 ^c	12 ^c
2	[Rh(cod)Cl] ₂ (2)	PPh ₃ (8)	97	<1	6	75	16
3 ^d	[Rh(cod)Cl] ₂ (2)	P(<i>p</i> -CF ₃ -C ₆ H ₄) ₃ (8)	92	<1	2	41	47
4	[Rh(cod)Cl] ₂ (2)	P(<i>p</i> -OMe-C ₆ H ₄) ₃ (8)	81	<1	14	37	26
5	[Rh(cod)Cl] ₂ (2)	P(<i>o</i> -OMe-C ₆ H ₄) ₃ (8)	79	2	7	15	37
6	[Rh(cod)Cl] ₂ (2)	PPh ₂ Cy (8)	quant.	<1	25	40	25
7 ^e	[Rh(cod)Cl] ₂ (2)	PCy ₃ (8)	68	18	9	17	18
8	Rh(PPh ₃) ₃ Cl (4)		70	<1	5	44	20
9	[Rh(cod) ₂]OTf (4)	PPh ₃ (8)	93	<1	3	50	25
10 ^f	[Rh(cod) ₂]OTf (2)	PPh ₃ (8)	quant.	<1	3	50	47
11 ^{e,f}	[Rh(cod)Cl] ₂ (2)	PPh ₃ (8)	quant.	<1	12	47	36
12 ^e	[Rh(cod)Cl] ₂ (2)	PPh ₃ (4)	42 ^g	<1 ^g	15 ^g	25 ^g	2 ^g
			quant. ^h	<1 ^h	43 ^h	42 ^h	12 ^h
				<1 ⁱ	43 ⁱ	43 ⁱ	13 ⁱ
				<1	39	42	13

^aPyridine (0.4 mmol, 1 equiv), HBpin (0.8 mmol, 2 equiv), cat. [Rh] (2~4 mol%), and P ligand (4~8 mol%) in C₆D₆ (0.5 mL) at 23 °C for 24 h unless otherwise specified. ^bDetermined by crude ¹H NMR based on an internal standard 1,3,5-trimethoxybenzene (0.1 mmol). ^cCrude yields after another 8 h-reaction with additional HBpin (1 equiv). ^d22% of the piperidin-N-tosyl-2-imine bearing a C(sp³)-B bond in the 4 (**G'**) or 3 (**R'**) position was obtained as a mixture upon the reaction with TsN₃ following the Rh catalysis in one-pot. ^e3 equivalents of HBpin applied. ^fAt 50 °C. Crude yields in 4 h^g, 10 h^h, and 16 hⁱ.

III. ¹H NMR for Entry 1 in Table 1 (Crude yields of A, B, G, and R)



In glove box, HBpin (0.8 mmol, 2 equiv) was added to a solution of bis(1,5-cyclooctadiene)-dirhodium(I) dichloride (0.008 mmol, 2 mol%) and triphenylphosphine (0.016 mmol, 4 mol%) in deuterated benzene (0.5 mL) in a 5 mL screw-cap vial. After shaking briefly, pyridine (0.4 mmol) was added to the above solution, and the whole mixture solution was carefully transferred to a medium-walled J. Young NMR tube to conduct the catalytic reaction at 23 °C for 24 h. At the end of the catalytic reaction, an internal standard 1,3,5-

trimethoxybenzene (0.1 mmol) was added to calculate the crude ^1H NMR yields of **1,2-DHP** (<1%), **1,4-DHP** (21%), **G** (50%), and **R** (11%). After measuring the ^1H NMR, another HBpin (0.4 mmol, 1equiv) was added into the catalytic reaction mixture to react at 23 °C for another 8 h. Then, the crude ^1H NMR yields of each products were determined on the basis of the internal standard: **1,2-DHP** (<1%), **1,4-DHP** (20%), **G** (51%), and **R** (12%).

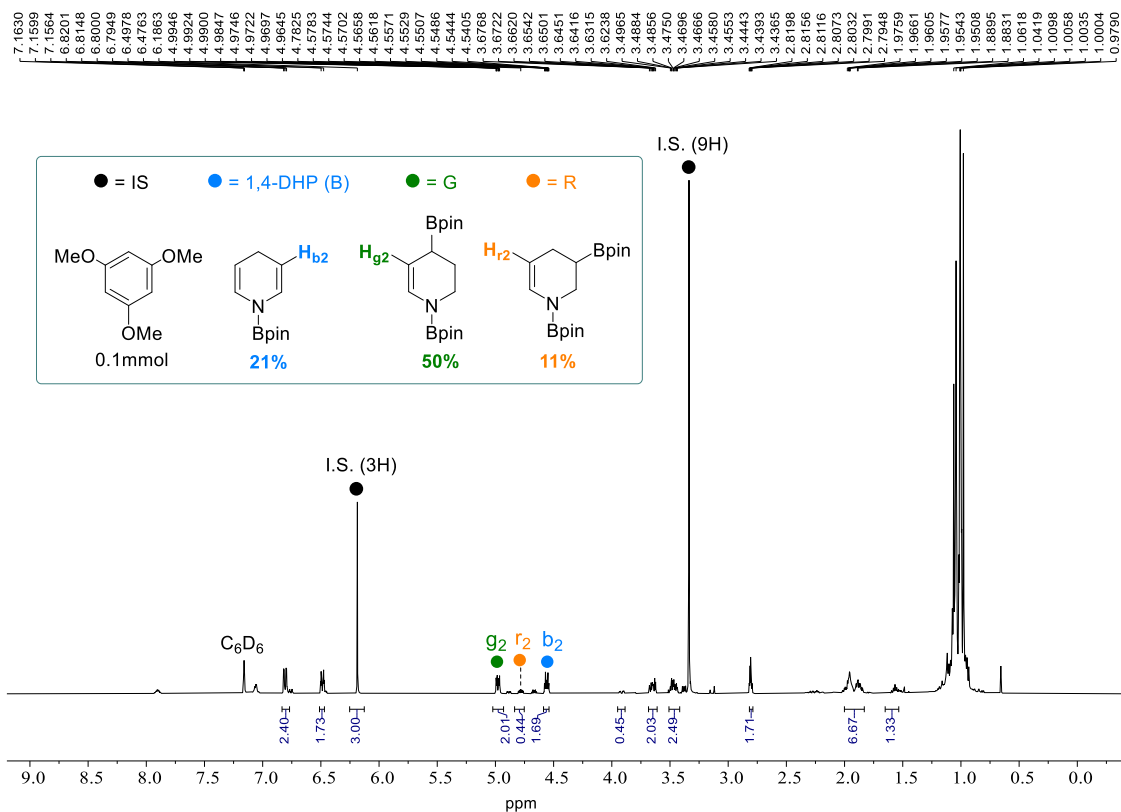


Fig. S1 ^1H NMR spectrum of the crude reaction mixture for entry 1 in Table 1.

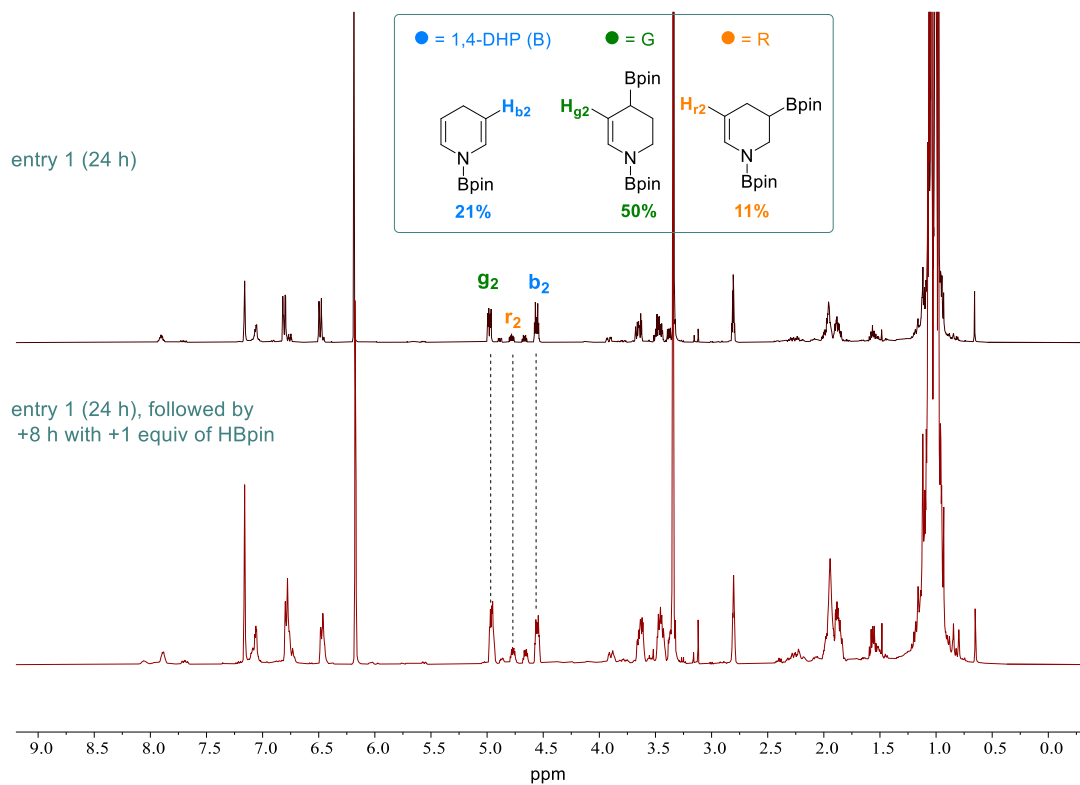
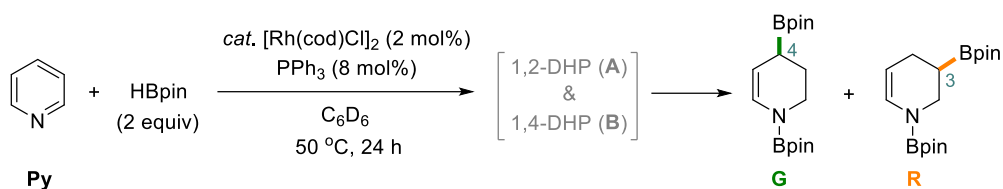
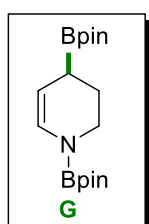


Fig. S2 Overlay of two ^1H NMR spectra for entry 1 in Table 1.

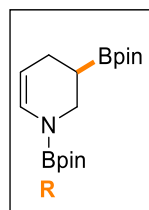
IV. Full NMR Assignments of G and R (Table S1, entry 10)



In glove box, HBpin (0.8 mmol, 2 equiv) was added to a solution of bis(1,5-cyclooctadiene)-dirhodium(I) dichloride (0.008 mmol, 2 mol%) and triphenylphosphine (0.032 mmol, 8 mol%) in deuterated benzene (0.5 mL) in a 5 mL screw-cap vial. After shaking briefly, pyridine (0.4 mmol) was added to the above solution, and the whole mixture solution was carefully transferred to a medium-walled J. Young NMR tube to conduct the catalytic reaction at 50 °C for 24 h. At the end of the reaction, an internal standard 1,3,5-trimethoxybenzene (0.1 mmol) was added to directly calculate the crude ^1H NMR yields of reduction products. The mass of **G/R** from the crude mixture was confirmed by both Bruker MALDI-TOF and Shimadzu GC mass spectrometers. **MALDI-TOF**: Calculated for $\text{C}_{17}\text{H}_{32}\text{B}_2\text{NO}_4$ $[\text{M}+\text{H}]^+$: 336.2517, Found: 336.0582. **GC-MS (EI mode)**: Calculated for $\text{C}_{17}\text{H}_{31}\text{B}_2\text{NO}_4$ $[\text{M}]^+$: 335.2439, Found: 335.2500.



Crude yield: 50%; ^1H NMR (400 MHz, C_6D_6) δ 6.71 (d, $J = 8.1$ Hz, 1H), 4.90 (dd, $J = 8.1, 3.3$ Hz, 1H), 3.68 – 3.50 (m, 1H), 3.48 – 3.22 (m, 1H), 1.96 – 1.81 (m, 3H), 1.12 – 0.91 (m, 24H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, C_6D_6) δ 128.82, 102.01, 82.67, 43.46, 24.69, 24.17, 18.53; ^{11}B NMR (128 MHz, C_6D_6) δ 33.67, 23.79.



Crude yield: 47%; ^1H NMR (400 MHz, C_6D_6) δ 6.71 (d, $J = 8.1$ Hz, 1H), 4.73 (ddd, $J = 7.9, 4.6, 3.0$ Hz, 1H), 3.83 (ddd, $J = 12.4, 3.4, 1.3$ Hz, 1H), 3.50 – 3.18 (m, 1H), 2.34 – 2.09 (m, 2H), 1.57 – 1.30 (m, 1H), 1.12 – 0.91 (m, 24H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, C_6D_6) δ 128.82, 101.88, 82.67, 41.93, 24.69, 23.68, 18.59; ^{11}B NMR (128 MHz, C_6D_6) δ 33.67, 23.79.

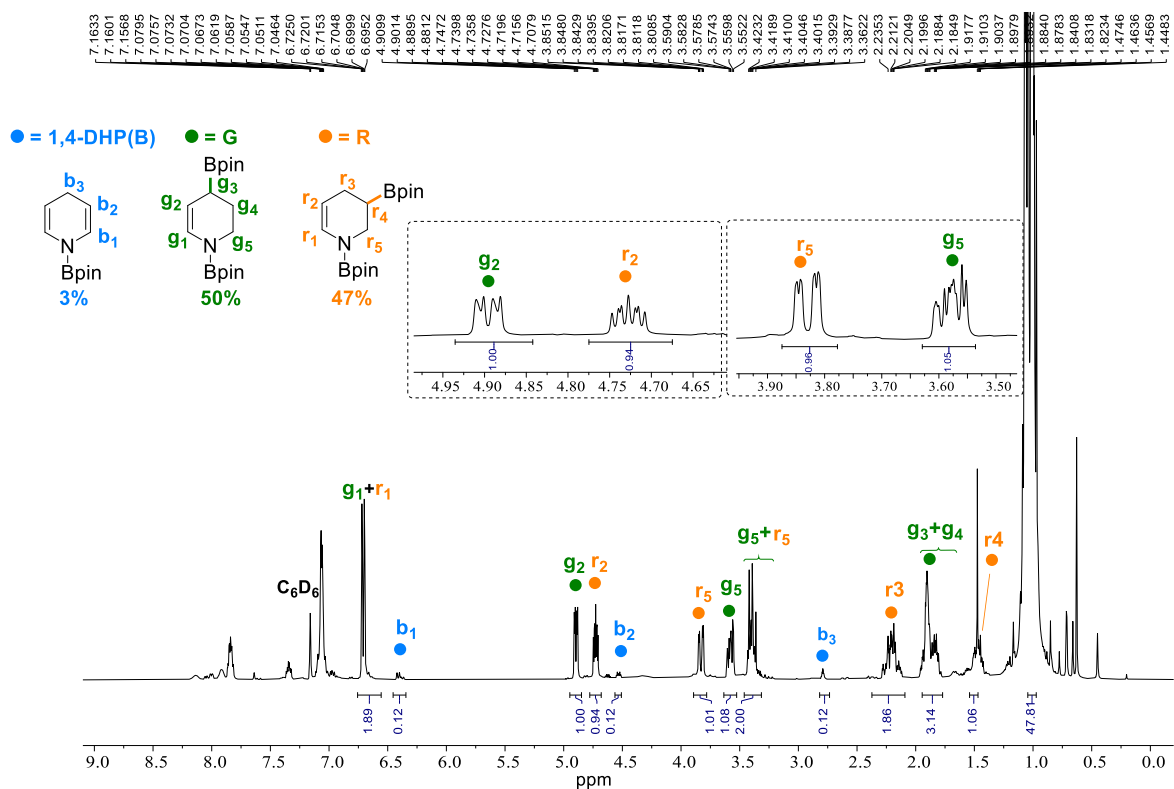


Fig. S3 ¹H NMR spectrum of the crude reaction mixture for entry 10 in Table S1.

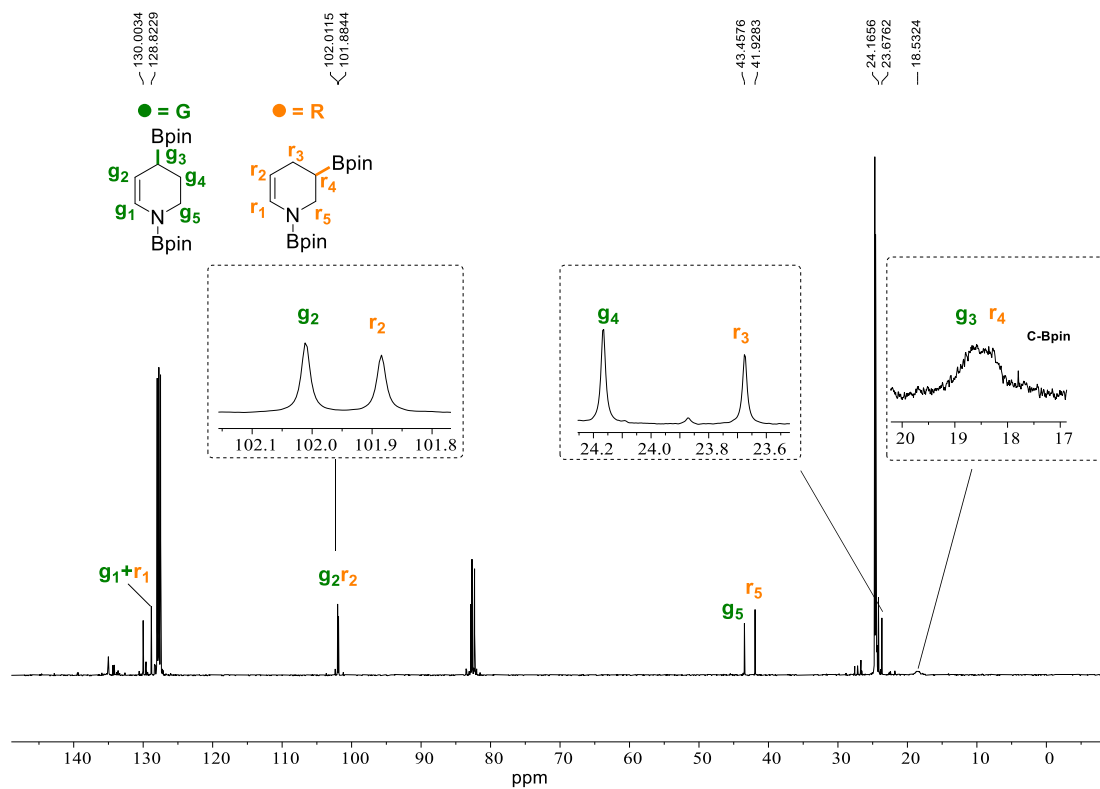


Fig. S4 ¹³C{¹H} NMR spectrum of the crude reaction mixture for entry 10 in Table S1.

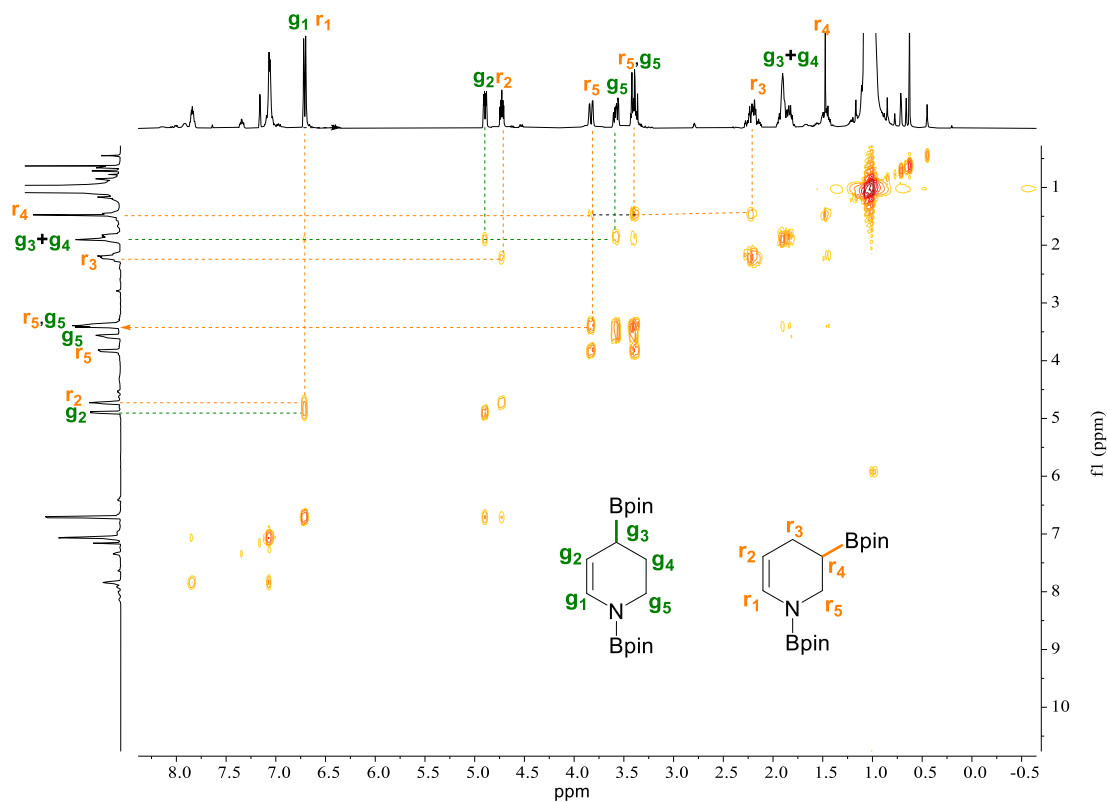


Fig. S5 ^1H - ^1H COSY spectra of the crude reaction mixture for entry 10 in Table S1.

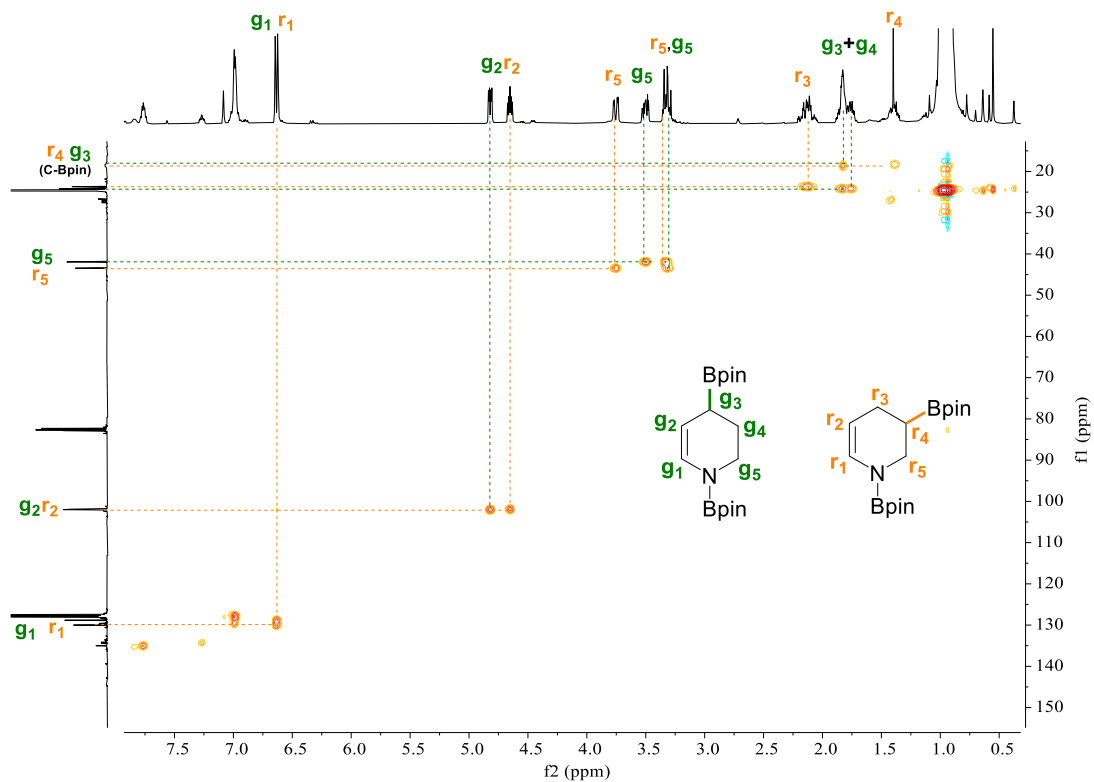


Fig. S6 ^1H - ^{13}C HSQC spectra of the crude reaction mixture for entry 10 in Table S1.

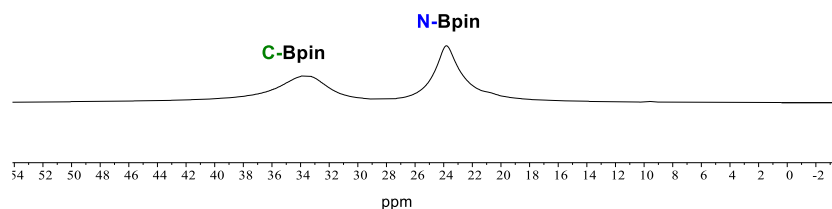
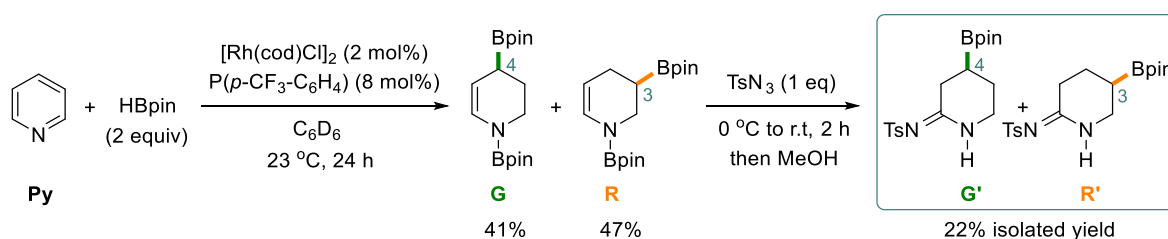


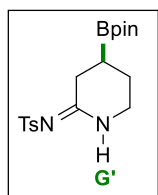
Fig. S7 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of the crude reaction mixture for entry 10 in Table S1.

V. Generation of **G'** and **R'** in One-Pot (Table 1, entry 3)^{S1}

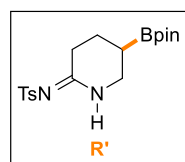


The catalytic reaction procedure using tris(4-trifluoromethylphenyl)phosphine as a ligand was the same as described in the general procedure (*vide supra*). To the resulting mixture containing **G** (41%) and **R** (47%) was added tosyl azide (0.4 mmol, 1.0 equiv) at 0 °C, which was then warmed up to r.t. to react for 2 h. After being quenched with MeOH, the solvent was removed under reduced pressure and the crude products were purified by column chromatography on silica gel to give the mixture of **G'** and **R'** as a colorless solid in 22% (34 mg) of the combined isolated yield. **G'** and **R'** could not be clearly and completely separated due to their similar polarities.

One-pot gram-scale double hydroboration-amidation: In glove box, HBpin (36 mmol, 3 equiv) was added to a solution of bis(1,5-cyclooctadiene)dirhodium(I) dichloride (0.048 mmol, 0.4 mol%) and $\text{P}(p\text{-CF}_3\text{-C}_6\text{H}_4)_3$ (0.096 mmol, 0.8 mol%) in benzene (10 mL) in a 20 mL screw-cap vial. After shaking briefly, pyridine (12 mmol, 1 equiv) was added to the above solution, and the whole mixture solution was stirred at 23 °C for 40 h. After that, all volatiles from the crude mixture were removed under reduced pressure, followed by adding CH_2Cl_2 (10 mL) and subsequently tosyl azide (24 mmol, 2 equiv) at 0 °C. The resulting solution was warmed up to r.t. and reacted overnight. After being quenched with MeOH (~5 mL), the solvent was removed under reduced pressure and the crude products were purified by column chromatography on silica gel to give the mixture of **G'** and **R'** in 21% (0.95 g) of the combined isolated yield.



$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.53 (s, 1H), 7.78 (d, $J = 8.3$ Hz, 2H), 7.24 (d, $J = 8.3$ Hz, 2H), 3.37–3.43 (m, 1H), 3.26–3.33 (m, 1H), 2.52–2.58 (m, 1H), 2.38–2.44 (m, 4H), 1.94–1.82 (m, 1H), 1.77–1.58 (m, 1H), 1.33 (m, 1H), 1.19 (s, 12H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.34, 142.38, 140.12, 129.22, 129.08, 126.24, 83.77, 77.38, 77.26, 77.06, 76.74, 42.69, 32.23, 24.86, 24.71, 24.69, 24.60, 22.83, 21.47, 14.96; $^{11}\text{B NMR}$ (128 MHz, CDCl_3) δ 33.00; **MALDI-TOF:** Calculated for $\text{C}_{18}\text{H}_{27}\text{BKN}_2\text{O}_4\text{S}$ $[\text{M}+\text{K}]^+$: 417.1422, Found: 417.0321.



$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.52 (s, 1H), 7.78 (d, $J = 8.3$ Hz, 2H), 7.25 (d, $J = 8.1$ Hz, 2H), 3.50–3.39 (m, 1H), 3.39–3.28 (m, 1H), 2.59–2.47 (m, 1H), 2.46–2.33 (m, 4H), 1.96–1.84 (m, 1H), 1.64 (m, 1H), 1.35 (m, 1H), 1.20 (s, 12H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.16, 142.45, 140.04, 129.25, 126.28, 83.90, 43.88, 31.20, 24.74, 24.69, 21.47, 21.09, 17.47. $^{11}\text{B NMR}$ (128 MHz, CDCl_3) δ 33.19; **MALDI-TOF:** Calculated for $\text{C}_{18}\text{H}_{27}\text{BKN}_2\text{O}_4\text{S}$ $[\text{M}+\text{K}]^+$: 417.1422, Found: 417.0359.

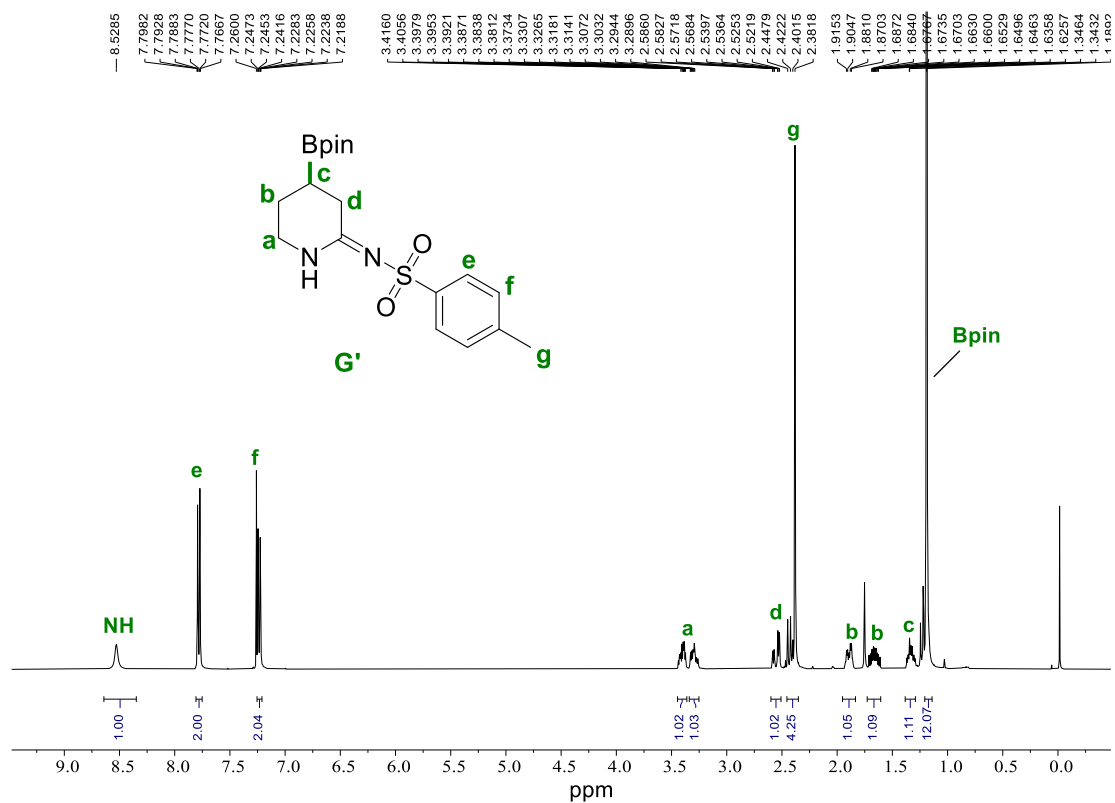


Fig. S8 ^1H NMR spectrum of the product **G'** after chromatographic purification on silica-gel.

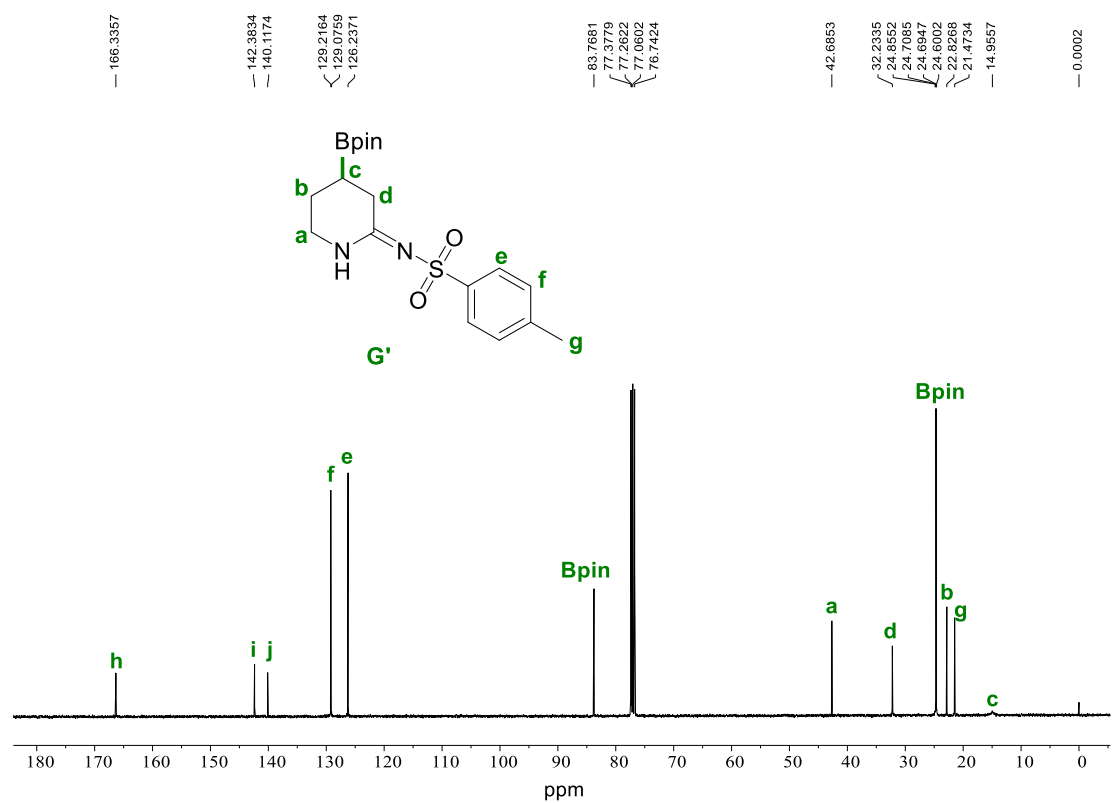


Fig. S9 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the product **G'** after chromatographic purification on silica-gel.

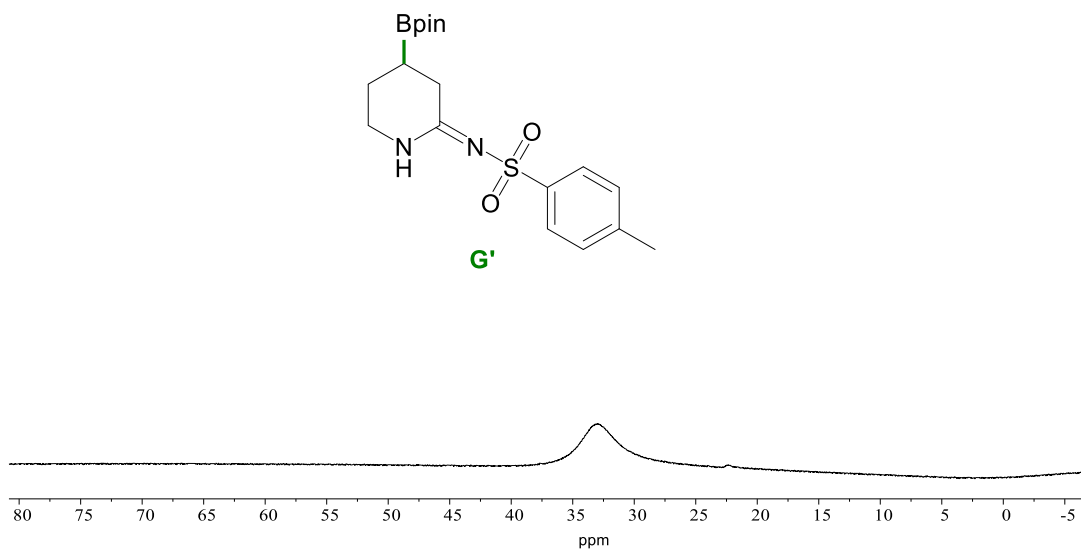


Fig. S10 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of the product **G'** after chromatographic purification on silica-gel.

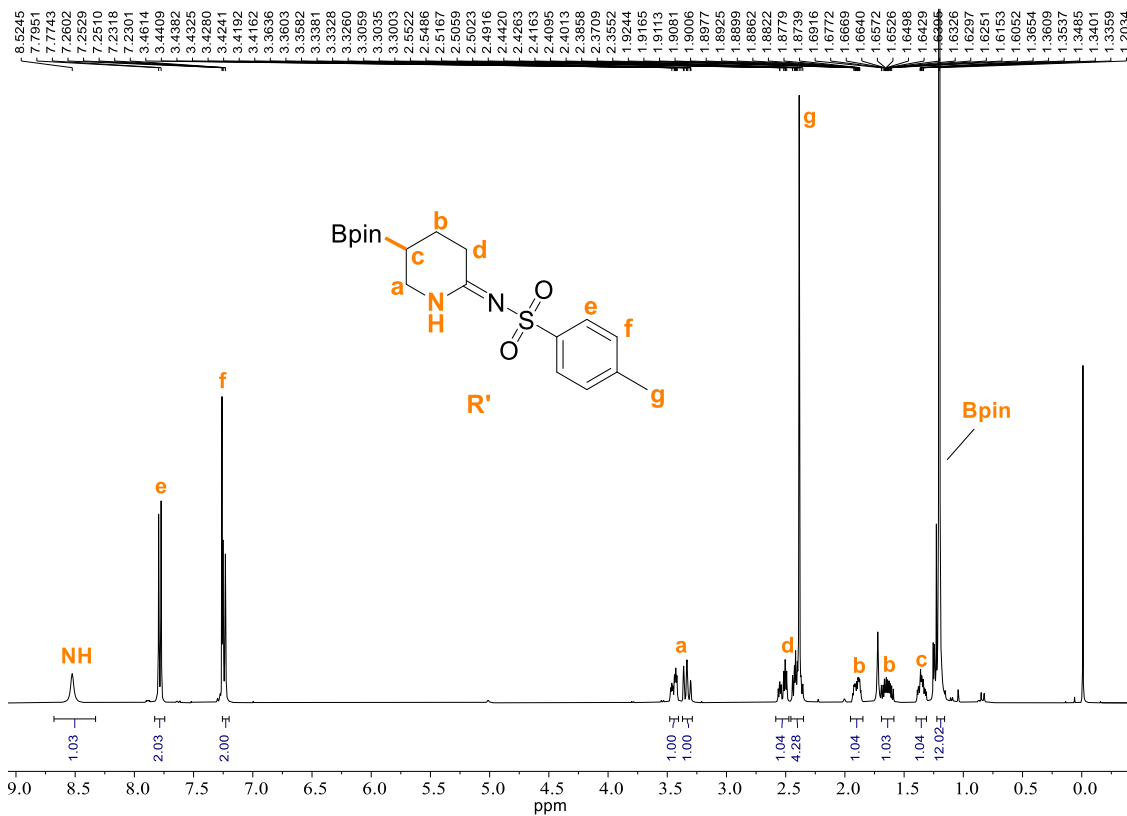


Fig. S11 ^1H NMR spectrum of the product **R'** after chromatographic purification on silica-gel.

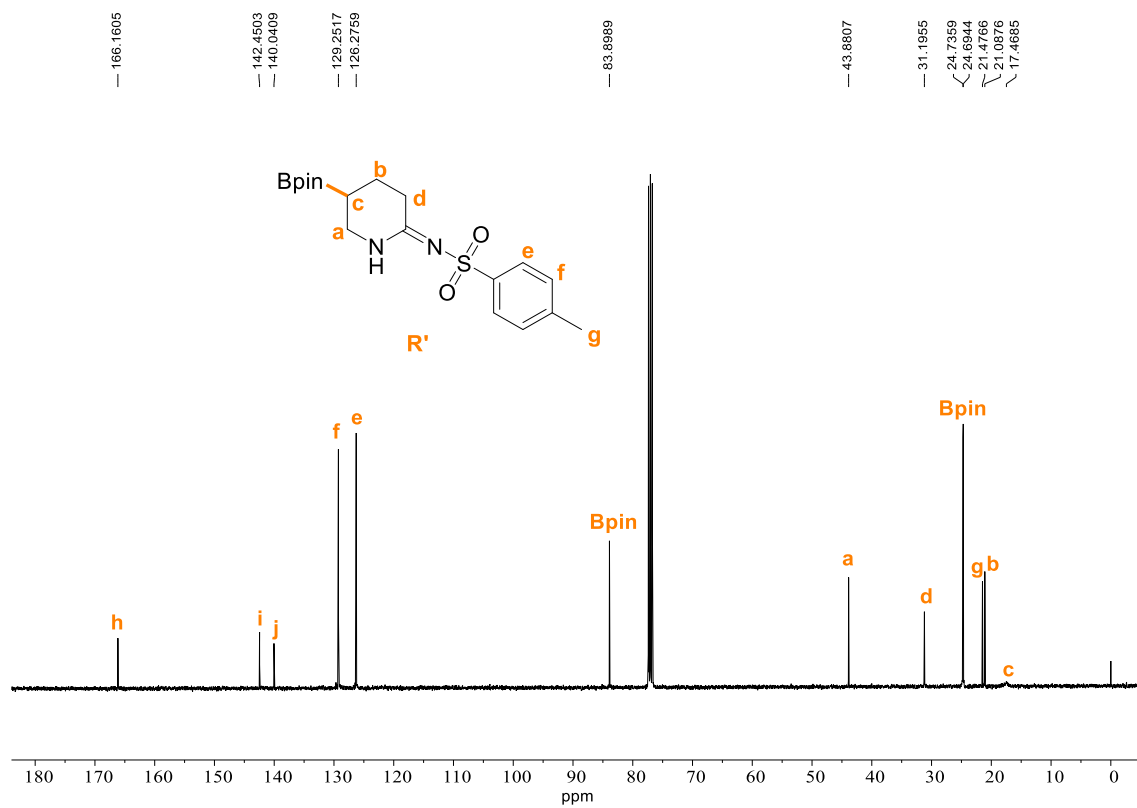


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the product **R'** after chromatographic purification on silica-gel.

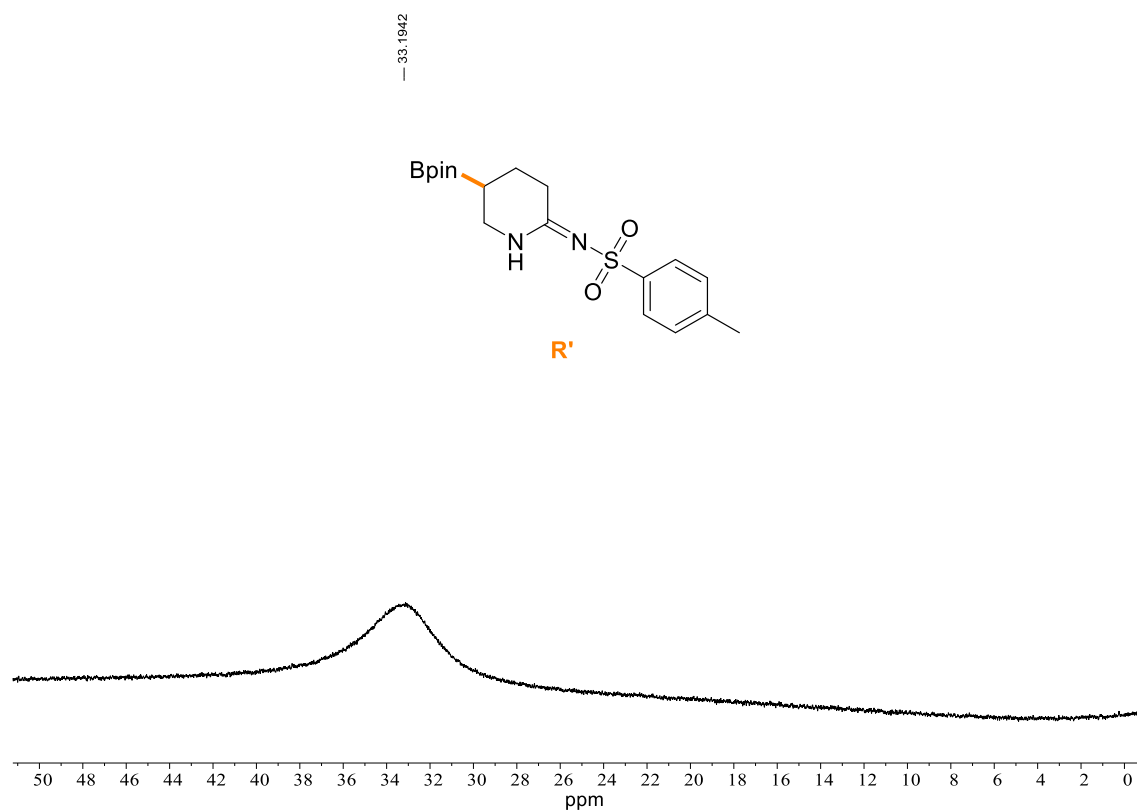
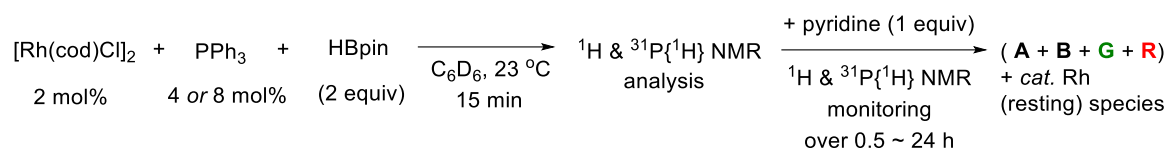


Fig. S13 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of the product **R'** after chromatographic purification on silica-gel.

VI. Mechanistic Experiments (Fig. 1)



The catalytic reaction procedure using triphenylphosphine as a ligand (4 or 8 mol%) was the same as described in the general procedure. For the catalysis with 4 mol% of PPh₃ (**Table 1**, entry 1), the reaction progress was monitored by ¹H and ³¹P{¹H} NMR at 0.5 h, 2 h, 6 h, and 24 h, while similarly the reaction with 8 mol% of PPh₃ ligand (**Table 1**, entry 2) was followed by ¹H and ³¹P{¹H} NMR at 2 h and 24 h. Prior to the addition of pyridine (1 equiv), the mixture of [Rh(cod)Cl]₂, PPh₃, and HBpin was analyzed by ¹H and ³¹P{¹H} NMR within 15 min. The known species Rh(cod)(PPh₃)Cl [**Rh(I)**]^{S2} and (*trans*-PPh₃)₂RhCl(H)(Bpin) [**Rh(III)**]^{S3} were clearly observed. The species **Rh(III)** completely disappeared in both ¹H and ³¹P NMR within 0.5 h upon the addition of pyridine (1 equiv), while instead, new peaks assignable to an isomeric mixture of the Rh(III) coordinating to pyridine molecule(s) [**Rh(III)-Py**] (Py = pyridine) were observed in ¹H NMR spectra (at δ -16.5 and -17.1 as broad singlets) (**Table 1**, entries 1 and 2). The two broad hydride peaks assigned to [**Rh(III)-Py**] completely disappeared upon addition of another 1 equiv HBpin after the 24 h-reaction where pyridine was quantitatively consumed out to be the hydroboration products (**Table 1**, entry 2).

VI-1. ¹H NMR monitoring of the catalytic reaction (Fig. 1)

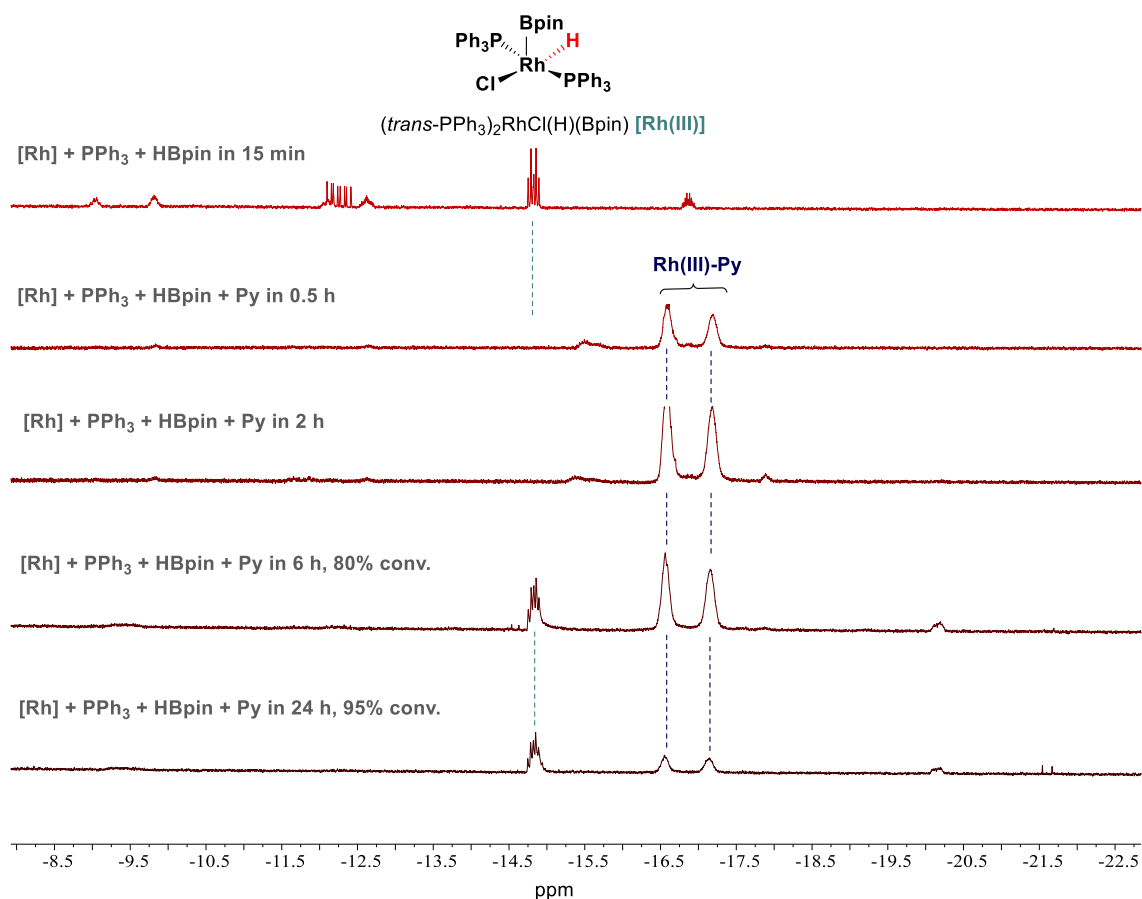


Fig. S14 Overlay of the Rh-H region of the ¹H NMR spectra at variable reaction times (**Table 1**, entry 1; P/Rh = 1).

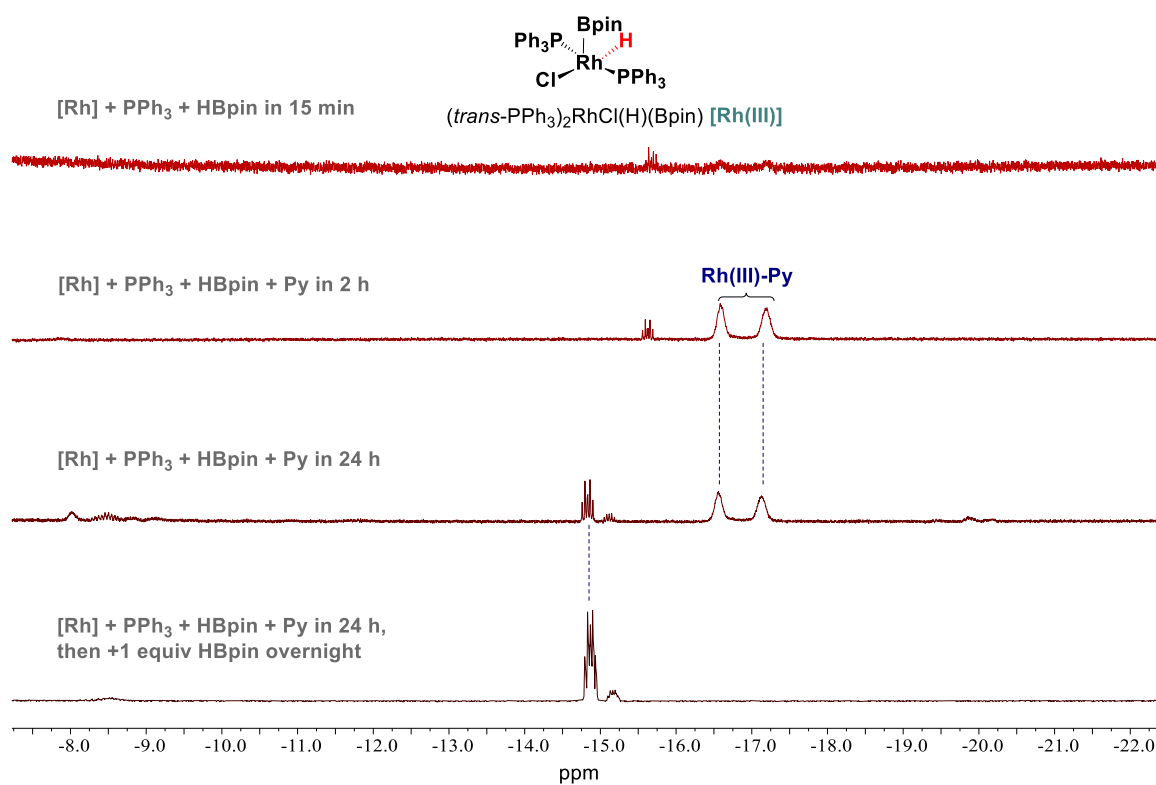


Fig. S15 Overlay of the Rh–H region of the ¹H NMR spectra at variable reaction times (Table 1, entry 2; P/Rh = 2).

VI -2. ³¹P{¹H} NMR monitoring of the catalytic reaction (Fig. 1)

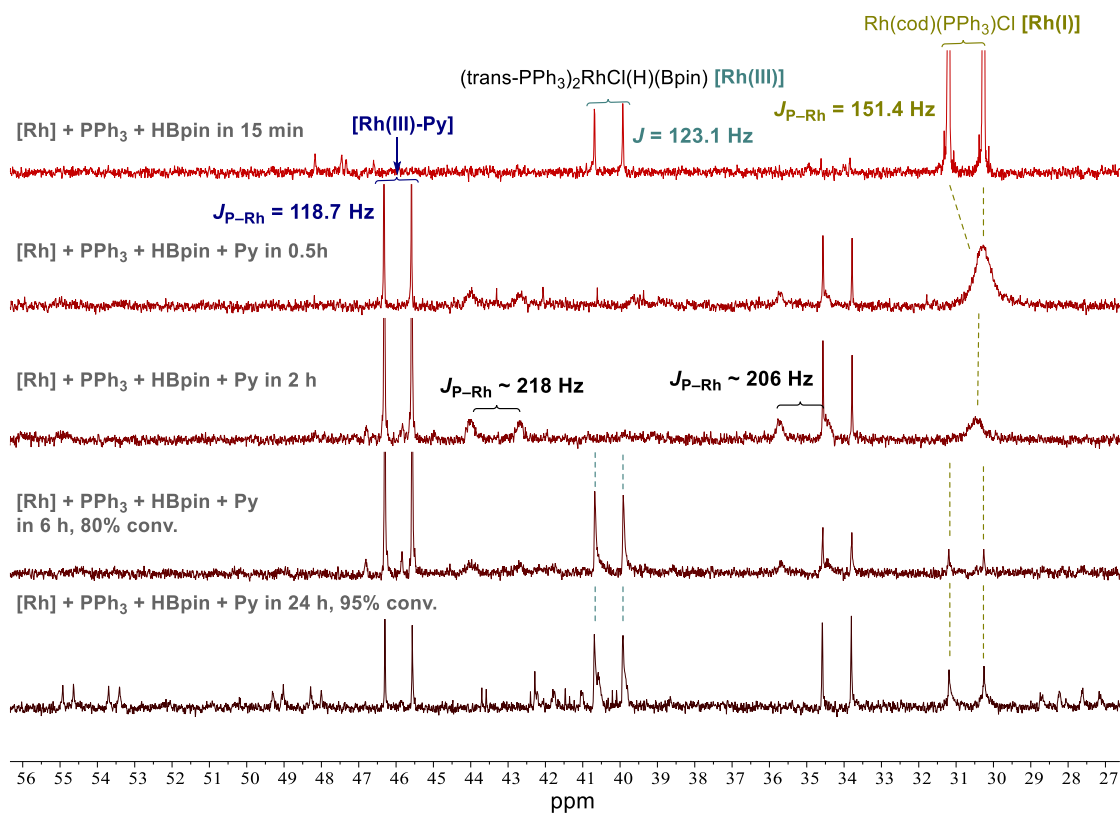


Fig. S16 Overlay of the ³¹P{¹H} NMR spectra at variable catalytic reaction times (Table 1, entry 1; P/Rh = 1)

VI -3. Variable-temperature ^1H NMR of the catalytic solution (Fig. 1)

The catalytic reaction conditions were modified from the standard conditions of entry 1 in Table 1 for the mechanistic study purpose – two-folds loadings of the Rh precatalyst and PPh_3 ligand. The ^1H , $^{31}\text{P}\{^1\text{H}\}$ NMR, and ^1H - ^{31}P gHMBC^{S4} optimized for $^n\text{J}_{\text{P-H}}$ of 100 Hz were measured over the catalytic reaction solution at 1 h at 23 °C. Then, $^{31}\text{P}\{^1\text{H}\}$ NMR was immediately taken at 50 °C within 0.5 h. As a result, the two Rh hydride peaks in the ^1H NMR were found to correlate with the ^{31}P peak at δ 46 (at 23 °C) and coalesce into a broad single peak (*ca.* δ -17.0) at 50 °C.

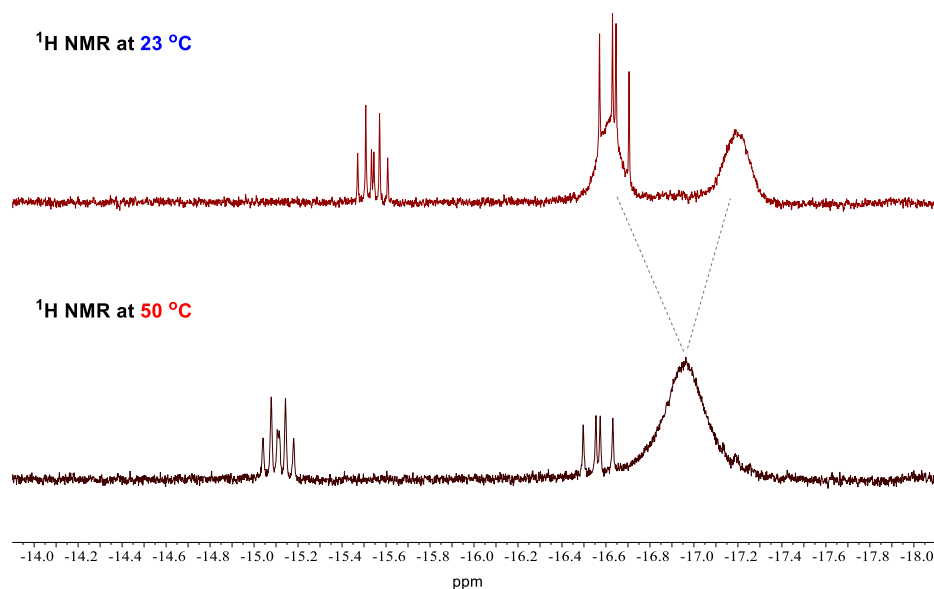


Fig. S17 Overlay of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra at 23 °C (in 1 h) and then 50 °C within 0.5 h.

VI -4. ^1H - ^{31}P two-dimensional correlation NMR of the catalytic solution (Fig. 1)

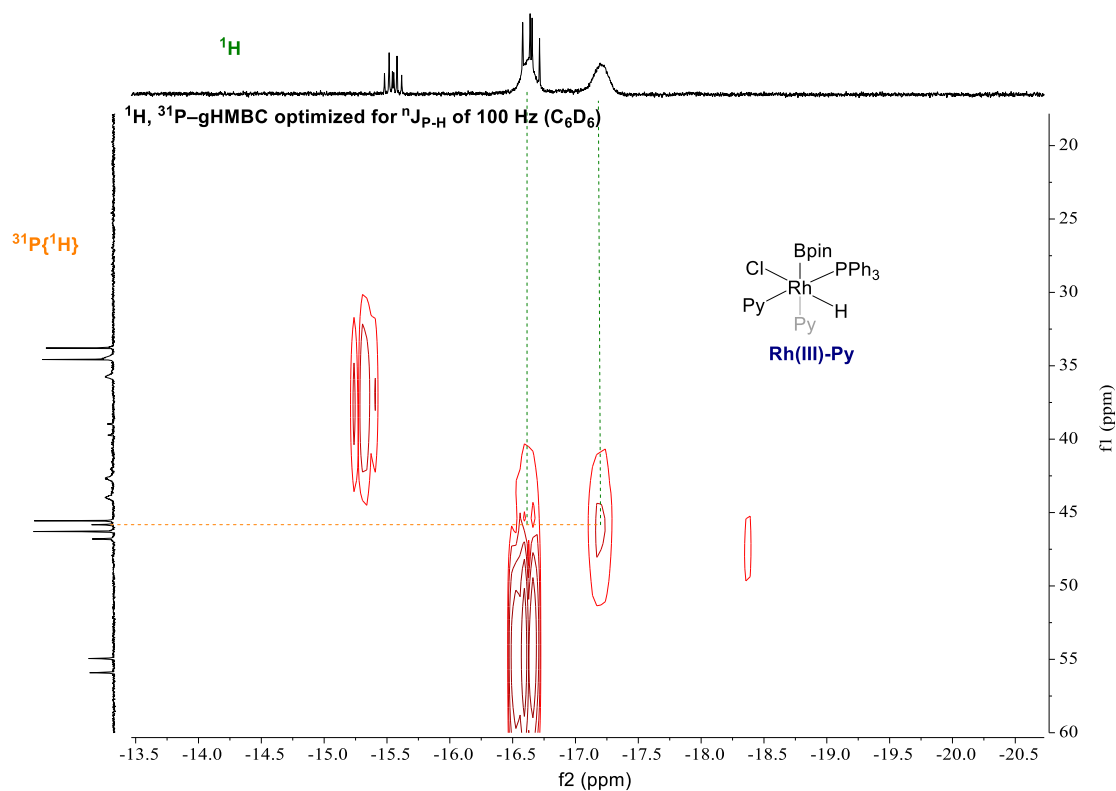


Fig. S18 The ^1H - ^{31}P gHMBC correlation between Rh-H and Rh-PPh₃ moieties.

VI-5. MALDI-TOF Mass analysis of the catalytic solution (Fig. 1)

The catalytic solution for MALDI-TOF Mass measurement was prepared according to the general procedure using $P(p\text{-CF}_3\text{-C}_6\text{H}_4)_3$ as a phosphine ligand (Table 1, entry 3). An aliquot of the catalytic reaction solution at 4 h was subjected for the MALDI-TOF analysis. The Rh species bearing two pyridine molecules and a single phosphine [$\text{PAr}_3 = P(p\text{-CF}_3\text{-C}_6\text{H}_4)_3$] in addition to Bpin and Cl ligands, was identified.

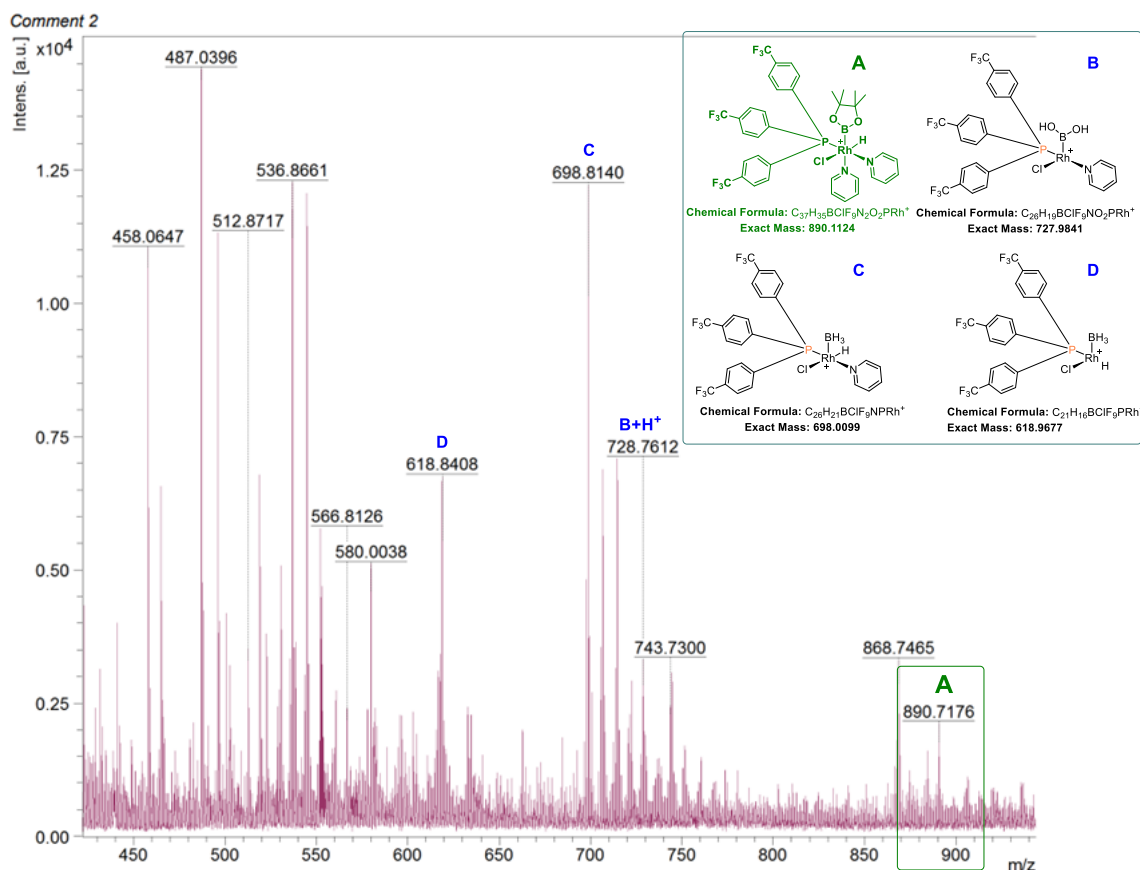
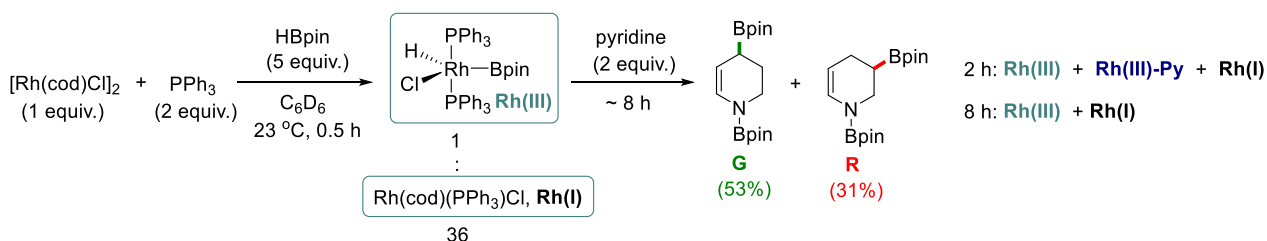


Fig. S19 MALDI-TOF spectrum of the catalytic reaction solution at 4 h (Fig. 1).

VI-6. ^1H NMR monitoring of the stoichiometric reaction (Fig. 2a-b)



In glove box, bis(1,5-cyclooctadiene)-dirhodium(I) dichloride (0.032 mmol, 1 equiv) and triphenylphosphine (0.128 mmol, 2 equiv) in deuterated benzene (0.5 mL) were mixed in a J. Young NMR tube. Then, HBpin (0.16 mmol, 5 equiv) was added to the catalyst solution to react for 0.5 h at 23 °C. After measuring the ^1H and ^{31}P NMR, pyridine (0.128 mmol, 2 equiv) was then added to the above reaction solution. This reaction mixture was subjected to ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR monitoring over 8 h at 23 °C. The identical Rh species were also observed in this stoichiometric reaction as observed in the catalytic reaction, e.g. [Rh(I)], [Rh(III)], and [Rh(III)-Py]. The signals due to the pyridine adduct [Rh(III)-Py] completely disappeared upon quantitative conversion of pyridine in 8 h.

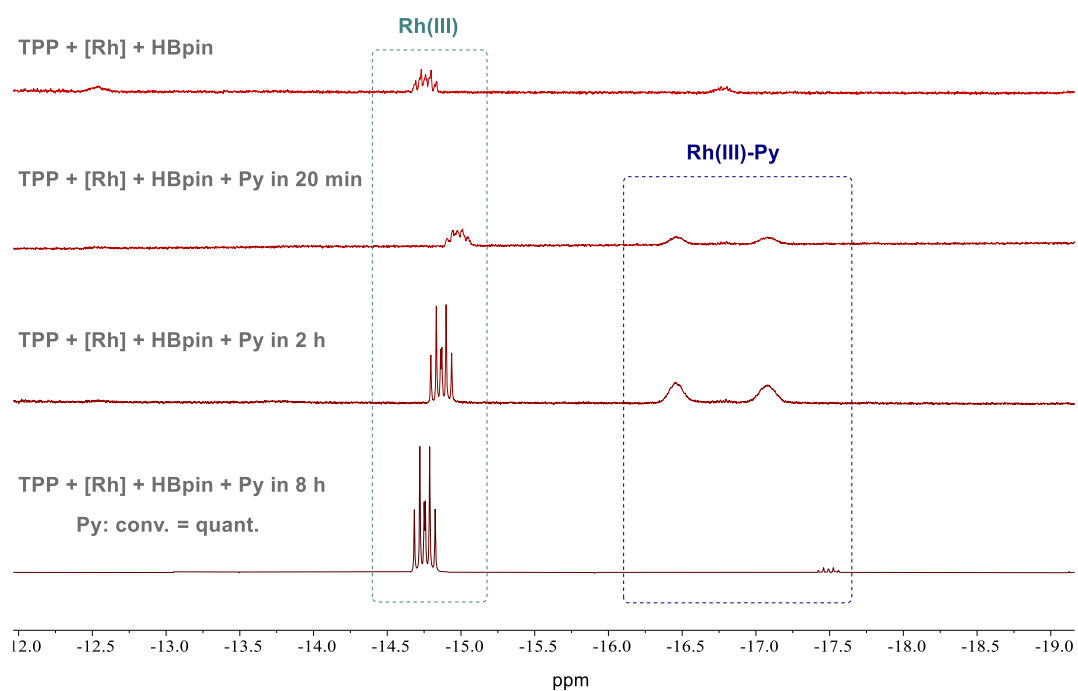


Fig. S20 Overlay of the Rh-H region of the ^1H NMR spectra at variable reaction times of the stoichiometric reaction.

VI -7. $^{31}\text{P}\{^1\text{H}\}$ NMR monitoring of the stoichiometric reaction (Fig. 2c-d)

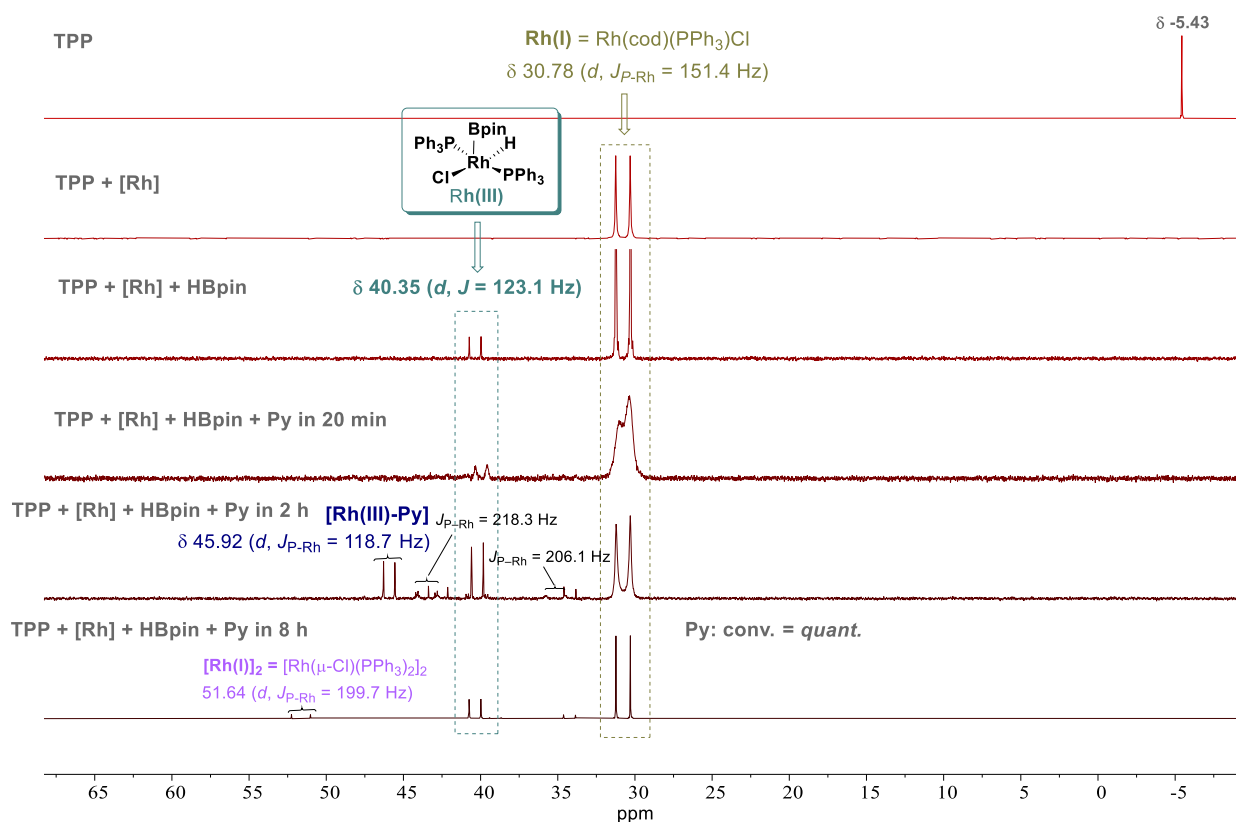


Fig. S21 Overlay of the $^{31}\text{P}\{^1\text{H}\}$ NMR spectra at variable stoichiometric reaction times.

VII. Density Functional Theory (DFT) Calculations

VII-1. Computational details

All calculations were carried out using DFT^{SS} as implemented in the Jaguar 9.1 suite^{S6} of ab initio quantum chemistry programs. Geometry optimizations were performed with the B3LYP including Grimme's D3 dispersion correction.^{S7} The 6-31G** basis set was used for main group atoms and Rh was represented using the Los Alamos LACVP basis set that includes relativistic effective core potentials. The energies of optimized structures were reevaluated by additional single-point calculations on each optimized geometry using Dunning's correlation consistent triple- ζ basis set cc-pVTZ(-f)^{S8} which includes a double set of polarization functions. For Rh, we used a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with the triple- ζ quality. Solvation energies were evaluated by a self-consistent reaction field (SCRF)^{S9} approach based on accurate numerical solutions of the Poisson-Boltzmann equation. In the results reported, solvation calculations were carried out at the same level of theory as the geometry optimization, employing a dielectric constant of $\epsilon = 2.284$ for benzene. As is the case for all continuum models, the solvation energies are subject to empirical parameterization of the atomic radii that are used to generate the solute surface. We employed the standard set of Van der Waals radii in Jaguar for H(1.150 Å), B(2.042 Å), C(1.900 Å), N(1.600 Å), O(1.600 Å), P(2.074 Å), Cl(1.974 Å) and Rh(1.464 Å).^{S10} Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP basis to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. The intermediates were confirmed with no imaginary frequency, while transition states showed a single imaginary frequency.

The energy components have been computed with the following protocol. The free energy in solution-phase, $G(\text{sol})$, has been calculated as follows, with $T = 298.15$ K to match the experimental conditions.

$$\begin{aligned}G^0(\text{sol}) &= G^0(\text{gas}) + G^{\text{solv}} \\G^0(\text{gas}) &= H(\text{gas}) - TS(\text{gas}) \\H(\text{gas}) &= E(\text{SCF}) + \text{ZPE} \\ \Delta E(\text{SCF}) &= \sum E(\text{SCF}) \text{ for products} - \sum E(\text{SCF}) \text{ for reactants} \\ \Delta G^0(\text{sol}) &= \sum G^0(\text{sol}) \text{ for products} - \sum G^0(\text{sol}) \text{ for reactants}\end{aligned}$$

VII-2. Inner-sphere pathway from **1b**

To generate dihydropyridine from pyridine, the dearomatization of pyridine is necessarily required in the reaction including C–H bond and N–B bond formation. Initially, we considered the inner-sphere hydride transfer to the C2-site of coordinated pyridine in **1b** as proposed by Suginome^{S11} (Fig. S22, pink dashed line), however it was discarded showing a prohibitive barrier of over 31.1 kcal/mol.

We also investigated the pathway forming a Lewis acid-base adduct **2** from **1b**. As illustrated in the gray dashed line, the coordinated pyridine in **1b** is migrated from Rh(III) to Bpin, rendering another Lewis acid–base adduct **1c** more unstable than the adduct **1b**. It is attributed by the weaker interaction of the nitrogen lone pair of pyridine with the empty p orbital of B rather than that with the empty d orbital of Rh(III).^{S12} The reductive elimination via **1c-TS** with a barrier of 15.2 kcal mol⁻¹ regenerates the original H–B bond with Rh(I) catalyst in **2**. Given these calculated results in which the pyridine migration transition state (**1b-TS**) is higher than oxidative coupling (**2-TS**), we concluded the pathway for direct formation of **2** from **1** would be faster.

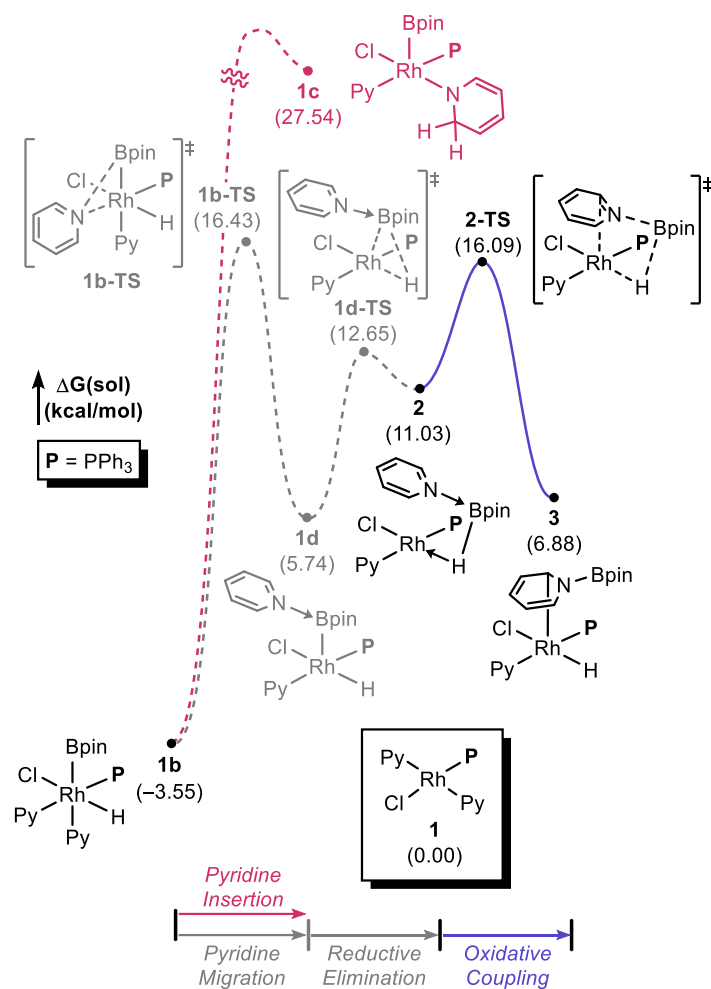


Fig. S22 The DFT-calculated energy profile for dearomatization initiated by hydride insertion (pink dashed line) and dearomatization initiated by pyridine migration from **1b** (gray dashed line).

VII-3. Reductive elimination from 3 without dissociating pyridine

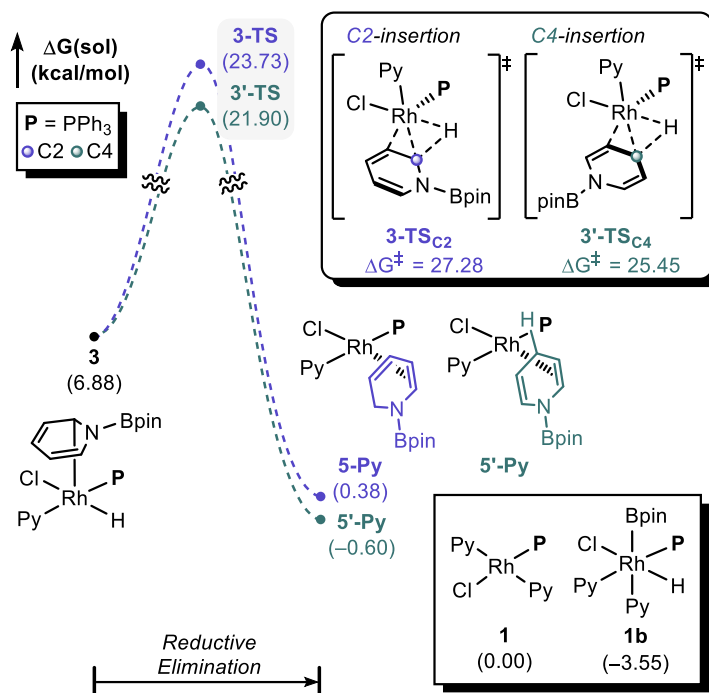


Fig. S23 The DFT-calculated energy profile for reductive elimination from 3.

VII-4. Detailed analysis on regioselective reductive elimination in the 1st-hydroboration

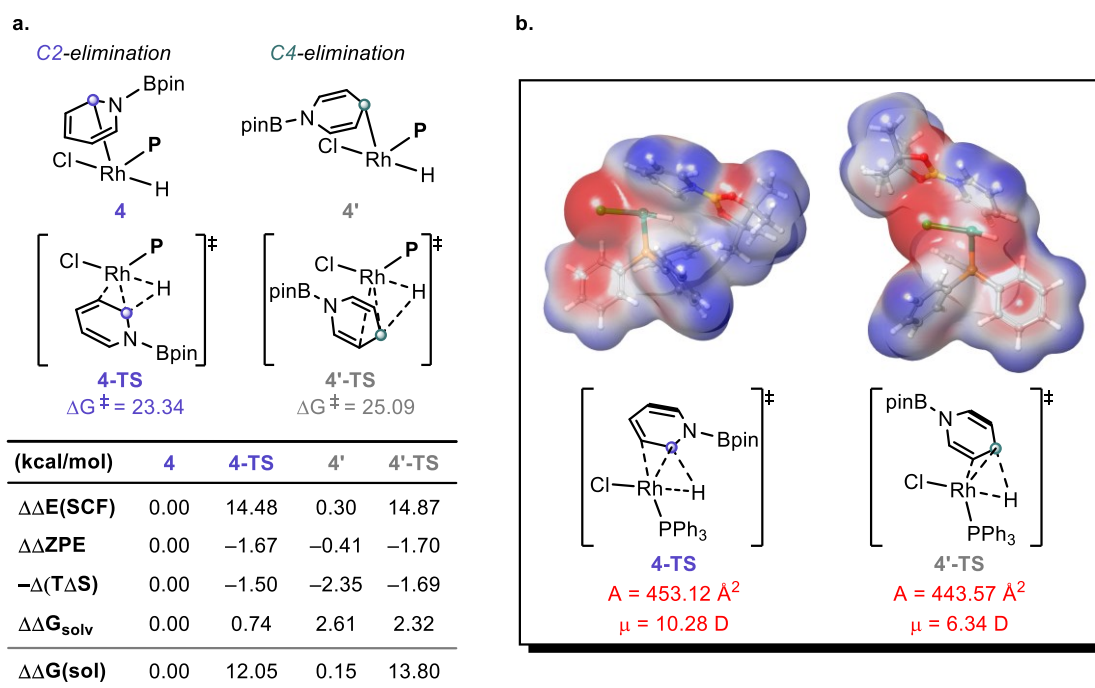


Fig. S24 (a) The free energy decomposition of the intermediates and transition states for the 1st reductive elimination with the intermediates 4 as a reference, and (b) the electrostatic potential maps of 4-TS and 4'-TS with surface areas and dipole moments.

A detailed comparison of energy components indicated that the energy difference between **4-TS** and **4'-TS** ($\Delta\Delta G^\ddagger$) mainly arises from the solvation energy ($\Delta\Delta G_{\text{solv}} = 1.58 \text{ kcal mol}^{-1}$, see Fig. S24†). Accordingly, the structural property of two regioisomers was evaluated, indicating that the greater solvation energy of **4-TS** is reflected by its larger surface area presumably because the bulky BPin moiety has spatially more deviated from the center of its 3D structure; 453.12 \AA^2 of **4-TS** and 443.57 \AA^2 of **4'-TS**. It is noteworthy that **A** favors forming a stable η^4 -Rh complex **5** at $-0.1 \text{ kcal mol}^{-1}$.

VII-5. Detailed analysis on regioselective reductive elimination in the 2nd-hydroboration

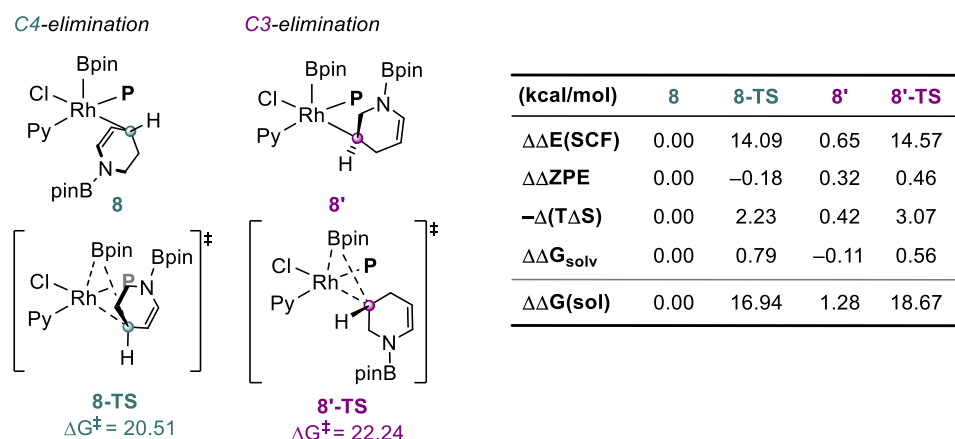


Fig. S25 Free energy decomposition of the intermediates and transition states for 2nd reductive elimination.

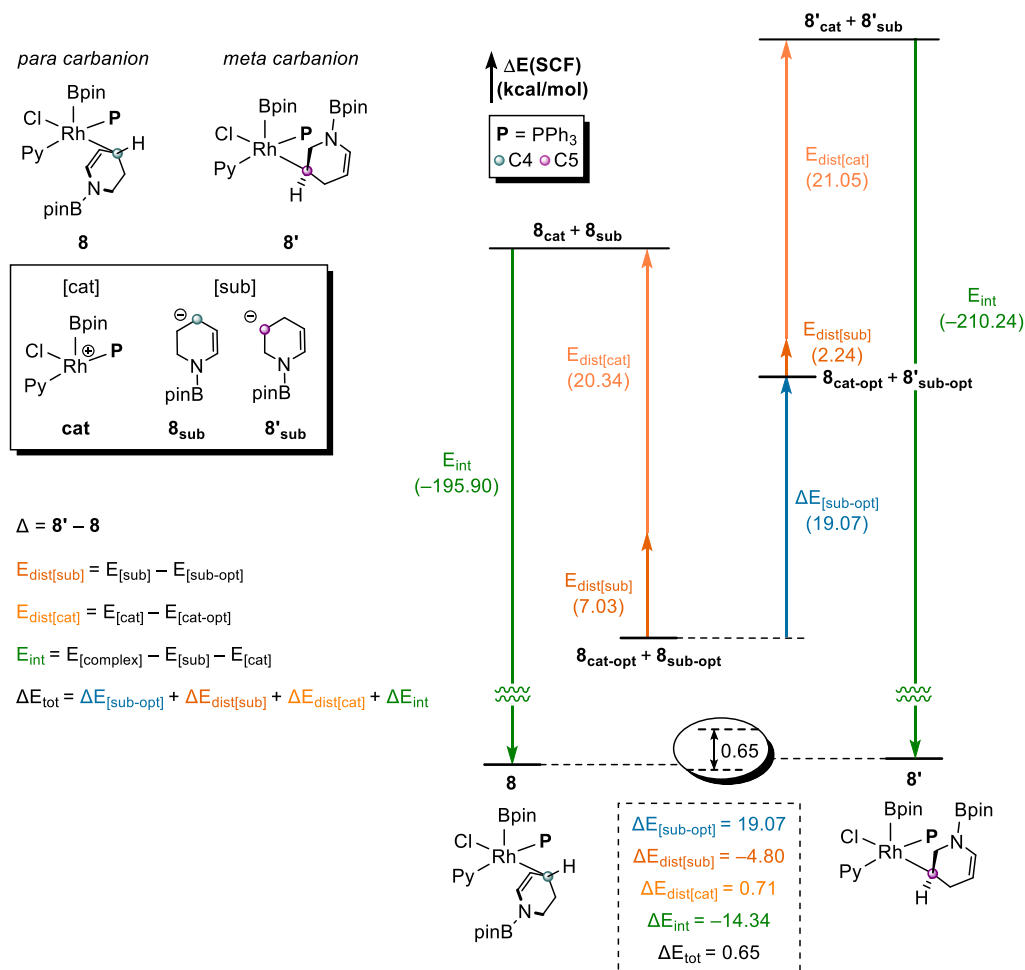


Fig. S26 Distortion interaction analysis of **8** and **8'**.

The significant difference between **8** and **8'** is the carbanion character of the substrate unit. The substrate part of **8** (para carbanion) is conjugated with the double bond (C5=C6), while the substrate part of **8'** (meta carbanion) is isolated. We hypothesized that the delocalization effect of conjugated substrates would effectively stabilize the total energy of its intermediates compared to that of the isolated substrates. To elucidate the hypothesis, we conducted the distortion interaction analysis^{S13} of the **8** and **8'**, dividing into the catalyst segment [cat] and the *N*-tetrahydropyridine segment [sub] (see Fig. S26†). We considered not only the distortion energy ($E_{\text{dist[cat]}}$ and $E_{\text{dist[sub]}}$) and interaction energy (E_{int}) of each intermediate but also the relative stability of the substrate unit ($\Delta E_{\text{[sub-opt]}}$) obtained from the structurally relaxed substrate [sub-opt]. When defining Δ , the difference between para carbanion and meta carbanion is used, and the total energy gap (ΔE_{tot}) is same as the sum of $\Delta E_{\text{dist[sub]}}$, $\Delta E_{\text{dist[cat]}}$, ΔE_{int} , and $\Delta E_{\text{[sub-opt]}}$. Comparing **8** and **8'** with *N*-Bpin-1,2,3,4-tetrahydropyridinyl (**Py**) as substrate fragment, it is appreciable that $\Delta E_{\text{[sub-opt]}}$ of 19.1 kcal mol⁻¹ significantly contributes to the positive ΔE_{tot} of 0.7 kcal mol⁻¹, despite $\Delta E_{\text{dist[sub]}}$, $\Delta E_{\text{dist[cat]}}$, and ΔE_{int} evaluated by -4.8, 0.7, and -14.3 kcal mol⁻¹, respectively.

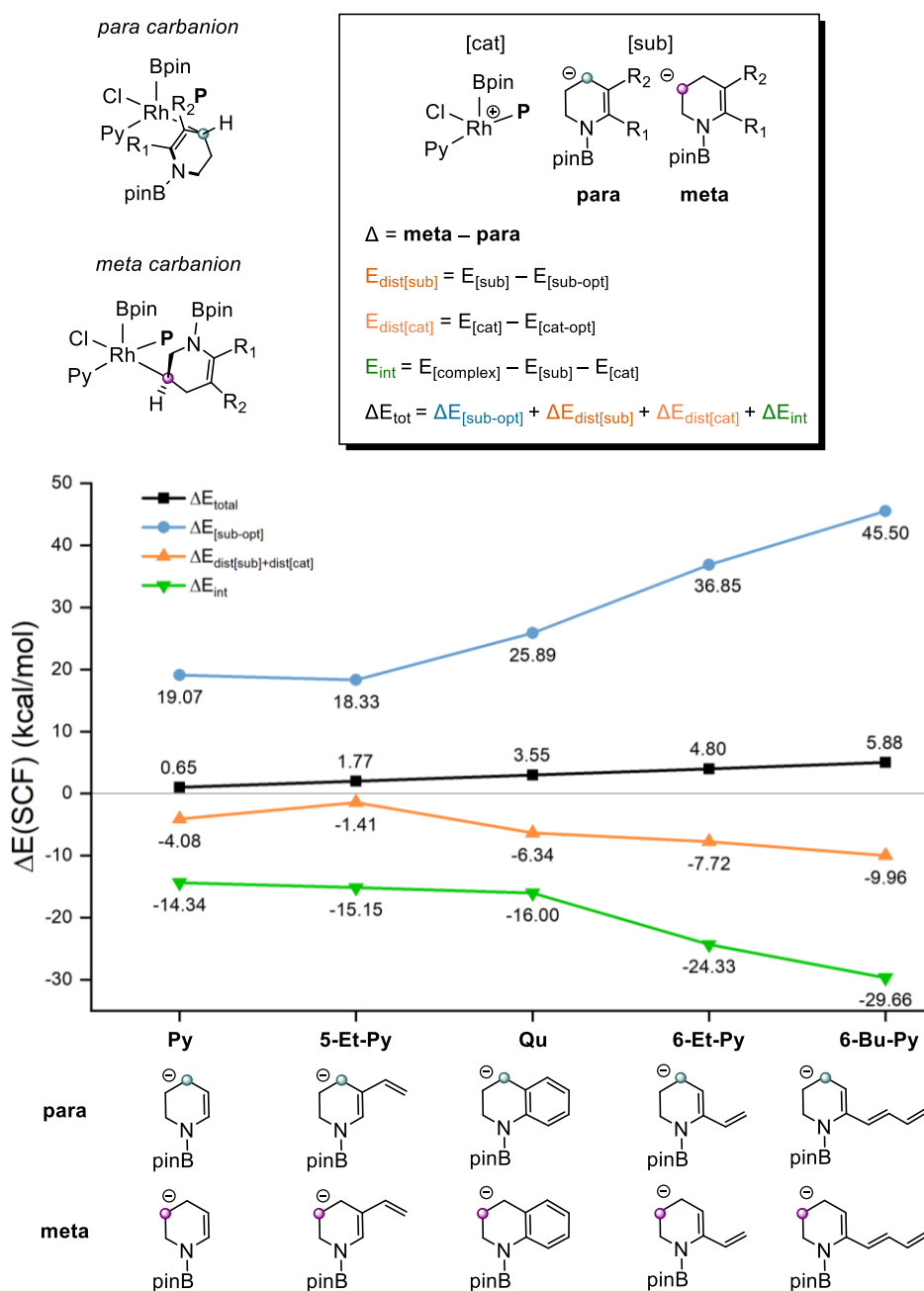


Fig. S27 Distortion interaction analysis of five models with various conjugated systems.

To get more clear evidence for the regioselectivity, we also performed same analysis for various model intermediates with an extended conjugation at C5- or C6-site of Py such as *N*-Bpin-6-vinyl-1,2,3,4-tetrahydropyridinyl (**6-Et-Py**), *N*-Bpin-5-vinyl-1,2,3,4-tetrahydropyridinyl (**5-Et-Py**), *N*-Bpin-6-(buta-1,3-dien-1-yl)-1,2,3,4-tetrahydropyridinyl (**6-Bu-Py**), and *N*-Bpin-1,2,3,4-

tetrahydroquinolinyl (**Qu**). As shown in Fig. S27†, comparing the two intermediates bearing para carbanion and meta carbanion, the gap of total energy (ΔE_{tot}) increased in the order of **Py**, **5-Et-Py**, **Qu**, **6-Et-Py**, and **6-Bu-Py** ($\Delta E_{\text{tot}} = 0.6, 1.8, 3.5, 4.8,$ and $5.9 \text{ kcal mol}^{-1}$). ΔE_{int} and ΔE_{dist} exhibit a tendency to decrease gradually, but $\Delta E_{\text{[sub-opt]}}$ tends to significantly increase. When the larger conjugation effect exists, it is natural that the interaction between Rh catalyst and the conjugated substrate becomes weaker, and the para carbanion is more stabilized rather than meta carbanion. But it's noteworthy that $\Delta E_{\text{[sub-opt]}}$ overwhelms the other terms such as $E_{\text{dist[cat]}}$, $E_{\text{dist[sub]}}$, and ΔE_{int} , leading to larger ΔE_{tot} . Consequently, the analysis can provide insight into how the delocalized effect of conjugated substrate units in an intermediate can affect the kinetic preference of 2nd regioselective hydroboration.

VII-6. Consideration of the rhodaboration pathway for 1,2-dihydropyridine

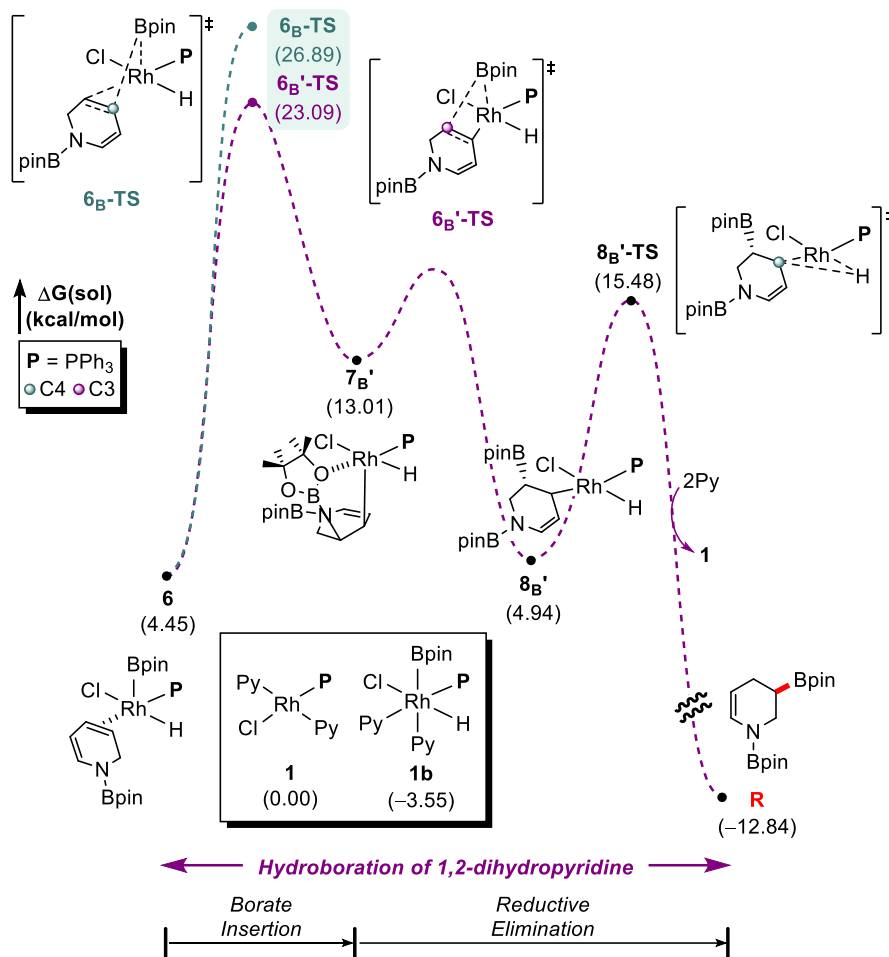


Fig. S28 The DFT-calculated energy profile for the 2nd-hydroboration via rhodaboration.

VII-7. Hydroboration of N-boryl-1,4-dihydropyridine

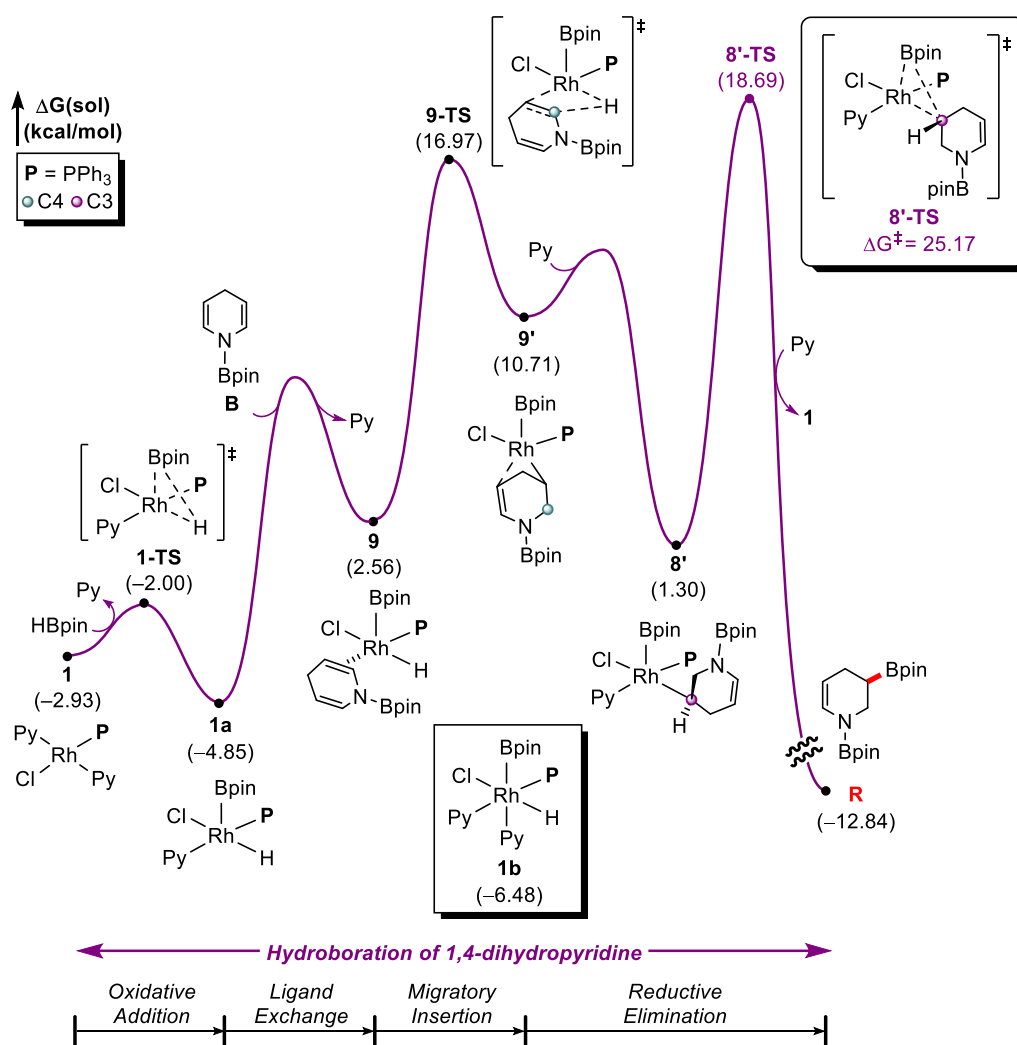


Fig. S29 The DFT-calculated energy profile for the 2nd-hydroboration of 1,4-dihydropyridine.

VII-8. Cartesian coordinates of DFT-optimized structures

Pyridine

C	-1.182272548	0.000000000	-3.068317780
C	-1.182272548	1.198347000	-2.355873780
C	-1.182272548	1.142246000	-0.961077780
N	-1.182272548	0.000000000	-0.262047780
C	-1.182272548	-1.142246000	-0.961077780
C	-1.182272548	-1.198347000	-2.355873780
H	-1.182272548	0.000000000	-4.15459780
H	-1.182272548	2.157005000	-2.865090780
H	-1.182272548	2.060344000	-0.375913780
H	-1.182272548	-2.060344000	-0.375913780
H	-1.182272548	-2.157005000	-2.865090780

HBpin

C	-0.458686154	-1.225304200	-3.500716814
O	0.594690176	-1.432520685	-2.514289217
B	0.056390650	-1.159940234	-1.286727732
O	-1.299500161	-0.979818388	-1.303698834
C	-1.766647345	-1.359577226	-2.631496170
H	0.707146594	-1.085606300	-0.294928645
C	-2.274208612	-2.801857126	-2.517930419
H	-2.702287513	-3.153250199	-3.461282264
H	-1.467858239	-3.479630234	-2.224632596
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H	0.635307856	-2.101683892	-5.137934759
H	-0.289919384	-3.281037426	-4.202277606
H	-1.125420485	-2.187325967	-5.325932472
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H	0.761685814	0.254966396	-4.472799101
H	-0.963565920	0.403749517	-4.867684549
H	-0.356894712	0.940522844	-3.285421160
C	-2.906756230	-0.427668046	-3.031372566
H	-3.231075722	-0.633615553	-4.056827410
H	-3.759710160	-0.584919951	-2.365402816
H	-2.612794000	0.620479822	-2.960205788

A

C	-0.882350336	0.097695754	-3.185067169
O	0.101296033	-0.607629440	-2.380781095
B	-0.350796829	-0.545081737	-1.078716643
O	-1.644373275	-0.077279200	-0.962782151
C	-2.185074788	-0.045239528	-2.311387308
C	-2.910791523	-1.377628694	-2.535181825
H	-3.411392370	-1.406598927	-3.507524788
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H	-3.663014363	-1.505310560	-1.752204248
C	-0.949626443	-0.560820420	-4.558696987
H	-0.001412699	-0.414271432	-5.083678084
H	-1.128042422	-1.634190204	-4.478246570
H	-1.747125556	-0.114292480	-5.161698581
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H	0.607906369	1.551274212	-3.727543506

H	-1.052584312	2.135271330	-3.964262326
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C	-0.056746319	-0.912699850	1.334029403
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H	1.774224191	-2.561486754	-0.224284223
H	-1.135763996	-0.826779617	1.410925668
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H	2.177075987	-1.100345601	-1.126317892

B

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B	-0.298878803	-0.390889128	-1.081392594
O	-1.632741960	-0.060597405	-0.974725720
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H	-2.888280987	1.934437880	-2.175161935
C	2.255665462	-1.133862935	2.381704097
C	2.726031616	-1.125098643	0.946394561
C	1.912719890	-0.895534149	-0.090286558
N	0.532480422	-0.647716205	0.048703050
C	0.018588494	-0.644982216	1.360771080
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H	2.492816375	-2.098969637	2.860920078
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H	2.810013836	-0.386196356	2.974361056

G

C	-1.438718048	-0.110995815	-3.302257267
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 C 2.793226064 0.004226025 0.392608803
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 C 0.195036633 -0.799971542 1.059934341
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 O 3.927904458 1.477685449 2.726228164
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 C 4.458972764 3.470238735 3.996405561
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 H 5.744480076 0.259069063 4.268082885
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 H 5.227278293 3.791032972 3.287417716
 H 3.508874829 3.906713554 3.684726806
 H 2.509652685 1.062868453 0.372499882

R

C -0.375610820 -0.164293763 -3.097782382
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 B 0.091684779 -0.643369802 -0.927864429
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C	-1.738385127	-0.823824724	7.391904621
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C	-3.976788199	-4.939512040	3.265046479
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C	-3.399808019	-4.669581769	0.248113397
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C	0.818672415	-3.797189652	-0.102566527
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C	-4.856930419	-3.524302109	4.251860864
C	-2.917823191	-4.222424916	5.508960917
C	-4.278600813	-4.342369805	5.222398873
H	-4.540445104	-1.945427018	2.827735432
H	-1.086595459	-3.193942383	5.060407055
H	-5.919258101	-3.601592616	4.036812273
H	-2.460318563	-4.849726562	6.269227339
H	-4.886809721	-5.064306693	5.761286814

2

Rh	-2.410247349	1.037106749	2.475489725
Cl	-4.820832495	0.668024897	2.380195623
H	-0.809030365	1.307100057	2.602115536

P	-2.055259942	-1.195877458	2.316423348
C	-3.044609326	5.829316169	3.662171715
C	-4.085300762	5.103623250	3.086379646
C	-3.880711277	3.766933005	2.753390407
N	-2.703715074	3.143179135	2.960769519
C	-1.694001283	3.849828428	3.514044636
C	-1.826295980	5.185272939	3.879162338
H	-3.177931636	6.872081698	3.936350923
H	-5.053117943	5.557217611	2.897494236
H	-4.664045453	3.146682290	2.330203482
H	-0.752607936	3.326448322	3.628655407
H	-0.982118328	5.704444737	4.321551322
C	-3.203252536	3.167351797	-1.664841990
C	-2.540103168	4.038953419	-0.801959719
C	-1.616104997	3.526875264	0.097525584
N	-1.376087367	2.202595771	0.181500892
C	-1.977731988	1.355303917	-0.683047954
C	-2.896156121	1.805881529	-1.614543555
H	-3.937458790	3.542574048	-2.371215615
H	-2.728018664	5.106926660	-0.820820477
H	-1.056015714	4.143674880	0.787551097
H	-1.699712391	0.316641116	-0.589994065
H	-3.368291400	1.086952379	-2.274105514
C	1.905540389	2.127387396	1.401375285
O	0.582734241	2.661997729	1.597768503
C	1.650855067	0.897380035	0.447263932
C	2.455096375	1.710591363	2.771764036
C	2.785289299	3.224056609	0.801238401
B	-0.364033204	1.612536854	1.323220373
O	0.333122034	0.471778093	0.835351018
C	2.605344479	-0.279219539	0.648219052
C	1.611175210	1.294219852	-1.038560206
H	3.645415415	0.025590172	0.487277119
H	2.506316532	-0.699510799	1.650680421
H	2.369929155	-1.070276465	-0.071496604
H	2.415149906	2.573257465	3.443984009
H	1.851640105	0.910450024	3.200864201
H	3.493009617	1.367817075	2.709266394
H	2.916054230	4.031346443	1.528534355
H	3.776196856	2.833104513	0.545149775
H	2.333968364	3.649840928	-0.097037334
H	2.607741449	1.529388145	-1.425973960
H	1.204549634	0.455733407	-1.612321189
H	0.964104373	2.159957453	-1.202562757
C	-3.198927049	-2.263298015	3.291163694
C	-3.750208697	-1.750931066	4.472418460
C	-3.451348041	-3.596869515	2.940264804
C	-4.532092631	-2.562927529	5.293433530
C	-4.240974616	-4.404349152	3.758414552
C	-4.779980624	-3.890118986	4.939175597
H	-3.584067757	-0.709193126	4.727059484
H	-3.044001357	-4.005773192	2.020411729
H	-4.959585936	-2.152411416	6.204158213
H	-4.435855696	-5.434640969	3.472085027
H	-5.395511488	-4.519752326	5.576281753
C	-0.441050699	-1.859954768	2.918749138
C	0.290773164	-1.111055910	3.847323503
C	0.018541886	-3.140219867	2.573494288

C	1.472069932	-1.614164943	4.395854250
C	1.204995383	-3.638457384	3.110909093
C	1.939520143	-2.874648094	4.021180157
H	-0.073360323	-0.128972827	4.134788903
H	-0.547130982	-3.752728275	1.878534501
H	2.029709014	-1.015507205	5.111168798
H	1.553375878	-4.626580423	2.821892261
H	2.863222784	-3.263729535	4.440942479
C	-2.242386736	-1.847426842	0.607153220
C	-1.153368240	-2.104039519	-0.240056603
C	-3.546139083	-1.918617540	0.085710792
C	-1.366951706	-2.444525571	-1.577865857
C	-3.752818920	-2.263594211	-1.248806703
C	-2.664485441	-2.529472419	-2.085119240
H	-0.142703241	-1.998853769	0.134905947
H	-4.390493884	-1.673405251	0.723667075
H	-0.515057068	-2.639560867	-2.224390490
H	-4.766251535	-2.318921512	-1.637499783
H	-2.827630906	-2.796604762	-3.125990486

[Py]

C	-1.935578950	0.000000000	0.136389871
C	-2.094006468	1.190816204	0.844118472
C	-1.758049725	-1.188425961	0.848124753
H	-1.939007950	-0.001264079	-0.949336109
C	-2.097243586	1.157554188	2.231185027
H	-2.211198659	2.141209511	0.334949189
N	-1.990573545	-0.004568832	2.906809243
H	-2.203211455	2.042012891	2.845009589
C	-1.788157791	-1.157668735	2.231003859
H	-1.661569479	-2.040235631	2.839136584
H	-1.612770841	-2.139429556	0.348846243

[Cat]

Rh	-2.410247349	1.037106749	2.475489725
Cl	-4.820832495	0.668024897	2.380195623
H	-0.809030365	1.307100057	2.602115536
P	-2.055259942	-1.195877458	2.316423348
C	-3.044609326	5.829316169	3.662171715
C	-4.085300762	5.103623250	3.086379646
C	-3.880711277	3.766933005	2.753390407
N	-2.703715074	3.143179135	2.960769519
C	-1.694001283	3.849828428	3.514044636
C	-1.826295980	5.185272939	3.879162338
H	-3.177931636	6.872081698	3.936350923
H	-5.053117943	5.557217611	2.897494236
H	-4.664045453	3.146682290	2.330203482
H	-0.752607936	3.326448322	3.628655407
H	-0.982118328	5.704444737	4.321551322
C	1.905540389	2.127387396	1.401375285
O	0.582734241	2.661997729	1.597768502
C	1.650855067	0.897380035	0.447263932
C	2.455096375	1.710591363	2.771764036
C	2.785289299	3.224056609	0.801238401
B	-0.364033204	1.612536854	1.323220373
O	0.333122034	0.471778093	0.835351018

C	2.605344479	-0.279219539	0.648219052
C	1.611175210	1.294219852	-1.038560206
H	3.645415415	0.025590172	0.487277119
H	2.506316532	-0.699510799	1.650680421
H	2.369929155	-1.070276465	-0.071496604
H	2.415149906	2.573257465	3.443984009
H	1.851640105	0.910450024	3.200864201
H	3.493009617	1.367817075	2.709266394
H	2.916054230	4.031346443	1.528534355
H	3.776196856	2.833104513	0.545149775
H	2.333968364	3.649840928	-0.097037334
H	2.607741449	1.529388145	-1.425973960
H	1.204549634	0.455733407	-1.612321189
H	0.964104373	2.159957453	-1.202562757
C	-3.198927049	-2.263298015	3.291163694
C	-3.750208697	-1.750931066	4.472418460
C	-3.451348041	-3.596869515	2.940264803
C	-4.532092631	-2.562927529	5.293433530
C	-4.240974616	-4.404349152	3.758414552
C	-4.779980624	-3.890118986	4.939175597
H	-3.584067757	-0.709193126	4.727059484
H	-3.044001357	-4.005773192	2.020411729
H	-4.959585936	-2.152411416	6.204158213
H	-4.435855696	-5.434640969	3.472085027
H	-5.395511488	-4.519752325	5.576281753
C	-0.441050699	-1.859954768	2.918749138
C	0.290773163	-1.111055910	3.847323503
C	0.018541886	-3.140219867	2.573494288
C	1.472069932	-1.614164943	4.395854250
C	1.204995383	-3.638457384	3.110909093
C	1.939520143	-2.874648094	4.021180157
H	-0.073360323	-0.128972827	4.134788903
H	-0.547130982	-3.752728275	1.878534501
H	2.029709014	-1.015507205	5.111168798
H	1.553375878	-4.626580423	2.821892260
H	2.863222784	-3.263729535	4.440942479
C	-2.242386736	-1.847426842	0.607153220
C	-1.153368240	-2.104039519	-0.240056603
C	-3.546139083	-1.918617540	0.085710792
C	-1.366951706	-2.444525571	-1.577865857
C	-3.752818920	-2.263594211	-1.248806703
C	-2.664485441	-2.529472419	-2.085119240
H	-0.142703241	-1.998853769	0.134905947
H	-4.390493883	-1.673405251	0.723667075
H	-0.515057068	-2.639560867	-2.224390490
H	-4.766251535	-2.318921512	-1.637499782
H	-2.827630906	-2.796604762	-3.125990486

2-TS

Rh	-2.506952941	1.049072279	2.210792438
Cl	-4.947140905	0.605843883	2.166315133
H	-0.879861740	1.298560755	2.303387992
P	-2.124583226	-1.201329570	2.143388893
C	-3.164645007	5.873097845	3.327961402
C	-4.235814211	5.088068363	2.907254091
C	-4.014711461	3.750737809	2.588691837
N	-2.798064630	3.180715705	2.672412714

H	3.712719797	3.776570995	1.388788241
H	4.512623150	2.259475960	0.940588007
H	3.616401798	3.192550016	-0.277913323
H	3.676022701	0.875935390	-1.207897573
H	2.177227455	0.065365653	-1.707722807
H	2.232519592	1.832427810	-1.607643725
C	-3.232252121	-2.297115042	3.191349096
C	-3.941894560	-1.755586434	4.269855060
C	-3.283093826	-3.680266371	2.962463160
C	-4.683554274	-2.586223645	5.110572997
C	-4.033046500	-4.506408463	3.797083067
C	-4.732202935	-3.960253794	4.876059492
H	-3.942160693	-0.682822124	4.428647574
H	-2.745316211	-4.113054531	2.124043287
H	-5.236246658	-2.153306940	5.939701517
H	-4.071813714	-5.575404028	3.605219105
H	-5.316893775	-4.604399203	5.527420176
C	-0.500867608	-1.777285856	2.766409668
C	0.116005763	-1.069420409	3.808321055
C	0.093993483	-2.967054621	2.320521915
C	1.297806647	-1.535324467	4.387249215
C	1.284898612	-3.423989642	2.887672167
C	1.890920793	-2.712152315	3.925062560
H	-0.333658761	-0.144821665	4.157176480
H	-0.366422333	-3.539123187	1.521483313
H	1.758636174	-0.971675514	5.194017609
H	1.737218362	-4.341055816	2.519532639
H	2.816028806	-3.070870869	4.367743768
C	-2.329405413	-1.873948533	0.474325064
C	-1.252088983	-1.875144190	-0.426199966
C	-3.610458723	-2.214541538	0.009263996
C	-1.447102285	-2.249554558	-1.757330273
C	-3.797096588	-2.588967265	-1.320941060
C	-2.716800090	-2.614634360	-2.207278630
H	-0.269898523	-1.554173402	-0.095511990
H	-4.459405778	-2.160996501	0.683974727
H	-0.604597231	-2.246238726	-2.444001795
H	-4.792720369	-2.852548605	-1.667444427
H	-2.867333745	-2.903900248	-3.243714641

4

Rh	-3.304900817	0.879408319	-0.455188194
Cl	-3.768822047	3.309656083	-0.410310783
H	-2.951736618	-0.618095566	-0.729926725
P	-1.561726214	0.864684683	0.932394926
C	-5.753584866	-0.577425516	-1.632807753
C	-5.532039951	-1.904364056	-1.150668558
C	-5.281888880	-2.096638198	0.177395344
N	-5.122892496	-1.047098105	1.047922624
C	-5.028887765	0.284874339	0.534253375
C	-5.616373927	0.499390176	-0.785217150
H	-6.096648692	-0.427214611	-2.652594745
H	-5.638020006	-2.761308605	-1.805024675
H	-5.215124488	-3.082106236	0.624566766
H	-5.225171331	1.028836213	1.300117327
H	-5.920033969	1.500816637	-1.069472438
C	-5.127524894	-2.403326064	4.436909353

O	-4.953602529	-2.554288033	2.994509590
C	-4.676395926	-0.908736307	4.684407428
C	-4.265885290	-3.452847365	5.130814918
C	-6.613138479	-2.646163092	4.724248039
B	-4.989486878	-1.291965848	2.470115076
O	-4.939356614	-0.283121067	3.386920480
C	-3.178637509	-0.772628992	4.954839082
C	-5.480357543	-0.157019078	5.739329917
H	-2.920483048	-1.168838298	5.941267295
H	-2.595598531	-1.302446736	4.202685919
H	-2.899362768	0.282351540	4.916546152
H	-4.645683203	-4.451887218	4.898072464
H	-3.228032823	-3.395873172	4.798751315
H	-4.298911515	-3.319742790	6.217054751
H	-6.890075682	-3.636671831	4.353002985
H	-6.825101130	-2.605572740	5.796635536
H	-7.239275302	-1.906213643	4.217240872
H	-5.376440437	-0.640021139	6.716442898
H	-5.101149196	0.865336794	5.822462959
H	-6.539747017	-0.106721302	5.482863464
C	-1.611574521	2.106431284	2.289497467
C	-2.814463502	2.281658375	2.988553757
C	-0.486657421	2.852042404	2.667338005
C	-2.883772329	3.171795588	4.058696594
C	-0.561803592	3.747245090	3.736871301
C	-1.757963246	3.907791637	4.437081919
H	-3.692707844	1.714571187	2.707897037
H	0.446140991	2.744138562	2.122146910
H	-3.824304745	3.299821653	4.588016177
H	0.316153257	4.322847873	4.017321640
H	-1.815829706	4.608583165	5.265237843
C	-0.030693742	1.279098701	0.001812741
C	-0.045697308	2.473879572	-0.742080730
C	1.099980926	0.452156952	-0.042641188
C	1.066485341	2.835187101	-1.500393136
C	2.206920730	0.819485057	-0.811222640
C	2.194761378	2.010452152	-1.537794218
H	-0.931592697	3.106372805	-0.726248776
H	1.121834730	-0.475734515	0.519861165
H	1.048193468	3.760723683	-2.068851991
H	3.078806042	0.171314908	-0.839970056
H	3.057525280	2.292613544	-2.134806613
C	-1.155154049	-0.690383061	1.835431442
C	-0.217297001	-0.680773667	2.882718300
C	-1.783577733	-1.896027397	1.500006382
C	0.088894344	-1.854299317	3.568747680
C	-1.487985651	-3.068846290	2.198933903
C	-0.550312181	-3.051561500	3.231578660
H	0.264435284	0.248865762	3.169513510
H	-2.504898256	-1.905848787	0.690037292
H	0.817538394	-1.833317877	4.374422153
H	-1.997802056	-3.991494766	1.937726138
H	-0.318539316	-3.964066378	3.774476102

4-TS

Rh	-5.274481412	1.585444777	1.598671780
Cl	-6.794531122	0.888632519	3.330326741

H	2.850616740	-6.810757721	-2.521756828
C	0.800387318	-1.035668107	-0.459443588
C	1.261318929	-0.954020168	0.862762915
C	-0.582615246	-1.074792546	-0.692800442
C	0.362660978	-0.922311350	1.928514329
C	-1.480825670	-1.032570358	0.374325390
C	-1.011615358	-0.960139849	1.686635161
H	2.328121758	-0.903737412	1.051538090
H	-0.962111547	-1.133045367	-1.707542258
H	0.736562297	-0.860552883	2.946943097
H	-2.549322949	-1.055895205	0.178131858
H	-1.712905255	-0.928346561	2.516022759
C	1.084751003	-0.662324037	-3.318960383
C	0.257560134	-1.547096541	-4.025906756
C	1.188400616	0.669994531	-3.740074873
C	-0.470131395	-1.097098844	-5.127831630
C	0.455532529	1.117379804	-4.837803330
C	-0.375461172	0.235646950	-5.531714812
H	0.188105156	-2.586870306	-3.720317730
H	1.859551097	1.345895287	-3.217863698
H	-1.107038746	-1.788979016	-5.672314970
H	0.544500168	2.151007226	-5.159799288
H	-0.940369603	0.584028975	-6.392088494

4'-TS

Rh	-3.955235115	0.163744986	0.600554071
Cl	-4.232096188	1.393054662	-1.468765747
H	-3.529114616	-0.805222194	1.806622359
P	-2.065825870	1.302570823	1.134113948
C	-4.980056574	-0.881214696	2.270805896
C	-5.417974200	0.139818954	3.251442086
C	-6.256651617	1.126777178	2.881934794
N	-6.724254323	1.234213114	1.563944024
C	-6.475792203	0.189398369	0.683909469
C	-5.812397153	-0.963377109	1.064460919
H	-4.693547398	-1.835431764	2.713786009
H	-5.060339344	0.087965936	4.273697422
H	-6.593974469	1.909652826	3.549639182
H	-6.933478729	0.291456726	-0.291691630
H	-5.865822982	-1.859492062	0.456243425
C	-7.867852279	4.650927180	0.933055919
O	-7.143069782	3.666491327	1.745113803
C	-7.742062289	4.037504137	-0.509899629
C	-7.213051055	6.016142143	1.101069587
C	-9.306969833	4.673944616	1.458857344
B	-7.201759129	2.496765620	1.034144331
O	-7.727591979	2.604318665	-0.218287179
C	-6.408627722	4.364579250	-1.189596248
C	-8.915600985	4.328883584	-1.436316876
H	-6.383724650	5.405034895	-1.528898486
H	-5.561653619	4.185752786	-0.522155254
H	-6.276791506	3.703734178	-2.048964440
H	-7.303658711	6.346880934	2.140412973
H	-6.156237724	5.991935277	0.836589812
H	-7.715298678	6.752670195	0.465018415
H	-9.292325960	4.901769973	2.528386125
H	-9.905489071	5.435200826	0.950030012

H	-9.790187346	3.702286796	1.321275354
H	-9.017389660	5.407557174	-1.595245785
H	-8.739788187	3.856212284	-2.406266459
H	-9.853672326	3.942414773	-1.033562788
C	-2.406728729	3.108293863	1.211817794
C	-3.589557358	3.513759752	1.848761756
C	-1.532955670	4.079395386	0.709520067
C	-3.878296516	4.866035521	2.010536957
C	-1.838345027	5.435845888	0.847807007
C	-3.004147837	5.832390162	1.504479492
H	-4.281377492	2.765032121	2.220218022
H	-0.618439842	3.780361255	0.207207280
H	-4.792121306	5.154403081	2.519453630
H	-1.159204777	6.182618909	0.445093085
H	-3.232965316	6.888878182	1.618795388
C	-0.552876653	1.150937756	0.101831013
C	-0.700938466	0.906242284	-1.271847360
C	0.734346637	1.292780652	0.644013141
C	0.426872523	0.812488753	-2.087933506
C	1.857277387	1.192857750	-0.177209932
C	1.705177596	0.953663165	-1.544516249
H	-1.697338315	0.802356288	-1.691381556
H	0.860493096	1.476887614	1.706686580
H	0.303713853	0.624753245	-3.151056774
H	2.850086700	1.300670485	0.251567679
H	2.581054601	0.874171538	-2.183086028
C	-1.429177697	0.939982515	2.829983382
C	-1.250124478	1.926576614	3.808022083
C	-1.115073579	-0.391797033	3.146253757
C	-0.780785696	1.585539928	5.079544404
C	-0.637119221	-0.728860587	4.410126474
C	-0.473906266	0.260503197	5.384577189
H	-1.478400565	2.962830845	3.582976019
H	-1.246232395	-1.166603402	2.394662773
H	-0.653797748	2.361374356	5.829970197
H	-0.394336485	-1.763480809	4.637417741
H	-0.108458722	-0.002360715	6.373582559

5

Rh	-3.167833893	3.615165851	2.157586897
Cl	-3.013800990	3.432349918	4.542607366
P	-1.554437959	2.001525564	1.738522465
C	-1.918481631	0.272561986	2.282508855
C	-1.446526586	-0.854551192	1.590374885
C	-2.626296036	0.090264140	3.480375234
C	-1.676055536	-2.137402331	2.088268195
C	-2.849844008	-1.195749453	3.975401941
C	-2.377555018	-2.311739700	3.282714926
H	-0.905013812	-0.736635660	0.657408028
H	-2.984327792	0.956475875	4.029123661
H	-1.307205200	-3.000458831	1.540318138
H	-3.398486988	-1.321061030	4.904829825
H	-2.556617545	-3.311640144	3.668836186
C	0.090653364	2.319371472	2.497601890
C	1.129983791	1.379727138	2.404604261
C	0.311107044	3.522963044	3.179033115
C	2.372566733	1.646742118	2.974140035

C	1.558615347	3.786975022	3.748938811
C	2.589024655	2.853168573	3.646314754
H	0.966246345	0.435799341	1.893463352
H	-0.502868936	4.232647321	3.282591212
H	3.170435170	0.912788925	2.899011613
H	1.718170650	4.719840936	4.282397842
H	3.557540185	3.058459224	4.094584932
C	-1.173350472	1.806067408	-0.053569886
C	-2.077860941	1.120326390	-0.884576964
C	-0.047614672	2.409105643	-0.632463681
C	-1.851073414	1.035493978	-2.258295935
C	0.172181138	2.325072875	-2.009161560
C	-0.725539715	1.637272620	-2.826936133
H	-2.962038815	0.655751821	-0.457097002
H	0.664782741	2.938666328	-0.007393084
H	-2.557406166	0.497340249	-2.884909301
H	1.052359266	2.794586121	-2.440353157
H	-0.549864959	1.569670215	-3.896877785
C	-7.026631765	0.089663437	1.654963030
O	-7.144823132	1.530400332	1.455277652
C	-6.086845636	-0.337362380	0.464344281
C	-8.422291811	-0.521158391	1.622326225
C	-6.376400733	-0.109725876	3.028248131
B	-6.005347118	1.910450908	0.792652360
O	-5.282713377	0.859966114	0.267559591
N	-5.560289472	3.265999803	0.690805405
C	-6.845865989	-0.581642229	-0.844028774
C	-5.146817832	-1.497435824	0.773271478
H	-7.430617640	-1.505359088	-0.803856851
H	-7.520450197	0.250259526	-1.066908603
H	-6.124150007	-0.663348704	-1.661672650
H	-8.999514338	-0.164871375	2.480062226
H	-8.959949321	-0.245105742	0.713552451
H	-8.363671938	-1.613194242	1.679323979
H	-6.987447958	0.389677914	3.784952829
H	-6.298539221	-1.170134454	3.285420739
H	-5.375005479	0.326522883	3.057288285
H	-5.716426834	-2.396905491	1.030382157
H	-4.537153462	-1.723315556	-0.106936497
H	-4.472241783	-1.260079992	1.595770842
C	-3.894041358	5.544432339	1.417483064
C	-4.948907532	5.102960957	2.216680149
C	-3.530906673	4.679512116	0.322872564
H	-3.276165770	6.397263369	1.680567200
C	-6.082845074	4.288836422	1.618373300
H	-5.145456571	5.593214117	3.164610037
H	-6.775213772	4.955816768	1.082307021
H	-6.652292395	3.790871535	2.405770224
C	-4.246666316	3.458810845	0.239086269
H	-3.911834351	2.711497632	-0.467784618
H	-2.700537991	4.886733669	-0.341695233

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Rh	-3.685394291	0.440466998	2.298328065
Cl	-3.358373948	-1.274523478	0.692653153
H	-4.848739355	-0.772774313	4.948836179
P	-1.753577857	1.474817577	2.068641000

C	-5.310637079	0.215014513	4.810766279
C	-4.311229939	1.195215421	4.217084587
C	-4.714948504	2.100950930	3.220306097
N	-5.992715182	2.045576587	2.607080697
C	-6.828094068	0.963895343	2.954817078
C	-6.549960394	0.107989640	3.949128291
H	-5.581856351	0.552475424	5.826397687
H	-3.477247058	1.491217028	4.847737688
H	-4.217219473	3.049615198	3.093797425
H	-7.717087714	0.875123014	2.340772840
H	-7.252847504	-0.693256260	4.152845209
C	-6.531626965	3.098154117	-0.823410361
O	-7.060507307	2.512680837	0.409194017
C	-5.613352994	4.248353548	-0.269722902
C	-7.699367195	3.561194685	-1.684391380
C	-5.732653891	1.995924431	-1.529763813
B	-6.096063546	2.743037967	1.356264833
O	-5.157397346	3.683697910	0.991785158
C	-6.391497001	5.525065747	0.065877818
C	-4.388816103	4.565769332	-1.119890778
H	-6.705169364	6.053446266	-0.839315231
H	-7.279012812	5.296923936	0.663257521
H	-5.747785568	6.188840676	0.649780470
H	-8.277003734	2.694593684	-2.017706958
H	-8.367870482	4.223222248	-1.131360983
H	-7.333667490	4.089650310	-2.571295290
H	-6.386120990	1.136375906	-1.701211740
H	-5.346862476	2.339856271	-2.494435719
H	-4.890834950	1.661552931	-0.916891912
H	-4.688291566	4.887650226	-2.123053736
H	-3.819658356	5.378934150	-0.658970518
H	-3.728659730	3.703187312	-1.207186302
C	-1.436493400	2.200983945	0.394665938
C	-0.645311976	3.349939535	0.224570027
C	-1.933492929	1.547645374	-0.743608404
C	-0.368870988	3.838831398	-1.052756063
C	-1.645669104	2.036267871	-2.019245189
C	-0.869518921	3.185388052	-2.180196644
H	-0.245339479	3.874073650	1.085956358
H	-2.534894794	0.651956058	-0.628843340
H	0.240250655	4.732015669	-1.163582044
H	-2.038046231	1.515430951	-2.888281452
H	-0.653401907	3.567464885	-3.174044875
C	-0.270618528	0.430014050	2.366140265
C	1.018321134	0.973959039	2.239509479
C	-0.420093695	-0.913965325	2.728827279
C	2.139618414	0.184997192	2.483387076
C	0.707898801	-1.701679272	2.969046328
C	1.985121611	-1.154993533	2.850492495
H	1.146052310	2.012339049	1.948435698
H	-1.415527794	-1.339769111	2.798321080
H	3.133336708	0.613160544	2.384235448
H	0.583705897	-2.745488252	3.242916202
H	2.860847641	-1.770335898	3.038597806
C	-1.515088899	2.895332366	3.210501335
C	-2.123352707	4.131653478	2.929396035
C	-0.841467383	2.730670447	4.429729325
C	-2.042284330	5.181496895	3.842963438

C	-0.766742580	3.783313071	5.343065540
C	-1.364137849	5.010514469	5.051842025
H	-2.669339503	4.268939731	1.999961205
H	-0.369552776	1.781367902	4.664467442
H	-2.514742979	6.131895911	3.610783377
H	-0.238653886	3.642648933	6.282220532
H	-1.304952546	5.828249695	5.764672681

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Rh	-2.122864252	2.813662435	2.106499278
Cl	-4.239554138	3.536025894	1.111009795
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P	-1.118159945	3.106168243	0.069114033
C	0.708062853	5.726440766	3.197236296
O	0.210367779	4.688524930	2.312923931
C	-0.469674312	5.850646258	4.228391249
C	0.979051557	6.973524578	2.361813745
C	2.000885856	5.194280343	3.824226182
B	-0.781472814	3.990498022	2.980075925
O	-0.966239191	4.480613256	4.268211636
C	-1.612527749	6.737078098	3.717353260
C	-0.057624331	6.258105191	5.637839328
H	-1.331029015	7.794702529	3.728709255
H	-1.901407920	6.461567196	2.699042442
H	-2.482958535	6.600298426	4.364782547
H	1.805179605	6.780373259	1.671511526
H	0.109210916	7.248452539	1.763494244
H	1.255600177	7.816492238	3.004482669
H	2.692670852	4.916745541	3.023643298
H	2.484078817	5.945648791	4.456181198
H	1.798876420	4.304552619	4.427694588
H	0.419163266	7.244198106	5.629733272
H	-0.942125601	6.311407165	6.279090880
H	0.635116195	5.536630303	6.074842145
C	-2.136436055	2.359791086	-1.264675403
C	-2.226329920	2.933489980	-2.539018491
C	-2.811667881	1.159659001	-1.000120875
C	-2.973458402	2.306462871	-3.538132920
C	-3.555377045	0.536836510	-1.999320237
C	-3.635876578	1.108053888	-3.271536746
H	-1.720183997	3.870545327	-2.750373580
H	-2.779618481	0.715238124	-0.011763981
H	-3.040914309	2.760547669	-4.523029501
H	-4.077845863	-0.387415456	-1.772074989
H	-4.220784470	0.625623723	-4.049999857
C	0.527398491	2.297923440	-0.184323071
C	0.871897427	1.765708179	-1.437851016
C	1.468494077	2.232788542	0.853672259
C	2.122466674	1.182268493	-1.644520336
C	2.718654459	1.652586268	0.643439730
C	3.049963041	1.122518434	-0.604665373
H	0.160890325	1.796027896	-2.256456236
H	1.233457896	2.650935535	1.821847686
H	2.367234798	0.770843281	-2.620085752
H	3.433250209	1.612021564	1.461230535
H	4.022388163	0.664549793	-0.764496809
C	-0.834027173	4.835866008	-0.484815943

C	0.365279814	5.239153324	-1.085945687
C	-1.855855266	5.775934706	-0.280459455
C	0.542051321	6.566780643	-1.479039925
C	-1.672857836	7.099931064	-0.677640367
C	-0.474706523	7.499993794	-1.275429848
H	1.168136836	4.525487790	-1.237499253
H	-2.784753921	5.463032205	0.188107154
H	1.478480866	6.870486716	-1.939793463
H	-2.469012265	7.821521452	-0.515585272
H	-0.333789568	8.534130107	-1.578537133
C	-2.012217874	-2.683804610	0.441798762
O	-2.907676608	-1.646274190	0.936553815
C	-0.623469812	-2.233690623	1.034316250
C	-2.081829555	-2.707140574	-1.081512933
C	-2.512422748	-4.012403360	1.021143263
B	-2.315161523	-1.144435369	2.078423480
O	-1.017902637	-1.556585689	2.263263414
N	-2.998055576	-0.276012667	2.977826617
C	0.089893496	-1.202770391	0.156568792
C	0.320170530	-3.375325254	1.395391476
H	0.489823984	-1.659195631	-0.753733272
H	-0.584635171	-0.395736242	-0.134011352
H	0.918514018	-0.757591370	0.712365819
H	-3.080666765	-3.021192538	-1.399721209
H	-1.886438681	-1.722856236	-1.508107998
H	-1.355734364	-3.419705559	-1.487071593
H	-3.558193209	-4.152289672	0.733564295
H	-1.931981148	-4.859758238	0.644055312
H	-2.456725428	-4.010142277	2.113726545
H	0.561185457	-3.968954305	0.507178093
H	1.252191775	-2.966921193	1.796150424
H	-0.114520900	-4.033236888	2.149920210
C	-3.948856478	2.158569712	3.938660767
C	-2.674454209	1.779775582	4.268359714
C	-4.848469687	1.209290108	3.310908384
H	-4.299303658	3.164501447	4.143605014
C	-2.324725914	0.312909368	4.147696372
H	-2.040589795	2.413055531	4.874154474
H	-1.250790979	0.159465112	4.039691976
H	-2.657102020	-0.219936175	5.057055234
C	-4.330511000	0.072688086	2.789423143
H	-4.892313181	-0.577512162	2.126725038
H	-5.870628599	1.488650068	3.094196265

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Rh	-2.131435963	2.693928553	2.104921684
Cl	-4.143367946	4.052480134	1.414400939
H	-0.871952217	1.812973368	2.365436015
P	-1.164578076	3.089242798	0.033548868
C	0.638467015	5.635778675	3.307553589
O	0.145536953	4.623231556	2.387313130
C	-0.657031504	5.986214845	4.126847452
C	1.218786430	6.782870714	2.485825970
C	1.725764834	4.967185968	4.155338061
B	-1.014432455	4.095064967	2.917229124
O	-1.393637269	4.727308973	4.082893321
C	-1.534385857	7.035646417	3.433703599

C	-0.419382135	6.358243434	5.585600627	H	1.140416294	-0.973851788	0.980592760
H	-1.078290890	8.029844025	3.478396644	H	-2.825080137	-2.923155338	-1.483411060
H	-1.707873603	6.773201297	2.386729642	H	-1.605824285	-1.644271533	-1.434152738
H	-2.505172695	7.070672577	3.934836192	H	-1.105283482	-3.349098556	-1.508322094
H	2.107638710	6.437187556	1.949606274	H	-3.465293432	-4.156456796	0.547398240
H	0.504092753	7.142502736	1.744051149	H	-1.864724512	-4.923667527	0.488835546
H	1.511332195	7.614643563	3.135998005	H	-2.430997587	-4.151141927	1.985653274
H	2.495777452	4.564671465	3.490761107	H	0.665094824	-4.134289853	0.538942293
H	2.197085952	5.676992101	4.841865976	H	1.323409820	-3.250312092	1.927424010
H	1.309621053	4.139609881	4.737209373	H	-0.101238130	-4.277629093	2.136462432
H	0.210194728	7.251798725	5.657553736	C	-3.640954806	2.170335530	3.851398488
H	-1.376143766	6.574762236	6.069011605	C	-2.390240168	1.709883530	4.218124152
H	0.061262047	5.545777359	6.133769566	C	-4.576217825	1.255996670	3.201919114
C	-2.270633476	2.381480469	-1.244541510	H	-3.966525422	3.170123219	4.111968998
C	-2.579600919	3.044509414	-2.437278480	C	-2.141903704	0.214774286	4.172521898
C	-2.809323359	1.108070917	-1.000848687	H	-1.754885732	2.304263885	4.865739307
C	-3.415336712	2.437064200	-3.376823381	H	-1.079982801	-0.019016655	4.091409497
C	-3.640612170	0.505590500	-1.941142230	H	-2.514631425	-0.228868652	5.112299460
C	-3.945276767	1.169967022	-3.132148450	C	-4.133532416	0.055681893	2.765817444
H	-2.174662651	4.032884551	-2.630438828	H	-4.727873250	-0.589558051	2.127476078
H	-2.591694902	0.578879399	-0.078014893	H	-5.564579594	1.604781596	2.934835056
H	-3.653939581	2.959085367	-4.299504379				
H	-4.051356809	-0.477694317	-1.732407956				
H	-4.598267033	0.703562083	-3.864839972				
C	0.437542802	2.236040166	-0.280295521				
C	0.725750374	1.674681688	-1.532787473				
C	1.416411461	2.205930432	0.723761622				
C	1.967132407	1.083040755	-1.772737848				
C	2.657812391	1.621674842	0.477131374				
C	2.935751524	1.055131640	-0.769045739				
H	-0.020547792	1.693751923	-2.320827256				
H	1.207350347	2.657630410	1.685878330				
H	2.175190080	0.644482014	-2.745028129				
H	3.408990485	1.605932161	1.262439789				
H	3.901771090	0.593660933	-0.955897064				
C	-0.808266451	4.813558443	-0.501245476				
C	0.439922666	5.172997951	-1.030896189				
C	-1.797746017	5.797409149	-0.345711701				
C	0.695423982	6.494850306	-1.397350915				
C	-1.535136264	7.115942206	-0.717283670				
C	-0.289588395	7.470305777	-1.240935171				
H	1.220733026	4.430227570	-1.147981776				
H	-2.759732840	5.527234510	0.080470474				
H	1.668953074	6.760437136	-1.801028762				
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H	-0.087626967	8.499976552	-1.524415598				
C	-1.850826232	-2.737986411	0.432385565				
O	-2.729083939	-1.697992478	0.949899675				
C	-0.477963049	-2.388089610	1.121542869				
C	-1.840205174	-2.652827887	-1.090610323				
C	-2.430981810	-4.079609582	0.894002053				
B	-2.169618417	-1.279692281	2.142125188				
O	-0.907148035	-1.773549292	2.369897315				
N	-2.840416215	-0.401207215	3.035174222				
C	0.321428818	-1.333361129	0.353883027				
C	0.399235549	-3.590743606	1.451804664				
H	0.745310311	-1.738450015	-0.569319876				
H	-0.297820310	-0.471638565	0.098252721				
H	1.140416294	-0.973851788	0.980592760				
H	-2.825080137	-2.923155338	-1.483411060				
H	-1.605824285	-1.644271533	-1.434152738				
H	-1.105283482	-3.349098556	-1.508322094				
H	-3.465293432	-4.156456796	0.547398240				
H	-1.864724512	-4.923667527	0.488835546				
H	-2.430997587	-4.151141927	1.985653274				
H	0.665094824	-4.134289853	0.538942293				
H	1.323409820	-3.250312092	1.927424010				
H	-0.101238130	-4.277629093	2.136462432				
C	-3.640954806	2.170335530	3.851398488				
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H	-3.966525422	3.170123219	4.111968998				
C	-2.141903704	0.214774286	4.172521898				
H	-1.754885732	2.304263885	4.865739307				
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H	-2.514631425	-0.228868652	5.112299460				
C	-4.133532416	0.055681893	2.765817444				
H	-4.727873250	-0.589558051	2.127476078				
H	-5.564579594	1.604781596	2.934835056				
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6-TS							
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C	0.579510627	5.782281130	3.352175795				
O	0.068899243	4.735920555	2.478631090				
C	-0.736211712	6.293009438	4.042925685				
C	1.305804858	6.812158938	2.493100609				
C	1.549144900	5.104538885	4.327207499				
B	-1.152967766	4.332868174	2.979885988				
O	-1.558697428	5.086520989	4.054494430				
C	-1.487322029	7.329975163	3.198953179				
C	-0.568377003	6.779679603	5.476960065				
H	-0.968410621	8.293995157	3.196649591				
H	-1.602627674	6.988463585	2.166631773				
H	-2.486977636	7.467936190	3.618733857				
H	2.199608399	6.359253097	2.053247822				
H	0.675542278	7.163875062	1.675123470				
H	1.618151024	7.669128837	3.099952988				
H	2.322861068	4.585575125	3.753778203				
H	2.034073420	5.830732239	4.986863264				
H	1.026978246	4.367156363	4.944424617				
H	0.118023745	7.632517462	5.516091409				
H	-1.536811833	7.101848297	5.869580515				
H	-0.184781727	5.990541014	6.126471210				
C	-2.205978987	2.311537172	-1.119769021				
C	-2.318728746	2.823232273	-2.419690241				
C	-2.900299718	1.140079135	-0.782358280				
C	-3.107553528	2.167211961	-3.366320872				
C	-3.688287686	0.487979082	-1.728409835				
C	-3.792790554	1.000615435	-3.023499607				
H	-1.797876969	3.736821554	-2.689848809				
H	-2.835244951	0.729806046	0.220133542				
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H	-4.217669979	-0.415733943	-1.442998406
H	-4.410907218	0.496420238	-3.761467690
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C	0.902915026	1.813999794	-1.270336894
C	1.297820436	2.114668749	1.094577294
C	2.160798341	1.227034272	-1.406298775
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H	0.262927277	1.917026774	-2.141390322
H	0.971819699	2.485570729	2.059138180
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H	3.970282008	0.623320974	-0.398699173
C	-0.845576627	4.789929421	-0.468194530
C	0.427207242	5.205448780	-0.881656733
C	-1.912131132	5.703593409	-0.500912744
C	0.630959797	6.512384795	-1.326923556
C	-1.701266189	7.007661416	-0.948059557
C	-0.430903450	7.416813077	-1.361464565
H	1.265025364	4.517828795	-0.847595256
H	-2.893919110	5.398081328	-0.151562063
H	1.623935937	6.823292275	-1.641256810
H	-2.533086551	7.706566991	-0.966411348
H	-0.269357766	8.434662546	-1.706769074
C	-2.030366956	-2.851165664	0.263292417
O	-2.820325074	-1.801061015	0.894666086
C	-0.569368251	-2.475750552	0.709366502
C	-2.266298144	-2.811923505	-1.242526073
C	-2.512132395	-4.184305581	0.847577419
B	-2.083239297	-1.373705435	1.982124592
O	-0.797072550	-1.865093550	2.012245891
N	-2.595287354	-0.485448083	2.964404708
C	0.067784465	-1.406849071	-0.183141983
C	0.374243143	-3.659690959	0.887803903
H	0.358472976	-1.816090700	-1.155350800
H	-0.615206542	-0.571420878	-0.352973909
H	0.960245630	-1.012224126	0.307264790
H	-3.302581526	-3.086166437	-1.462271361
H	-2.085631233	-1.817766604	-1.651958893
H	-1.610808012	-3.528386258	-1.749219563
H	-3.589608696	-4.273902696	0.683886556
H	-2.015973974	-5.034802280	0.370159911
H	-2.325141599	-4.230994980	1.924445314
H	0.490719682	-4.203424195	-0.055727678
H	1.359501255	-3.299550980	1.197586616
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C	-3.216524641	2.087141308	4.056371823
C	-1.884202631	1.566749620	4.138076040
C	-4.236397971	1.215406814	3.466016536
H	-3.509543844	2.950473524	4.642819420
C	-1.744105042	0.047025484	4.025446785
H	-1.209918370	2.032596917	4.854841259
H	-0.714056636	-0.257304846	3.832611284
H	-2.050513572	-0.373860581	4.996896711
C	-3.897130618	0.039569278	2.889887778
H	-4.597013054	-0.549513818	2.307410445
H	-5.246863676	1.590680917	3.364746424

6'-TS

Rh	-2.937572142	3.302528744	1.628470113
Cl	-5.001619769	4.513373076	1.420319403
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C	-1.010661579	5.424800371	4.646969588
O	-1.304502584	4.199917178	3.912216096
C	-0.931443456	6.490329401	3.493464117
C	0.281328371	5.223872950	5.430080647
C	-2.190700909	5.656196351	5.597999921
B	-1.943555477	4.580252800	2.746558387
O	-1.843958705	5.931268175	2.503933884
C	0.450111443	6.569399204	2.837123133
C	-1.427137202	7.883273515	3.867485779
H	1.178042394	7.052091310	3.496838952
H	0.819039962	5.577247445	2.568855267
H	0.373538458	7.151021839	1.915294204
H	0.132717950	4.455671136	6.194607551
H	1.096476760	4.903185432	4.779178317
H	0.576430373	6.152060956	5.931263996
H	-2.304980910	4.777484225	6.239077499
H	-2.031003646	6.531615565	6.234569535
H	-3.120496948	5.792198947	5.038353017
H	-0.827255124	8.300388696	4.683771561
H	-1.336630802	8.548025447	3.003484662
H	-2.474605082	7.865992190	4.172463776
C	-0.169927220	4.617311396	-0.257877090
C	0.335734040	5.791472044	-0.828934158
C	0.709434389	3.748341777	0.407144656
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H	-0.333536641	6.473241972	-1.344028683
H	0.321695414	2.841457547	0.863929688
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H	3.623682823	5.454545373	-0.005438562
C	-2.739094987	5.540170914	-1.223868639
C	-2.956635843	5.548955528	-2.608924169
C	-3.138695646	6.645166157	-0.454235484
C	-3.554292264	6.653383335	-3.219016022
C	-3.725215633	7.748523631	-1.073001580
C	-3.935830439	7.756846573	-2.453948160
H	-2.661985425	4.696628594	-3.213279381
H	-2.994584494	6.631294765	0.620286900
H	-3.720299500	6.649511003	-4.293068057
H	-4.032631644	8.598490536	-0.469883004
H	-4.401404949	8.615468796	-2.930317677
C	-1.911620023	2.774154985	-1.587810162
C	-0.913850479	2.643496500	-2.565398351
C	-2.936381257	1.819375435	-1.528618938
C	-0.952224581	1.580131873	-3.468552560
C	-2.977102459	0.760053088	-2.433249363
C	-1.982724520	0.638476533	-3.405446451
H	-0.105640131	3.367503186	-2.616828875
H	-3.718414251	1.895856497	-0.783355651
H	-0.174054932	1.486018963	-4.221477433

H	-3.788454225	0.041868130	-2.360652558
H	-2.005693984	-0.188160279	-4.110639319
C	-6.873092217	1.400994192	-1.263943132
O	-5.811703539	0.680365327	-0.562337290
C	-7.942298822	1.613695088	-0.122372690
C	-7.337369392	0.541810309	-2.435319025
C	-6.275740134	2.718619464	-1.773297713
B	-5.943102513	1.019049673	0.771535136
O	-7.127249771	1.630606326	1.079718464
N	-4.918702766	0.767461933	1.734816209
C	-8.911519718	0.433960430	0.017729187
C	-8.704200242	2.933181707	-0.198715182
H	-9.610509032	0.385328652	-0.822991008
H	-8.368604186	-0.514127206	0.076751762
H	-9.485215758	0.555052930	0.940581460
H	-6.523485731	0.444573899	-3.160086792
H	-7.628130590	-0.459753278	-2.113517470
H	-8.188113508	1.009629736	-2.941835786
H	-5.444258052	2.501144155	-2.448069227
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H	-9.252267406	3.010511520	-1.144081581
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C	-2.399631638	1.433491720	2.870252540
C	-3.600292119	2.142476981	3.289525166
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C	-4.924218521	1.449925062	3.040772348
H	-3.543411561	2.717441526	4.210131293
H	-5.737141686	2.176507667	3.045192431
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C	-3.791432722	0.001867508	1.450738887
H	-3.924008347	-0.765135121	0.693074398
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Rh	-1.983420773	2.395504038	1.346630305
Cl	-4.225464715	3.129631298	0.646353356
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C	-0.751145332	4.986329054	4.420727602
O	-0.654318115	3.765331475	3.636037936
C	-1.243634235	6.036072870	3.357100597
C	0.618900560	5.278743267	5.023847442
C	-1.781956655	4.717682716	5.522837340
B	-1.491413347	3.902553673	2.540182360
O	-1.951094323	5.195528919	2.405041592
C	-0.099098352	6.717725686	2.599169686
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H	0.422316501	7.441514813	3.233283988
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H	-0.513690667	7.245646282	1.736158240
H	0.880211501	4.494858845	5.740958481
H	1.391568737	5.306150919	4.253389434
H	0.613477515	6.237960593	5.552654360
H	-1.457368452	3.852115623	6.107537724

H	-1.886648674	5.572650831	6.197554100
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H	-2.508526260	7.756008367	3.073535717
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C	-1.747258305	4.740983755	-1.366799780
C	-1.599945460	4.787904571	-2.761470529
C	-2.557247933	5.690142960	-0.724770082
C	-2.241710263	5.780454595	-3.504111264
C	-3.189164386	6.682718354	-1.473832045
C	-3.034470015	6.732340956	-2.860868207
H	-0.985800504	4.051582579	-3.270849993
H	-2.696252679	5.641911017	0.348184543
H	-2.121705862	5.807103682	-4.583991358
H	-3.818132776	7.411567543	-0.970004094
H	-3.535469369	7.504055064	-3.439505314
C	-0.364352992	2.214953624	-1.577363535
C	0.914872989	2.140318689	-2.143946784
C	-1.321679236	1.245589607	-1.914938287
C	1.227167991	1.109062815	-3.033112445
C	-1.006789959	0.215840539	-2.797157618
C	0.270980420	0.145995793	-3.359189354
H	1.667858998	2.879556917	-1.888797123
H	-2.309016297	1.282119496	-1.471294510
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H	-1.757954616	-0.537003290	-3.015849902
H	0.523319456	-0.659801977	-4.043298567
C	0.732427324	4.329730929	0.046721462
C	1.564707196	3.754122067	1.018520532
C	1.140868517	5.513750036	-0.583652165
C	2.780895274	4.347421005	1.352781107
C	2.355493397	6.110722422	-0.241894646
C	3.176963218	5.531383659	0.726125817
H	1.243293486	2.853869888	1.526182483
H	0.506684251	5.976562722	-1.332355427
H	3.411531024	3.892081534	2.111484687
H	2.655885258	7.034059236	-0.729732908
H	4.118783244	6.002266455	0.994511737
C	-5.980318988	-0.576271044	-0.448510395
O	-5.126355901	-0.194802434	0.664301667
C	-4.980699681	-0.579868629	-1.672694331
C	-7.108268567	0.446179566	-0.552547548
C	-6.531942655	-1.967774513	-0.118391331
B	-3.836808184	-0.415034606	0.278146654
O	-3.692624645	-0.833035624	-1.025806662
N	-2.716088804	-0.221139017	1.161028395
C	-4.877427193	0.782265727	-2.368563060
C	-5.219693943	-1.683930802	-2.697297528
H	-5.798722119	1.016612116	-2.910279289
H	-4.679455797	1.584113048	-1.651249975
H	-4.057237634	0.753346116	-3.091959434
H	-7.758724704	0.363205973	0.323201288
H	-6.708940440	1.461123466	-0.580353471
H	-7.714065668	0.266078050	-1.447337979
H	-7.054178710	-1.922046610	0.841118611
H	-7.236227000	-2.312768331	-0.881634747
H	-5.723798787	-2.700316858	-0.030829182
H	-6.211884857	-1.580600806	-3.148708942

H	-4.475650303	-1.608960987	-3.496020148
H	-5.139181724	-2.676428844	-2.250430029
C	-0.522508907	1.064992618	2.243269985
C	-0.202966087	-0.039004585	1.241308904
C	-1.733159704	0.969436132	3.020015395
H	0.330042240	1.500892307	2.756614225
C	-1.434097317	-0.925565386	0.967429779
H	0.600468489	-0.679976002	1.633187358
H	-1.420639215	-1.780968842	1.657092277
H	-1.418563943	-1.312816059	-0.052716876
C	-2.868725743	0.522342820	2.339451631
H	-3.876539834	0.626366323	2.724147882
H	-1.825943566	1.439029353	3.991559379

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Rh	-2.845683397	2.658446255	0.843427769
Cl	-4.639122993	4.265029322	1.406771345
H	-1.956532592	0.978803451	-1.714298267
P	-1.711797709	4.056549059	-0.504727629
C	0.449899305	3.152747501	3.430700796
O	-0.182369370	3.278777008	2.128343150
C	-0.773270117	3.314481360	4.405301507
C	1.523871634	4.230123557	3.547809017
C	1.074188186	1.753459745	3.478414142
B	-1.525948313	2.972446802	2.274113911
O	-1.876377497	2.822383235	3.595160843
C	-1.085471226	4.777426356	4.739817557
C	-0.697511106	2.476087506	5.677898683
H	-0.330025488	5.206656975	5.405768039
H	-1.139180264	5.382777908	3.832039482
H	-2.058555150	4.825736671	5.235527330
H	2.327033194	4.028747565	2.832053388
H	1.119167658	5.218928774	3.325556906
H	1.957483576	4.238398414	4.553731557
H	1.775083685	1.647412775	2.645156951
H	1.617914725	1.583107707	4.412412370
H	0.305882671	0.981729793	3.374663043
H	0.191277399	2.738630181	6.262283022
H	-1.579444830	2.664248442	6.296886948
H	-0.669519759	1.408990980	5.450927569
C	-0.930486686	5.532862932	0.260944225
C	-1.681023937	6.249301208	1.206986028
C	0.363245371	5.960019166	-0.061861227
C	-1.130969437	7.371549631	1.825915011
C	0.910120168	7.079732863	0.569260497
C	0.168485417	7.785293411	1.518167183
H	-2.684513965	5.916198896	1.461940600
H	0.953204552	5.416522663	-0.792366479
H	-1.718589864	7.917276154	2.559105866
H	1.918883429	7.396658409	0.318262460
H	0.596838897	8.654574237	2.009655630
C	-2.853571305	4.763176008	-1.757385591
C	-3.969220946	4.022484327	-2.173951941
C	-2.611397595	6.021023019	-2.327382638
C	-4.824025531	4.531296595	-3.150566732
C	-3.471685949	6.528287625	-3.300721134
C	-4.578198315	5.784610065	-3.713988285

H	-4.181816989	3.055396812	-1.727157215
H	-1.756193963	6.607408974	-2.005509393
H	-5.690801944	3.953957952	-3.459726867
H	-3.279572070	7.507020047	-3.731722434
H	-5.251249960	6.183934400	-4.467849545
C	-0.387544065	3.273919604	-1.512939678
C	0.735472366	2.725569391	-0.868150192
C	-0.501506060	3.150137772	-2.905359891
C	1.721012149	2.074296877	-1.607652807
C	0.486477418	2.488675120	-3.638813585
C	1.599633595	1.949224236	-2.994479464
H	0.823737777	2.815353832	0.209136587
H	-1.360369568	3.567804708	-3.420287689
H	2.585570612	1.657884755	-1.097445738
H	0.382355290	2.398789752	-4.716750502
H	2.366559706	1.434934334	-3.566882403
C	-6.562211698	1.255492972	3.957055811
O	-6.054545977	1.184686279	2.595415624
C	-5.240831612	1.428281598	4.809163329
C	-7.287199095	-0.068274935	4.224038314
C	-7.530766271	2.431389592	4.038858893
B	-4.726155353	0.875323131	2.687742731
O	-4.236235450	0.792183575	3.960379447
N	-3.918350544	0.652383809	1.508393712
C	-5.245619349	0.710492437	6.154100437
C	-4.825114041	2.892778775	4.983979945
H	-6.039580313	1.105259367	6.796875342
H	-5.388924267	-0.365559680	6.039792565
H	-4.287385487	0.874571501	6.655498705
H	-8.067649546	-0.202980761	3.469797093
H	-6.597184111	-0.914535090	4.154644236
H	-7.755113225	-0.078303277	5.213171507
H	-8.414299501	2.222232385	3.428125627
H	-7.858432590	2.591287024	5.071753246
H	-7.066309109	3.343217376	3.661199427
H	-5.507665112	3.415107433	5.662250310
H	-3.816935969	2.920377928	5.401359243
H	-4.796702833	3.416640803	4.025222476
C	-2.314345496	0.347518901	-0.892548998
C	-1.814948072	0.867332087	0.456901697
C	-3.827889750	0.317013957	-0.887975110
H	-1.918078348	-0.662429754	-1.100958690
C	-2.532753060	0.094285415	1.563945046
H	-0.728170070	0.868107661	0.541342493
H	-2.134089571	0.290612283	2.560594011
H	-2.573172507	-0.996236700	1.404283489
C	-4.541558634	0.504914757	0.237739506
H	-5.622777176	0.580942668	0.252391038
H	-4.362633943	0.171354664	-1.822256705

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Rh	-3.346165953	1.754886316	2.734309442
Cl	-2.988206722	3.790758102	4.144632310
H	-5.355171968	-2.316641674	4.514053937
C	-0.431871660	2.312584617	-0.207161216
O	-0.901370719	1.814827348	1.076957838
C	-1.671759377	2.050760349	-1.137050984

C	0.832597541	1.549736771	-0.588053030
C	-0.124967972	3.803014456	-0.019782975
B	-2.284231505	1.895313063	1.081709415
O	-2.772701915	2.117331557	-0.194446534
C	-1.688943514	0.643593023	-1.745437751
C	-1.904955858	3.104430846	-2.217370248
H	-0.926367368	0.530976573	-2.522590790
H	-1.522336994	-0.119105598	-0.980189567
H	-2.670333285	0.460550506	-2.192383688
H	1.630790986	1.786012800	0.121456366
H	0.670585456	0.470183974	-0.570024623
H	1.170293305	1.836189408	-1.589896018
H	0.597977700	3.914771335	0.792717292
H	0.296834672	4.243593806	-0.928851277
H	-1.027262333	4.356074451	0.251656085
H	-1.042166345	3.169919874	-2.889246336
H	-2.780492994	2.831512655	-2.814897070
H	-2.093144414	4.086541650	-1.780464076
C	-6.184641632	1.750643531	0.617831382
P	-5.109424674	2.811960341	1.677951513
C	-6.320763816	3.469222509	2.898248175
C	-4.723591430	4.267549901	0.619752806
C	-5.766066060	1.378534438	-0.671726920
C	-7.377295361	1.211740191	1.122216493
C	-6.531368192	0.500674821	-1.436941687
H	-4.832525093	1.768087645	-1.058180105
C	-7.717058738	-0.031691583	-0.926008260
H	-6.196373102	0.226852735	-2.434115149
C	-8.135362641	0.324874474	0.355234021
H	-9.057057493	-0.082571120	0.761760742
H	-8.309140471	-0.720236295	-1.522812390
C	-7.260809937	4.442126807	2.530039743
C	-6.355286193	2.946132893	4.197268867
C	-8.217878703	4.879838223	3.443919102
H	-7.241872946	4.864997474	1.530537978
C	-7.317058335	3.380272841	5.108994572
H	-5.622403785	2.208438066	4.503453887
C	-8.249383459	4.348342125	4.734531185
H	-8.937332769	5.638514397	3.148013711
H	-7.329624061	2.969289458	6.114634386
H	-8.994638719	4.691869249	5.446798737
C	-5.489083850	4.594607723	-0.508782231
C	-3.639288172	5.084832290	0.972694168
C	-5.167532188	5.713126120	-1.279968583
H	-6.330860016	3.974058331	-0.798296140
C	-3.325795077	6.202826400	0.200693584
H	-3.054168457	4.847917450	1.856129021
C	-4.084700498	6.519228679	-0.928397977
H	-5.765929123	5.951989903	-2.155224609
H	-2.484099594	6.828159573	0.485827638
H	-3.833993348	7.388474427	-1.530615802
H	-7.722687845	1.487665957	2.113265416
O	-3.779847762	-3.663568397	5.889793886
C	-2.892591594	-4.080818554	6.957642949
C	-1.594419241	-4.495480601	6.167228162
C	-3.559668450	-5.209720919	7.737259469
C	-2.673826548	-2.861732157	7.862691088
O	-1.637114375	-3.610296183	5.020330660

N	-3.425994449	-2.520157581	3.736298743
C	-1.656317750	-5.931472800	5.632594873
C	-0.284537689	-4.260121228	6.913741493
H	-1.549110049	-6.668292967	6.434309134
H	-2.600768363	-6.112949271	5.111872776
H	-0.841369469	-6.075541223	4.917731403
H	-4.446187128	-4.829511987	8.253163598
H	-3.874613269	-6.018713451	7.076019859
H	-2.875075379	-5.616062643	8.489678960
H	-3.647434722	-2.498015631	8.203528224
H	-2.065983133	-3.108609061	8.738494321
H	-2.185573444	-2.053851622	7.311277861
H	-0.256887492	-4.839572479	7.842791321
H	0.557403821	-4.574855116	6.289793020
H	-0.151183031	-3.203510260	7.152522386
C	-3.976942886	-0.182191390	2.092070669
C	-4.868265170	-0.573649678	3.288545515
C	-4.815806338	-2.078577510	3.594385299
H	-5.902569514	-0.260577729	3.107280363
C	-2.866400616	-1.136886470	1.854564877
H	-4.561167630	-0.063488980	1.179447211
H	-2.214619174	-0.962846939	1.003258977
H	-4.541524976	-0.057569671	4.206072367
C	-2.583816600	-2.167629285	2.669185997
H	-1.699709558	-2.787403825	2.552818246
H	-5.281190511	-2.632658842	2.766656190
B	-2.963677901	-3.254636769	4.849336045
N	-1.827158653	0.835795282	4.011381284
C	-2.077496356	0.912076132	5.332236917
C	-0.700279436	0.222705477	3.607929505
C	-1.231061100	0.363693896	6.289825823
C	0.204267895	-0.337404773	4.504950681
C	-0.063673304	-0.271439952	5.869452223
H	-2.971023918	1.453776708	5.619923526
H	-0.530011460	0.198598693	2.542090444
H	-1.483423600	0.451818707	7.341282580
H	1.101525935	-0.817274219	4.128557321
H	0.622451778	-0.705377840	6.591327924

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Rh	-2.834317290	4.266214875	3.401487405
Cl	-3.840649115	6.296639284	4.433586978
H	-4.614279771	1.947288914	2.618124833
P	-2.707313530	5.365062061	1.368309417
C	1.237871171	4.260421951	4.444179977
O	-0.172006049	3.976594041	4.671954352
C	1.356764948	4.151045061	2.877325678
C	2.053170428	3.231175081	5.221780653
C	1.488015537	5.678553282	4.968608604
B	-0.866454354	4.235230728	3.503795855
O	0.003313047	4.445360113	2.449778206
C	1.684895055	2.734743930	2.385580123
C	2.286436835	5.172246469	2.224480387
H	2.717806355	2.461449767	2.624627205
H	1.021783677	1.987838943	2.826186061
H	1.567067276	2.698408841	1.298101226
H	1.912077410	3.387183294	6.295703948

H	0.029685803	2.445151065	-0.895002547
H	-1.673180271	0.638012524	-0.621071619
H	-2.190700510	1.575377995	0.772724436
H	-0.175046915	-0.715067818	0.728020065
H	1.783346802	2.599620134	0.860772442
H	1.642938915	1.305822649	2.997265600

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C	-1.633860635	0.122826419	-2.204697898
H	-2.263889176	0.437482725	-3.058618118
C	-2.422440220	-0.334158001	4.239755610
O	-2.480930733	-0.840511255	2.902078648
C	-1.006976967	0.349583823	4.274045160
C	-2.602081997	-1.492900818	5.220131687
C	-3.564762815	0.681137256	4.407781858
B	-1.645425974	-0.020100814	2.111547755
O	-0.857976101	0.811216351	2.929021732
C	0.121490491	-0.658138686	4.550797193
C	-0.889579713	1.541904697	5.223457103
H	-3.611733413	-1.905159271	5.123648667
H	-1.891294348	-2.295689198	5.014350945
H	-2.465930454	-1.156168505	6.254585573
H	-4.507295226	0.188969151	4.151562912
H	-3.633235811	1.063198454	5.432378057
H	-3.427021066	1.523050627	3.723682153
N	-1.606242731	-0.030227319	0.725102163
C	-0.597490018	0.761124484	-0.086321992
C	-2.420079539	-0.876493076	-0.046468704
H	0.127196877	-1.000528668	5.591703905
H	0.024503843	-1.526089282	3.892536721
H	1.078340842	-0.175296784	4.333013322
H	-1.091801049	1.242464457	6.258424299
H	0.124427209	1.951625944	5.175104351
H	-1.584286555	2.335800631	4.942531385
C	-1.230503345	1.295949924	-1.329662500
C	-2.419293833	-0.884186657	-1.388935284
H	-0.804108031	-0.479186575	-2.697517360
H	-0.506994948	1.950764254	-1.848476417
H	-3.043558810	-1.627151503	-1.888984853
H	-0.214328728	1.554866170	0.567505139
H	0.252970282	0.011401688	-0.187500298
H	-3.022694204	-1.573957181	0.533535625

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Rh	-2.250095999	0.040176975	0.966924335
Cl	-2.834970549	2.002646495	-0.086567220
B	-3.890006290	0.076736523	2.123899047
P	-0.864882614	0.852743731	2.591931451
N	-3.241414137	-1.186599622	-0.480284180
O	-5.105368487	0.476478547	1.669214414
C	-5.997435764	0.501937486	2.840642845
C	-5.297241807	-0.520998484	3.809950593
C	-7.395301729	0.105998042	2.384764545
C	-5.978130875	1.940017342	3.363257281
O	-3.884879056	-0.400816249	3.404611454
C	-5.696365197	-1.975565089	3.551028281

C	-5.390358197	-0.180886893	5.291313372
H	-7.792711626	0.870493373	1.712120127
H	-7.391768565	-0.847201761	1.853382067
H	-8.068810489	0.025612489	3.244030921
H	-6.272326719	2.615218768	2.555959716
H	-6.674743120	2.067475363	4.196728254
H	-4.976571042	2.223312716	3.698364365
H	-6.721860882	-2.169893374	3.876685106
H	-5.615152208	-2.223774945	2.488522160
H	-5.028482849	-2.635863478	4.111518833
H	-6.436850639	-0.156297825	5.611625833
H	-4.872233000	-0.943612905	5.879378875
H	-4.928781224	0.782938081	5.509818514
C	-0.340997836	-0.893091355	2.447765454
C	-1.269110790	-1.908292865	2.797773487
C	0.816852940	-1.240889923	1.713127176
C	0.517581305	1.940989559	2.178844485
C	-1.425612322	1.247352895	4.265694073
C	1.432495796	2.326887044	3.173716998
C	0.689982619	2.372435119	0.853603884
C	-1.138150581	0.432840158	5.368499518
C	-2.184498281	2.417311532	4.431571579
C	-1.024779707	-3.236850427	2.417878989
H	-2.134470663	-1.671128991	3.406471164
C	1.041803474	-2.563623612	1.352518319
H	1.528385282	-0.470289033	1.432887597
C	0.118328483	-3.564998136	1.695333935
H	-1.732977409	-4.008399162	2.704881399
H	0.306580241	-4.595253026	1.408756560
H	1.941404356	-2.822954980	0.802307395
C	2.522472923	3.124385632	2.835008018
H	1.288848253	2.011605570	4.203156897
C	1.785546961	3.171073423	0.526695495
H	-0.039991302	2.111236302	0.094066931
C	2.700160450	3.543722866	1.513251056
H	3.230711699	3.423101261	3.601724841
H	1.915689009	3.511703159	-0.495895861
H	3.548655140	4.170492332	1.255265321
C	-1.616358709	0.786034022	6.631216986
H	-0.551754402	-0.472445789	5.245561640
C	-2.652675389	2.765049412	5.697055297
H	-2.416290989	3.046145717	3.575359355
C	-2.373966275	1.947268815	6.797039452
H	-1.393939873	0.153825377	7.485613777
H	-3.237458603	3.671069913	5.824395635
H	-2.743528734	2.218145650	7.781368499
C	-4.378544718	-0.803110799	-1.094358989
C	-2.691408848	-2.379093237	-0.790131766
C	-5.000571176	-1.607166118	-2.044043307
H	-4.776338750	0.160077258	-0.799759032
C	-3.255753674	-3.230106387	-1.731140533
H	-1.776933932	-2.642537744	-0.266256356
C	-4.433023192	-2.837742093	-2.370819282
H	-5.914255700	-1.264233164	-2.517249903
H	-2.778633209	-4.178112834	-1.955271740
H	-4.898480643	-3.481813932	-3.110661035

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Rh	-3.346165953	1.754886316	2.734309442
Cl	-2.988206722	3.790758102	4.144632310
C	-0.431871660	2.312584617	-0.207161216
O	-0.901370719	1.814827348	1.076957838
C	-1.671759377	2.050760349	-1.137050984
C	0.832597541	1.549736771	-0.588053030
C	-0.124967971	3.803014456	-0.019782975
B	-2.284231505	1.895313063	1.081709414
O	-2.772701915	2.117331556	-0.194446534
C	-1.688943514	0.643593023	-1.745437751
C	-1.904955858	3.104430846	-2.217370248
H	-0.926367368	0.530976572	-2.522590790
H	-1.522336994	-0.119105598	-0.980189567
H	-2.670333284	0.460550506	-2.192383688
H	1.630790986	1.786012800	0.121456366
H	0.670585456	0.470183974	-0.570024623
H	1.170293305	1.836189408	-1.589896018
H	0.597977700	3.914771335	0.792717292
H	0.296834672	4.243593806	-0.928851277
H	-1.027262333	4.356074451	0.251656084
H	-1.042166345	3.169919874	-2.889246336
H	-2.780492994	2.831512655	-2.814897070
H	-2.093144414	4.086541650	-1.780464076
C	-6.184641632	1.750643531	0.617831382
P	-5.109424674	2.811960341	1.677951513
C	-6.320763816	3.469222509	2.898248175
C	-4.723591429	4.267549901	0.619752806
C	-5.766066060	1.378534438	-0.671726920
C	-7.377295361	1.211740191	1.122216493
C	-6.531368192	0.500674821	-1.436941687
H	-4.832525093	1.768087645	-1.058180105
C	-7.717058738	-0.031691583	-0.926008260
H	-6.196373102	0.226852735	-2.434115149
C	-8.135362641	0.324874474	0.355234021
H	-9.057057493	-0.082571120	0.761760742
H	-8.309140471	-0.720236295	-1.522812390
C	-7.260809937	4.442126807	2.530039743
C	-6.355286193	2.946132893	4.197268867
C	-8.217878703	4.879838223	3.443919102
H	-7.241872946	4.864997474	1.530537978
C	-7.317058335	3.380272840	5.108994572
H	-5.622403785	2.208438066	4.503453887
C	-8.249383459	4.348342125	4.734531185
H	-8.937332769	5.638514397	3.148013711
H	-7.329624061	2.969289458	6.114634386
H	-8.994638719	4.691869248	5.446798737
C	-5.489083850	4.594607723	-0.508782231
C	-3.639288172	5.084832290	0.972694168
C	-5.167532187	5.713126120	-1.279968583
H	-6.330860016	3.974058331	-0.798296140
C	-3.325795077	6.202826400	0.200693584
H	-3.054168457	4.847917450	1.856129021
C	-4.084700498	6.519228679	-0.928397977
H	-5.765929123	5.951989903	-2.155224609
H	-2.484099593	6.828159573	0.485827638
H	-3.833993348	7.388474427	-1.530615802
H	-7.722687845	1.487665957	2.113265416

N	-1.827158653	0.835795282	4.011381283
C	-2.077496356	0.912076132	5.332236917
C	-0.700279436	0.222705477	3.607929505
C	-1.231061100	0.363693896	6.289825823
C	0.204267895	-0.337404773	4.504950681
C	-0.063673304	-0.271439952	5.869452222
H	-2.971023918	1.453776708	5.619923526
H	-0.530011460	0.198598693	2.542090444
H	-1.483423600	0.451818707	7.341282580
H	1.101525935	-0.817274219	4.128557321
H	0.622451778	-0.705377840	6.591327924

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Rh	-2.834317290	4.266214875	3.401487405
Cl	-3.840649115	6.296639284	4.433586978
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C	1.237871171	4.260421951	4.444179977
O	-0.172006049	3.976594041	4.671954352
C	1.356764948	4.151045061	2.877325678
C	2.053170428	3.231175081	5.221780653
C	1.488015537	5.678553282	4.968608604
B	-0.866454353	4.235230728	3.503795855
O	0.003313047	4.445360113	2.449778206
C	1.684895055	2.734743930	2.385580123
C	2.286436834	5.172246469	2.224480387
H	2.717806355	2.461449767	2.624627205
H	1.021783677	1.987838943	2.826186061
H	1.567067276	2.698408840	1.298101225
H	1.912077410	3.387183294	6.295703947
H	1.736812058	2.214724762	4.978798819
H	3.121232367	3.334762667	5.001643779
H	1.202366856	5.723066280	6.023293279
H	2.542008272	5.959926445	4.879910283
H	0.882123949	6.407462747	4.422724398
H	3.311677047	5.057627254	2.592667954
H	2.293452917	5.018327131	1.141090215
H	1.950814810	6.193892467	2.410236457
C	-4.330325322	6.149691333	1.025143862
C	-4.439409085	7.428221897	0.466881400
C	-5.496895519	5.427502662	1.319134134
C	-5.696782086	7.976752418	0.210331958
C	-6.750275393	5.973148065	1.053689442
C	-6.852199580	7.252181128	0.501248326
H	-3.545426857	8.001077134	0.242416627
H	-5.423435147	4.436482973	1.759907262
H	-5.771222441	8.974326920	-0.213871786
H	-7.647151358	5.406091719	1.287534940
H	-7.829759021	7.683179389	0.303114044
C	-2.403944240	4.379261504	-0.161561685
C	-3.398656212	4.201631243	-1.134305303
C	-1.158196619	3.754555140	-0.344517529
C	-3.155736210	3.411234712	-2.259573301
C	-0.920917108	2.968583831	-1.470013788
C	-1.919264922	2.790603608	-2.429808111
H	-4.364933533	4.680809088	-1.020463338
H	-0.384644824	3.894585254	0.399644798
H	-3.937650636	3.284500204	-3.003589095

H	0.046842657	2.489736906	-1.594727629
H	-1.733468850	2.173092104	-3.304527238
C	-1.489956861	6.739103613	1.255102576
C	-0.832259176	7.049501489	0.057307550
C	-1.216900687	7.493378421	2.406957830
C	0.100875629	8.087319950	0.015582727
C	-0.286578535	8.530625184	2.357511755
C	0.379662513	8.826554180	1.165465734
H	-1.033629729	6.476592667	-0.841875651
H	-1.740192318	7.268956886	3.331703567
H	0.610953514	8.313950442	-0.916976230
H	-0.082162840	9.108128822	3.255206157
H	1.108380393	9.632313845	1.132073282
N	-3.325669448	3.371423515	5.311988467
C	-2.502450068	3.109720856	6.341701368
C	-4.646991808	3.168043056	5.472230212
C	-2.974446665	2.625000599	7.558850660
C	-5.191956496	2.675428661	6.651150706
C	-4.338959993	2.397222762	7.718928110
H	-1.452364673	3.300993891	6.161818823
H	-5.279397581	3.426293819	4.629200172
H	-2.272120087	2.431236927	8.363098431
H	-6.263825747	2.525365664	6.726590288
H	-4.732920757	2.017285376	8.657221176

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C	-1.245048081	0.000000000	1.900160779
H	-2.294219867	-0.138002138	2.171406438
C	-2.544945408	-0.308360057	6.051595132
O	-2.312367712	-0.496311902	4.633073175
B	-0.991269663	-0.148334115	4.410537246
C	-1.099711749	-0.490589219	6.651631640
C	-3.571001595	-1.334999973	6.521098254
C	-3.089311069	1.114226252	6.233408617
O	-0.257149058	-0.008291531	5.575422896
C	-0.734294624	-1.961143052	6.887596729
C	-0.813209006	0.337432249	7.900936445
H	-4.539834810	-1.128702855	6.056948527
H	-3.274293595	-2.348844712	6.247273153
H	-3.696182110	-1.286091766	7.608229427
H	-3.982002586	1.230827118	5.612217314
H	-3.358107022	1.317407438	7.274523052
H	-2.352889432	1.854102711	5.908778677
N	-0.447669449	0.073910411	3.127122082
C	0.910593641	0.371550382	2.930141963
H	-1.272889966	-2.381356179	7.742277484
H	-0.954171216	-2.564146121	6.002094750
H	0.338918269	-2.028820784	7.086493692
H	-1.500247310	0.069768507	8.710872467
H	0.208588158	0.147505601	8.243125059
H	-0.907573556	1.405355119	7.696332943
C	0.441326058	1.583900255	0.802743948
C	-1.047112268	1.270305798	1.058589465
C	1.344775059	1.000539170	1.824813212
H	0.753445418	1.261575573	-0.190724066
H	-1.583113297	1.180716569	0.107099453
H	-1.530632162	2.090541405	1.613904972

H	-0.919962514	-0.874197417	1.318076353
H	2.415274753	1.134124023	1.698258742
H	1.574653012	0.054403240	3.728734497

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H	-1.035796303	0.000000000	-6.434348065
C	-0.267638494	0.297595864	-5.697538564
O	-0.456023479	-1.009010409	-0.641810017
C	-0.613379630	-0.472432145	0.695686568
C	-1.953456055	0.342263520	0.569158668
C	0.601727399	0.425408328	0.967999121
C	-0.653458325	-1.630131211	1.687937021
B	-1.117438113	-0.138757361	-1.490989433
O	-1.913891423	0.777632342	-0.814494132
C	-3.201385889	-0.535762996	0.728050729
H	1.513013136	-0.160515382	0.819116611
H	0.625353227	1.272103583	0.275575792
H	0.598937401	0.811479962	1.992254492
H	0.317330959	-2.134093626	1.704865104
H	-0.867790809	-1.266345362	2.698679993
H	-1.410509931	-2.365783733	1.411229799
N	-0.988764716	-0.154652190	-2.894467237
C	-1.731029892	0.785199019	-3.748451115
C	-0.142271326	-1.037327730	-3.579544751
H	-1.980525464	1.282511962	2.523182058
H	-1.255323654	2.286993228	1.248881469
H	-3.008983056	2.070439826	1.312987733
H	-3.348965983	-0.845587850	1.767297352
H	-4.077554804	0.034613839	0.406840419
H	-3.129189634	-1.430720356	0.103256700
C	-0.786697803	1.413385243	-4.778298664
C	0.162316801	-0.902774579	-4.879278652
H	0.589107465	0.656702228	-6.280542205
H	0.067286180	1.808446548	-4.221274602
H	0.787131864	-1.657702895	-5.349349198
H	-2.528897359	0.230714809	-4.258718932
H	-2.207427577	1.528952566	-3.109854041
H	0.245439334	-1.853333668	-2.976986797
C	-2.048318348	1.570488627	1.468592241

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Rh	-3.075060967	1.934145117	2.174067580
Cl	-3.252005404	2.919284356	4.370423441
H	-0.484139320	-1.736542093	-0.848073702
C	-0.814246689	4.008824324	-0.501769137
O	-0.986472781	2.704447569	0.109640025
C	-2.190764898	4.214121732	-1.229434461
C	0.401288648	3.951812591	-1.420624881
C	-0.582076817	5.016995526	0.632133890
B	-2.353981129	2.530170612	0.361954909
O	-3.087168871	3.454352920	-0.383270229
C	-2.221430324	3.606200802	-2.635975976
C	-2.688806262	5.657965042	-1.271973107
H	-1.647908928	4.219316207	-3.339342491
H	-1.827586570	2.589756061	-2.649495983
H	-3.259285942	3.562446394	-2.979082476

H	-3.525116762	-0.434003896	6.624538482
H	-7.517654585	0.912178751	3.826725982
H	-6.578988464	-0.419246922	4.514474195
H	-7.320359916	0.791363880	5.585826797
H	-6.535301192	3.148215670	3.524553803
H	-6.574935972	3.284825954	5.295890043
H	-5.080156321	3.632153400	4.405385609
H	-5.457731215	2.015286040	7.367140916
H	-3.696723748	1.864124860	7.511373041
H	-4.389688667	3.179218920	6.552753011
C	-3.119800339	-2.320972800	2.223842693
C	-4.456369625	-1.898401142	2.253319083
C	-2.820160881	-3.644671801	1.866799325
C	-5.476018975	-2.800814431	1.952322869
C	-3.845722695	-4.539887261	1.561753287
C	-5.175983291	-4.119595349	1.608141148
H	-4.697868935	-0.867349999	2.481575726
H	-1.787304487	-3.976837305	1.821276761
H	-6.508407477	-2.462116303	1.969381261
H	-3.603844542	-5.562294578	1.283754728
H	-5.974667091	-4.815919872	1.365846552
C	-1.492081371	-1.521086490	4.485654515
C	-0.923753986	-0.552154896	5.323698021
C	-1.790976366	-2.784744023	5.019340742
C	-0.641912376	-0.844435401	6.657886993
C	-1.523359080	-3.070109285	6.358006796
C	-0.944520807	-2.102323947	7.180802850
H	-0.736578275	0.440559635	4.932376925
H	-2.246137892	-3.546423421	4.395590845
H	-0.204763832	-0.079017892	7.293661172
H	-1.770851342	-4.049630662	6.758142015
H	-0.738712947	-2.324916479	8.224575796
C	-0.306995239	-1.810034900	1.850729919
C	0.848488396	-2.220347375	2.525222349
C	-0.322015342	-1.806245488	0.444806936
C	1.977764287	-2.620030276	1.804212241
C	0.802768341	-2.213175679	-0.267804454
C	1.958373516	-2.617925551	0.409356131
H	0.870028540	-2.227166920	3.610893781
H	-1.210580684	-1.459237060	-0.077688196
H	2.871266030	-2.935100428	2.337178667
H	0.783549729	-2.201018691	-1.354036635
H	2.837715702	-2.928476363	-0.148523969

Ic

Rh	-2.400123126	0.629744534	2.100829845
Cl	-4.329827590	0.029055079	3.429187637
H	-0.379200169	2.259625160	3.140187510
P	-1.154676560	-1.137302987	2.939810277
C	1.890874470	2.208093121	0.684518917
C	1.011139164	1.809096774	-0.383240266
C	-0.233567843	1.337850092	-0.020156339
N	-0.734246023	1.455579596	1.229040761
C	-0.098493494	2.458666502	2.097908111
C	1.401247560	2.414449397	1.932226921
H	2.964152719	2.246009278	0.501195553
H	1.362969371	1.691912929	-1.401724686

H	-0.847940739	0.790869758	-0.730070699
H	-0.506913500	3.464394604	1.851594185
H	2.041761236	2.574997201	2.794474622
C	-4.509884450	4.961269054	0.850411179
C	-4.800891257	4.349512051	2.067840207
C	-4.239417451	3.107776643	2.351070359
N	-3.412982136	2.479149786	1.493367500
C	-3.133292630	3.068695957	0.314957592
C	-3.664844198	4.303217857	-0.041407787
H	-4.933035125	5.930356114	0.601084679
H	-5.455354467	4.818096098	2.795469692
H	-4.456836229	2.576470611	3.270445526
H	-2.469375343	2.529257815	-0.342815542
H	-3.408807336	4.736340120	-1.002769890
C	-3.738014705	-0.806657918	-1.592754831
O	-3.262805373	0.230689429	-0.684366038
C	-2.998366043	-2.081964590	-1.048349508
C	-3.368759592	-0.404498115	-3.015867223
C	-5.259185391	-0.871847675	-1.422009112
B	-2.890620569	-0.390736747	0.487586628
O	-2.861091481	-1.762769931	0.368124588
C	-1.580768680	-2.252321594	-1.606006648
C	-3.779504878	-3.385428754	-1.169738063
H	-1.600508674	-2.540880419	-2.661545706
H	-0.997685916	-1.333502394	-1.503218663
H	-1.064671311	-3.029673983	-1.038582211
H	-3.917312909	0.499121694	-3.296951745
H	-2.301275421	-0.196667449	-3.108142605
H	-3.633735107	-1.198738187	-3.721885729
H	-5.679490283	0.116874325	-1.625084690
H	-5.711591862	-1.591805265	-2.110752514
H	-5.523567586	-1.146649623	-0.397030297
H	-3.975691677	-3.621553510	-2.221132457
H	-3.193659416	-4.202335747	-0.738872556
H	-4.731096457	-3.333058180	-0.638144934
C	-2.025967966	-2.529319266	3.763645291
C	-1.479758428	-3.114252418	4.916068274
C	-3.208215697	-3.053547675	3.221617835
C	-2.105868330	-4.206740890	5.516770178
C	-3.825779979	-4.149389065	3.823966372
C	-3.280847135	-4.727557810	4.972087435
H	-0.566846655	-2.716701212	5.348817339
H	-3.639393275	-2.603646144	2.338009676
H	-1.674981654	-4.647515750	6.411604345
H	-4.744961864	-4.543226058	3.399076540
H	-3.771034209	-5.575662040	5.442354854
C	0.072510344	-1.971966488	1.861154695
C	1.097341935	-1.229568764	1.253284834
C	-0.018353970	-3.349100062	1.604008651
C	2.010369435	-1.856331347	0.404694579
C	0.899602064	-3.969151678	0.755748548
C	1.914685374	-3.225146830	0.149218365
H	1.192162159	-0.168269846	1.445528170
H	-0.805730406	-3.937817403	2.061158733
H	2.789373554	-1.260145843	-0.061700411
H	0.817589683	-5.036465639	0.567570952
H	2.624454883	-3.709989890	-0.515632379
C	-0.212626988	-0.354450698	4.312017686

C	-0.971438599	0.337932618	5.274376777
C	1.182789266	-0.375922162	4.426475210
C	-0.337465923	1.004186698	6.322057231
C	1.810948583	0.295682208	5.477913583
C	1.056524331	0.991768459	6.422829699
H	-2.057130693	0.345595655	5.201546462
H	1.783707129	-0.911722834	3.700582480
H	-0.934076531	1.535147091	7.058585921
H	2.894703849	0.274527251	5.553048248
H	1.550355615	1.516931543	7.235554856

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Rh	-2.686958366	2.123163939	2.344503785
Cl	-1.186601432	1.237153668	4.025187828
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P	-2.279175715	0.248592471	1.041823414
C	-2.081959319	4.315967859	4.768276918
C	-2.921201860	4.161541665	3.578152941
C	-2.349532352	4.450733803	2.345222916
N	-0.990960851	4.653892199	2.186770451
C	-0.064253178	4.422159797	3.324803204
C	-0.763161287	4.516568429	4.653211148
H	-2.560288587	4.296477715	5.742626883
H	-3.998781673	4.218003719	3.666265464
H	-2.947235237	4.735481905	1.488719358
H	0.375087481	3.417653063	3.230321199
H	-0.133374548	4.661378108	5.525881791
C	-0.312728480	4.851418952	-1.392133858
O	-1.221500115	4.948401754	-0.257643555
C	1.073864281	5.245300727	-0.749132925
C	-0.804722767	5.795377634	-2.484568504
C	-0.351544607	3.400113977	-1.878733670
B	-0.448218153	4.812052024	0.872359952
O	0.903490538	4.840787425	0.638409472
C	1.324998838	6.757924410	-0.739982974
C	2.277706248	4.504064181	-1.321544452
H	1.524987108	7.139269534	-1.745948891
H	0.466233033	7.295557255	-0.327207092
H	2.192779467	6.969024960	-0.109096093
H	-1.772857175	5.449443243	-2.858298502
H	-0.931075303	6.812972598	-2.111147153
H	-0.101559761	5.813087345	-3.323987241
H	-1.375562181	3.141586402	-2.159457948
H	0.288249654	3.252819879	-2.753644196
H	-0.031678241	2.711703807	-1.094759607
H	2.385101739	4.712184624	-2.391496981
H	3.188413957	4.838146036	-0.815941336
H	2.183866871	3.426359494	-1.178478264
C	-3.364883841	0.094683734	-0.437793853
C	-4.012967929	-1.096047660	-0.780982516
C	-3.529659216	1.223444307	-1.255408794
C	-4.810358741	-1.157854329	-1.927118941
C	-4.318549615	1.158240007	-2.400984661
C	-4.963048046	-0.034818164	-2.740431105
H	-3.900818128	-1.974268902	-0.153626101
H	-3.045203045	2.156839146	-0.983976654
H	-5.313501731	-2.086909793	-2.181809156

H	-4.437287664	2.040005518	-3.025263177
H	-5.584418537	-0.085439881	-3.630531407
C	-2.375907792	-1.385796408	1.857636564
C	-1.575148183	-2.466897588	1.465006114
C	-3.309930790	-1.552002947	2.889810213
C	-1.716632146	-3.705275755	2.092121169
C	-3.450005197	-2.792302282	3.508910198
C	-2.654839942	-3.869571742	3.112409523
H	-0.839734246	-2.343485619	0.675713560
H	-3.920723011	-0.710330687	3.195248172
H	-1.090360842	-4.538920413	1.785979558
H	-4.173695215	-2.914919813	4.310046576
H	-2.761209270	-4.833894398	3.602206032
C	-0.604656666	0.303802945	0.265734012
C	0.478881114	0.831804720	0.985593196
C	-0.392001788	-0.162445590	-1.042709751
C	1.744642425	0.899036180	0.401689101
C	0.876670087	-0.097116618	-1.619257291
C	1.947572173	0.437824800	-0.900576702
H	0.327830138	1.177386962	2.003138901
H	-1.218317769	-0.566843331	-1.618090451
H	2.570718091	1.320692716	0.967313970
H	1.024921256	-0.458551712	-2.633390328
H	2.933582360	0.496289644	-1.353907210
C	-6.728212979	1.046213026	1.716281764
O	-5.297717337	0.802471821	1.786201745
B	-4.682485211	2.000505410	2.114721219
O	-5.610466713	2.962107756	2.490749222
C	-6.884173384	2.282982050	2.671000191
H	-3.651533123	2.620449234	1.157913208
C	-6.974975345	1.887244182	4.149628392
H	-7.936655374	1.420881360	4.384135897
H	-6.172361858	1.193961068	4.416714687
H	-6.865035603	2.784986424	4.764174698
C	-7.456414218	-0.217591882	2.160280535
H	-7.265426277	-1.019247470	1.440824080
H	-7.112260777	-0.554077270	3.139911149
H	-8.537438040	-0.046407950	2.205941032
C	-7.053787033	1.367911159	0.252706780
H	-6.698358961	0.549394977	-0.378208979
H	-8.130387612	1.492721500	0.098290298
H	-6.544568730	2.280726759	-0.068380006
C	-8.005721393	3.247604149	2.302537550
H	-8.976666819	2.741873191	2.340323249
H	-8.025783466	4.078820803	3.013414469
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Rh	-2.374572244	1.035998371	2.462173394
Cl	-4.801509937	0.707509608	2.248263060
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P	-2.044113700	-1.204068508	2.317949011
C	-2.985671524	5.805240789	3.772808262
C	-4.028689812	5.100365793	3.175293839
C	-3.826752751	3.774908932	2.798320397
N	-2.650153629	3.142814705	2.983327067
C	-1.638944223	3.829158307	3.558116694

H	-6.839992683	4.848559766	0.255074536
H	-6.030863169	3.340036294	0.732027874
H	-5.754123420	6.561592247	2.009548594
H	-4.418651597	6.011517977	3.041864358
H	-4.743218460	5.183944660	1.520247689
C	0.291616884	1.339055149	2.730505477
C	1.178695311	2.338020435	3.168159062
C	0.797001515	0.089957219	2.344313511
C	2.549174297	2.091296962	3.212045523
C	2.172685381	-0.149175416	2.388695241
C	3.049067522	0.846386629	2.819849341
H	0.797450981	3.307335075	3.475514734
H	0.111620657	-0.699209446	2.049070732
H	3.226805980	2.869286060	3.554101662
H	2.554471277	-1.123321154	2.095591164
H	4.118215601	0.653994783	2.858237517
C	-1.656500300	2.655014575	1.057410193
C	-0.583229066	2.899965712	0.190493997
C	-2.929231203	3.137665304	0.703629816
C	-0.778516530	3.609548439	-0.998164124
C	-3.120467088	3.851235121	-0.476624490
C	-2.043949294	4.088388420	-1.336940746
H	0.408393210	2.537114803	0.441421843
H	-3.769105856	2.949431742	1.365271193
H	0.065743866	3.788186997	-1.659149426
H	-4.114060585	4.209741357	-0.733537522
H	-2.192644660	4.637677576	-2.262518520
C	-1.755327695	2.917715911	3.929263714
C	-1.974874687	4.281486026	3.700183941
C	-1.740849409	2.447973920	5.253801283
C	-2.184027716	5.154293794	4.771026703
C	-1.944790322	3.320402630	6.321048575
C	-2.173186094	4.678660598	6.081863597
H	-1.986593496	4.667792214	2.686696860
H	-1.576942614	1.388899139	5.438975351
H	-2.348119994	6.211626535	4.577385301
H	-1.929275657	2.940525491	7.339117418
H	-2.336910952	5.359484076	6.912781864

3'-TS

Rh	-3.246641237	-0.090061596	2.811329703
Cl	-2.136027206	-2.217009883	2.265767277
H	-4.160105131	1.304435319	2.761392079
P	-1.775171136	0.402522649	4.613556585
C	-0.269250235	2.409430501	-0.478414592
C	-0.935228656	3.092329518	0.538619284
C	-1.773573459	2.374292237	1.384415992
N	-1.970514553	1.049082160	1.266735298
C	-1.326599580	0.392129657	0.286738874
C	-0.472412738	1.036670624	-0.605865597
H	0.399896918	2.936729279	-1.152595618
H	-0.798011849	4.158008246	0.690403520
H	-2.292551358	2.858763057	2.205681023
H	-1.495919300	-0.680049400	0.258782683
H	0.028403379	0.462221298	-1.378777377
C	-5.398460231	0.754152788	2.184462809
C	-5.135891950	-0.670219245	2.176191799

C	-4.923163133	-1.169267723	3.525896844
N	-5.701357299	-0.606926933	4.593838852
C	-6.388504246	0.574353525	4.392412786
C	-6.280805626	1.273335461	3.241433882
H	-5.435038864	1.257321260	1.219313287
H	-5.176706738	-1.281714394	1.282926708
H	-4.710727646	-2.221520392	3.674174062
H	-6.981345460	0.912683441	5.233717231
H	-6.778874598	2.227526216	3.117850724
C	-5.715507984	-1.242470461	8.172114851
O	-6.236330932	-0.556662975	6.995306539
C	-5.375801795	-2.663208856	7.593059456
C	-6.784929284	-1.225035150	9.257214779
C	-4.470413545	-0.469433281	8.619892097
B	-5.647882694	-1.171111258	5.916745052
O	-5.009218408	-2.346388130	6.213779231
C	-6.595603339	-3.588568737	7.520560096
C	-4.206981784	-3.366060738	8.271057078
H	-6.892616860	-3.936954284	8.514367377
H	-7.447670961	-3.080322506	7.059603058
H	-6.344079322	-4.458170683	6.907501805
H	-6.951247630	-0.196933210	9.591476342
H	-7.734017997	-1.621281196	8.892001220
H	-6.464553231	-1.817093074	10.120905685
H	-4.735075758	0.580136556	8.768014448
H	-4.068089256	-0.866106999	9.557063241
H	-3.685396854	-0.506731651	7.860519959
H	-4.423802643	-3.520598787	9.333577571
H	-4.046608520	-4.345333144	7.810682077
H	-3.283488054	-2.795489134	8.174883005
C	-1.037868851	-1.026452821	5.517080192
C	0.241367108	-0.974889023	6.095327749
C	-1.784732888	-2.206692245	5.627702853
C	0.752959234	-2.073753187	6.786102599
C	-1.267438882	-3.305297325	6.315567655
C	-0.001515484	-3.243405018	6.899516525
H	0.847883817	-0.079695295	5.992980139
H	-2.759466736	-2.274062527	5.163829732
H	1.744687031	-2.017701811	7.227412934
H	-1.855345190	-4.216069763	6.380564899
H	0.400550270	-4.103687517	7.427837339
C	-2.445175701	1.449743491	5.981654319
C	-1.779583593	1.594365228	7.210912809
C	-3.641266625	2.150399930	5.778942901
C	-2.290656750	2.431832169	8.200794726
C	-4.156150243	2.985892398	6.772481430
C	-3.479734998	3.133163038	7.982842029
H	-0.860983545	1.047123856	7.396927327
H	-4.176170494	2.031584483	4.842301332
H	-1.762523678	2.535179489	9.145036467
H	-5.088925175	3.515738345	6.598923117
H	-3.878220731	3.783654228	8.756948570
C	-0.269776345	1.326681068	4.095723501
C	0.566458927	0.684557143	3.164274439
C	0.021837182	2.640846524	4.480704739
C	1.675244774	1.343959692	2.643064471
C	1.133253709	3.301554247	3.949251855
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H	0.326101882	-0.325976060	2.841476176
H	-0.613430989	3.152496182	5.197366426
H	2.311896267	0.838134276	1.922346748
H	1.350506816	4.321187249	4.257558001
H	2.824962734	3.172081882	2.620358004

5-Py

Rh	0.290745083	1.182905149	0.057962801
Cl	0.729268002	1.734879762	-2.279539245
P	1.970961114	-0.364067248	-0.091474415
C	2.052817049	-1.599562462	1.280702694
C	1.374700433	-2.825809171	1.193286201
C	2.679310615	-1.262070842	2.492014966
C	1.334849353	-3.691617210	2.287071175
C	2.641666452	-2.131161601	3.581585919
C	1.967184939	-3.349161624	3.482733081
H	0.876006291	-3.106265801	0.271651450
H	3.216807667	-0.321583508	2.577602276
H	0.808842218	-4.638834910	2.201272081
H	3.139352050	-1.855082757	4.507482035
H	1.935908729	-4.026302463	4.332028527
C	3.683563891	0.302101739	-0.159203705
C	4.800920382	-0.463762191	0.214481722
C	3.877192560	1.612634959	-0.620295921
C	6.084911326	0.074488291	0.136032765
C	5.164604776	2.145140514	-0.699566959
C	6.268816151	1.381604294	-0.319378518
H	4.668467177	-1.479158721	0.575371837
H	3.020496983	2.199129316	-0.935765220
H	6.940525981	-0.527090119	0.431526800
H	5.301832008	3.160783420	-1.060770606
H	7.269589388	1.801662362	-0.378131872
C	1.808520510	-1.440476526	-1.573239167
C	0.516720429	-1.818157224	-1.973270819
C	2.914717359	-1.914558966	-2.287456371
C	0.344891138	-2.674435504	-3.059619403
C	2.735580462	-2.762053634	-3.381546049
C	1.452060615	-3.146346168	-3.767866808
H	-0.348113006	-1.441177847	-1.434482539
H	3.918187487	-1.615496186	-2.002927523
H	-0.657383457	-2.962473898	-3.362992985
H	3.601651051	-3.116537487	-3.934302391
H	1.313758303	-3.804574596	-4.621673761
C	-3.423229948	-2.589038985	-0.303023662
O	-2.339503904	-1.704997153	0.083356213
C	-4.656763693	-1.610206156	-0.309905047
C	-3.522200597	-3.671252971	0.780260122
C	-3.084335785	-3.214233830	-1.651493290
B	-2.920479628	-0.684438591	0.817390065
O	-4.296752805	-0.652583885	0.723153418
N	-2.168347049	0.228840545	1.591571690
C	-5.989229206	-2.251072259	0.062003958
C	-4.783423970	-0.825534632	-1.621840269
H	-6.244164048	-3.048728490	-0.643960184
H	-5.960925359	-2.669757733	1.069583161
H	-6.783199428	-1.499072062	0.029994869
H	-2.548062712	-4.158941406	0.878197679

H	-3.780489800	-3.232632468	1.748791718
H	-4.269648880	-4.430353281	0.529832190
H	-3.909457490	-3.840676791	-2.006836421
H	-2.873494958	-2.451322800	-2.403188143
H	-2.193955205	-3.841679625	-1.550475505
H	-3.820133698	-0.399951841	-1.917673191
H	-5.147007693	-1.457025312	-2.437989377
H	-5.490629563	-0.004353200	-1.474099523
C	-0.566622647	2.148926150	2.946316677
C	0.073714497	1.041165507	2.227186007
C	-1.899290230	2.280536259	2.981208499
H	0.068207915	2.854313684	3.478363580
C	-0.762872420	0.088637956	1.602396613
H	1.021048572	0.698817436	2.629407596
H	-0.452823096	-0.945223039	1.519448248
H	-3.610252977	0.988282559	2.928172383
C	-2.839927149	1.369980074	2.241464153
H	-3.384683006	1.952352208	1.483205943
H	-2.368835076	3.090175178	3.535171344
N	-1.271006666	2.651222718	-0.165063027
C	-2.290762424	2.335713555	-0.983635836
C	-1.181834086	3.907339276	0.299111317
C	-3.271646625	3.253040435	-1.342165193
C	-2.111535801	4.891054734	-0.027586274
C	-3.180866940	4.557507872	-0.856573348
H	-2.295370222	1.318460730	-1.355257713
H	-0.341925722	4.112354598	0.951414822
H	-4.082461239	2.945362043	-1.994152383
H	-1.993078594	5.895475363	0.365901358
H	-3.926116974	5.301153426	-1.124305181

5'-Py

Rh	0.305709555	-1.154171969	-0.074979714
Cl	0.894209331	-1.865800678	2.180344198
H	-0.036392945	-3.148987533	-2.629128566
P	1.956722533	0.423875690	0.086919834
C	1.974217702	1.702896114	-1.246176844
C	2.563010414	1.410040985	-2.487844711
C	1.276986518	2.911923601	-1.103136592
C	2.462969519	2.303482236	-3.553281043
C	1.175652898	3.803738145	-2.171752938
C	1.765958329	3.503005610	-3.399465856
H	3.118841722	0.485601734	-2.617017717
H	0.806791118	3.157097569	-0.156334954
H	2.929072350	2.060370544	-4.504324424
H	0.633603860	4.736661840	-2.041451037
H	1.684918225	4.198076630	-4.230615508
C	3.692035218	-0.188019283	0.080504728
C	3.944449340	-1.526080074	0.417016445
C	4.772124287	0.649837456	-0.246415853
C	5.252000289	-2.013838915	0.420353089
C	6.076251495	0.156788397	-0.243094914
C	6.318273041	-1.177861795	0.088280191
H	3.117743953	-2.170668901	0.695521031
H	4.593675052	1.686607361	-0.514873195
H	5.434463054	-3.051921562	0.684473378
H	6.901844413	0.814396449	-0.501755370

H	7.334539661	-1.563065150	0.087201794
C	1.786506721	1.432727461	1.613813990
C	2.886060698	1.900868662	2.341731775
C	0.488093261	1.749086321	2.046249222
C	2.693366864	2.681162658	3.482581824
C	0.302540207	2.536603125	3.181286392
C	1.403247793	3.002307666	3.903351772
H	3.894528713	1.647594579	2.031741369
H	-0.370825110	1.374368332	1.496003088
H	3.554357183	3.031282161	4.045635589
H	-0.704554578	2.772793631	3.512633089
H	1.255054260	3.605934750	4.794871369
C	-4.717044983	1.473446117	0.335169556
O	-4.329722260	0.595596401	-0.757851020
C	-3.472569290	2.434000122	0.449233111
C	-4.908116221	0.590861598	1.574599481
C	-6.028481344	2.159149574	-0.032196952
B	-2.952770292	0.620883264	-0.807076765
O	-2.386022951	1.574318171	0.016324268
N	-2.165170778	-0.247194790	-1.608565002
C	-3.164131267	2.933685112	1.856721850
C	-3.526729094	3.607995316	-0.536258375
H	-2.962119392	2.106891901	2.540292727
H	-2.276787785	3.572488516	1.830720243
H	-3.999873437	3.521194279	2.250990581
H	-3.967779286	0.121900772	1.876797743
H	-5.292314559	1.165620592	2.422492613
H	-5.625426787	-0.199558920	1.336501533
H	-6.830426802	1.417163216	-0.085319719
H	-6.299629276	2.901864052	0.725564357
H	-5.961497810	2.654597732	-1.001997330
H	-2.545622023	4.090658274	-0.559880086
H	-3.757514174	3.260006622	-1.547427436
H	-4.274858169	4.350222079	-0.242076246
C	-0.459114965	-2.201685829	-2.995044678
C	-1.964504201	-2.242940066	-2.955356411
C	0.102966155	-1.014120912	-2.227996330
H	-0.120381521	-2.134382708	-4.042023640
C	-2.706800743	-1.332855384	-2.314604399
H	-2.472173246	-3.042763725	-3.486717094
H	-3.790130081	-1.380216320	-2.289068189
C	-0.751992444	-0.074522087	-1.613681075
H	-0.467651774	0.967184829	-1.535670203
H	1.038742087	-0.630836001	-2.621166234
N	-1.216317525	-2.649131443	0.137153930
C	-2.346802217	-2.308356652	0.777858728
C	-0.993753259	-3.945891405	-0.128487360
C	-3.312906821	-3.239907178	1.138078590
C	-1.908045939	-4.941760147	0.199840695
C	-3.093968573	-4.583632553	0.838747257
H	-2.457136883	-1.256183657	1.006163728
H	-0.051658512	-4.177763129	-0.611772879
H	-4.212498193	-2.910771999	1.647721466
H	-1.685502785	-5.976524192	-0.039166179
H	-3.827575641	-5.338087887	1.107860125

VII-9. Vibrational frequencies of DFT-optimized structures

Pyridine

385.71	420.35	613.29	668.66	719.16	763.89
898.89	958.22	998.52	1011.25	1014.40	1050.11
1085.56	1099.40	1182.63	1251.53	1309.78	1389.12
1482.02	1524.02	1636.71	1642.58	3161.92	3164.33
3187.18	3203.80	3212.35			

HBpin

95.62	230.49	246.02	284.56	291.62	295.94
323.54	334.19	361.57	372.65	398.18	449.28
512.82	522.62	583.39	665.82	748.83	806.22
868.45	904.88	938.01	947.34	965.47	978.76
1023.00	1031.46	1065.06	1144.78	1183.61	1192.05
1207.02	1244.76	1273.03	1302.94	1383.08	1415.82
1418.92	1428.65	1438.61	1485.02	1494.30	1497.16
1502.08	1518.15	1520.83	1523.16	1541.91	2714.60
3051.27	3053.90	3055.94	3060.33	3124.17	3124.92
3132.32	3133.29	3137.25	3137.52	3154.21	3154.33

A

43.72	58.62	102.17	106.90	122.29	207.15
222.45	236.34	265.32	274.08	308.25	325.60
332.59	337.89	363.10	378.35	385.63	413.23
455.59	524.45	530.46	541.79	585.77	597.53
630.10	662.26	677.08	722.16	768.89	812.28
861.29	877.00	939.19	942.73	944.51	947.83
952.50	974.88	975.57	984.70	1004.74	1022.08
1030.38	1045.52	1107.65	1146.02	1160.04	1188.68
1192.85	1206.01	1250.37	1270.93	1279.07	1294.87
1304.69	1367.14	1371.42	1415.53	1417.71	1422.37
1428.16	1437.57	1461.23	1486.31	1493.33	1498.41
1501.73	1507.99	1516.96	1518.55	1524.23	1525.49
1541.48	1644.69	1716.34	2931.68	3050.33	3052.21
3055.17	3059.08	3106.80	3123.11	3123.50	3130.50
3131.79	3135.14	3135.67	3152.84	3153.91	3173.13
3198.68	3204.62	3226.26			

B

50.92	58.64	98.48	108.01	115.29	198.30
222.02	237.34	262.01	273.54	306.19	324.03
329.18	340.09	380.66	382.53	414.58	427.36
447.84	515.34	524.03	531.32	585.65	601.53
638.64	656.51	674.53	751.74	759.27	813.62
861.88	877.62	896.98	940.38	946.74	971.29
972.11	973.89	980.53	987.20	1007.14	1009.87
1021.52	1030.86	1106.12	1143.88	1152.12	1188.63
1191.96	1216.81	1249.22	1256.45	1270.43	1299.62
1325.26	1367.73	1379.12	1415.43	1416.93	1419.74

1428.18 1437.73 1450.58 1485.71 1493.54 1497.86
1501.89 1503.43 1508.30 1518.50 1522.74 1523.88
1541.60 1710.59 1775.42 2963.45 2966.21 3050.80
3052.81 3055.77 3059.74 3124.15 3124.77 3131.28
3131.82 3135.63 3136.39 3152.00 3152.56 3188.39
3189.17 3226.24 3228.22

G

12.18 19.60 36.66 52.23 81.34 87.95
104.17 111.06 120.18 147.27 171.63 224.92
228.04 234.41 238.57 258.96 270.46 285.36
287.69 298.52 305.32 320.41 324.64 326.09
334.92 336.73 340.51 354.94 374.80 377.28
384.19 393.50 403.28 435.56 443.83 454.17
513.92 523.42 525.27 534.70 541.22 555.08
586.30 587.78 604.33 660.06 673.49 674.36
718.20 756.90 779.87 807.72 839.65 859.21
864.67 870.77 880.74 926.13 939.41 939.94
945.99 947.92 960.02 969.04 973.27 976.81
985.71 990.94 1021.71 1022.43 1024.15 1030.25
1034.25 1042.77 1082.21 1114.31 1143.16 1146.57
1172.12 1180.39 1191.29 1191.59 1192.41 1195.57
1234.73 1247.59 1249.94 1269.76 1272.19 1289.20
1302.06 1302.64 1307.07 1310.80 1349.62 1363.37
1368.52 1390.09 1403.22 1414.61 1415.53 1416.93
1418.19 1427.25 1428.12 1436.81 1438.00 1442.73
1485.91 1486.22 1493.57 1493.78 1497.37 1498.14
1498.52 1501.74 1501.75 1513.50 1518.12 1518.49
1519.15 1520.35 1523.64 1524.17 1533.18 1541.39
1541.98 1725.84 2946.90 3009.09 3049.11 3049.88
3051.12 3052.11 3053.62 3053.82 3054.58 3057.92
3058.72 3098.96 3115.83 3121.25 3122.11 3122.50
3123.23 3129.34 3130.27 3130.91 3131.64 3133.72
3134.63 3135.17 3136.08 3152.02 3152.59 3152.80
3153.22 3193.18 3214.09

R

13.09 16.01 44.17 66.00 74.87 100.86
106.32 121.91 127.29 142.31 220.77 226.59
233.95 239.84 244.05 252.38 267.45 283.61
287.90 303.51 311.26 313.92 326.73 331.56
337.59 339.57 345.66 374.67 377.04 384.02
388.84 401.78 416.29 435.78 447.85 474.75
506.06 520.02 527.51 532.53 544.46 561.95
585.74 586.96 599.69 660.22 674.79 678.16
713.12 740.82 806.42 832.21 853.81 866.16
869.17 880.98 896.30 930.19 937.59 939.70
941.80 945.84 948.78 956.77 968.14 975.10
979.03 981.98 992.05 1022.55 1023.19 1029.34
1034.21 1054.31 1074.71 1121.04 1141.92 1145.15
1150.74 1180.98 1183.97 1191.75 1192.10 1193.69
1235.24 1248.12 1249.03 1263.23 1271.41 1271.62
1277.97 1298.77 1305.29 1310.04 1345.46 1351.02
1366.89 1384.06 1414.32 1415.08 1417.79 1418.81
1422.30 1427.36 1427.68 1437.13 1437.93 1441.77
1485.42 1486.28 1492.02 1494.05 1496.70 1497.38

1498.89 1501.32 1502.27 1514.25 1516.83 1518.36
1519.66 1520.27 1523.31 1525.83 1532.56 1541.65
1541.96 1722.39 3000.31 3016.05 3035.30 3049.75
3049.87 3051.75 3053.25 3054.49 3055.60 3058.55
3063.31 3072.30 3121.66 3122.31 3123.24 3123.63
3130.22 3130.59 3132.08 3134.14 3134.42 3134.48
3134.86 3137.74 3148.68 3150.87 3152.47 3153.88
3166.51 3186.88 3208.69

I

13.53 28.13 32.59 34.45 40.89 42.75
48.30 54.24 64.56 65.93 71.94 80.68
82.93 101.20 122.85 137.29 163.81 183.09
187.46 190.76 206.81 213.10 235.12 237.45
251.07 259.64 262.94 265.73 276.84 297.21
400.95 404.32 406.25 412.12 422.24 439.64
447.11 461.38 469.87 478.62 502.90 525.24
545.58 630.87 631.37 633.23 648.65 656.87
663.34 664.49 696.32 702.69 704.92 708.86
711.05 712.39 714.05 721.01 760.23 765.62
769.04 769.85 771.65 866.17 870.31 876.06
877.86 880.32 934.34 943.22 951.17 952.05
957.56 979.00 982.92 986.18 987.53 997.33
1002.18 1005.60 1005.83 1006.03 1011.65 1014.03
1015.05 1017.30 1035.89 1043.30 1051.82 1053.33
1053.98 1058.89 1058.92 1095.31 1097.48 1100.61
1104.46 1108.02 1113.03 1113.96 1115.02 1116.91
1119.36 1186.21 1186.74 1196.95 1197.94 1198.45
1217.05 1224.90 1227.34 1242.45 1252.89 1306.28
1309.07 1321.80 1327.43 1332.71 1359.55 1364.40
1368.20 1380.10 1390.29 1473.77 1475.73 1479.03
1487.97 1489.12 1519.36 1521.94 1524.66 1526.21
1528.27 1624.50 1625.88 1626.61 1628.04 1629.24
1644.91 1646.09 1647.46 1657.36 1658.27 3159.60
3171.88 3173.65 3174.97 3178.38 3182.03 3184.99
3188.44 3191.34 3191.60 3191.83 3193.93 3200.01
3200.52 3202.95 3205.77 3208.81 3211.16 3212.09
3215.41 3216.80 3239.25 3239.99 3246.68 3247.02

I-TS

-87.90 16.52 26.00 31.03 33.59 39.64
40.50 49.93 50.45 53.54 58.56 63.60
67.90 69.29 98.30 108.23 124.53 136.60
158.20 165.77 180.01 201.14 204.02 216.05
225.91 229.99 236.81 244.73 249.36 252.58
257.98 266.66 272.76 296.70 304.61 325.94
336.15 337.05 372.85 379.90 398.27 407.41
408.48 409.69 413.10 445.56 448.25 451.11
456.03 466.75 509.88 517.30 523.98 527.78
542.64 586.80 625.17 629.91 631.49 633.22
650.78 664.67 679.16 699.60 705.98 706.66
708.83 711.20 714.99 718.45 763.38 767.43
767.61 773.69 800.27 847.90 860.60 867.30
872.97 879.60 884.96 887.28 936.98 939.94
943.37 947.22 948.65 963.76 973.44 979.98
986.46 988.06 989.67 992.78 1001.77 1005.58

1008.69 1013.07 1013.86 1014.83 1016.06 1022.90
1034.10 1042.36 1051.00 1054.03 1055.37 1056.04
1100.52 1104.00 1114.07 1115.09 1116.35 1118.48
1122.35 1125.22 1127.14 1152.11 1187.44 1191.46
1197.64 1198.15 1198.31 1204.62 1224.63 1228.02
1233.46 1246.72 1254.24 1270.24 1276.18 1309.65
1313.67 1327.20 1330.53 1334.29 1365.95 1371.61
1373.57 1389.03 1414.30 1417.88 1428.38 1438.03
1475.28 1477.31 1478.88 1486.45 1491.96 1493.22
1497.41 1501.07 1517.99 1519.35 1522.35 1525.05
1527.65 1530.18 1531.49 1540.22 1627.07 1629.78
1631.43 1632.46 1646.96 1647.53 1648.80 1661.23
1953.25 3046.36 3048.62 3051.37 3055.32 3118.32
3119.49 3126.21 3128.61 3130.15 3134.65 3148.50
3158.61 3172.20 3174.47 3175.36 3180.63 3184.50
3186.04 3188.50 3191.07 3195.32 3197.88 3199.87
3203.86 3205.04 3208.01 3208.28 3214.20 3216.83
3226.25 3237.49 3240.36

1a

13.84 20.23 25.44 29.67 34.73 38.40
47.65 50.96 53.51 56.88 61.32 64.23
74.80 86.77 97.70 114.68 122.80 133.38
154.10 171.34 173.96 200.26 207.11 214.07
224.34 228.90 235.43 247.90 249.17 256.28
264.13 276.05 286.63 297.67 306.06 327.20
337.13 367.94 379.74 397.81 407.42 408.65
412.38 413.21 418.91 443.75 449.35 459.31
465.00 497.93 515.20 523.84 527.40 545.61
547.67 586.78 613.83 630.22 631.29 632.11
649.33 664.96 677.64 701.57 704.75 707.11
708.10 713.25 717.21 721.41 763.85 766.23
767.54 774.93 799.97 849.38 860.60 863.71
875.23 877.12 883.56 888.65 938.47 939.61
940.45 948.05 948.89 968.71 971.39 979.17
983.92 984.15 993.53 1000.29 1000.74 1002.22
1013.43 1013.63 1015.89 1016.25 1018.02 1022.78
1033.05 1040.88 1051.63 1054.67 1055.05 1056.01
1100.33 1104.18 1114.72 1116.25 1117.15 1120.03
1123.31 1124.72 1130.11 1159.09 1187.67 1192.56
1197.77 1197.97 1199.35 1211.34 1225.41 1228.80
1231.65 1246.91 1255.07 1270.87 1283.96 1309.42
1311.90 1328.09 1331.26 1335.28 1366.63 1370.14
1375.03 1388.08 1415.01 1417.64 1427.19 1437.01
1475.92 1477.22 1479.30 1485.95 1491.77 1492.49
1497.42 1500.91 1516.75 1519.13 1523.38 1523.54
1527.88 1530.43 1530.73 1539.71 1628.33 1630.19
1630.88 1631.34 1647.58 1648.06 1648.86 1661.18
2093.68 3047.68 3050.48 3052.22 3056.65 3119.40
3120.84 3128.91 3130.78 3131.68 3143.15 3148.53
3150.52 3173.68 3175.09 3175.24 3179.31 3184.57
3185.14 3189.54 3190.14 3194.66 3195.06 3201.10
3203.35 3203.50 3208.55 3209.33 3214.08 3215.15
3226.05 3235.09 3250.90

1b

14.22 21.88 23.20 30.30 35.23 37.57
42.04 47.21 50.82 57.56 58.70 61.33
63.58 74.15 81.63 91.25 99.15 108.73
115.30 121.07 128.16 140.63 148.61 157.34
168.37 173.03 185.78 203.21 207.24 218.45
226.69 234.04 237.19 250.06 254.49 256.84
263.32 272.79 278.90 299.76 304.47 326.41
335.77 369.27 378.06 391.70 400.07 408.53
410.19 411.44 416.82 426.79 440.82 443.93
448.18 459.74 470.65 502.33 513.94 525.34
527.47 546.34 586.71 597.52 630.66 631.60
632.39 633.56 649.17 665.04 666.33 676.39
679.45 700.35 703.55 704.54 707.97 712.39
713.63 715.06 718.87 762.40 763.72 766.74
768.14 773.02 798.75 856.07 856.65 861.81
872.13 880.03 881.69 884.24 893.00 936.63
938.13 938.85 942.81 947.04 959.01 962.03
971.47 976.22 980.66 984.68 988.83 989.17
997.68 999.27 1002.34 1008.39 1010.21 1014.85
1015.55 1016.55 1017.65 1022.45 1027.99 1032.95
1041.60 1052.02 1052.67 1053.72 1055.37 1056.07
1095.99 1099.18 1100.28 1104.54 1112.76 1114.77
1117.48 1118.75 1120.03 1122.48 1125.13 1159.13
1184.44 1186.41 1191.09 1195.82 1197.45 1198.01
1208.13 1225.74 1228.70 1230.46 1245.80 1252.89
1255.85 1269.25 1269.64 1308.84 1311.32 1312.06
1326.20 1328.66 1336.72 1363.54 1370.34 1373.21
1388.62 1389.77 1413.85 1416.21 1426.13 1435.65
1474.37 1475.65 1479.16 1485.74 1489.46 1491.84
1492.48 1497.49 1500.63 1516.71 1518.78 1521.91
1522.75 1525.26 1527.23 1530.35 1530.84 1539.34
1626.81 1628.97 1631.50 1631.79 1632.02 1645.75
1648.34 1648.74 1652.34 1660.72 2094.85 3044.95
3047.31 3049.14 3053.48 3115.73 3117.32 3125.55
3127.87 3130.34 3135.26 3146.23 3149.07 3170.31
3171.96 3173.93 3176.51 3182.52 3183.25 3183.42
3186.31 3187.84 3191.12 3193.34 3193.53 3197.49
3198.34 3201.72 3202.30 3203.78 3206.29 3207.49
3212.75 3215.25 3217.39 3231.30 3245.80 3280.20

2

10.71 16.42 26.22 32.03 33.35 41.52
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2-TS

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4-TS

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4'-TS

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5-TS

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8-TS

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 789.78 815.98 855.15 860.64 861.55 864.60
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8'-TS

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1b-TS

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 408.61 409.38 415.85 417.41 428.60 432.78
 446.03 455.20 463.27 498.96 513.07 523.99
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1c

24.77 25.55 27.90 38.20 39.89 45.88
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1d

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1d-TS

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3-TS

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3171.13 3172.50 3173.99 3179.31 3179.98 3180.26
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3'-TS

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413.22 417.27 422.61 433.08 438.60 443.81
452.32 456.57 478.22 508.97 524.82 526.69
528.78 530.28 555.34 586.95 619.36 626.46
630.58 630.94 633.52 634.70 652.99 665.06
675.61 680.20 698.86 710.19 710.52 711.24
712.47 714.56 715.91 729.95 761.81 762.41
765.50 770.00 782.00 808.99 852.79 866.40
869.11 870.98 872.60 890.49 902.42 934.94
939.54 941.13 942.61 944.96 946.85 951.19
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1013.45 1014.34 1016.19 1017.68 1023.60 1028.44
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1197.11 1222.25 1225.08 1226.49 1250.35 1254.75
1274.18 1303.61 1310.54 1323.77 1324.64 1328.70
1334.26 1348.85 1362.82 1365.73 1369.96 1379.94
1390.09 1402.87 1417.95 1420.87 1428.97 1431.24
1441.06 1446.40 1472.97 1475.65 1478.05 1486.70
1489.02 1489.84 1493.91 1498.55 1502.60 1518.45
1521.42 1522.12 1524.00 1525.44 1527.36 1528.26
1541.35 1626.23 1628.21 1629.01 1629.98 1644.64
1645.80 1647.41 1653.22 1656.51 1790.79 3049.96
3053.81 3055.24 3060.42 3119.99 3123.51 3129.36
3134.90 3136.48 3147.11 3150.15 3163.29 3168.74
3169.35 3172.27 3172.55 3174.39 3183.55 3185.07
3185.27 3185.85 3194.72 3195.41 3195.67 3196.40
3200.95 3202.06 3203.13 3206.29 3208.11 3210.46
3216.23 3216.55 3217.78 3227.97 3236.86 3259.54

5-Py

10.12 16.55 27.82 33.63 37.02 43.31
46.06 50.61 54.88 60.92 64.60 68.99
78.55 84.61 88.53 92.59 109.85 113.94
121.08 128.84 137.55 149.18 165.45 171.40
204.03 206.50 212.20 224.01 226.54 236.62
241.54 246.42 254.15 255.33 260.03 265.87
274.03 278.00 288.76 308.85 326.49 332.61
340.46 353.72 378.67 389.21 399.56 409.27
411.95 414.95 419.65 434.80 440.99 453.27
466.89 471.23 486.94 507.68 525.30 525.72
532.93 545.21 552.18 585.03 599.29 624.35
628.18 631.57 633.12 644.40 663.95 668.77

672.13 695.96 704.28 707.73 711.91 713.11
717.21 719.83 735.45 761.71 765.46 769.94
770.79 800.51 859.54 863.95 869.02 870.26
872.47 874.58 879.33 912.02 931.82 940.04
940.65 944.59 948.39 950.39 951.38 968.39
980.20 983.00 984.62 986.23 987.15 988.49
991.12 1004.12 1005.72 1008.26 1008.44 1010.43
1014.33 1016.43 1018.39 1024.16 1031.74 1038.40
1046.39 1051.43 1054.86 1055.11 1055.45 1083.87
1098.19 1099.58 1114.55 1114.68 1117.69 1118.82
1121.36 1123.32 1146.57 1165.17 1185.57 1187.05
1192.97 1198.59 1198.98 1199.82 1206.90 1228.58
1228.74 1231.01 1246.63 1250.73 1266.40 1270.97
1300.84 1307.18 1313.16 1322.96 1331.86 1334.34
1359.69 1369.76 1370.59 1372.07 1379.29 1383.63
1414.88 1417.65 1419.46 1428.23 1437.42 1442.91
1473.80 1476.22 1479.63 1482.84 1486.49 1489.09
1493.31 1498.68 1501.16 1518.11 1518.31 1521.33
1524.34 1525.33 1528.28 1529.42 1530.49 1540.13
1543.59 1626.77 1629.53 1631.35 1631.68 1647.14
1647.57 1648.91 1657.21 1713.89 2995.57 3008.23
3047.32 3049.84 3052.43 3056.30 3120.62 3121.95
3127.42 3129.27 3131.52 3131.93 3147.90 3149.48
3158.58 3172.49 3172.67 3173.08 3180.10 3181.87
3184.02 3186.52 3189.96 3190.08 3192.67 3194.79
3199.96 3200.73 3202.47 3203.61 3207.57 3208.85
3210.39 3211.47 3214.15 3222.05 3235.90 3239.45

5'-Py

5.84 14.12 27.98 33.89 37.54 40.98
45.53 51.08 55.27 59.24 65.04 71.24
82.98 85.21 87.40 95.59 112.59 113.63
116.75 127.49 135.75 149.14 164.87 191.79
204.17 207.70 215.13 222.16 229.73 240.38
241.72 246.22 252.06 254.98 259.92 275.11
278.04 280.41 294.17 311.64 322.64 332.33
344.28 378.38 384.56 399.36 405.88 409.90
412.15 416.64 419.04 437.05 448.74 449.80
464.79 472.59 474.06 507.84 524.26 525.56
532.93 542.17 555.48 585.74 609.56 623.78
628.04 631.70 633.06 646.26 661.51 667.64
671.02 695.90 707.50 708.10 711.90 713.00
717.22 719.83 742.19 761.77 765.19 769.91
770.05 809.73 858.96 860.94 868.76 869.75
872.00 873.94 882.63 888.16 932.71 939.66
941.14 944.79 948.76 949.58 956.34 961.83
968.13 979.44 981.14 983.87 986.05 987.98
989.68 990.94 1003.88 1006.73 1007.57 1009.37
1010.40 1014.55 1016.41 1024.14 1032.14 1041.42
1051.26 1052.15 1054.84 1055.25 1055.97 1098.34
1098.84 1101.26 1114.13 1114.60 1117.58 1118.96
1121.05 1123.01 1146.71 1163.11 1185.36 1187.13
1192.46 1198.52 1198.86 1199.93 1211.77 1227.93
1228.51 1230.63 1244.16 1245.80 1249.91 1270.90
1300.29 1313.91 1323.71 1328.15 1331.84 1334.75
1353.04 1369.53 1369.87 1371.96 1378.83 1382.74
1393.76 1415.47 1418.42 1428.52 1437.87 1442.77

1473.99 1476.12 1479.56 1485.30 1486.18 1490.52
1493.69 1497.77 1499.22 1501.84 1518.00 1519.49
1522.52 1524.30 1528.18 1529.21 1530.37 1539.11
1543.25 1627.27 1629.80 1631.48 1632.66 1647.16
1647.84 1649.04 1659.70 1742.39 2978.66 3005.60
3048.98 3052.19 3054.24 3058.37 3122.23 3124.30
3129.26 3131.53 3133.54 3134.74 3148.35 3153.19
3173.67 3173.84 3174.17 3181.16 3183.96 3184.85
3186.09 3190.42 3190.92 3191.78 3192.08 3195.36
3201.38 3202.57 3203.28 3207.25 3208.24 3209.65
3213.61 3214.44 3216.83 3220.72 3226.72 3243.43

VII-10. Energy components of DFT-optimized structures

Table S2. Computed Energy Components for Optimized Structures

Components	E(SCF) (eV)	ZPE (kcal/mol)	S(gas) (cal/mol·K)	Gsolv (kcal/mol)
	B3LYP-D3 /cc-pVTZ(-f)	B3LYP-D3 /LACVP/6-31G**	B3LYP-D3 /LACVP/6-31G**	B3LYP-D3 /LACVP/6-31G**
Pyridine	-6758.45	55.804	67.27	-2.5
HBpin	-11211.934	120.078	90.98	-2.27
A	-17971.105	178.464	119.06	-2.73
B	-17971.231	178.519	118.90	-2.54
G	-29184.231	301.690	169.11	-4.46
R	-29184.346	301.942	166.41	-3.47
1	-57231.52	288.488	203.46	-10.22
1-TS	-61685.037	350.412	222.694	-7.28
1a	-61685.096	351.048	227.708	-7.91
1b	-68444.33	408.063	252.097	-7.96
2	-68443.771	409.191	248.88	-8.36
[Py]	-6758.402			
[Cat]	-61683.709			
2-TS	-68443.673	408.193	239.203	-7.44
3	-68444.007	409.283	243.822	-8.66
4	-61684.776	352.196	216.772	-10.04
4-TS	-61684.148	350.525	221.801	-9.3
4'	-61684.763	351.789	224.648	-7.43
4'-TS	-61684.131	350.493	222.429	-7.72
5	-61685.218	353.573	222.943	-7.24
5'	-61684.885	353.763	221.416	-6.96
5-TS	-72897.44	473.177	263.14	-7.52
6	-72897.63	473.998	268.38	-7.85

6-TS	-72897.23	472.845	265.59	-8.37
6'-TS	-72897.161	472.954	264.67	-7.01
7	-72898.146	476.633	263.16	-7.41
7'	-72897.636	476.004	263.48	-7.15
8	-79657.003	533.363	294.70	-9.26
8'	-79656.975	533.679	293.28	-9.37
8_{sub-opt}	-17987.038			
8'_{sub-opt}	-17986.211			
8_{cat-opt}	-61662.657			
8_{cat}	-61661.775			
8'_{cat}	-61661.744			
8_{sub}	-17986.733			
8'_{sub}	-17986.114			
8-TS	-79656.392	533.188	287.21	-8.47
8'-TS	-79656.371	533.825	284.40	-8.70
1b-TS	-68443.458	407.624	248.257	-8.79
1c	-68443.189	409.715	245.306	-6.86
1d	-72897.643	473.889	267.059	-6.54
1d-TS	-68443.771	408.663	241.785	-8.32
3-TS	-68443.135	407.312	245.70	-9.39
3'-TS	-68443.347	407.498	240.52	-8.06
5-Py	-68444.308	411.009	247.014	-9
5'-Py	-68444.468	411.138	238.693	-8.9

VIII. References

- S1. (a) S. Joung, D. G. Jo, V. D. Cao, H. Kim, C. Kim and S. Yun, Utilization of borane-catalyzed hydrosilylation as a dearomatizing tool: Six-membered cyclic amidine synthesis from isoquinolines and pyridines, *Synthesis*, 2020, **53**, 754–764; (b) V. D. Cao, S. H. Mun, S. H. Kim, G. U. Kim, H. G. Kim and S. Joung, Synthesis of cyclic amidines from quinolines by a borane-catalyzed dearomatization strategy, *Org. Lett.*, 2020, **22**, 515–519.
- S2. E. Tomás-Mendivil, R. García-Álvarez, C. Vidal, P. Crochet and V. Cadierno, Exploring rhodium(I) complexes [RhCl(COD)(PR₃)] (COD = 1,5-Cyclooctadiene) as catalysts for nitrile hydration reactions in water: The aminophosphines make the difference, *ACS Catal.*, 2014, **4**, 1901–1910.
- S3. (a) K. Burgess, W. A. Van der Donk, S. A. Westcott, T. B. Marder, R. T. Baker and J. C. Calabrese, Reactions of catecholborane with Wilkinson's catalyst: Implications for transition metal-catalyzed hydroborations of alkenes, *J. Am. Chem. Soc.*, 1992, **114**, 9350–9359; (b) C. B. Fritsch, S. M. Wernitz, C. M. Vogels, M. P. Shaver, A. Decken, A. Bell and S. A. Westcott, 4,4,5,5-Tetraphenyl-1,3,2-dioxaborolane: A bulky borane for the transition metal catalysed hydroboration of alkenes, *Eur. J. Inorg. Chem.*, 2008, **2008**, 779–785.
- S4. J. E. Perea-Buceta, I. Fernández, S. Heikkinen, K. Axenov, A. W. T. King, T. Niemi, M. Nieger, M. Leskelä and T. Repo, Diverting hydrogenations with Wilkinson's catalyst towards highly reactive rhodium(I) species, *Angew. Chem., Int. Ed.*, 2015, **54**, 14321–14325.
- S5. R. G. Parr, Density functional theory of atoms and molecules, *Horizons of Quantum Chemistry*, 1980, 5–15.
- S6. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. A. Friesner, Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences, *Int. J. Quantum Chem.*, 2013, **113**, 2110–2142.
- S7. (a) J. C. Slater and J. C. Phillips, Quantum theory of molecules and solids Vol. 4: The self-consistent field for molecules and solids, *Physics Today*, 1974, **27**, 49–50; (b) S. H. Vosko, L. Wilk and M. Nusair, Accurate spin-dependent electron liquid correlation energies for local spin density calculations: a critical analysis, *Can. J. Phys.*, 1980, **59**, 1200; (c) A. D. Becke, Density-functional exchange-energy approximation with correct asymptotic behavior, *Phys. Rev. A Gen. Phys.*, 1988, **38**, 3098–3100; (d) C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, *Phys. Rev. B*, 1988, **37**, 785–789; (e) A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.*, 1993, **98**, 5648–5652; (f) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H–Pu, *J. Chem. Phys.*, 2010, **132**, 154104.
- S8. T. H. Dunning, Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen, *J. Chem. Phys.*, 1989, **90**, 1007–1023.
- S9. (a) B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff and B. Honig, New model for calculation of solvation free energies: Correction of self-consistent reaction field continuum dielectric theory for short-range hydrogen-bonding effects, *J. Phys. Chem.*, 1996, **100**, 11775–11788. (b) M. Friedrichs, R. Zhou, S. R. Edinger and R. A. Friesner, Poisson–Boltzmann analytical gradients for molecular modeling calculations, *J. Phys. Chem. B*, 1999, **103**, 3057–3061; (c) S. R. Edinger, C. Cortis, P. S. Shenkin and R. A. Friesner, Solvation free energies of peptides: Comparison of approximate continuum solvation models with accurate solution of the Poisson–Boltzmann equation, *J. Phys. Chem. B*, 1997, **101**, 1190–1197.

- S10. A. A. Rashin and B. Honig, Reevaluation of the Born Model of Ion Hydration, *J. Phys. Chem.*, 1985, **89**, 5588–5593.
- S11. K. Oshima, T. Ohmura and M. Suginome, Regioselective synthesis of 1,2-dihydropyridines by rhodium-catalyzed hydroboration of pyridines, *J. Am. Chem. Soc.*, 2012, **134**, 3699–3702.
- S12. A. Ariafard, E. S. Tabatabaie, A. T. Monfared, S. H. A. Assar, C. J. T. Hyland and B. F. Yates, Theoretical investigation into the palladium-catalyzed silaboration of pyridines, *Organometallics*, 2012, **31**, 1680–1687.
- S13. (a) K. Morokuma, Molecular orbital studies of hydrogen bonds. III. C=O···H–O Hydrogen Bond in H₂CO···H₂O and H₂CO···2H₂O, *J. Chem. Phys.*, 1971, **55**, 1236–1244; (b) F. M. Bickelhaupt, and K. N. Houk, Analyzing reaction rates with the distortion/interaction-activation strain model, *Angew. Chem., Int. Ed.*, 2017, **56**, 10070–10086.

X. Appendix I

X-Ray crystallographic data for G' and R'

Structural Analysis of G' and R'

The data collection for X-ray single crystal structure analysis was performed at room temperature on a Bruker D8 QUEST diffractometer equipped with I μ s 3.0 Mo x-ray tube ($\lambda = 0.71073 \text{ \AA}$) and Photon II detector. The Parabar oil coated crystals were mounting on goniometer for diffraction experiment. The diffraction data were integrated, scaled, and reduced by using the Bruker APEX4 software. The crystal structures were solved by SHELX structure solution program and refined by full-matrix least-squares calculations with the SHELXL. The thermal ellipsoid of crystal structure by ORTEP drawing is set at a 30% probability level. The single crystals of compounds for X-ray crystal structure analysis were obtained by a diffusion method in separate vials using dichloromethane and n-pentane as an eluent.

Crystallographic Data for **G'** (CCDC 2217742):

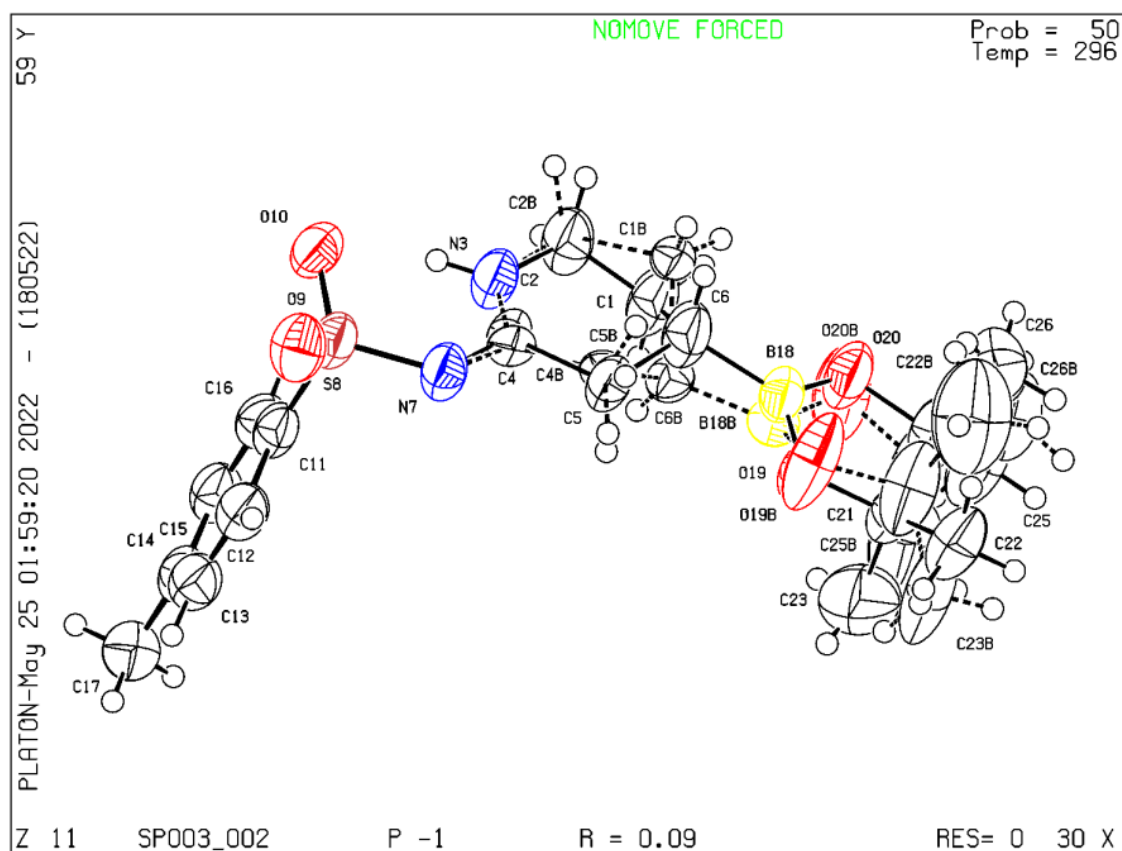


Fig. S30 Molecular structure of complex **G'**

Table S3. Crystal data and structure refinement for **G'**.

Empirical formula	C ₁₈ H ₂₇ B N ₂ O ₄ S	
Formula weight	378.28	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	a = 6.4445(15) Å	α = 80.205(7)°
	b = 11.458(3) Å	β = 85.649(7)°
	c = 13.656(3) Å	γ = 82.844(7)°
Volume	984.4(4) Å ³	
Z	2	
Density (calculated)	1.276 Mg/m ³	
Absorption coefficient	0.189 mm ⁻¹	
F(000)	404	
Crystal size	0.323 x 0.048 x 0.043 mm ³	

Theta range for data collection	2.547 to 26.020°.
Index ranges	-7<=h<=7, -14<=k<=14, -16<=l<=16
Reflections collected	32379
Independent reflections	3803 [R(int) = 0.0677]
Completeness to theta = 25.242°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.6733
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3803 / 217 / 363
Goodness-of-fit on F ²	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0892, wR2 = 0.2382
R indices (all data)	R1 = 0.1182, wR2 = 0.2708
Largest diff. peak and hole	0.775 and -0.325 e·Å ⁻³

Table S4. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **G'**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(3)	2295(5)	5648(3)	8592(2)	64(1)
C(1)	2735(11)	7075(7)	7086(5)	77(2)
C(2)	1650(20)	6832(12)	8061(9)	80(5)
C(4)	4000(20)	5020(9)	8438(9)	60(3)
C(5)	5630(30)	5399(12)	7556(9)	61(4)
C(6)	4987(11)	6715(6)	7074(5)	75(2)
B(18)	6116(14)	7060(8)	6016(6)	62(3)
O(19)	7728(14)	6395(5)	5600(5)	95(3)
O(20)	5450(12)	8049(6)	5399(5)	85(2)
C(21)	8087(10)	6951(6)	4570(4)	70(2)
C(22)	10484(10)	6918(8)	4343(5)	93(2)
C(23)	7114(18)	6219(10)	3956(7)	145(4)
C(24)	7006(11)	8197(6)	4576(5)	77(2)
C(25)	5842(14)	8760(11)	3643(6)	126(3)
C(26)	8357(14)	9084(7)	4821(7)	119(3)
C(1B)	3510(30)	7432(14)	7424(12)	46(4)
C(2B)	1580(60)	6860(40)	8130(20)	52(11)
C(4B)	4180(40)	4940(20)	8380(30)	34(7)

C(5B)	5320(80)	5510(40)	7610(30)	45(7)
C(6B)	4310(30)	6369(15)	6708(11)	45(4)
B(18B)	5850(40)	6830(30)	5810(20)	66(9)
O(19B)	7950(40)	6520(30)	5662(17)	107(9)
O(20B)	5240(40)	7890(30)	5261(19)	106(8)
C(21B)	8560(30)	7230(20)	4717(16)	109(10)
C(22B)	9940(50)	8100(30)	5050(30)	175(12)
C(23B)	9670(50)	6450(30)	4010(20)	145(11)
C(24B)	6550(30)	7930(20)	4359(16)	108(10)
C(25B)	5470(40)	7450(30)	3570(20)	133(9)
C(26B)	6810(50)	9220(20)	3930(20)	118(9)
N(7)	4720(5)	3920(3)	8926(2)	60(1)
S(8)	3411(1)	3249(1)	9853(1)	58(1)
O(9)	4885(4)	2496(2)	10483(2)	73(1)
O(10)	1884(4)	4041(2)	10335(2)	68(1)
C(11)	2008(6)	2296(3)	9338(2)	55(1)
C(12)	2949(6)	1158(3)	9241(3)	61(1)
C(13)	1871(7)	388(3)	8861(3)	66(1)
C(14)	-177(6)	739(3)	8542(3)	62(1)
C(15)	-1061(6)	1879(3)	8642(3)	65(1)
C(16)	-22(6)	2650(3)	9037(3)	61(1)
C(17)	-1331(8)	-92(4)	8122(3)	80(1)

Table S5. Bond lengths [Å] and angles [°] for **G⁺**.

N(3)-C(4)	1.263(10)
N(3)-C(4B)	1.417(19)
N(3)-C(2)	1.453(13)
N(3)-C(2B)	1.46(5)
N(3)-H(3)	0.8600
C(1)-C(2)	1.456(14)
C(1)-C(6)	1.458(9)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(4)-N(7)	1.364(9)

C(4)-C(5)	1.577(18)
C(5)-C(6)	1.558(12)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-B(18)	1.578(8)
C(6)-H(6)	0.9800
B(18)-O(20)	1.336(7)
B(18)-O(19)	1.357(8)
O(19)-C(21)	1.456(7)
O(20)-C(24)	1.450(6)
C(21)-C(23)	1.500(8)
C(21)-C(24)	1.510(9)
C(21)-C(22)	1.549(8)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(26)	1.511(9)
C(24)-C(25)	1.533(9)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(1B)-C(2B)	1.65(4)
C(1B)-C(6B)	1.70(2)
C(1B)-H(1BA)	0.9700
C(1B)-H(1BB)	0.9700
C(2B)-H(2BA)	0.9700
C(2B)-H(2BB)	0.9700
C(4B)-N(7)	1.296(19)
C(4B)-C(5B)	1.36(6)
C(5B)-C(6B)	1.56(2)
C(5B)-H(5BA)	0.9700

C(5B)-H(5BB)	0.9700
C(6B)-B(18B)	1.58(3)
C(6B)-H(6B)	0.9800
B(18B)-O(20B)	1.343(17)
B(18B)-O(19B)	1.368(18)
O(19B)-C(21B)	1.463(16)
O(20B)-C(24B)	1.440(16)
C(21B)-C(24B)	1.501(17)
C(21B)-C(23B)	1.509(12)
C(21B)-C(22B)	1.553(14)
C(22B)-H(22D)	0.9600
C(22B)-H(22E)	0.9600
C(22B)-H(22F)	0.9600
C(23B)-H(23D)	0.9600
C(23B)-H(23E)	0.9600
C(23B)-H(23F)	0.9600
C(24B)-C(26B)	1.524(14)
C(24B)-C(25B)	1.538(14)
C(25B)-H(25D)	0.9600
C(25B)-H(25E)	0.9600
C(25B)-H(25F)	0.9600
C(26B)-H(26D)	0.9600
C(26B)-H(26E)	0.9600
C(26B)-H(26F)	0.9600
N(7)-S(8)	1.604(3)
S(8)-O(9)	1.433(3)
S(8)-O(10)	1.452(3)
S(8)-C(11)	1.763(4)
C(11)-C(12)	1.391(5)
C(11)-C(16)	1.392(5)
C(12)-C(13)	1.376(6)
C(12)-H(12)	0.9300
C(13)-C(14)	1.410(6)
C(13)-H(13)	0.9300
C(14)-C(15)	1.383(5)
C(14)-C(17)	1.489(6)
C(15)-C(16)	1.373(6)

C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(4)-N(3)-C(2)	125.8(7)
C(4B)-N(3)-C(2B)	128.2(19)
C(4)-N(3)-H(3)	117.1
C(2)-N(3)-H(3)	117.1
C(2)-C(1)-C(6)	114.5(7)
C(2)-C(1)-H(1A)	108.6
C(6)-C(1)-H(1A)	108.6
C(2)-C(1)-H(1B)	108.6
C(6)-C(1)-H(1B)	108.6
H(1A)-C(1)-H(1B)	107.6
N(3)-C(2)-C(1)	112.7(9)
N(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2A)	109.0
N(3)-C(2)-H(2B)	109.0
C(1)-C(2)-H(2B)	109.0
H(2A)-C(2)-H(2B)	107.8
N(3)-C(4)-N(7)	128.5(8)
N(3)-C(4)-C(5)	122.8(8)
N(7)-C(4)-C(5)	108.7(8)
C(6)-C(5)-C(4)	109.3(11)
C(6)-C(5)-H(5A)	109.8
C(4)-C(5)-H(5A)	109.8
C(6)-C(5)-H(5B)	109.8
C(4)-C(5)-H(5B)	109.8
H(5A)-C(5)-H(5B)	108.3
C(1)-C(6)-C(5)	114.7(9)
C(1)-C(6)-B(18)	112.8(6)
C(5)-C(6)-B(18)	112.8(8)
C(1)-C(6)-H(6)	105.1
C(5)-C(6)-H(6)	105.1
B(18)-C(6)-H(6)	105.1
O(20)-B(18)-O(19)	112.4(5)

O(20)-B(18)-C(6)	121.4(6)
O(19)-B(18)-C(6)	126.1(6)
B(18)-O(19)-C(21)	108.1(5)
B(18)-O(20)-C(24)	107.2(5)
O(19)-C(21)-C(23)	105.6(6)
O(19)-C(21)-C(24)	102.0(4)
C(23)-C(21)-C(24)	115.3(7)
O(19)-C(21)-C(22)	108.0(6)
C(23)-C(21)-C(22)	112.0(6)
C(24)-C(21)-C(22)	112.9(6)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
O(20)-C(24)-C(21)	103.6(5)
O(20)-C(24)-C(26)	105.4(6)
C(21)-C(24)-C(26)	115.4(6)
O(20)-C(24)-C(25)	107.3(6)
C(21)-C(24)-C(25)	115.7(7)
C(26)-C(24)-C(25)	108.5(7)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5

C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(2B)-C(1B)-C(6B)	102.2(17)
C(2B)-C(1B)-H(1BA)	111.3
C(6B)-C(1B)-H(1BA)	111.3
C(2B)-C(1B)-H(1BB)	111.3
C(6B)-C(1B)-H(1BB)	111.3
H(1BA)-C(1B)-H(1BB)	109.2
N(3)-C(2B)-C(1B)	110(3)
N(3)-C(2B)-H(2BA)	109.8
C(1B)-C(2B)-H(2BA)	109.8
N(3)-C(2B)-H(2BB)	109.8
C(1B)-C(2B)-H(2BB)	109.8
H(2BA)-C(2B)-H(2BB)	108.2
N(7)-C(4B)-C(5B)	128(2)
N(7)-C(4B)-N(3)	121(2)
C(5B)-C(4B)-N(3)	111(2)
C(4B)-C(5B)-C(6B)	123(4)
C(4B)-C(5B)-H(5BA)	106.5
C(6B)-C(5B)-H(5BA)	106.5
C(4B)-C(5B)-H(5BB)	106.5
C(6B)-C(5B)-H(5BB)	106.5
H(5BA)-C(5B)-H(5BB)	106.5
C(5B)-C(6B)-B(18B)	117(3)
C(5B)-C(6B)-C(1B)	92(2)
B(18B)-C(6B)-C(1B)	111.8(16)
C(5B)-C(6B)-H(6B)	111.7
B(18B)-C(6B)-H(6B)	111.7
C(1B)-C(6B)-H(6B)	111.7
O(20B)-B(18B)-O(19B)	111.1(18)
O(20B)-B(18B)-C(6B)	116.8(19)
O(19B)-B(18B)-C(6B)	129(2)
B(18B)-O(19B)-C(21B)	105.5(15)
B(18B)-O(20B)-C(24B)	105.0(17)
O(19B)-C(21B)-C(24B)	104.5(13)
O(19B)-C(21B)-C(23B)	110.5(18)

C(24B)-C(21B)-C(23B)	114.6(19)
O(19B)-C(21B)-C(22B)	102.3(19)
C(24B)-C(21B)-C(22B)	109.0(18)
C(23B)-C(21B)-C(22B)	115(2)
C(21B)-C(22B)-H(22D)	109.5
C(21B)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
C(21B)-C(22B)-H(22F)	109.5
H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
C(21B)-C(23B)-H(23D)	109.5
C(21B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(21B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
O(20B)-C(24B)-C(21B)	102.4(14)
O(20B)-C(24B)-C(26B)	109.0(19)
C(21B)-C(24B)-C(26B)	112.3(18)
O(20B)-C(24B)-C(25B)	110.0(19)
C(21B)-C(24B)-C(25B)	117.1(18)
C(26B)-C(24B)-C(25B)	105.8(18)
C(24B)-C(25B)-H(25D)	109.5
C(24B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
C(24B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(24B)-C(26B)-H(26D)	109.5
C(24B)-C(26B)-H(26E)	109.5
H(26D)-C(26B)-H(26E)	109.5
C(24B)-C(26B)-H(26F)	109.5
H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5
C(4B)-N(7)-S(8)	127.9(11)
C(4)-N(7)-S(8)	121.9(5)
O(9)-S(8)-O(10)	116.22(17)

O(9)-S(8)-N(7)	107.41(17)
O(10)-S(8)-N(7)	113.70(16)
O(9)-S(8)-C(11)	106.55(17)
O(10)-S(8)-C(11)	107.21(17)
N(7)-S(8)-C(11)	104.94(16)
C(12)-C(11)-C(16)	119.3(4)
C(12)-C(11)-S(8)	119.0(3)
C(16)-C(11)-S(8)	121.6(3)
C(13)-C(12)-C(11)	120.2(4)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	121.1(3)
C(12)-C(13)-H(13)	119.4
C(14)-C(13)-H(13)	119.4
C(15)-C(14)-C(13)	117.2(4)
C(15)-C(14)-C(17)	121.8(4)
C(13)-C(14)-C(17)	121.0(4)
C(16)-C(15)-C(14)	122.4(4)
C(16)-C(15)-H(15)	118.8
C(14)-C(15)-H(15)	118.8
C(15)-C(16)-C(11)	119.8(3)
C(15)-C(16)-H(16)	120.1
C(11)-C(16)-H(16)	120.1
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for \mathbf{G}^4 . The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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N(3)	62(2)	58(2)	60(2)	8(2)	18(2)	6(2)
C(1)	77(4)	81(4)	57(3)	17(3)	10(3)	6(3)
C(2)	79(7)	55(6)	85(8)	16(5)	22(5)	18(5)
C(4)	67(7)	60(5)	47(4)	-1(4)	14(4)	-8(4)
C(5)	61(7)	60(6)	52(4)	2(4)	17(4)	0(5)
C(6)	81(4)	70(4)	60(3)	15(3)	12(3)	0(3)
B(18)	73(4)	55(4)	53(4)	2(3)	14(3)	-9(3)
O(19)	116(6)	70(3)	80(4)	6(3)	42(3)	6(3)
O(20)	99(5)	76(3)	62(3)	15(2)	30(3)	4(3)
C(21)	80(4)	83(4)	47(3)	-7(2)	12(3)	-21(3)
C(22)	76(4)	122(6)	70(4)	0(4)	19(3)	-4(4)
C(23)	179(9)	158(8)	118(6)	-58(6)	6(6)	-58(7)
C(24)	75(4)	88(4)	57(3)	13(3)	17(3)	-14(3)
C(25)	110(6)	173(8)	69(4)	35(5)	8(4)	3(6)
C(26)	132(6)	88(5)	134(6)	-9(4)	34(5)	-36(4)
C(1B)	54(9)	39(7)	42(8)	-6(5)	3(6)	-2(6)
C(2B)	57(16)	80(30)	27(11)	-12(13)	4(10)	-20(14)
C(4B)	9(9)	42(12)	51(12)	-16(8)	0(8)	8(8)
C(5B)	31(11)	36(9)	68(13)	-18(7)	9(9)	8(7)
C(6B)	46(8)	54(8)	38(6)	-10(6)	-6(5)	-9(6)
B(18B)	82(15)	49(12)	66(11)	-16(8)	14(10)	-9(10)
O(19B)	51(9)	176(18)	66(11)	46(10)	3(7)	5(9)
O(20B)	46(9)	146(15)	107(12)	41(10)	-9(7)	-13(9)
C(21B)	68(11)	160(20)	84(14)	32(12)	0(9)	-19(10)
C(22B)	112(17)	200(20)	190(20)	37(17)	-13(15)	-20(15)
C(23B)	120(19)	170(20)	105(15)	57(12)	47(13)	2(15)
C(24B)	78(14)	160(20)	69(12)	30(12)	13(9)	-5(12)
C(25B)	88(15)	180(20)	126(15)	16(14)	-21(12)	-28(14)
C(26B)	101(17)	138(16)	99(16)	25(12)	6(13)	-24(12)
N(7)	55(2)	57(2)	61(2)	3(1)	14(1)	-1(1)
S(8)	60(1)	58(1)	48(1)	5(1)	7(1)	-1(1)
O(9)	73(2)	74(2)	62(2)	13(1)	-12(1)	-1(1)
O(10)	75(2)	68(2)	56(1)	-6(1)	18(1)	-2(1)
C(11)	57(2)	53(2)	46(2)	7(1)	7(2)	3(2)
C(12)	61(2)	55(2)	57(2)	5(2)	2(2)	12(2)
C(13)	74(3)	56(2)	60(2)	1(2)	7(2)	7(2)
C(14)	67(2)	61(2)	52(2)	2(2)	13(2)	-5(2)

C(15)	57(2)	65(2)	64(2)	1(2)	6(2)	2(2)
C(16)	59(2)	58(2)	59(2)	-2(2)	7(2)	6(2)
C(17)	93(3)	71(3)	74(3)	-11(2)	7(2)	-12(2)

Table S7. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **G'**.

	x	y	z	U(eq)
H(3)	1437	5348	9052	77
H(1A)	2494	7923	6839	92
H(1B)	2128	6664	6632	92
H(2A)	1920	7420	8456	96
H(2B)	154	6914	7980	96
H(5A)	7023	5323	7804	73
H(5B)	5667	4880	7061	73
H(6)	5530	7201	7500	90
H(22A)	10759	7281	3666	139
H(22B)	11062	7348	4782	139
H(22C)	11116	6106	4440	139
H(23A)	7302	6545	3264	218
H(23B)	7771	5412	4071	218
H(23C)	5644	6231	4140	218
H(25A)	6830	8871	3082	189
H(25B)	4857	8245	3522	189
H(25C)	5109	9518	3740	189
H(26A)	9428	9221	4299	179
H(26B)	7506	9821	4879	179
H(26C)	8996	8774	5438	179
H(1BA)	4625	7554	7822	55
H(1BB)	3024	8184	7021	55
H(2BA)	1110	7343	8635	62
H(2BB)	408	6846	7723	62
H(5BA)	6241	4901	7329	54
H(5BB)	6212	5970	7896	54

H(6B)	3123	6051	6481	54
H(22D)	10432	8622	4481	263
H(22E)	9117	8561	5499	263
H(22F)	11110	7648	5387	263
H(23D)	10064	6930	3398	217
H(23E)	10908	6014	4307	217
H(23F)	8757	5895	3890	217
H(25D)	6358	7480	2967	199
H(25E)	5211	6643	3808	199
H(25F)	4166	7935	3428	199
H(26D)	7692	9255	3331	176
H(26E)	5467	9653	3792	176
H(26F)	7449	9573	4409	176
H(12)	4310	917	9434	74
H(13)	2503	-377	8814	80
H(15)	-2409	2132	8435	78
H(16)	-672	3406	9103	73
H(17A)	-464	-835	8113	120
H(17B)	-2590	-229	8526	120
H(17C)	-1683	252	7455	120

Crystallographic Data for **R'** (CCDC 2217744):

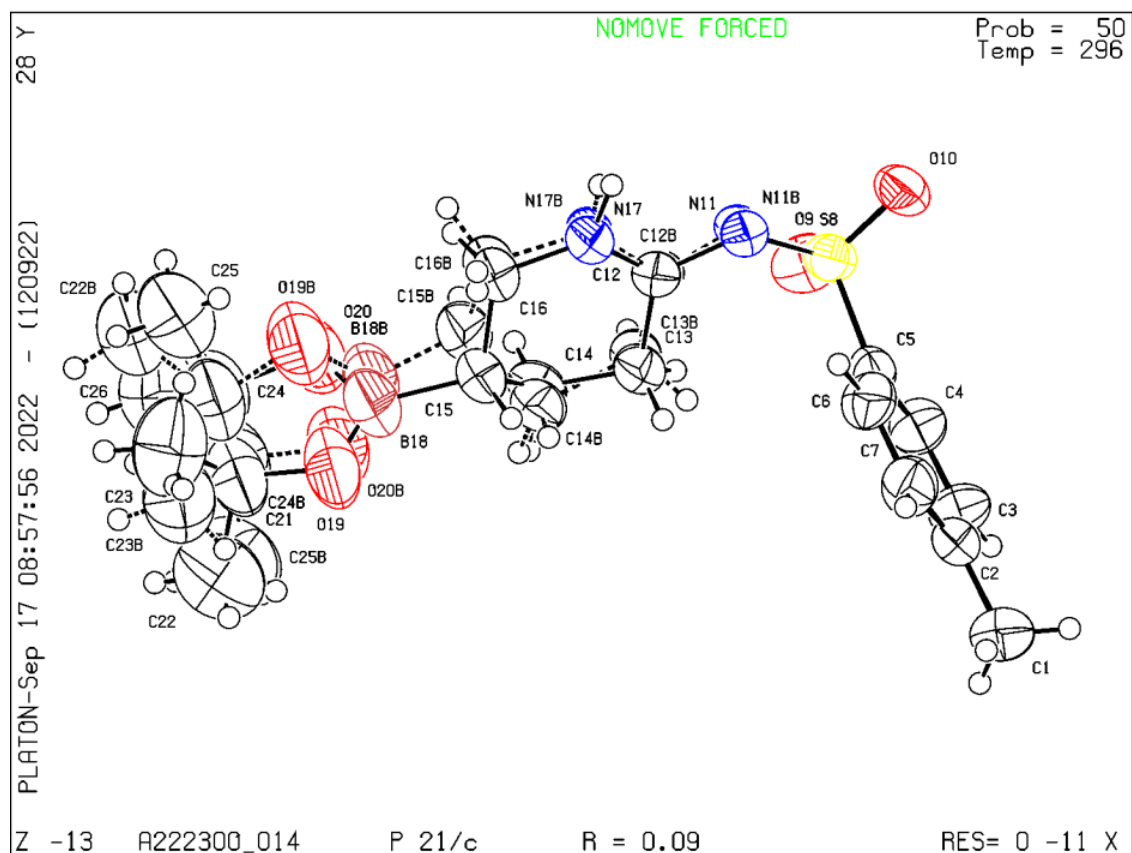


Fig. S31 Molecular structure of complex **R'**

Table S8. Crystal data and structure refinement for **R'**

Empirical formula	C ₁₈ H ₂₇ B N ₂ O ₄ S	
Formula weight	378.28	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 12.029(3) Å	α = 90°
	b = 14.490(4) Å	β = 95.143(7)°
	c = 11.877(3) Å	γ = 90°
Volume	2061.7(9) Å ³	
Z	4	
Density (calculated)	1.219 Mg/m ³	
Absorption coefficient	0.181 mm ⁻¹	
F(000)	808	
Crystal size	0.209 x 0.162 x 0.059 mm ³	

Theta range for data collection	2.703 to 25.727°.
Index ranges	-14<=h<=14, -17<=k<=17, -12<=l<=14
Reflections collected	33518
Independent reflections	3905 [R(int) = 0.0785]
Completeness to theta = 25.242°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.6645
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3905 / 765 / 387
Goodness-of-fit on F ²	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0875, wR2 = 0.2466
R indices (all data)	R1 = 0.1170, wR2 = 0.2773
Largest diff. peak and hole	0.732 and -0.523 e·Å ⁻³

Table S9. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **R'**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	11743(5)	4535(4)	4916(6)	94(2)
C(2)	11326(4)	5479(3)	4556(4)	65(1)
C(3)	10816(4)	5610(3)	3463(4)	73(1)
C(4)	10417(4)	6454(3)	3107(4)	64(1)
C(5)	10548(3)	7210(3)	3834(3)	50(1)
C(6)	11043(4)	7089(3)	4910(4)	65(1)
C(7)	11418(4)	6225(4)	5258(4)	71(1)
S(8)	10150(1)	8310(1)	3304(1)	58(1)
O(9)	9261(3)	8178(2)	2423(3)	78(1)
O(10)	11147(3)	8743(2)	2981(3)	76(1)
N(11)	9865(15)	8911(16)	4417(16)	50(3)
C(12)	8880(30)	8800(30)	4910(20)	51(2)
C(13)	8200(10)	7912(9)	4812(9)	57(2)
C(14)	7036(10)	8025(9)	5149(9)	68(2)
C(15)	7161(7)	8455(6)	6394(8)	65(2)
C(16)	7735(13)	9390(13)	6338(13)	61(2)
N(17)	8655(17)	9399(15)	5657(13)	52(2)
N(11B)	9697(19)	8960(20)	4230(20)	47(3)

C(12B)	8850(40)	8780(30)	4780(30)	51(2)
C(13B)	8022(14)	8017(12)	4504(12)	57(2)
C(14B)	7207(13)	7903(11)	5516(12)	66(2)
C(15B)	6716(9)	8821(9)	5730(11)	76(2)
C(16B)	7566(18)	9487(17)	6128(17)	63(2)
N(17B)	8560(20)	9450(20)	5454(18)	53(2)
B(18)	6023(14)	8536(13)	6969(15)	96(2)
O(19)	5713(6)	8116(7)	7725(8)	121(2)
O(20)	5086(8)	9056(8)	6365(9)	130(2)
C(21)	4575(10)	8281(9)	7896(11)	121(2)
C(22)	4007(16)	7383(12)	8038(19)	170(5)
C(23)	4600(16)	8908(13)	9089(12)	154(5)
C(24)	4224(10)	9030(10)	7142(11)	125(2)
C(25)	4352(15)	9943(12)	7672(16)	162(5)
C(26)	3109(12)	9075(15)	6552(16)	163(5)
B(18B)	5850(20)	8704(17)	6563(18)	101(2)
O(19B)	5555(9)	9333(9)	7314(11)	127(2)
O(20B)	5085(8)	8112(9)	6473(10)	121(2)
C(21B)	4577(12)	9065(11)	7840(14)	124(2)
C(22B)	3724(16)	9881(15)	7690(20)	151(5)
C(23B)	4420(20)	8362(16)	8974(16)	142(5)
C(24B)	4139(12)	8322(11)	7074(15)	125(3)
C(25B)	3790(18)	7391(13)	7160(20)	149(5)
C(26B)	3198(15)	8548(16)	6247(18)	145(5)

Table S10. Bond lengths [Å] and angles [°] for **R⁴**.

C(1)-C(2)	1.504(7)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(7)	1.364(7)
C(2)-C(3)	1.398(7)
C(3)-C(4)	1.367(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.395(5)
C(4)-H(4)	0.9300

C(5)-C(6)	1.372(6)
C(5)-S(8)	1.764(4)
C(6)-C(7)	1.381(7)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
S(8)-O(10)	1.437(3)
S(8)-O(9)	1.440(3)
S(8)-N(11B)	1.59(3)
S(8)-N(11)	1.64(2)
N(11)-C(12)	1.38(4)
C(12)-N(17)	1.29(3)
C(12)-C(13)	1.52(4)
C(13)-C(14)	1.50(2)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.599(15)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.52(2)
C(15)-B(18)	1.588(18)
C(15)-H(15)	0.9800
C(16)-N(17)	1.43(2)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
N(17)-H(17)	0.95(10)
N(11B)-C(12B)	1.28(5)
C(12B)-N(17B)	1.33(4)
C(12B)-C(13B)	1.50(5)
C(13B)-C(14B)	1.63(2)
C(13B)-H(13C)	0.9700
C(13B)-H(13D)	0.9700
C(14B)-C(15B)	1.49(2)
C(14B)-H(14C)	0.9700
C(14B)-H(14D)	0.9700
C(15B)-C(16B)	1.45(3)
C(15B)-B(18B)	1.51(2)
C(15B)-H(15B)	0.9800

C(16B)-N(17B)	1.50(3)
C(16B)-H(16C)	0.9700
C(16B)-H(16D)	0.9700
N(17B)-H(17B)	0.69(15)
B(18)-O(19)	1.173(17)
B(18)-O(20)	1.49(2)
O(19)-C(21)	1.422(12)
O(20)-C(24)	1.449(13)
C(21)-C(24)	1.445(12)
C(21)-C(22)	1.487(14)
C(21)-C(23)	1.680(13)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(26)	1.458(13)
C(24)-C(25)	1.467(14)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
B(18B)-O(20B)	1.25(2)
B(18B)-O(19B)	1.34(3)
O(19B)-C(21B)	1.434(14)
O(20B)-C(24B)	1.430(15)
C(21B)-C(24B)	1.476(16)
C(21B)-C(22B)	1.566(19)
C(21B)-C(23B)	1.711(17)
C(22B)-H(22D)	0.9600
C(22B)-H(22E)	0.9600
C(22B)-H(22F)	0.9600
C(23B)-H(23D)	0.9600
C(23B)-H(23E)	0.9600

C(23B)-H(23F)	0.9600
C(24B)-C(25B)	1.420(18)
C(24B)-C(26B)	1.468(17)
C(25B)-H(25D)	0.9600
C(25B)-H(25E)	0.9600
C(25B)-H(25F)	0.9600
C(26B)-H(26D)	0.9600
C(26B)-H(26E)	0.9600
C(26B)-H(26F)	0.9600
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(7)-C(2)-C(3)	117.6(4)
C(7)-C(2)-C(1)	122.7(5)
C(3)-C(2)-C(1)	119.6(5)
C(4)-C(3)-C(2)	121.5(4)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	119.6(4)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
C(6)-C(5)-C(4)	119.4(4)
C(6)-C(5)-S(8)	121.9(3)
C(4)-C(5)-S(8)	118.5(3)
C(5)-C(6)-C(7)	119.8(4)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-H(6)	120.1
C(2)-C(7)-C(6)	122.0(4)
C(2)-C(7)-H(7)	119.0
C(6)-C(7)-H(7)	119.0
O(10)-S(8)-O(9)	116.6(2)
O(10)-S(8)-N(11B)	105.8(10)
O(9)-S(8)-N(11B)	107.9(8)

O(10)-S(8)-N(11)	102.9(8)
O(9)-S(8)-N(11)	117.4(6)
O(10)-S(8)-C(5)	106.45(19)
O(9)-S(8)-C(5)	107.40(19)
N(11B)-S(8)-C(5)	112.9(9)
N(11)-S(8)-C(5)	105.1(7)
C(12)-N(11)-S(8)	121.9(16)
N(17)-C(12)-N(11)	117(3)
N(17)-C(12)-C(13)	119(2)
N(11)-C(12)-C(13)	123(2)
C(14)-C(13)-C(12)	113.2(17)
C(14)-C(13)-H(13A)	108.9
C(12)-C(13)-H(13A)	108.9
C(14)-C(13)-H(13B)	108.9
C(12)-C(13)-H(13B)	108.9
H(13A)-C(13)-H(13B)	107.8
C(13)-C(14)-C(15)	106.1(9)
C(13)-C(14)-H(14A)	110.5
C(15)-C(14)-H(14A)	110.5
C(13)-C(14)-H(14B)	110.5
C(15)-C(14)-H(14B)	110.5
H(14A)-C(14)-H(14B)	108.7
C(16)-C(15)-B(18)	111.4(11)
C(16)-C(15)-C(14)	108.2(9)
B(18)-C(15)-C(14)	114.4(9)
C(16)-C(15)-H(15)	107.6
B(18)-C(15)-H(15)	107.6
C(14)-C(15)-H(15)	107.6
N(17)-C(16)-C(15)	114.2(14)
N(17)-C(16)-H(16A)	108.7
C(15)-C(16)-H(16A)	108.7
N(17)-C(16)-H(16B)	108.7
C(15)-C(16)-H(16B)	108.7
H(16A)-C(16)-H(16B)	107.6
C(12)-N(17)-C(16)	127(2)
C(12)-N(17)-H(17)	110(6)
C(16)-N(17)-H(17)	123(6)

C(12B)-N(11B)-S(8)	124(2)
N(11B)-C(12B)-N(17B)	114(3)
N(11B)-C(12B)-C(13B)	126(3)
N(17B)-C(12B)-C(13B)	118(3)
C(12B)-C(13B)-C(14B)	110.2(17)
C(12B)-C(13B)-H(13C)	109.6
C(14B)-C(13B)-H(13C)	109.6
C(12B)-C(13B)-H(13D)	109.6
C(14B)-C(13B)-H(13D)	109.6
H(13C)-C(13B)-H(13D)	108.1
C(15B)-C(14B)-C(13B)	108.0(12)
C(15B)-C(14B)-H(14C)	110.1
C(13B)-C(14B)-H(14C)	110.1
C(15B)-C(14B)-H(14D)	110.1
C(13B)-C(14B)-H(14D)	110.1
H(14C)-C(14B)-H(14D)	108.4
C(16B)-C(15B)-C(14B)	111.8(13)
C(16B)-C(15B)-B(18B)	111.6(15)
C(14B)-C(15B)-B(18B)	108.6(14)
C(16B)-C(15B)-H(15B)	108.2
C(14B)-C(15B)-H(15B)	108.2
B(18B)-C(15B)-H(15B)	108.2
C(15B)-C(16B)-N(17B)	112.0(17)
C(15B)-C(16B)-H(16C)	109.2
N(17B)-C(16B)-H(16C)	109.2
C(15B)-C(16B)-H(16D)	109.2
N(17B)-C(16B)-H(16D)	109.2
H(16C)-C(16B)-H(16D)	107.9
C(12B)-N(17B)-C(16B)	128(3)
C(12B)-N(17B)-H(17B)	113(10)
C(16B)-N(17B)-H(17B)	118(10)
O(19)-B(18)-O(20)	110.7(13)
O(19)-B(18)-C(15)	129.5(14)
O(20)-B(18)-C(15)	118.4(12)
B(18)-O(19)-C(21)	113.5(12)
C(24)-O(20)-B(18)	103.6(10)
O(19)-C(21)-C(24)	105.6(9)

O(19)-C(21)-C(22)	109.1(12)
C(24)-C(21)-C(22)	128.0(13)
O(19)-C(21)-C(23)	105.5(11)
C(24)-C(21)-C(23)	95.7(10)
C(22)-C(21)-C(23)	110.5(12)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-O(20)	103.2(10)
C(21)-C(24)-C(26)	122.5(13)
O(20)-C(24)-C(26)	111.8(13)
C(21)-C(24)-C(25)	113.4(13)
O(20)-C(24)-C(25)	101.3(11)
C(26)-C(24)-C(25)	102.9(12)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(20B)-B(18B)-O(19B)	106.7(17)
O(20B)-B(18B)-C(15B)	124.4(18)

O(19B)-B(18B)-C(15B)	126.5(18)
B(18B)-O(19B)-C(21B)	112.2(14)
B(18B)-O(20B)-C(24B)	114.9(15)
O(19B)-C(21B)-C(24B)	101.0(11)
O(19B)-C(21B)-C(22B)	107.4(13)
C(24B)-C(21B)-C(22B)	106.5(14)
O(19B)-C(21B)-C(23B)	130.9(14)
C(24B)-C(21B)-C(23B)	89.6(12)
C(22B)-C(21B)-C(23B)	115.2(13)
C(21B)-C(22B)-H(22D)	109.5
C(21B)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
C(21B)-C(22B)-H(22F)	109.5
H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
C(21B)-C(23B)-H(23D)	109.5
C(21B)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(21B)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
C(25B)-C(24B)-O(20B)	95.1(13)
C(25B)-C(24B)-C(26B)	92.7(15)
O(20B)-C(24B)-C(26B)	108.3(15)
C(25B)-C(24B)-C(21B)	137.6(16)
O(20B)-C(24B)-C(21B)	102.0(11)
C(26B)-C(24B)-C(21B)	117.5(15)
C(24B)-C(25B)-H(25D)	109.5
C(24B)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25E)	109.5
C(24B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
C(24B)-C(26B)-H(26D)	109.5
C(24B)-C(26B)-H(26E)	109.5
H(26D)-C(26B)-H(26E)	109.5
C(24B)-C(26B)-H(26F)	109.5

H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **R**⁴. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	96(4)	66(3)	122(5)	23(3)	27(3)	7(3)
C(2)	62(2)	52(2)	86(3)	4(2)	31(2)	-4(2)
C(3)	87(3)	45(2)	89(3)	-17(2)	11(3)	-9(2)
C(4)	71(3)	58(2)	61(2)	-16(2)	3(2)	-7(2)
C(5)	53(2)	48(2)	51(2)	-8(2)	17(2)	-9(2)
C(6)	80(3)	60(2)	55(2)	-15(2)	12(2)	2(2)
C(7)	79(3)	80(3)	56(2)	5(2)	11(2)	9(2)
S(8)	71(1)	48(1)	56(1)	-2(1)	18(1)	-7(1)
O(9)	96(2)	71(2)	64(2)	1(2)	-10(2)	2(2)
O(10)	97(2)	59(2)	80(2)	-2(2)	46(2)	-14(2)
N(11)	52(5)	44(4)	54(5)	-1(4)	10(4)	-1(4)
C(12)	50(3)	44(3)	59(5)	2(4)	9(4)	-2(3)
C(13)	55(4)	55(4)	64(4)	0(3)	10(3)	-7(3)
C(14)	62(4)	67(4)	75(4)	3(4)	8(4)	-15(3)
C(15)	53(3)	68(3)	76(3)	5(3)	18(3)	-5(3)
C(16)	52(4)	64(4)	68(4)	1(3)	16(3)	-2(3)
N(17)	49(4)	50(3)	57(5)	1(4)	10(3)	-4(3)
N(11B)	46(5)	42(4)	53(6)	0(4)	6(4)	-5(4)
C(12B)	51(3)	45(3)	56(5)	0(4)	8(4)	-1(3)
C(13B)	55(4)	52(4)	65(5)	-1(4)	9(4)	-3(3)
C(14B)	59(4)	63(4)	75(5)	4(4)	10(4)	-9(3)
C(15B)	64(3)	79(4)	87(4)	0(3)	17(3)	-7(3)
C(16B)	58(4)	63(4)	70(5)	0(4)	15(4)	-2(4)
N(17B)	49(4)	50(4)	62(5)	-1(4)	15(4)	-5(3)
B(18)	77(4)	107(4)	110(4)	2(4)	35(4)	-10(3)
O(19)	89(3)	149(4)	133(4)	8(4)	53(3)	10(3)
O(20)	113(4)	152(4)	132(4)	15(4)	47(3)	-8(3)

C(21)	98(4)	145(4)	128(4)	9(4)	50(4)	2(4)
C(22)	159(8)	172(9)	180(9)	8(9)	23(8)	-27(8)
C(23)	142(8)	189(10)	133(8)	-21(8)	18(7)	32(9)
C(24)	102(4)	147(4)	134(4)	3(4)	50(4)	0(4)
C(25)	146(8)	168(9)	179(8)	5(8)	61(8)	-14(8)
C(26)	138(8)	181(9)	170(9)	-2(8)	16(8)	10(8)
B(18B)	80(4)	113(4)	114(4)	-8(4)	40(4)	-10(4)
O(19B)	103(4)	144(4)	139(4)	-18(4)	50(4)	-9(4)
O(20B)	95(3)	138(4)	138(4)	-15(4)	44(3)	-10(3)
C(21B)	103(4)	146(4)	131(4)	-2(4)	51(4)	-1(4)
C(22B)	127(9)	159(9)	173(9)	-2(8)	56(8)	-2(8)
C(23B)	129(8)	163(10)	139(8)	6(8)	34(8)	17(8)
C(24B)	102(4)	145(5)	135(4)	-6(4)	45(4)	-10(4)
C(25B)	143(9)	157(9)	151(10)	4(9)	35(9)	-41(8)
C(26B)	116(8)	163(10)	155(10)	-25(9)	3(8)	-7(9)

Table S12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **R'**.

	x	y	z	U(eq)
H(1A)	11976	4540	5710	141
H(1B)	12364	4372	4501	141
H(1C)	11155	4092	4765	141
H(3)	10747	5112	2968	88
H(4)	10060	6523	2385	76
H(6)	11127	7588	5404	78
H(7)	11742	6150	5993	86
H(13A)	8164	7694	4037	69
H(13B)	8581	7444	5287	69
H(14A)	6659	7434	5148	81
H(14B)	6610	8436	4629	81
H(15)	7659	8050	6869	78
H(16A)	7190	9842	6041	73
H(16B)	7998	9579	7100	73
H(17)	9190(70)	9880(70)	5690(70)	62
H(13C)	8415	7443	4405	69

H(13D)	7579	8157	3802	69
H(14C)	6619	7463	5299	79
H(14D)	7629	7680	6196	79
H(15B)	6342	9049	5016	91
H(16C)	7804	9364	6915	76
H(16D)	7248	10103	6079	76
H(17B)	8840(110)	9860(100)	5380(100)	64
H(22A)	3238	7491	8154	255
H(22B)	4050	7015	7372	255
H(22C)	4364	7065	8681	255
H(23A)	3849	9043	9251	231
H(23B)	4970	8564	9704	231
H(23C)	4994	9474	8993	231
H(25A)	4106	10409	7132	242
H(25B)	3911	9973	8306	242
H(25C)	5123	10044	7925	242
H(26A)	3044	9623	6096	245
H(26B)	2986	8542	6077	245
H(26C)	2563	9090	7094	245
H(22D)	3057	9723	8030	226
H(22E)	4048	10426	8038	226
H(22F)	3543	9995	6894	226
H(23D)	3649	8328	9106	213
H(23E)	4692	7755	8820	213
H(23F)	4843	8607	9632	213
H(25D)	3130	7367	7562	223
H(25E)	3632	7136	6421	223
H(25F)	4374	7040	7570	223
H(26D)	3242	9185	6033	217
H(26E)	3227	8166	5590	217
H(26F)	2509	8441	6576	217

Table S13. Hydrogen bonds for **R'** [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(17)-H(17)...O(10)#1	0.95(10)	2.60(10)	3.14(2)	116(7)

N(17)-H(17)...N(11)#1	0.95(10)	2.10(11)	3.03(3)	169(8)
N(17B)-H(17B)...O(10)#1	0.69(15)	2.81(14)	3.21(3)	120(13)
N(17B)-H(17B)...N(11B)#1	0.69(15)	2.47(14)	3.11(4)	157(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1