

Electronic Supporting Information for:

The Characterisation and Reactivity of a Rh^{III} η¹-σ-Alkane Complex and the Role of a Structurally Responsive Phosphine Ligand in Solid-State Molecular Organometallic Chemistry

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S1. Experimental Procedures

S1a. General Considerations

All manipulations, unless otherwise stated, were performed under standard Schlenk line and glovebox (<0.5 ppm H₂O/O₂) techniques under an argon (BOC, N4.8 purity), hydrogen (CK Gases, N5.0 purity), deuterium (CK Gases, N2.8 purity), propylene (CK Gases, N2.5 purity) or nitrogen atmosphere. Glassware and Celite were dried overnight at 140 °C and flame dried under vacuum before use. Pentane, hexane, CH₂Cl₂ and toluene were dried using a commercially available Grubbs-type purification system (Innovative Technology) and degassed with three freeze-pump-thaw cycles and dried over 3 Å molecular sieves under argon in resealable glass ampoules fitted with PTFE high vacuum stopcocks (Rotaflo HP or J Young). 1,2-F₂C₆H₄ (pre-treated with alumina), C₆D₆ and CD₂Cl₂ were dried over CaH₂, vacuum transferred, degassed with three freeze-pump-thaw cycles and stored over 3 Å molecular sieves. Tetrahydrofuran (THF) was dried over Na/benzophenone, distilled, degassed with three freeze-pump-thaw cycles and stored over 3 Å molecular sieves.

[Rh(NBD)₂][BAR^F₄]¹ was synthesised according to literature methods. All other chemicals were obtained from commercial sources and used without further purification.

Solution-state NMR spectroscopic data were collected on a Bruker AVIIIHD 500 MHz at the specified temperatures. Solution ¹H and ¹³C{¹H} NMR spectra were referenced to the residual solvent peaks. Assignments were aided with ¹H{³¹P} and 2-D solution NMR data. Solution ³¹P{¹H} NMR spectra were referenced externally to 85% H₃PO₄ in D₂O. Solid-state NMR samples were prepared in an argon-filled glovebox by pre-loading 15-30 mg, or 60-100 mg of crushed material into 1.9 mm or 4.0 mm zirconia solid-state NMR rotors, respectively. The rotors were sealed with Kel-F, vespel or zirconia caps. Solid-state NMR data were collected on Bruker Avance III HD spectrometers, operating at 100.56 or 100.63 MHz (¹³C{¹H}), and 161.99 or 162.04 MHz (³¹P{¹H}) at the specified MAS rates and temperatures. All ¹³C{¹H} CP MAS spectra were referenced externally to adamantane where the upfield methine resonance was taken to be δ_C 29.5, secondarily referenced to SiMe₄, δ_C 0.0. ³¹P{¹H} CP MAS spectra were externally referenced to triphenylphosphine (δ_P -9.3, relative to H₃PO₄) or calcium hydrogen phosphate (δ_P 1.4, relative to H₃PO₄). Solid-state NMR spectra were recorded at varied MAS rates to determine isotropic chemical shifts. Gas chromatography electron-ionisation mass spectrometry data were obtained by Mr Karl Heaton at the University of York Centre of Excellence in Mass Spectrometry. Elemental analyses were collected by Ms Orfhlaith McCullough at London Metropolitan University.

S1b. Synthesis of dtbbp (1,4-di-*tert*-butylphosphinobutane)

This preparation is adapted from literature methods but circumvents the usage of highly pyrophoric *tert*-butyllithium and does not require Kugelrohr distillation.^{2, 3}

A solution of di-*tert*-butylphosphine (2.5 mL, 1.98 g) in THF (20 mL) was cooled to -78 °C. A solution of *n*-butyllithium (6.4 mL, 2.1 M in hexanes) was added dropwise. After full addition of *n*-butyllithium, the reaction mixture changed colour from colourless to pale yellow. The reaction was stirred at -78 °C for 10 minutes before warming to ambient temperature. The reaction was stirred at ambient temperature for 18 hours, before cooling back to -78 °C. A solution of 1,4-dibromobutane (800 μ L, 1.45 g) in THF (5 mL) was then added dropwise *via* syringe. After full addition, the reaction mixture had become a cloudy white suspension. The reaction was stirred at -78 °C for 15 minutes before warming to ambient temperature and stirring for 18 hours. The volatiles were removed *in vacuo*, the product extracted into hexane (3 x 30 mL) and isolated through filtration through a thick pad of celite. The volatiles were then removed *in vacuo* to yield dtbbp as a white powder (1.97 g, 85 % yield).

Solution ^1H NMR (500 MHz, C_6D_6 , 298 K): δ_{H} 1.80 (second-order m, 4 H), 1.41 (second-order m, 4H) 1.11 [d, $^3J(\text{PH}) = 10.6$ Hz, 36 H].

Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, C_6D_6 , 298 K): δ_{P} 27.3.

Solution $^{13}\text{C}\{^1\text{H}\}$ NMR (125.80 MHz, C_6D_6 , 298 K): δ_{C} 32.8 (second-order m, CH_2), 31.3 [d, $^1J(\text{CP}) = 22$ Hz, CH_2], 29.9 [d, $^2J(\text{CP}) = 15$ Hz, $\text{C}(\text{CH}_3)_3$], 21.8 [d, $^1J(\text{CP}) = 23$ Hz, $\text{C}(\text{CH}_3)_3$].

Elemental Analysis *calc* for $\text{C}_{20}\text{H}_{44}\text{P}_2$: C 69.32; H 12.80; N 0.0; *found*: C 69.15; H 12.42; N 0.0.

S1c. Synthesis of [Rh(dtbpb)(NBD)][BAr^F₄], 1[BAr^F₄]

To a rapidly stirring solution of [Rh(NBD)₂][BAr^F₄] (1.00 g) in CH₂Cl₂ (50 mL) was dropwise added a solution of dtbpb (321 mg) in CH₂Cl₂ (15 mL). The reaction mixture was stirred at ambient temperature for 2 hours. The reaction mixture took on a slight colour change from red to plum red. The reaction mixture was precipitated by addition of hexane (300 mL) to form a bright red, microcrystalline solid. The supernatant was removed *via* cannula filtration. The product was extracted into CH₂Cl₂ (2 x 30 mL), cannula filtered and layered with hexane (250 mL) at ambient temperature to yield bright-red, block-like crystals of 1[BAr^F₄] (897 mg, 80 % yield).

Solution ¹H NMR (500 MHz, CD₂Cl₂, 298 K): δ_H 7.72 (br s, 8 H, *ortho*-BAr^F₄), 7.56 (s, 3 H, *para*-BAr^F₄), 5.05 (second-order m, 4 H, NBD C=CH), 3.89 (m, 2 H, NBD bridgehead CH₂), 1.91 (br s, FWHM = 27 Hz, 4 H, CH₂), 1.78 (br m, FWHM = 30 Hz, 4 H, CH₂), 1.56 (s, 2 H, NBD bridge CH), 1.40 [d, ³J(HP) = 13.2 Hz, 36 H, C(CH₃)₃].

Solution ³¹P{¹H} NMR (202.49 MHz, C₆D₆, 298 K): δ_P 34.6 [d, ¹J(PRh) = 148 Hz].

Solid-State ³¹P{¹H} CP MAS NMR (162.04 MHz, 10 kHz spin rate, 298 K): δ_P 48.2 [d, ¹J(PRh) = 144 Hz], 25.0 [d, ¹J(PRh) = 144 Hz].

Solid-State ¹³C{¹H} CP MAS NMR (100.66 MHz, 10 kHz spin rate, 298 K): δ_C 166.4, 163.6, 137.7, 135.2, 130.5, 125.1, 117.2 (BAr^F₄ resonances), 77.1, 75.8, 64.4, 51.8, 48.7 (NBD alkene resonances), 40.5, 38.8, 38.8, 37.3, 32.6, 32.0, 29.0, 28.7, 24.3, 21.7, 20.3, 16.2 (overlapping phosphine and NBD resonances).

ESI-MS m/z (CH₂Cl₂) found (calc): C₂₇H₅₂P₂Rh₁ 541.2587 (541.2599).

Elemental Analysis calc for C₅₉H₆₄B₁F₂₄P₂Rh₁: C 50.44; H 4.59; N 0; *found:* C 50.48; H 4.54; N 0.0

S1d. Synthesis of [RhH(dtbbp')(σ-NBA)][BAr^F₄], 2[BAr^F₄]

An ampoule was charged with **1[BAr^F₄]** (54 mg), evacuated (1×10^{-3} mbar) and back-filled with H₂ (1 bar gauge). Over the course of 2 hours the, bright red, crystalline **1[BAr^F₄]** gradually changed colour to sandy yellow. After 2 hours had elapsed, the ampoule was evacuated and back-filled with Ar) to yield **2[BAr^F₄]** as a sandy yellow, crystalline material in quantitative yield.

*Solution-state NMR spectroscopic data are reported under **3[BAr^F₄]**.*

Solid-State ³¹P{¹H} CP MAS NMR (162.05 MHz, 10 kHz spin rate, 298 K): δ_P 100.5 [dd, ¹J(PRh) = 125 Hz, ²J(PP) = 289 Hz], -8.5 (apparent t, J_{app} = 300 Hz).

Solid-State ¹³C{¹H} CP MAS NMR (100.66 MHz, 10 kHz spin rate, 298 K): δ_C 164.8, 163.0, 137.4, 135.4, 130.7, 125.4, 117.9, 117.8 (BAr^F₄ resonances), 43.3, 38.6, 37.8, 33.9, 30.0, 21.3 (overlapping phosphine and NBA resonances).

*Due to the sensitivity of **2[BAr^F₄]** satisfactory elemental analyses could not be obtained.*

S1e. Synthesis of $[\text{RhH}(\text{dtbpb}')(\kappa^1\text{-CD}_2\text{Cl}_2)][\text{BAr}^{\text{F}}_4], 3[\text{BAr}^{\text{F}}_4]$

A J. Youngs NMR tube was charged with $2[\text{BAr}^{\text{F}}_4]$ (25 mg) and CD_2Cl_2 (0.6 mL) was vacuum transferred onto the solids. Thawing of the resultant mixture formed a pale-yellow solution. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by layering a CD_2Cl_2 solution of $3[\text{BAr}^{\text{F}}_4]$ with heptane at $-30\text{ }^\circ\text{C}$.

Note: Solution NMR spectroscopic data listed below were recorded by vacuum transferring CD_2Cl_2 (0.6 mL) directly onto $2[\text{BAr}^{\text{F}}_4]$, without purification via recrystallisation to remove NBA. Recrystallised material often contained unidentified impurities due to slow but persistent decomposition of $3[\text{BAr}^{\text{F}}_4]$ in solution, which were chemically and physically inseparable. Elemental analysis was not successful for $3[\text{BAr}^{\text{F}}_4]$ due to the lack of long-term stability of the complex. Nevertheless, purity of freshly-prepared solutions is established to the limits NMR spectroscopy (see Figures S12-13).

Solution ^1H NMR (500 MHz, CD_2Cl_2 , 193 K): δ_{H} 7.72 (s, 8 H, *ortho*- BAr^{F}_4), 7.53 (s, 4 H, *para*- BAr^{F}_4), 2.88 (m, 1 H, phosphine backbone), 2.57 (m, 1 H, phosphine backbone), 2.20 (m, 1 H, phosphine backbone), 2.07 (m, 2 H, NBA methylene bridge), 1.67 (m, 1 H, phosphine backbone), 1.41 - 0.97 (m, 46 H, overlapping phosphine ^tBu methyl, backbone and NBA resonances), -28.43 [m, $^1J(\text{HRh}) = 64.0$ Hz, 1 H, Rh-*H*].

Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 193 K): δ_{P} 98.8 [dd, $^1J(\text{PRh}) = 127$ Hz, $^2J(\text{PP}) = 289$ Hz], -16.5 [dd, $^1J(\text{PRh}) = 90$ Hz, $^2J(\text{PP}) = 289$ Hz].

S1f. Addition of D₂ to 1[BAr^F₄]

A J. Youngs NMR tube was charged with **1[BAr^F₄]** (20 mg), evacuated (1×10^{-3} mbar), back-filled with D₂ gas (1 bar gauge) and sealed. After 2 hours, the NMR tube was degassed and CH₂Cl₂ (0.6 mL) was vacuum transferred onto the sandy yellow solids. The mixture was thawed, agitated and the volatiles vacuum transferred into a fresh J. Youngs NMR tube, yielding a CH₂Cl₂ solution of *endo-exo-d₄*-NBA.

Solution ²H NMR (76.79 MHz, CH₂Cl₂, 298 K): δ_H 1.39 (*exo* methylene NBA), 1.09 (*endo* methylene NBA).

GC-MS (EI-MS, CH₂Cl₂) *found* (*calc*): 100.12090 (100.11901, *d₄*-NBA).

S1g. Synthesis of [Rh(dtbbp)(NBE)][BAR^F₄], 4[BAR^F₄]

An ampoule was charged with **1**[BAR^F₄] (50 mg, 0.04 mmol), norbornene (NBE, 200 mg, 2.1 mmol, 60 equivalents) and 1,2-F₂C₆H₄ (7 mL), forming a bright red solution. The solution was degassed *via* three freeze-pump-thaw cycles and back-filled with H₂ (1 bar gauge, -196 °C). The reaction mixture was warmed to ambient temperature and stirred for 2 minutes, at which point the reaction mixture was wine-red/purple in colour. The reaction mixture was rapidly cooled to -196 °C and degassed *via* three freeze-pump-thaw cycles. As the reaction warmed to room temperature, the volatiles were removed under reduced pressure, keeping the temperature below 0 °C, to yield a wine-red solid which was washed with pre-cooled (-20 °C) hexane (3 x 5 mL). The solids were extracted into a pre-cooled (-30 °C) solution of NBE (2 mg, 0.02 mmol, 0.5 equivalents) in 1,2-F₂C₆H₄ (3 mL). The solution was layered with hexane at -30 °C to yield **4**[BAR^F₄] as a wine-red, crystalline solid (7 mg, 15% yield).

*Note: This reaction was found to be unpredictable. Trace impurities in 1,2-F₂C₆H₄ or in the starting materials likely contributed to the variation in yields obtained using this synthetic protocol. **4**[BAR^F₄] is unstable in solution at ambient temperature. Excess NBE was used in attempt to reduce solution decomposition of **4**[BAR^F₄] in the recrystallisation step.*

Solution ¹H NMR (500 MHz, CD₂Cl₂, 193 K): δ_H 7.72 (s, 8 H, *ortho*-BAR^F₄), 7.52 (s, 4 H, *para*-BAR^F₄), 4.99 (s, 1 H, C=CH), 4.57 (s, 1 H, C=CH), 3.53 (s, 1 H, NBE bridgehead), 3.39 (s, 1 H, NBE bridgehead), 2.06 – 1.66 (m, 7 H, multiple overlapping phosphine backbone), 1.58 – 0.88 (m, 45 H, overlapping NBE methylene and bridge, and ^tBu methyl resonances), -5.68 (s, 1 H, agostic NBE bridge CH).

Solution ³¹P{¹H} NMR (202.49 MHz, CD₂Cl₂, 193 K): δ_P 90.3 [dd, ¹J(PRh) = 220 Hz, ²J(PP) = 19 Hz], 30.0 [dd, ¹J(PRh) = 142 Hz, ²J(PP) = 18 Hz].

*Due to the instability and variable reaction outcomes in the synthesis of **4**[BAR^F₄], reliable elemental analyses were not obtained.*

S1h. Synthesis of $[\text{RhH}(\text{dtbpb})(\eta^3\text{-C}_3\text{H}_5)][\text{BAr}^{\text{F}}_4]$, 5 $[\text{BAr}^{\text{F}}_4]$

An ampoule was charged with 2 $[\text{BAr}^{\text{F}}_4]$ (125 mg) and evacuated (1×10^{-3} mbar). The ampoule was back-filled with propylene gas (1 bar gauge) and sealed. After 24 hours the ampoule was evacuated and placed under dynamic vacuum (1×10^{-3} mbar) for 18 hours to remove displaced NBA. The product was obtained in quantitative yield as a tan, crystalline solid.

Note: During the step involving addition propylene gas, the crystalline material tends to aggregate together, likely due egressed NBA on the surfaces of the crystals. Therefore, the sample should be evenly dispersed within the ampoule to allow for even gas diffusion throughout the sample.

Solid-State $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.00 MHz, 10 kHz spin rate, 293 K): δ_{P} 70.6, 64.1.

Solid-State $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.00 MHz, 10 kHz spin rate, 193 K): δ_{P} 73.7, 58.1.

Solid-State $^{13}\text{C}\{^1\text{H}\}$ CP TOSS MAS NMR (100.63 MHz, 10 kHz spin rate, 295 K): δ_{C} 165.3, 162.0, 136.0, 134.4, 130.4, 124.2 (BAr^{F}_4 resonances), 117.1, 37.4, 29.4 (phosphine resonances).

Solid-State $^{13}\text{C}\{^1\text{H}\}$ CP TOSS MAS NMR (100.63 MHz, 10 kHz spin rate, 193 K): δ_{C} 165.4, 161.5, 136.0, 133.9, 130.2, 124.2, 116.9, 107.0 (BAr^{F}_4 resonances), 68.0, 62.0 (C=C resonances), 37.2, 32.3, 29.5, 27.1, 25.4, 23.7, 22.4, 20.9, 19.0, 17.0 (phosphine resonances).

Solution ^1H NMR (500 MHz, CD_2Cl_2 , 193 K): δ_{H} 7.72 (s, 7 H, *ortho*- BAr^{F}_4), 7.53 (s, 4 H, *para*- BAr^{F}_4), 5.09 (m, 1 H, allyl CH), 4.82 (m, 2 H, allyl CH), 2.36 (apparent triplet, 2 H, allyl CH), 2.21 (m, 2 H, phosphine backbone CH_2), 2.04 (m, 2 H, phosphine backbone CH_2), 1.75 (m, 2 H, phosphine backbone CH_2), 1.52 – 0.65 (m, 36 H, overlapping ^iBu methyl environments), -32.55 [dt, $^1J(\text{HRh}) = 40$ Hz, $^2J(\text{HP}) = 20$ Hz, 1 H, Rh-*H*].

Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 193 K): δ_{P} 65.3 [d, $^1J(\text{PRh}) = 131$ Hz].

Elemental Analysis *calc* for $\text{C}_{55}\text{H}_{62}\text{B}_1\text{F}_{24}\text{Rh}_1\text{P}_2$: C 48.76; H 4.61; N 0.0; *found*: C 48.82; H 4.71; N 0.0

S2. NMR Spectroscopic Data

S2a. 1,4-di-*tert*-butylphosphinobutane (dtbpb)

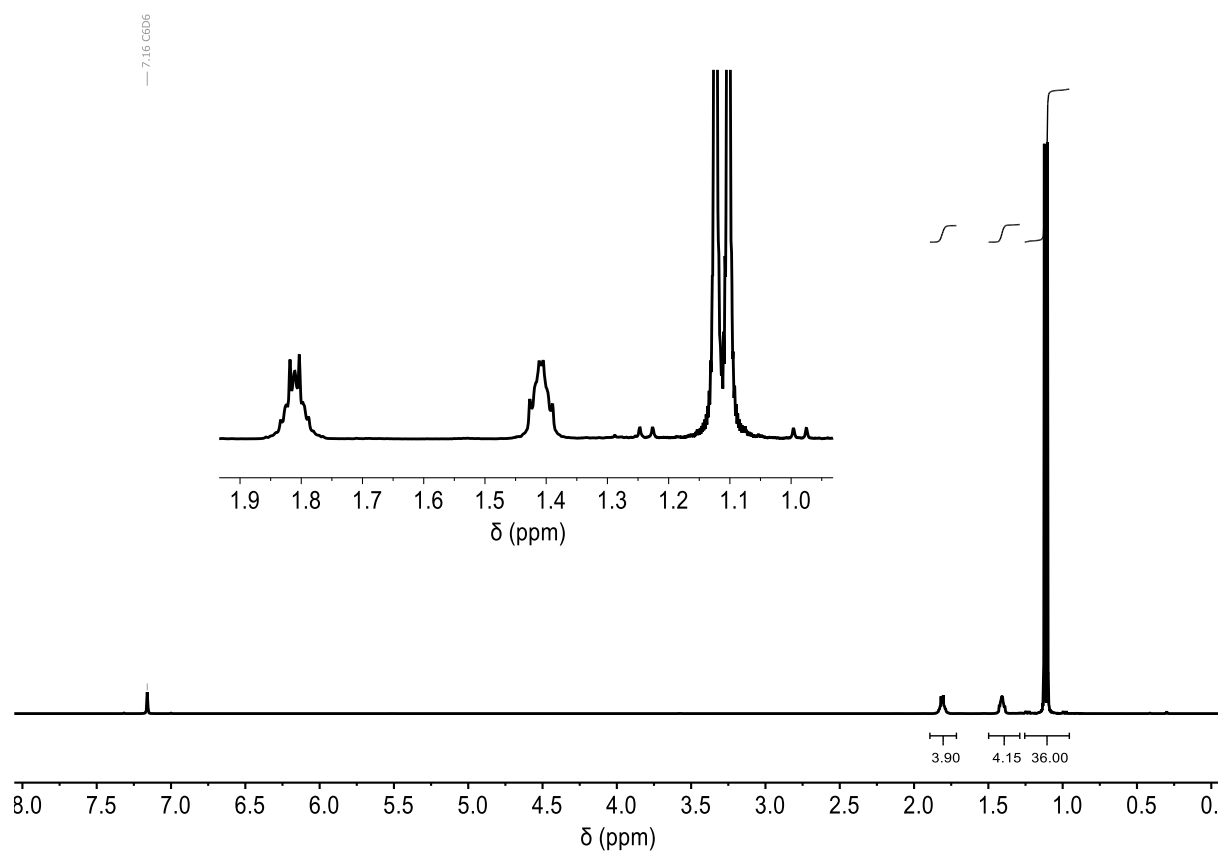


Figure S1: Solution ^1H NMR (500 MHz, C_6D_6 , 298 K) of 1,4-di-*tert*-butylphosphinobutane (dtbpb). Inset depicts the fine coupling of the resonances.

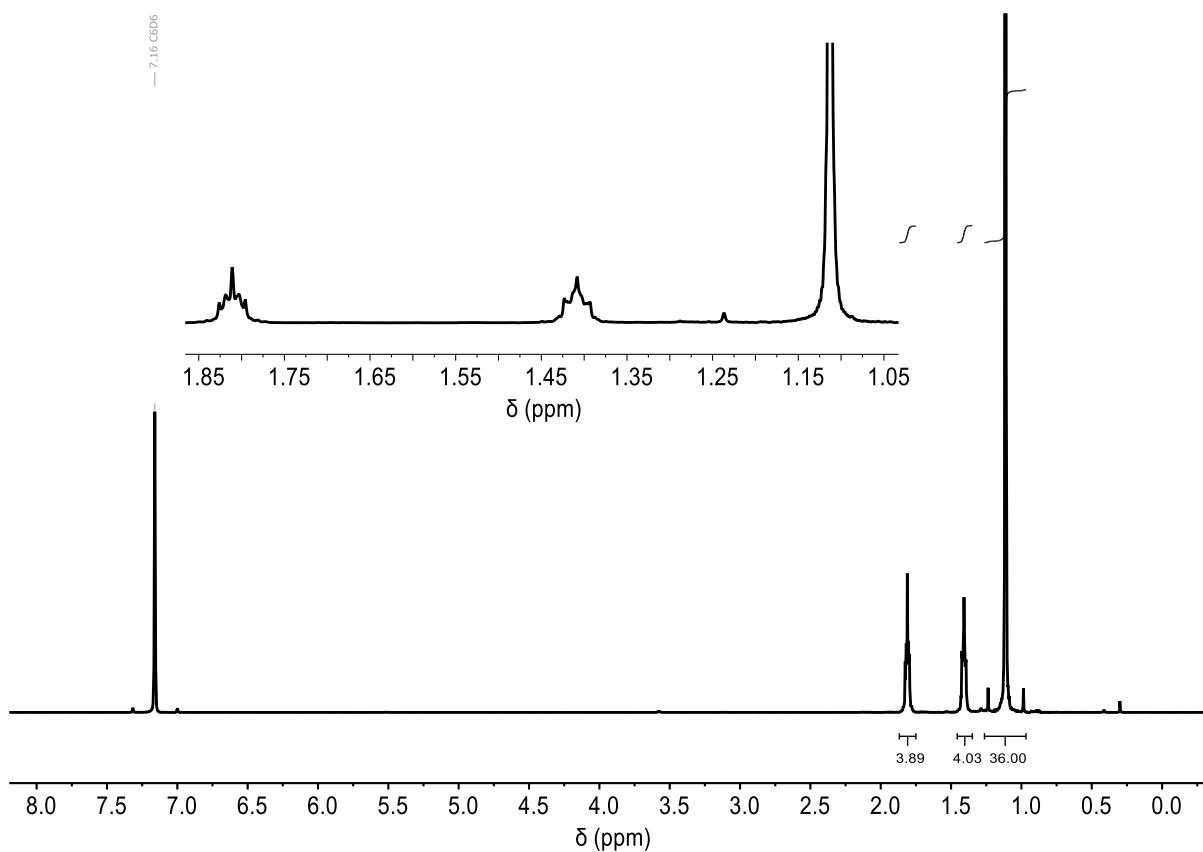


Figure S2: Solution $^1\text{H}\{^{31}\text{P}\}$ NMR (500 MHz, C_6D_6 , 298 K) of 1,4-di-*tert*-butylphosphinobutane (dtbpb). Inset depicts the fine coupling of the resonances.

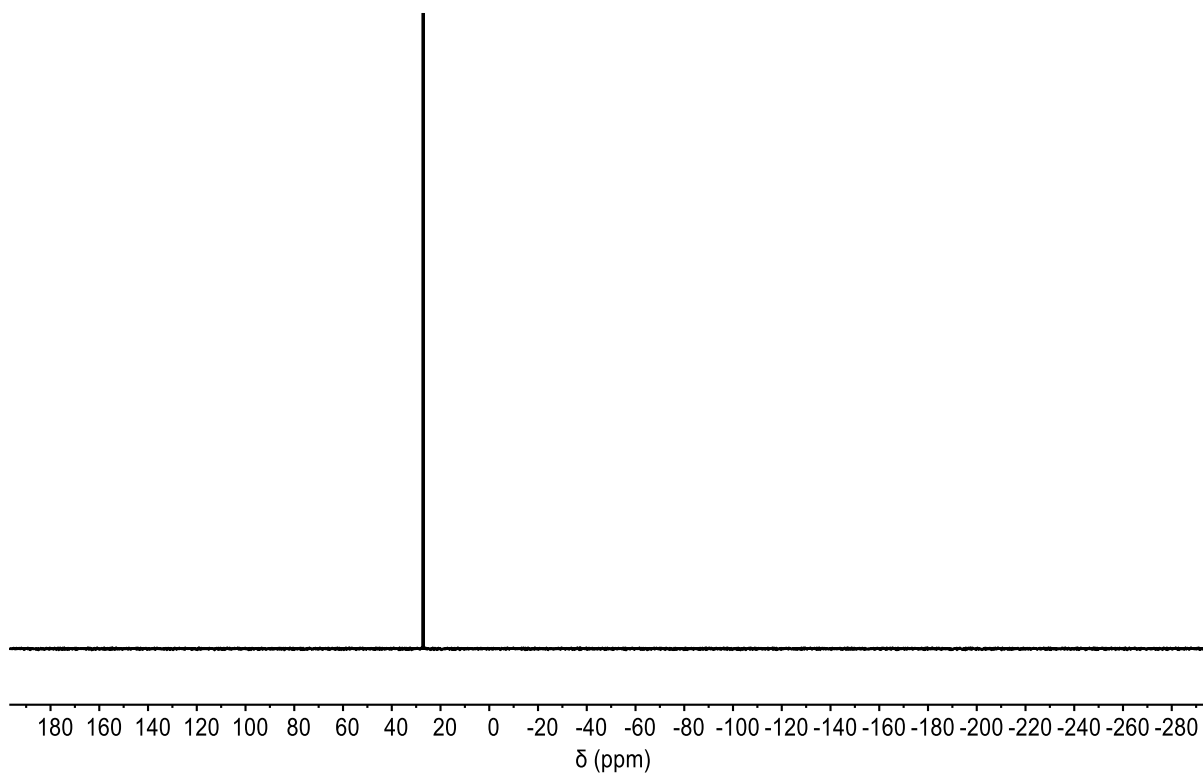


Figure S3: Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, C_6D_6 , 298 K) of 1,4-di-*tert*-butylphosphinobutane (dtbpb).

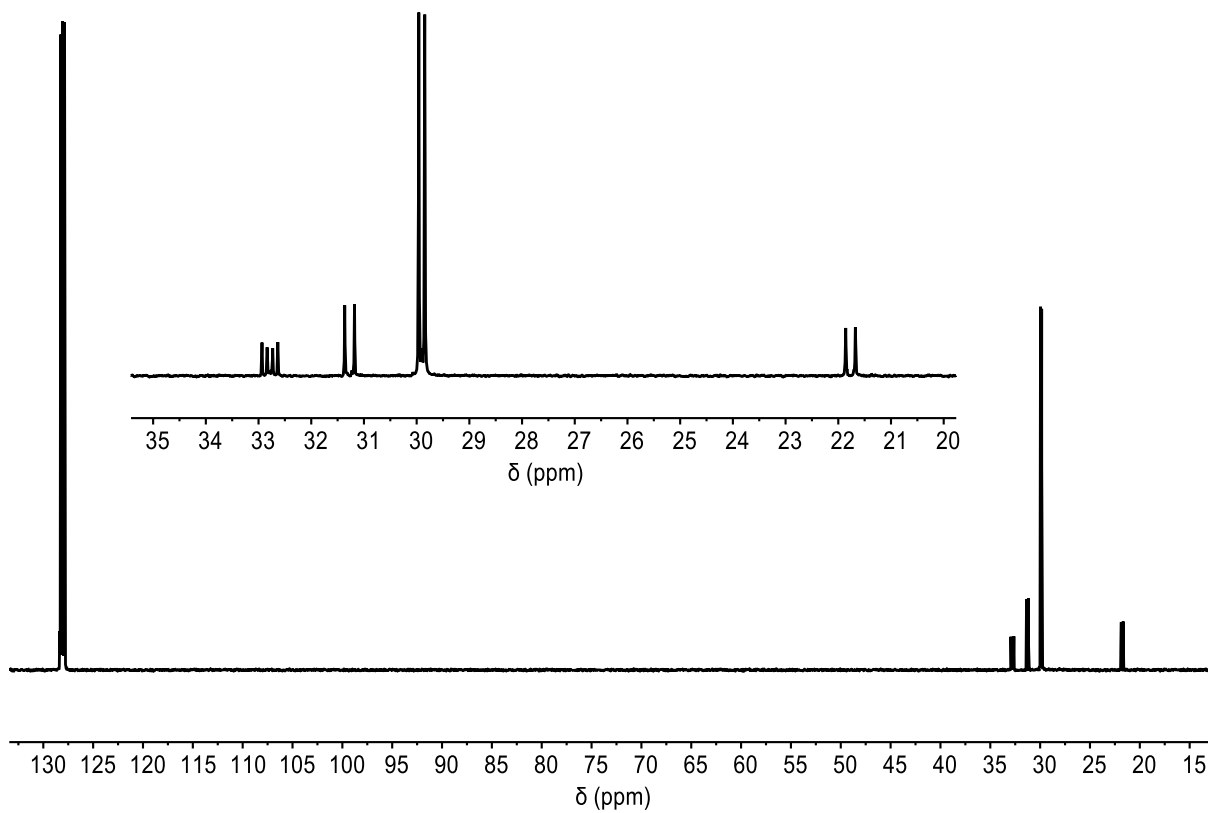


Figure S4: Solution $^{13}\text{C}\{^1\text{H}\}$ NMR (125.80 MHz, C_6D_6 , 298 K) of 1,4-di-*tert*-butylphosphinobutane (dtbpb). Inset depicts the fine coupling of the resonances.

S2b. [Rh(dtbpb)(NBD)][BAR^F₄], 1[BAR^F₄]

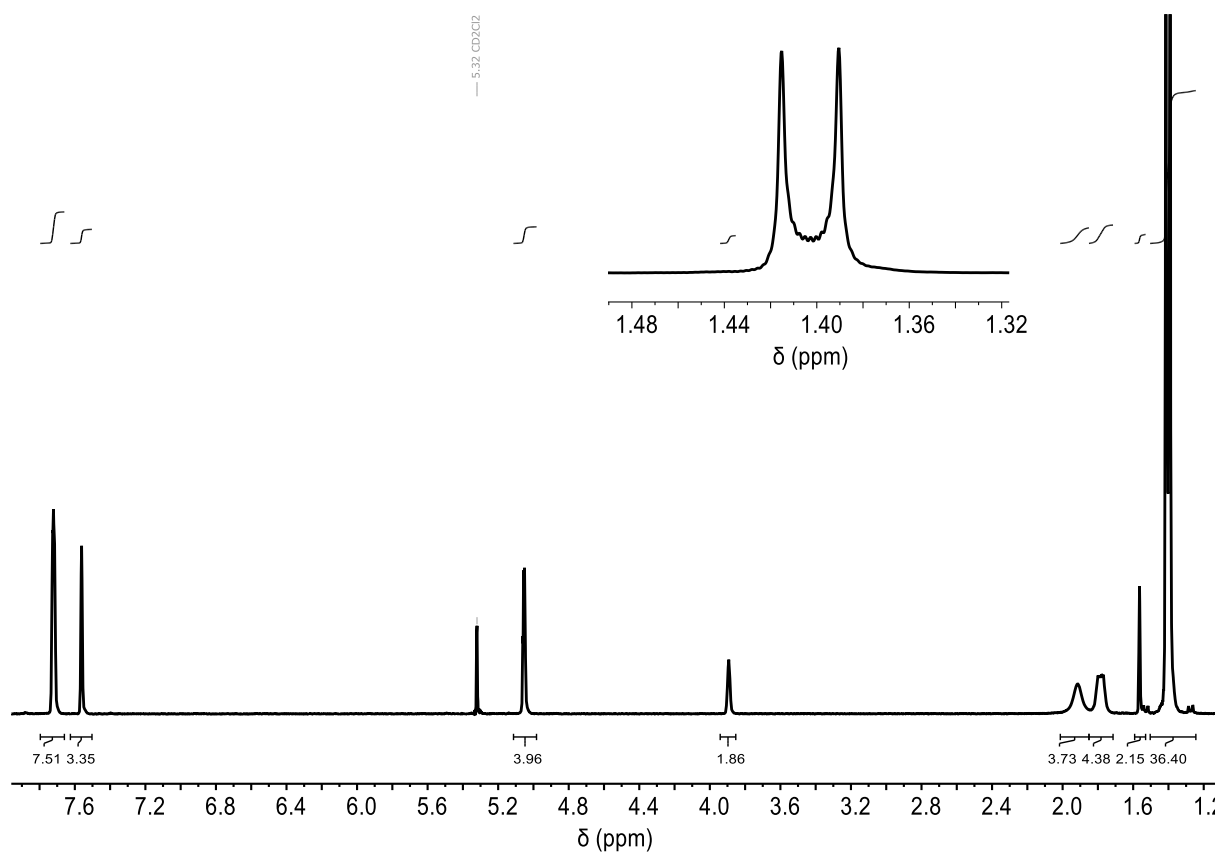


Figure S5: Solution ¹H NMR (500 MHz, CD₂Cl₂, 298 K) of 1[BAR^F₄]. Inset depicts ¹Bu methyl resonance.

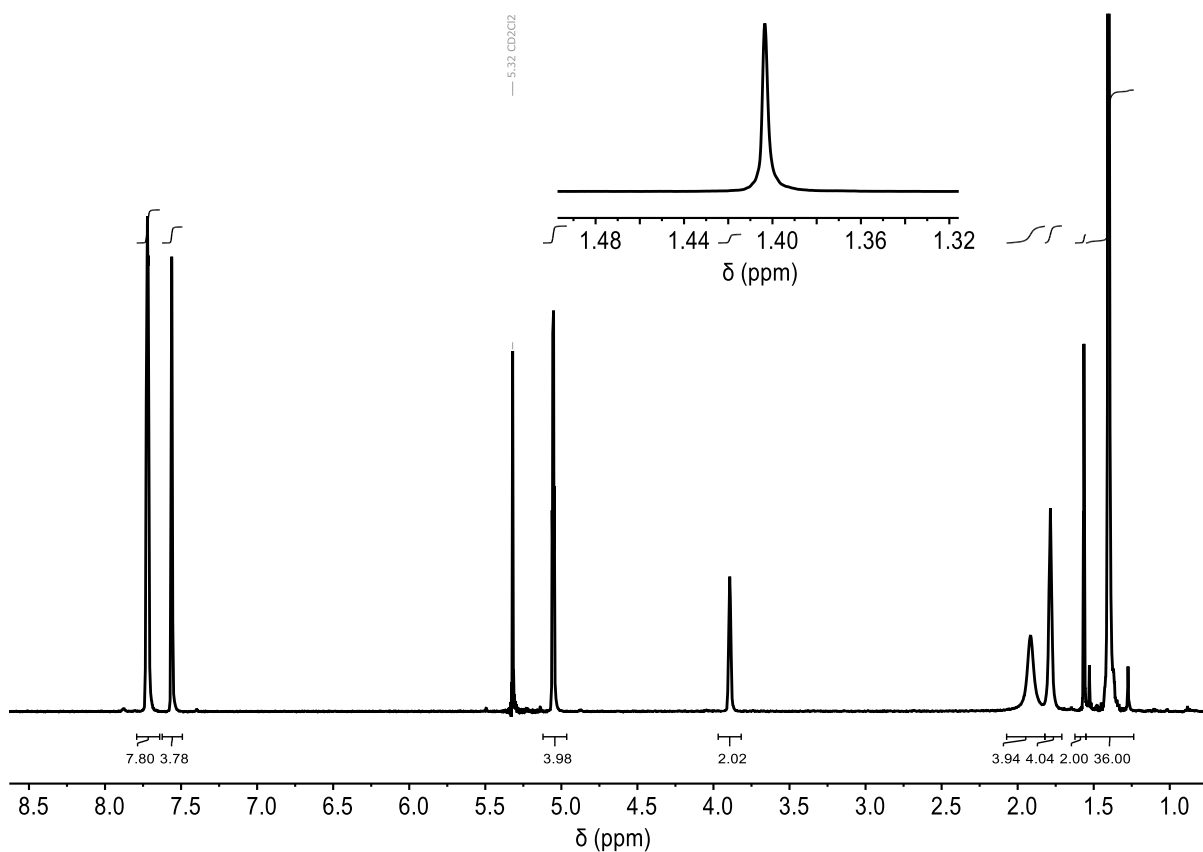


Figure S6: Solution $^1\text{H}\{^{31}\text{P}\}$ NMR (500 MHz, CD_2Cl_2 , 298 K) of $1[\text{BAr}^{\text{F}}_4]$. Inset depicts ^1Bu methyl resonance.

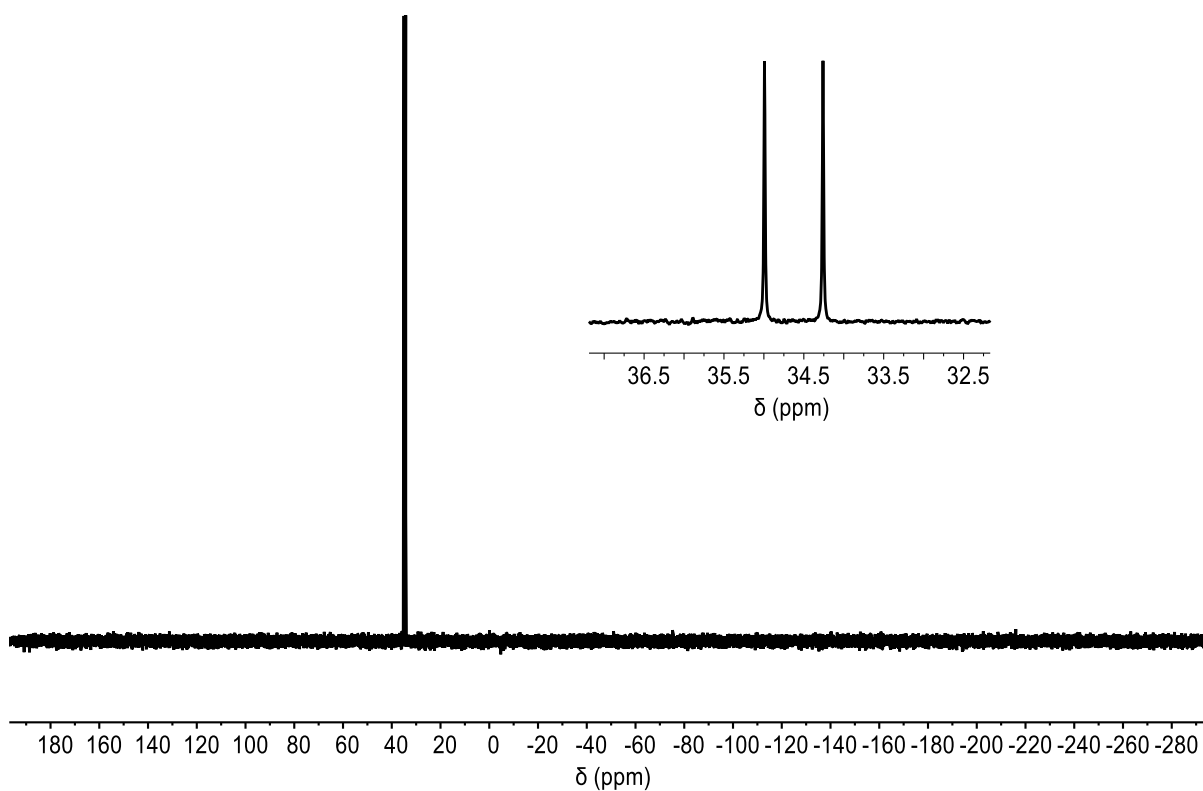


Figure S7: Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 298 K) of $1[\text{BAr}^{\text{F}}_4]$. Inset depicts doublet structure of resonance.

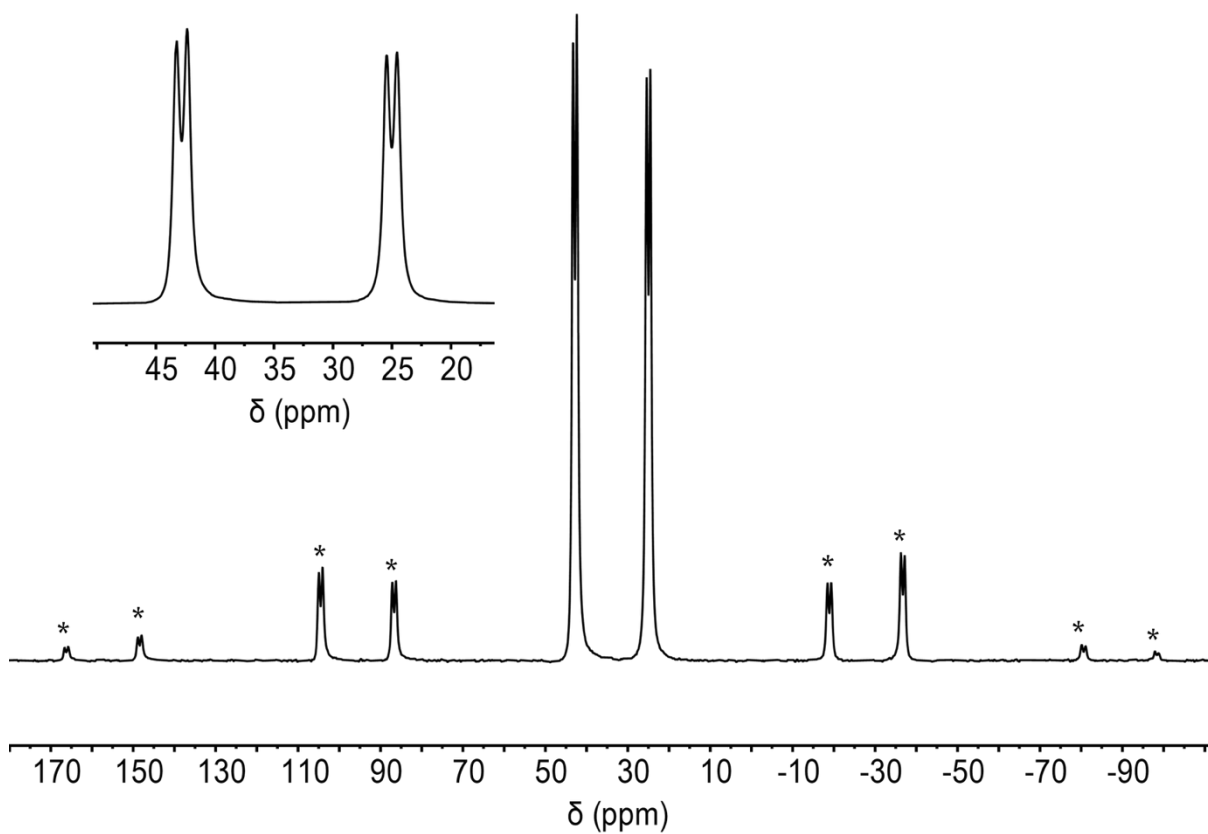


Figure S8: Solid-state $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.04 MHz, 10 kHz spin rate, 298 K) spectrum of $1[\text{BArF}_4]$. Inset depicts isotropic chemical shifts. Spinning side bands are noted with asterisks.

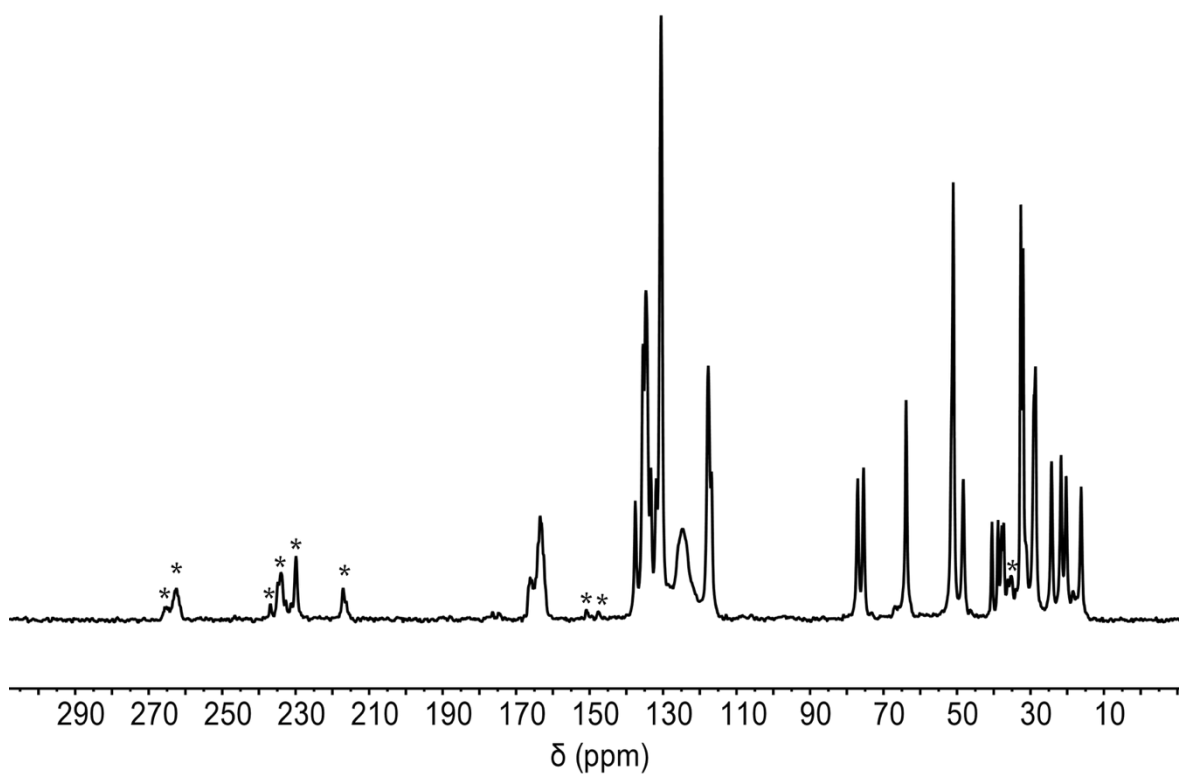


Figure S9: Solid-state $^{13}\text{C}\{^1\text{H}\}$ CP MAS NMR (100.66 MHz, 10 kHz spin rate, 298 K) spectrum of **1**[BArF₄]. Spinning side bands are noted with asterisks.

S2c. $[\text{RhH}(\text{dtbpb}^*)(\sigma\text{-NBA})][\text{BAR}^{\text{F}_4}]$, $2[\text{BAR}^{\text{F}_4}]$

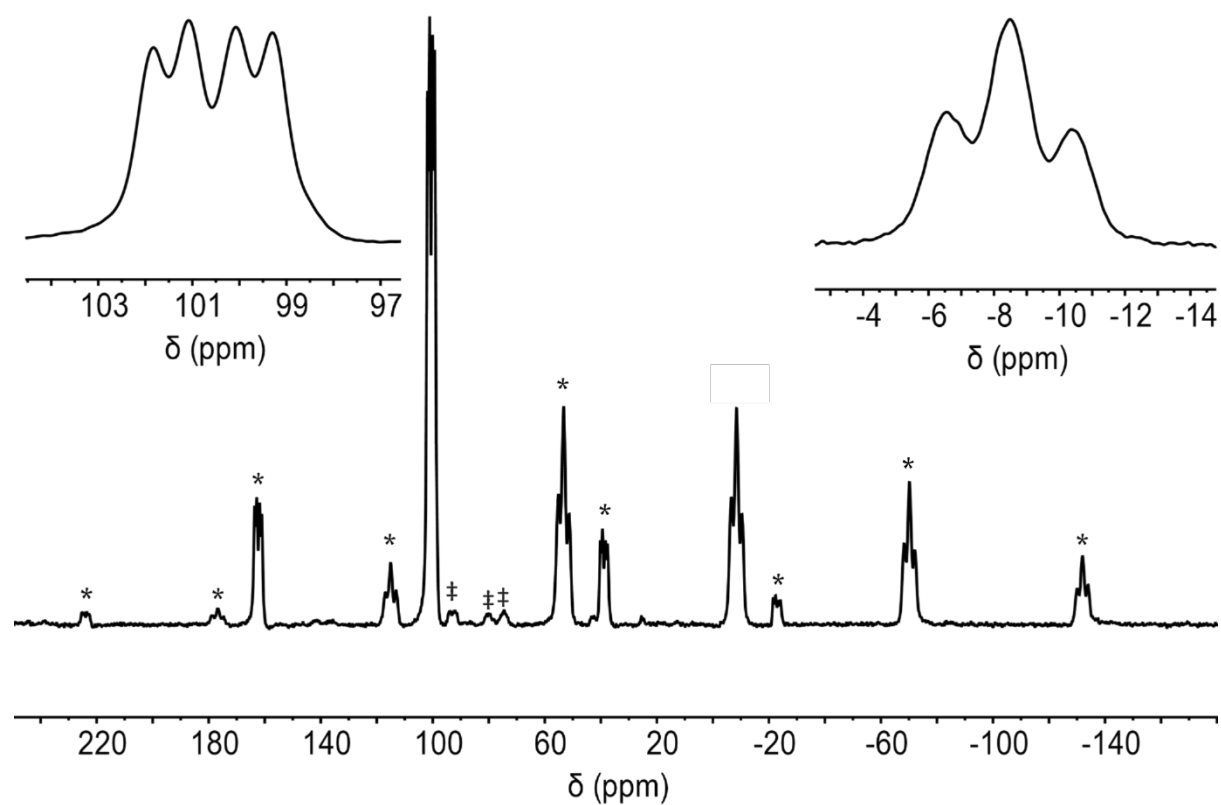


Figure S10: Solid-state $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.04 MHz, 10 kHz spin rate, 298 K) spectrum of $2[\text{BAR}^{\text{F}_4}]$. The insets depict the isotropic chemical shifts at δ_{P} 100.6 (*top left*) and -8.7 (*top right*). Spinning side bands are marked with asterisks. Unidentified impurities are denoted by ‡.

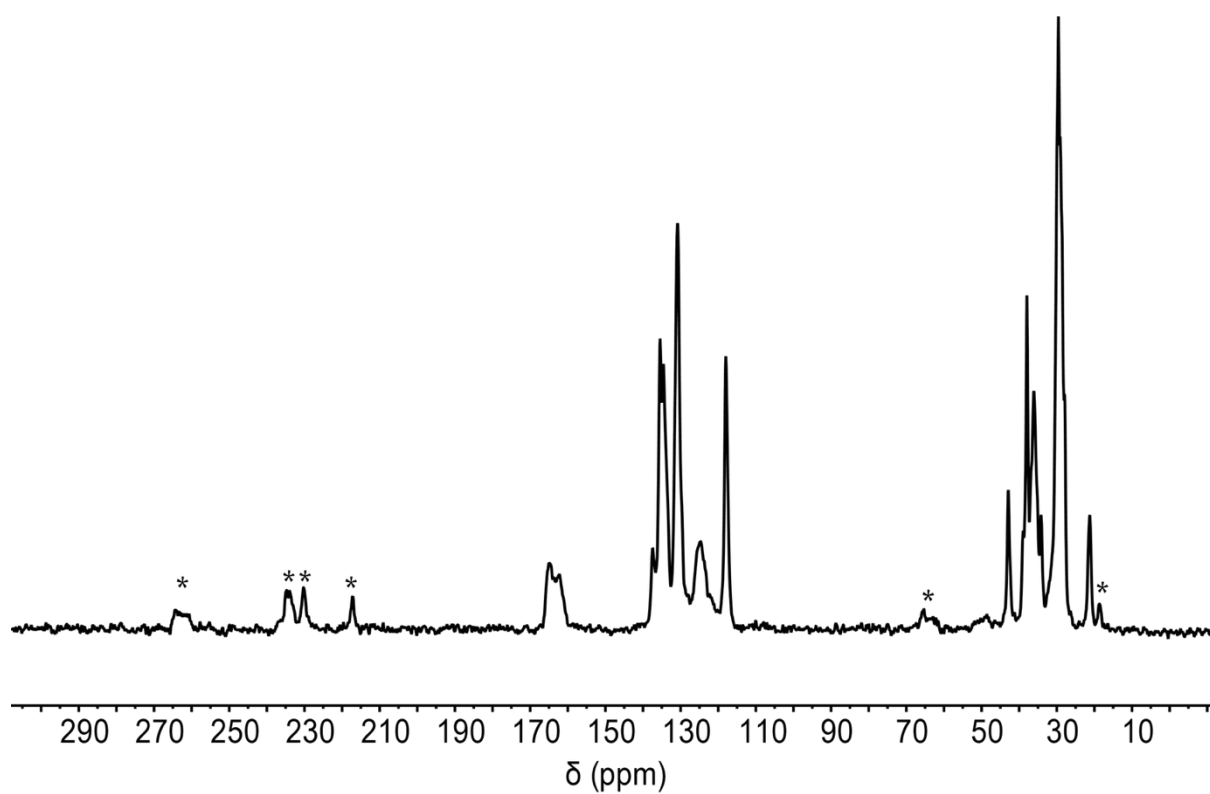


Figure S11: Solid-state $^{13}\text{C}\{^1\text{H}\}$ CP MAS NMR (100.66 MHz, 10 kHz spin rate, 298 K) spectrum of **2[BArF₄]**. Spinning side bands are marked with asterisks.

S2d. $[\text{RhH}(\text{dtbpb}')(\kappa^1\text{-CD}_2\text{Cl}_2)][\text{BAR}^{\text{F}_4}]$, $3[\text{BAR}^{\text{F}_4}]$

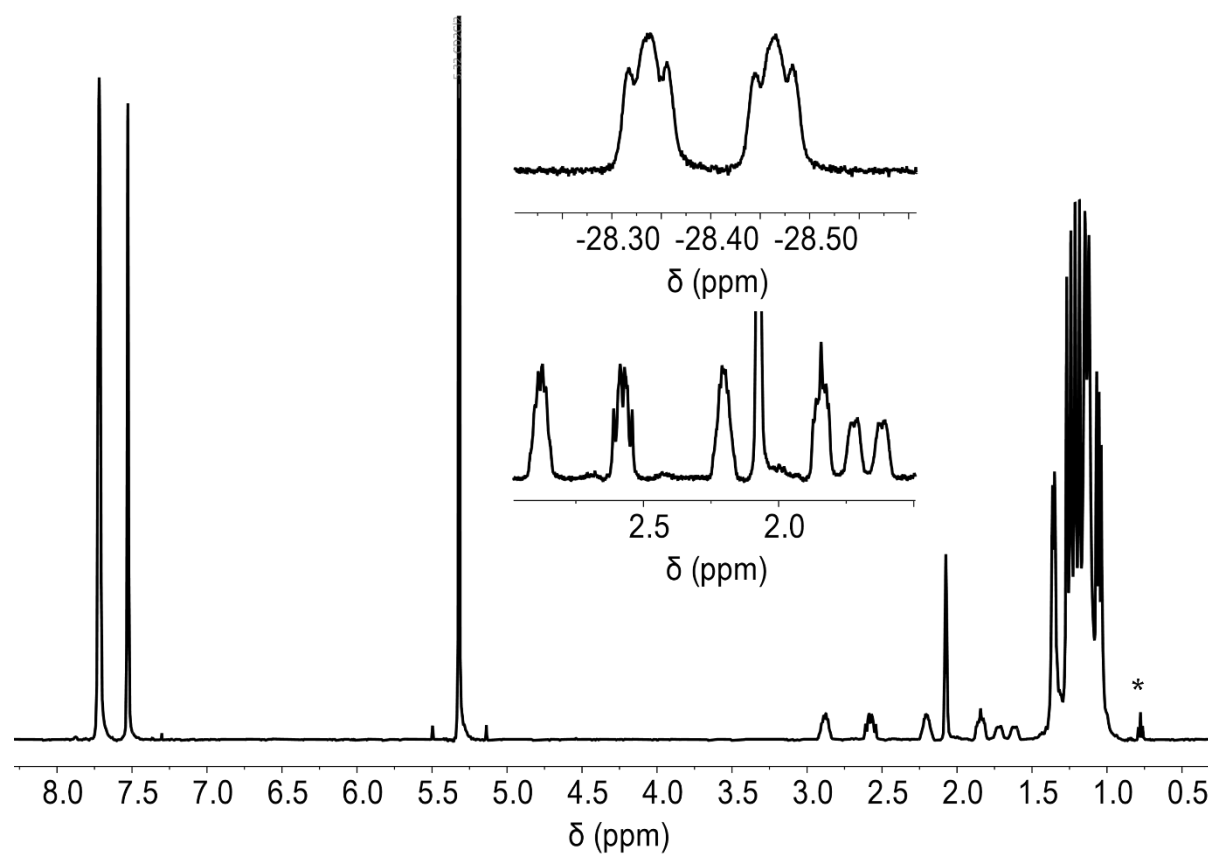


Figure S12: Solution ^1H NMR (500 MHz, CD_2Cl_2 , 193 K) spectrum of $3[\text{BAR}^{\text{F}_4}]$, synthesised immediately before running the NMR analysis without further purification, and thus egressed NBA resonances are observed (δ 2.08, 1.36, 1.05). Insets depict the hydride resonance at $\delta_{\text{H}} = -28.43$ (*top*) and phosphine resonances at $\delta_{\text{H}} = 3.0 - 1.5$ (*bottom*). Asterisk denotes minor pentane solvent impurity.

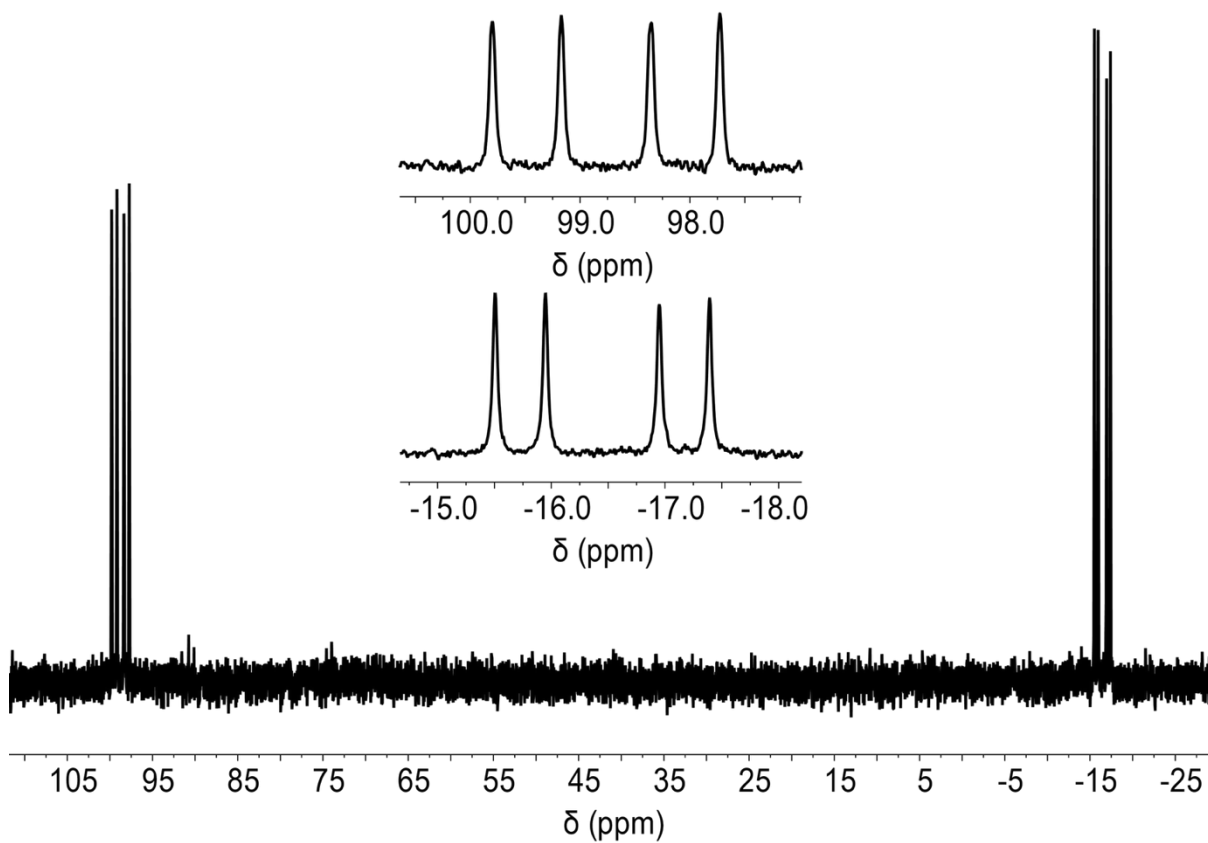


Figure S13: Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 193 K) spectrum of $3[\text{BAr}^{\text{F}}_4]$. Insets depict the doublet of doublet structure of the resonances at δ_{P} 98.9 (*top*) and -16.5 (*bottom*).

S2e. *Endo-exo-d₄*-NBA

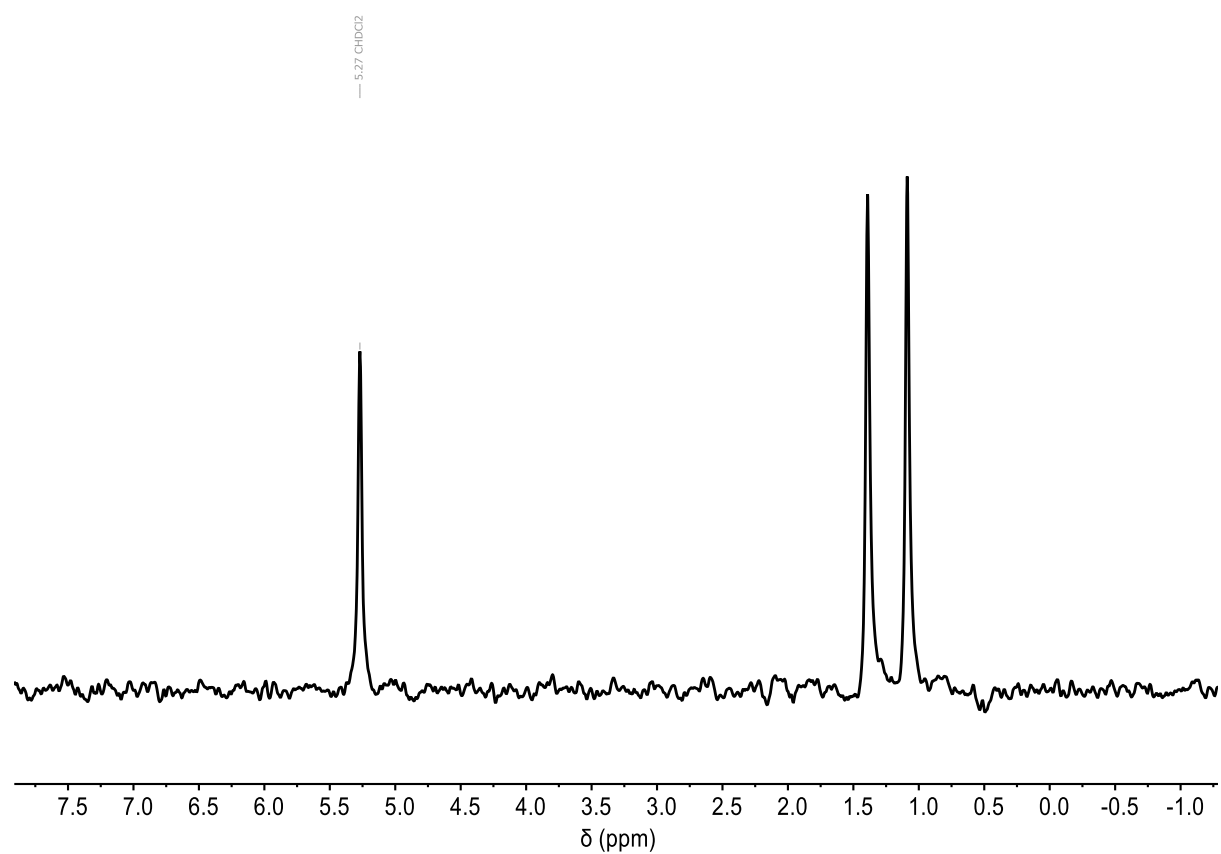


Figure S14: ^2H NMR (76.79 MHz, CH_2Cl_2 , 298 K) spectrum of *endo-exo-d₄*-NBA, formed through solid-state deuteration of **1**[BAr^{F}_4] followed by vacuum transfer of the volatiles.

S2f. [Rh(dtbpb)(NBE)][BAr^F₄], 4[BAr^F₄]

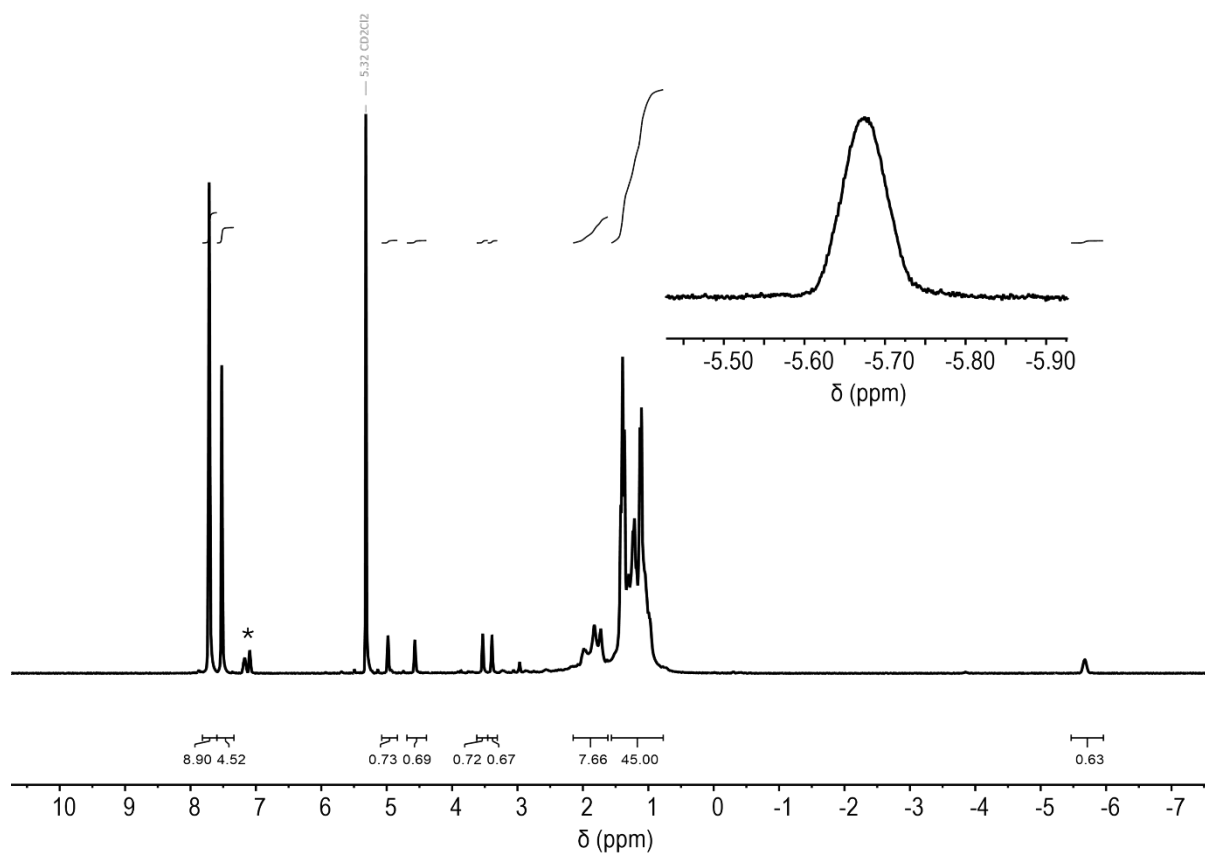


Figure S15: Solution ¹H NMR (500 MHz, CD₂Cl₂, 193 K) spectrum of 4[BAr^F₄]. Minor 1,2-F₂C₆H₄ impurity is noted with an asterisk. Inset shows the σ(C–H) agostic resonance at δ_H -5.68.

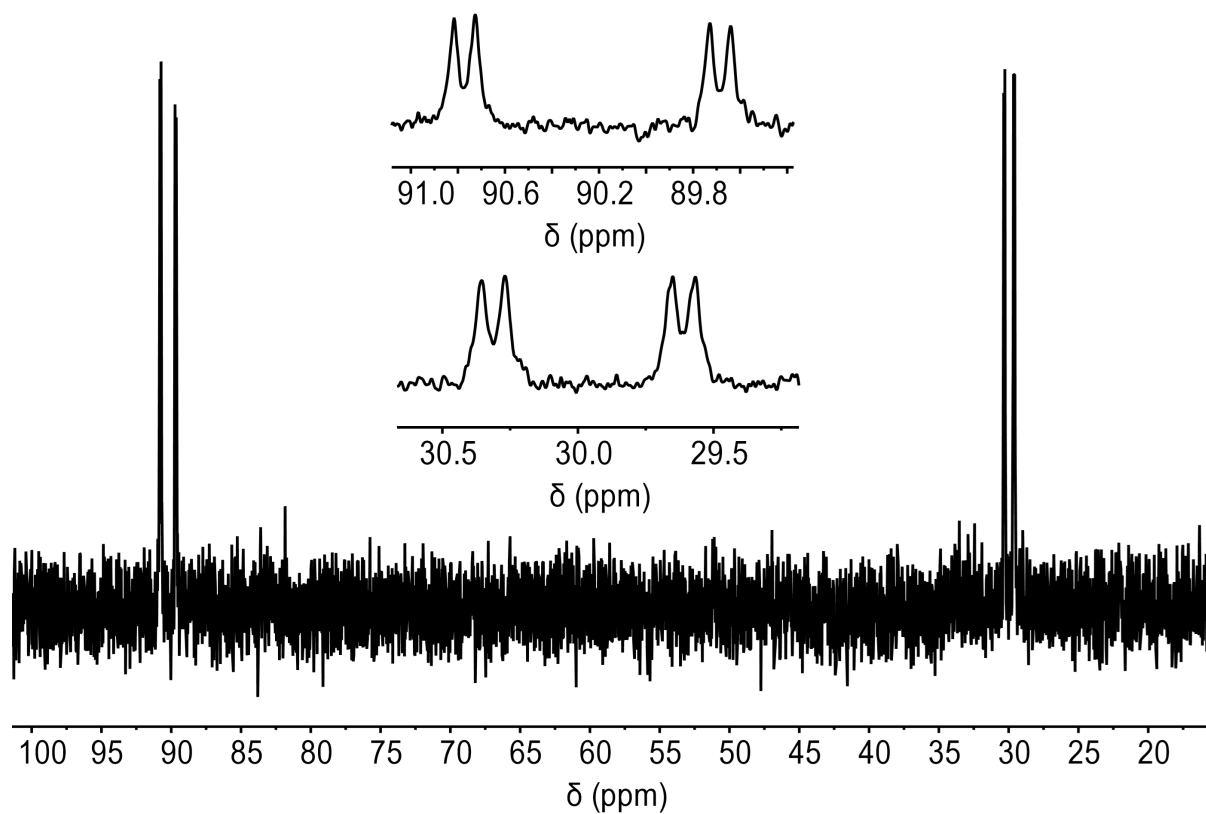


Figure S16: Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 193 K) spectrum of $4[\text{BAr}^{\text{F}}_4]$. Insets depict the doublet of doublets structure of the resonances at $\delta_{\text{P}} 90.3$ (*top*) and 30.0 (*bottom*).

S2g. $[\text{RhH}(\text{dtbpb})(\eta^3\text{-C}_3\text{H}_5)][\text{BAr}^{\text{F}}_4]$, $5[\text{BAr}^{\text{F}}_4]$

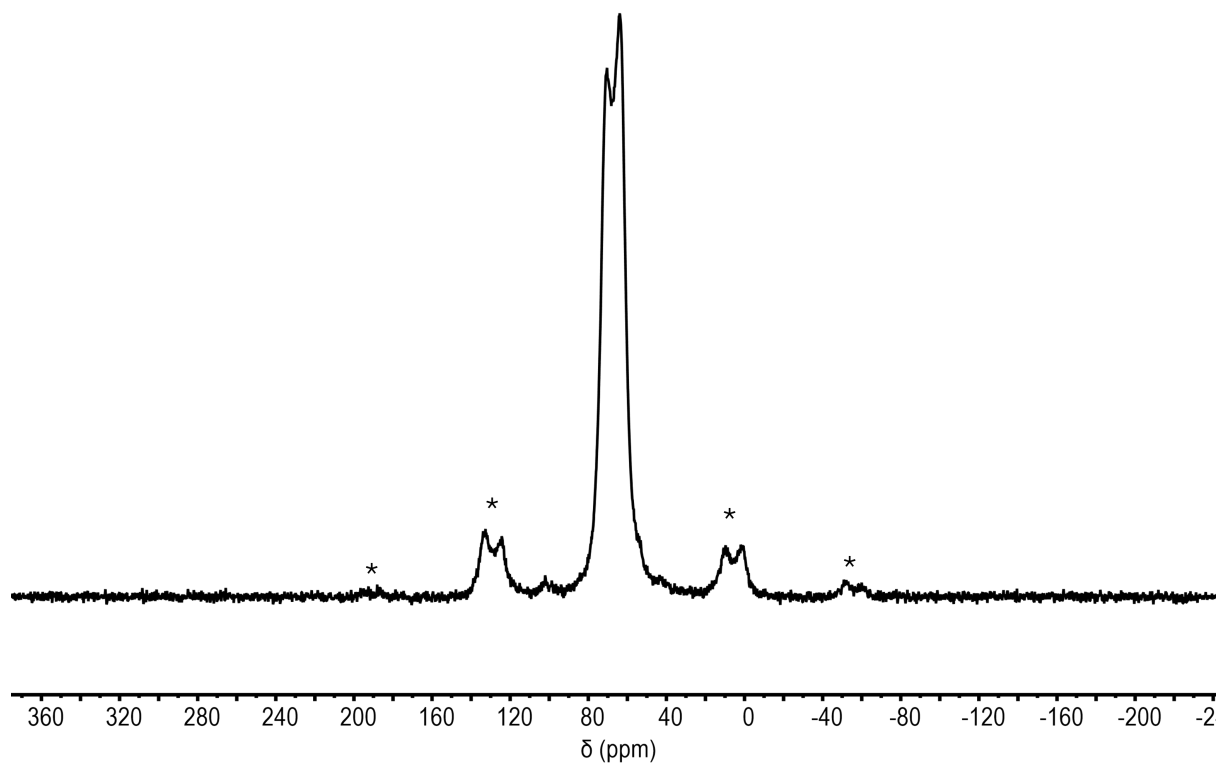


Figure S17: Solid-state $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.00 MHz, 10 kHz spin rate, 293 K) spectrum of $5[\text{BAr}^{\text{F}}_4]$. Spinning side bands are noted with asterisks.

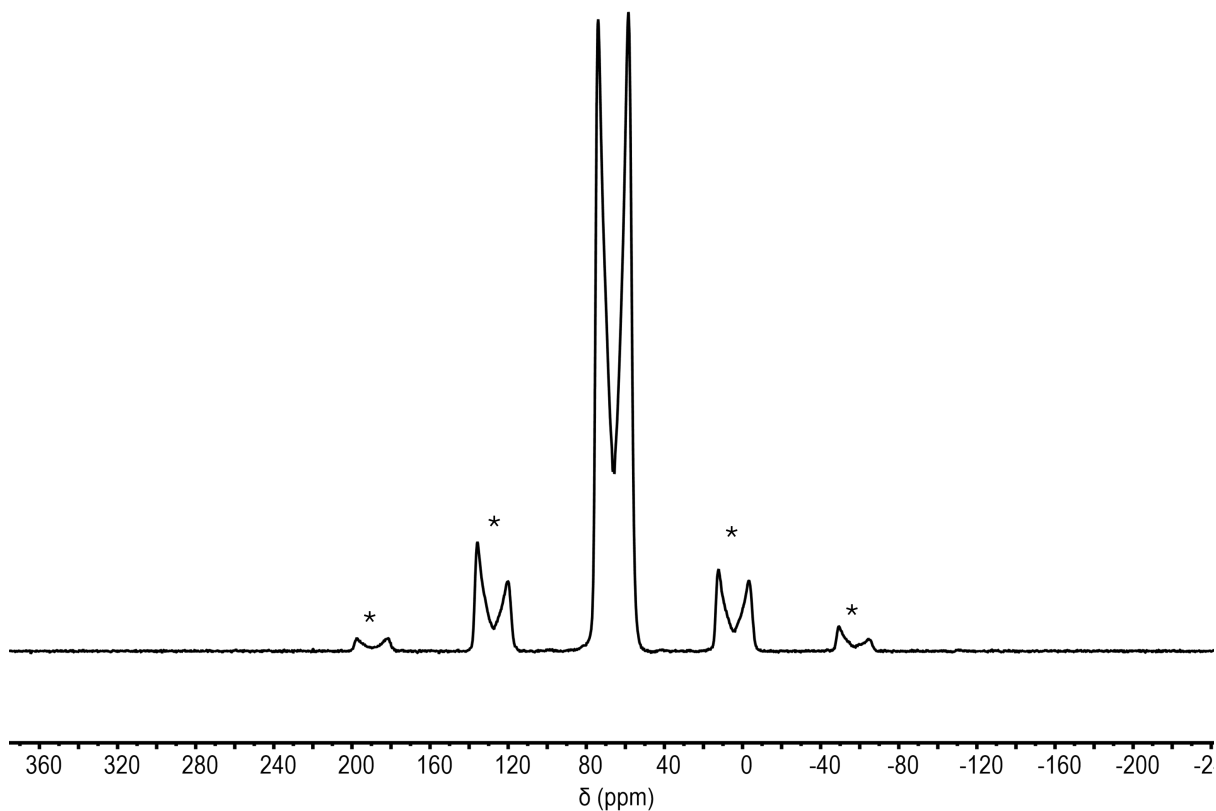


Figure S18: Solid-state $^{31}\text{P}\{^1\text{H}\}$ CP MAS NMR (162.00 MHz, 10 kHz spin rate, 193 K) spectrum of **5[BAr $^{\text{F}}_4$]**. Spinning side bands are noted with asterisks.

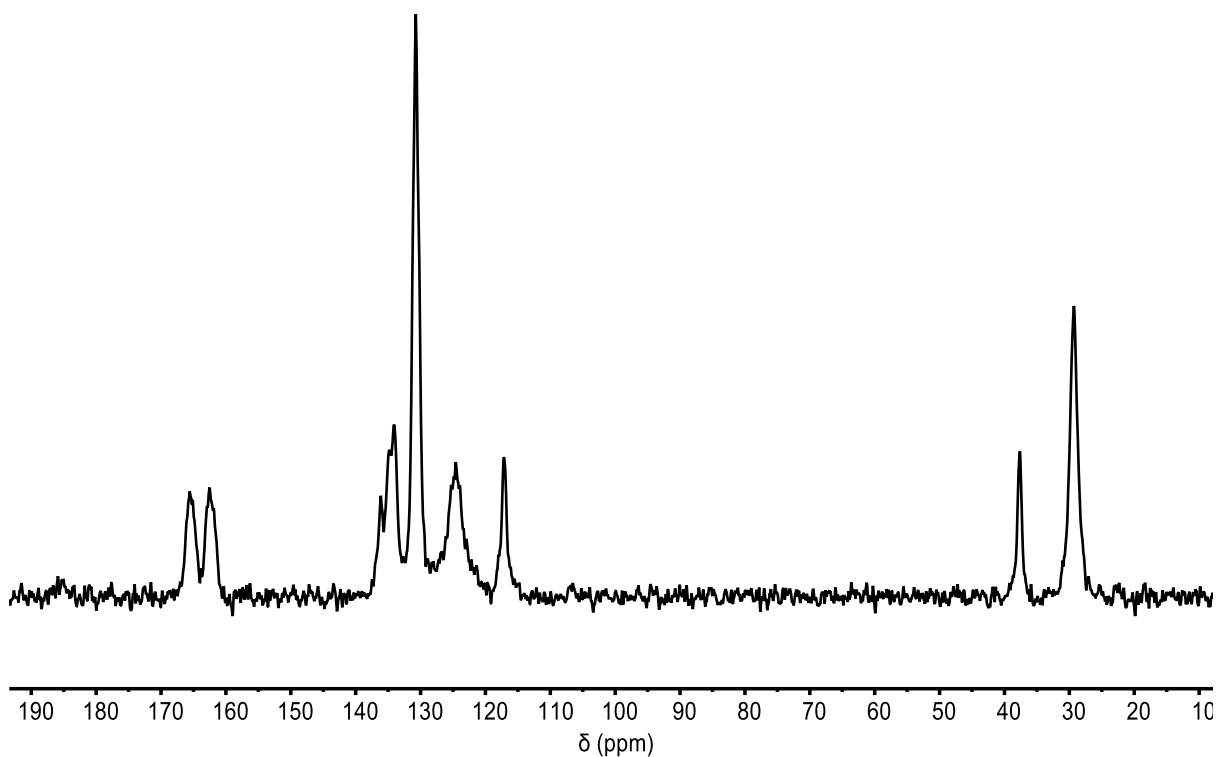


Figure S19: Solid-state $^{13}\text{C}\{^1\text{H}\}$ CP TOSS MAS NMR (100.63 MHz, 10 kHz spin rate, 295 K) spectrum of **5[BAr $^{\text{F}}_4$]**.

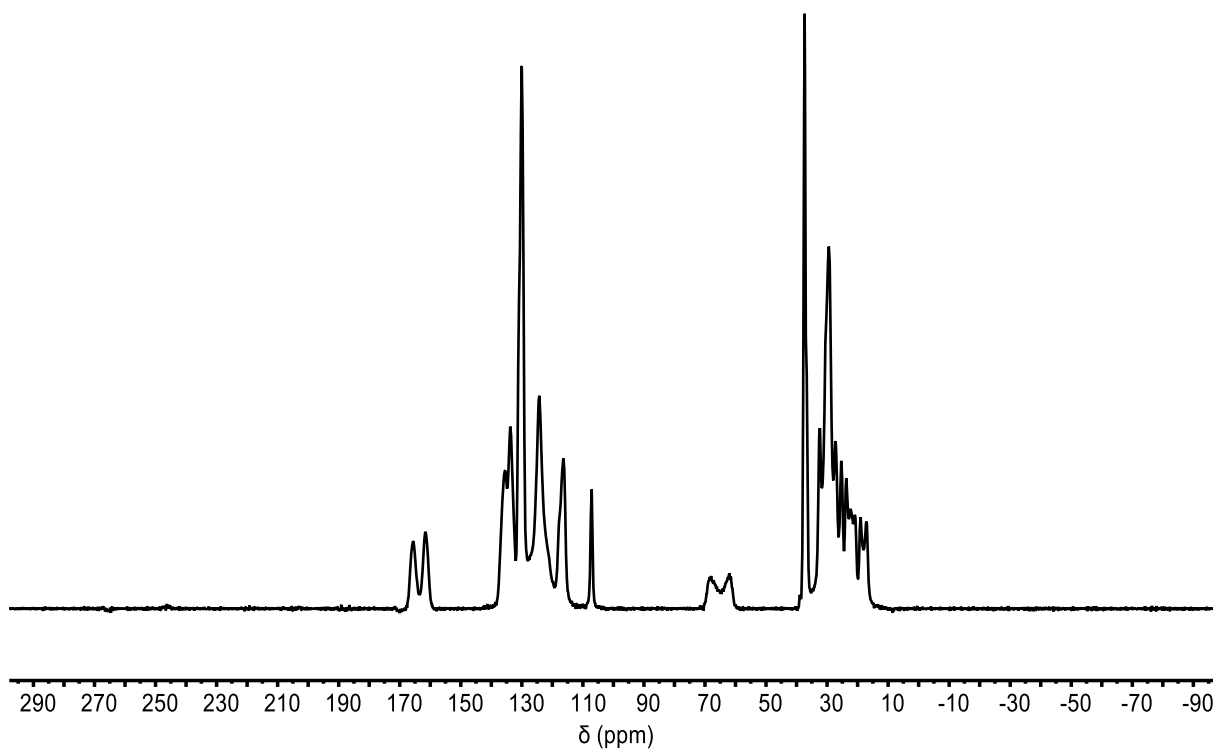


Figure S20: Solid-state $^{13}\text{C}\{^1\text{H}\}$ CP TOSS MAS NMR (100.63 MHz, 10 kHz spin rate, 193 K) spectrum of **5[BAr^F₄]**.

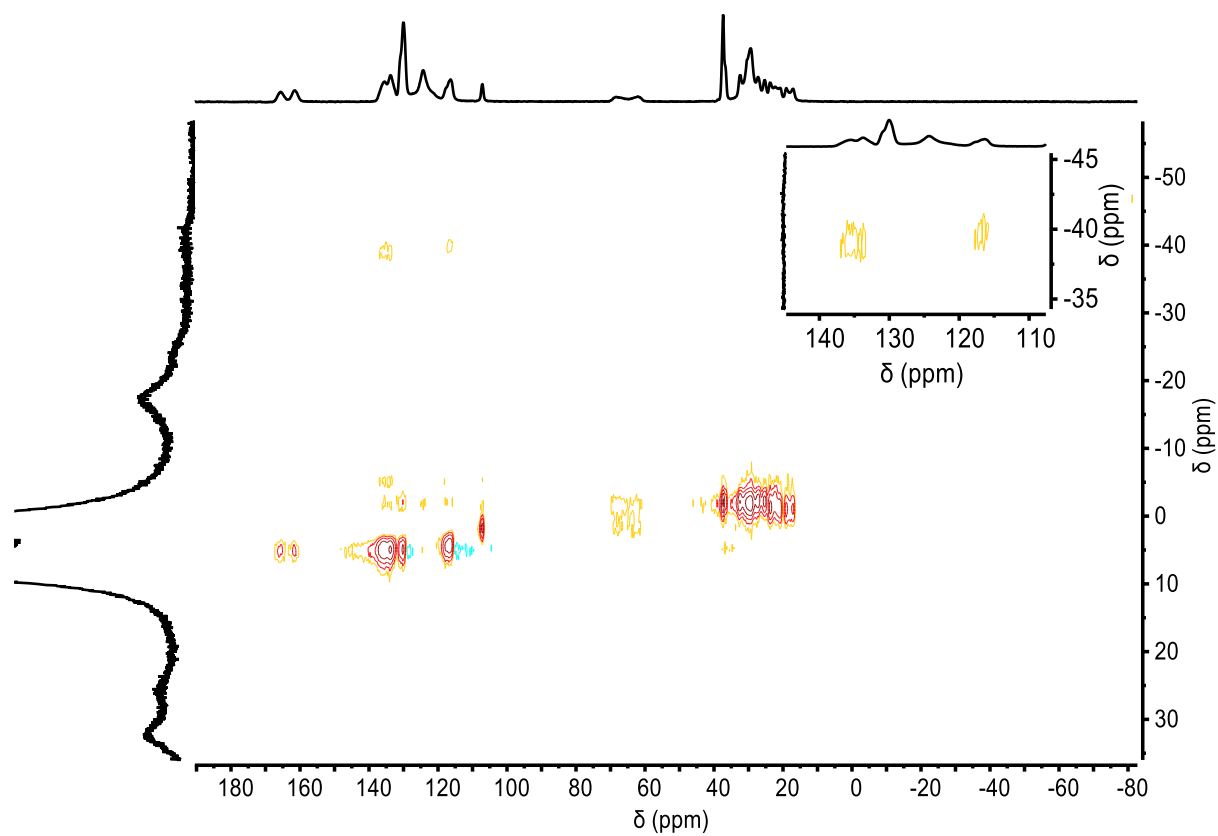


Figure S21: Solid-state ^{13}C - ^1H HETCOR (100.63 MHz/400.17 MHz, 10 kHz spin rate, 193 K) spectrum of $5[\text{BArF}_4]$. Inset depicts weak through-space interaction with the $[\text{BArF}_4]^-$ anions detecting the hydride resonance in the solid-state

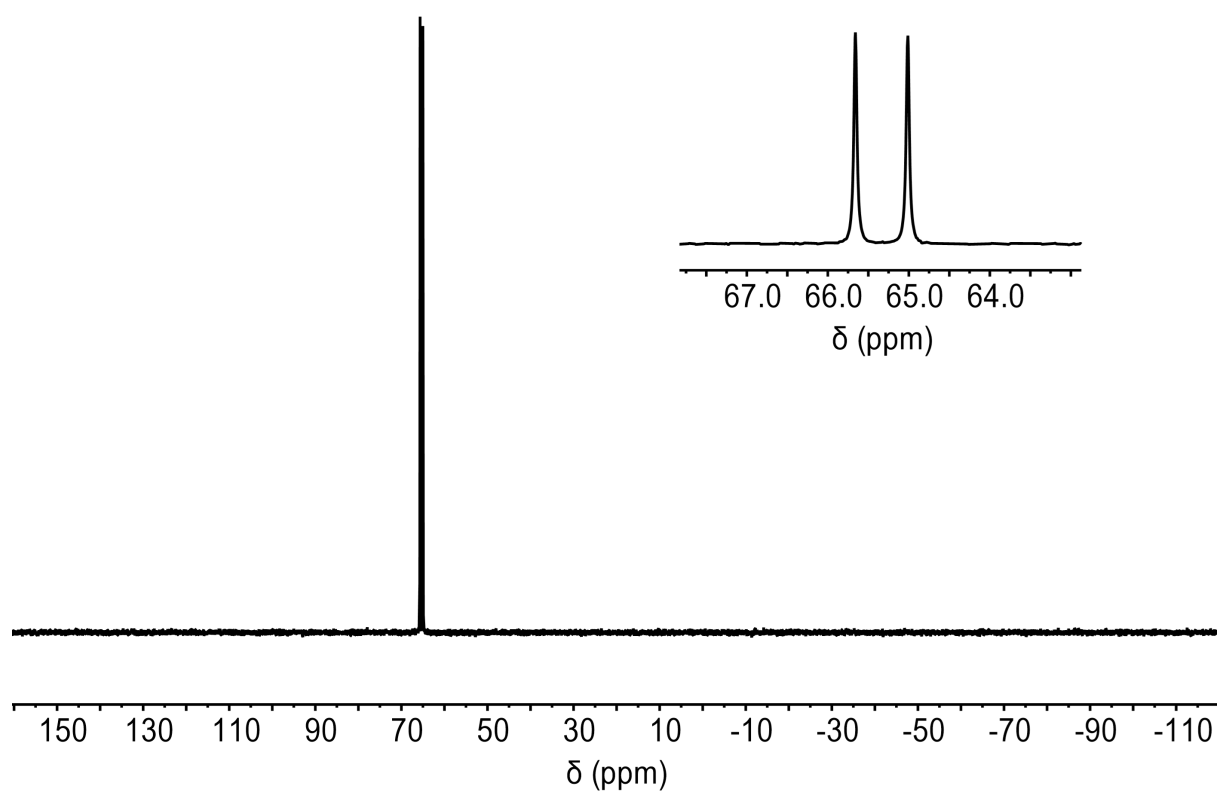


Figure S22: Solution $^{31}\text{P}\{^1\text{H}\}$ NMR (202.49 MHz, CD_2Cl_2 , 193 K) spectrum of **5[BAr $^{\text{F}}_4$]**. Inset depicts doublet structure of resonance.

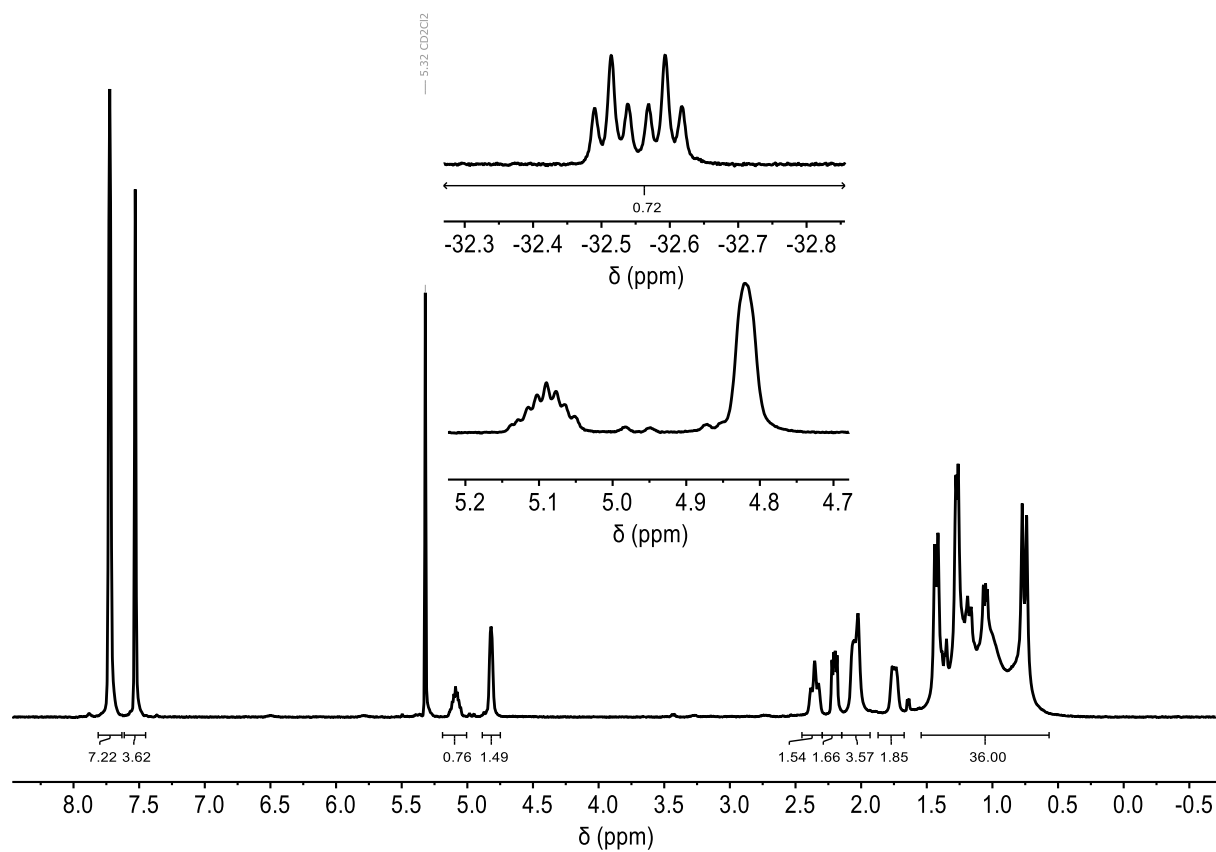


Figure S23: Solution ^1H NMR (500 MHz, CD_2Cl_2 , 193 K) spectrum of $5[\text{BAr}^{\text{F}}_4]$. Insets depict the hydride resonance ($\delta_{\text{H}} -32.55$, *top*) and two allyl resonances ($\delta_{\text{H}} 5.09$ and 4.82 , *bottom*).

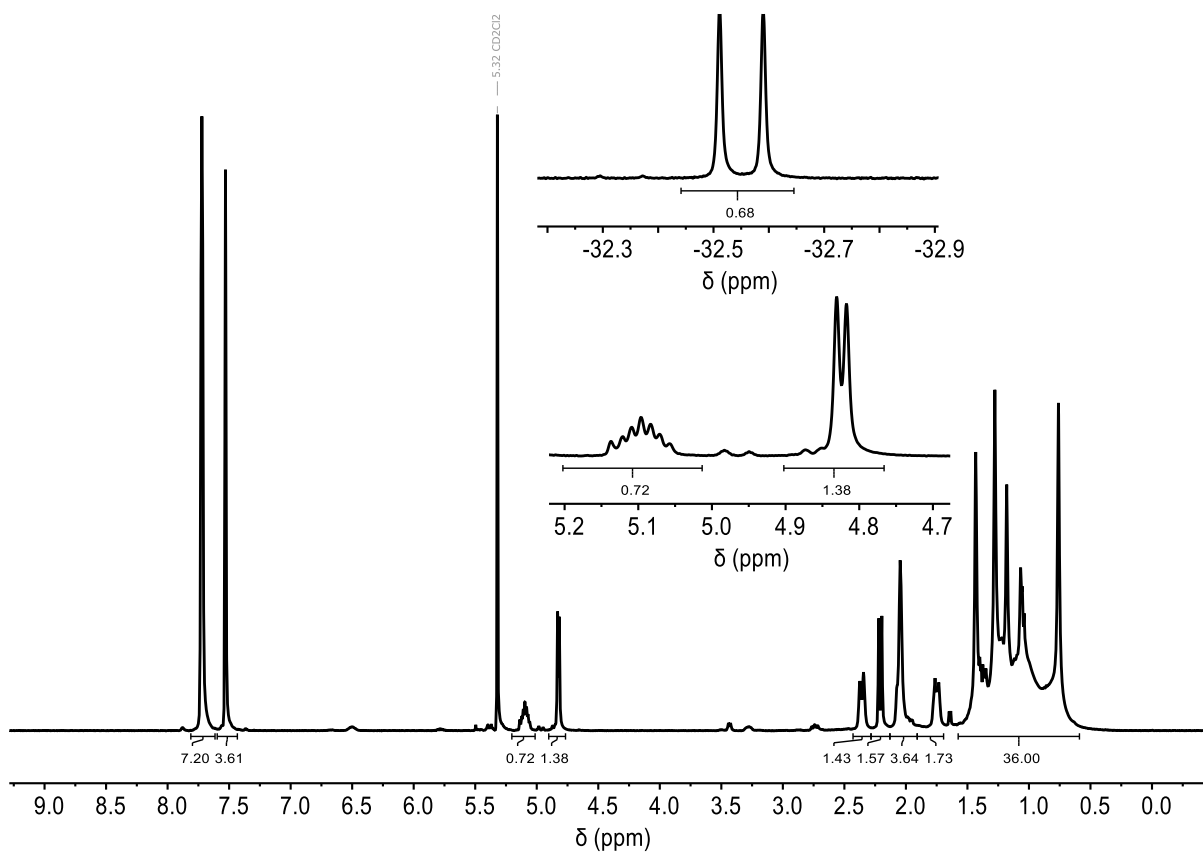


Figure S24: Solution ${}^1\text{H}\{{}^{31}\text{P}\}$ NMR (500 MHz, CD_2Cl_2 , 193 K) spectrum of $5[\text{BArF}_4]$. Insets depict the hydride resonance ($\delta_{\text{H}} -32.55$, *top*) and two allyl resonances ($\delta_{\text{H}} 5.09$ and 4.82 , *bottom*).

S3. Single Crystal X-Ray Diffraction

Single-crystal X-ray diffraction data were collected on a Rigaku SuperNova diffractometer with Cu-K α ($\lambda = 1.54184 \text{ \AA}$) radiation equipped with a nitrogen gas Oxford Cryosystems Cryostream unit⁴ at the University of York. Diffraction images from raw frame data were reduced using the CrysAlisPro suite of programmes. The structures were solved using SHELXT⁵ and refined by full convergence on F^2 against all independent reflections by full-matrix least-squares using SHELXL (version 2018/3)⁶ through the Olex2 GUI.⁷ All non-hydrogen atoms were refined anisotropically and hydrogen atoms were geometrically placed and allowed to ride on their parent atoms. Unlocated hydride atoms in **2**[BAr^F₄] and **5**[BAr^F₄] were added implicitly into the sum atom moieties and crystal densities adjusted appropriately. Bond lengths and angles of the NBA fragment in **2**[BAr^F₄] were lightly restrained (DFIX 1.55 0.01; DANG 2.6 0.02) to produce sensible alkyl C–C bonding geometries. The displacement parameters of the NBA ligand were also lightly restrained (SIMU 0.02 0.04; RIGU 0.004 0.004). Disorder of the –CF₃ groups of the [BAr^F₄][–] anions and ^tBu methyl groups of the phosphine ligand in all structures, as well as the CD₂Cl₂ ligand in **3**[BAr^F₄], were treated by introducing a split-site model and restraining the geometries and displacement parameters. Disordered solvent (heptane) in **3**[BAr^F₄] was treated with the Olex2 solvent mask implement.^{8, 9} Distances and angles were calculated using the full covariance matrix. Crystallographic data are available free of charge *via* the Cambridge Crystallographic Data Centre, under deposition numbers 2472635 - 2472641

S3a. F...F Distances

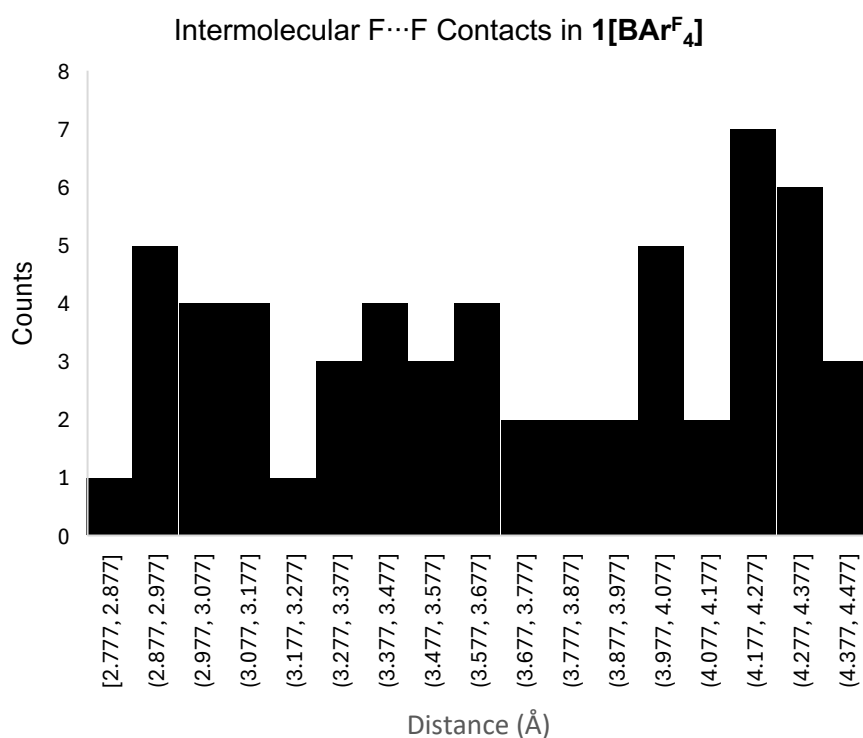


Figure S25: Intermolecular F...F distances in **1**[BAr^F₄].

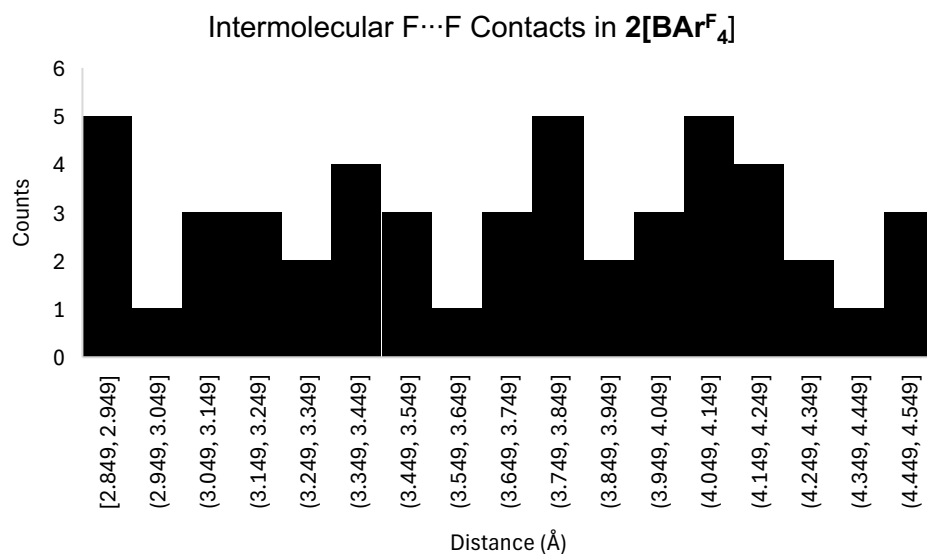


Figure S26: Intermolecular F...F distances in 2[BAr^F₄], showing small overall increases compared to 1[BAr^F₄] (Figure S25).

S3b. Variable Temperature Single Crystal X-Ray Diffraction of 2[BAr^F₄]

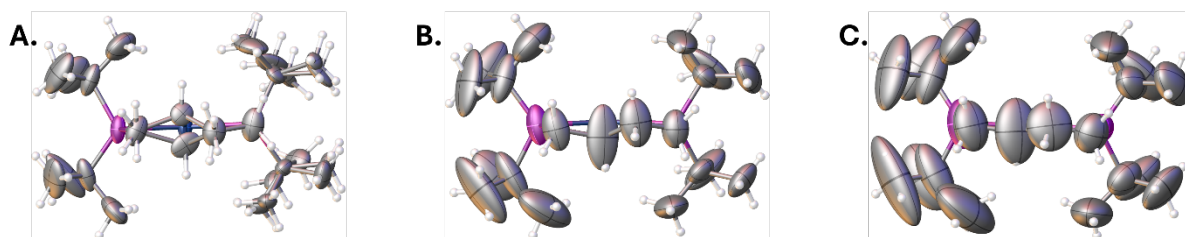


Figure S27: Influence on increasing temperature on the disorder of the phosphine backbone in 2[BAr^F₄]. NBA fragment omitted in each case for clarity. Thermal ellipsoids set at 50% probability. **A.** Solid-state structure at 110 K. **B.** Solid-state structure at 215 K. **C.** Solid-state structure at 298 K.

S3c. Crystallographic Data Tables

Table S1: Crystallographic data table for complexes **1[BAr^F₄]**, and **2[BAr^F₄]** at 110 K and 215 K.

	1[BAr^F₄]	2[BAr^F₄] (110 K)	2[BAr^F₄] (215 K)
CCDC Number	2472635	2472636	2472637
Formula	C ₅₉ H ₆₄ BF ₂₄ P ₂ Rh	C ₅₉ H ₆₇ BF ₂₄ P ₂ Rh	C ₅₉ H ₆₈ BF ₂₄ P ₂ Rh
M _w / g mol ⁻¹	1404.76	1408.79	1408.79
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
T / K	110.15	110.15	215.15
a / Å	21.39780(10)	22.0393(3)	22.2413(5)
b / Å	12.92970(10)	12.96270(10)	13.0869(2)
c / Å	23.21930(10)	23.7552(3)	24.0201(5)
α / °	90	90	90
β / °	112.0440(10)	112.901(2)	112.889(2)
γ / °	90	90	90
V / Å ³	5954.39(7)	6251.66(15)	6441.0(2)
Z	4	4	4
ρ _{calc} / g cm ⁻³	1.567	1.497	1.453
μ / mm ⁻¹	3.856	3.673	3.565
2θ range / °	7.104 – 153.998	6.998 – 142.916	7.848 – 136.492
Reflns collected	69849	45037	24466
R _{int}	0.0380	0.0373	0.0438
Completeness / %	100	100	99.9
Data/restr/param	12409 / 0 / 796	12063 / 241 / 990	11775 / 132 / 908
R ₁ [I > 2σ(I)]	0.0315	0.0560	0.0759
wR ₂ [all data]	0.0788	0.1569	0.2437
GooF	1.052	1.053	1.021
Largest pk/hole / eÅ ⁻³	0.87 / -0.62	2.19 / -1.71	2.23 / -0.59

Table S2: Crystallographic data table for complexes **2[BAr^F₄]** at 298 K, **3[BAr^F₄]** and **4[BAr^F₄]**.

	2[BAr^F₄] (298 K)	3[BAr^F₄]	4[BAr^F₄]
CCDC Number	2472638	2472639	2472640
Formula	C ₅₉ H ₆₈ BF ₂₄ P ₂ Rh	C _{56.75} H _{66.25} BCl ₂ F ₂₄ P ₂ Rh	C ₅₉ H ₆₆ BF ₂₄ P ₂ Rh
M _w / g mol ⁻¹	1408.79	1450.90	1406.77
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
T / K	298.15	110.15	110.15
a / Å	22.4113(8)	21.70260(10)	21.8071(2)
b / Å	13.1931(5)	27.81260(10)	12.76750(10)
c / Å	24.2050(6)	21.48550(10)	23.4341(3)
α / °	90	90	90
β / °	112.732(3)	103.0890(11)	112.080(10)
γ / °	90	90	90
V / Å ³	6600.9(4)	12631.83(11)	6049.13(11)
Z	4	8	4
ρ _{calc} / g cm ⁻³	1.418	1.526	1.545
μ / mm ⁻¹	3.478	4.416	3.796
2θ range / °	7.784 – 155.524	7.31 – 136.502	8.032 – 149.006
Reflns collected	38735	150980	40049
R _{int}	0.0863	0.0458	0.0519
Completeness / %	99.1	100	99.8
Data/restr/param	11961 / 220 / 958	23135 / 336 / 1664	12189 / 187 / 968
R ₁ [I > 2σ(I)]	0.0855	0.0570	0.0670
wR ₂ [all data]	0.3098	0.1598	0.1736
GooF	1.042	1.020	1.025
Largest pk/hole / eÅ ⁻³	1.82 / -0.71	1.93 / -1.01	1.82 / -1.54

Table S3: Crystallographic data table for complex **5[BAR^F₄]**.

5[BAR^F₄]	
CCDC Number	2472641
Formula	C ₅₅ H ₆₁ BF ₂₄ P ₂ Rh
M _w / g mol ⁻¹	1354.74
Crystal System	Monoclinic
Space Group	C 2/c
T / K	109.9(2)
a / Å	22.2182(11)
b / Å	12.5068(6)
c / Å	23.2112(10)
α / °	90
β / °	113.970(6)
γ / °	90
V / Å ³	5893.6(6)
Z	4
ρ _{calc} / g cm ⁻³	1.527
μ / mm ⁻¹	3.872
2θ range / °	8.3 – 142.74
Reflns collected	12631
R _{int}	0.0454
Completeness / %	99.7
Data/restr/param	5605 / 263 / 502
R ₁ [I > 2σ(I)]	0.0938
wR ₂ [all data]	0.2981
Goof	1.099
Largest pk/hole / eÅ ⁻³	1.69 / -0.80

S4. Computational Details

S4.1 Solid-State Periodic-DFT Calculations

All static Kohn-Sham DFT calculations were performed on periodic models of the studied rhodium complexes, employing the Gaussian Plane Wave (GPW) formalism as implemented in the QUICKSTEP¹⁰ module within the CP2K program suite (Version 2023.1).¹¹ Molecularly optimized basis sets of double- ζ quality plus polarization in their short-range variant (DZVP-MOLOPT-SR-GTH)¹² were used for all atomic species. The interaction between the core electrons and the valence shell (Rh: 17, B: 3, C: 4, P: 5, F: 7, H: 1 electrons) was described by Goedecker-Teter-Hutter (GTH) pseudo potentials.¹³⁻¹⁵ The generalized gradient approximation (GGA) to the exchange-correlation functional according to Perdew-Burke-Ernzerhof (PBE)¹⁶ was used in combination with Grimme's D3-correction for dispersion interactions.¹⁷ The auxiliary plane wave basis set was truncated at a cutoff of 500 Ry. The maximum force convergence criterion was set to 10^{-4} Eh·Bohr⁻¹, whilst default values were used for the remaining criteria. The convergence criterion for the self-consistent field (SCF) accuracy was set to 10^{-7} Eh and 10^{-8} Eh for geometry optimizations.

The Brillouin zone was sampled using the Γ -point. Initial coordinates were obtained from the experimental crystallographic data, with the hydrogen positions normalised where possible with Mercury.¹⁸ Periodic boundary conditions (PBC) were applied throughout in combination with fixed unit cell parameters obtained from experiment. The geometry of the η^1 -bridgehead complex **2**[BAR^F₄] was first partially optimised by relaxing only the H, F atoms (referred to in the following as the 'partially optimized structure'), then fully optimised without imposing any constraints.

S4.2 Molecular DFT Calculations

Inter-ion interactions were analysed between central rhodium cation and six nearest neighbour surrounding [BAR^F₄]⁻ anions, where ion-pair geometries were extracted from the periodic-DFT optimised structures. The ion-pair (IP) interaction energies were computed using Gaussian 16 (Revision A.03) program package¹⁹ and employed the PBE functional with and without Grimme's D3 dispersion correction. Stuttgart-Dresden (SDD)²⁰ relativistic effective core potentials (ECP) in combination with the associated basis sets were utilized to describe Rh and P, with polarization functions added for P ($\zeta = 0.387$).²¹ The 6-31G(d,p) basis sets^{22, 23} were used for remaining atoms. Extended wavefunction (.wfx) files suitable for bonding analysis were generated using single point calculations for the ion-pairs and cations extracted from periodic DFT structures.

Independent gradient model calculations for ion-pair (IP) interactions and extracted cations were performed with Multiwfn²⁴ with the Hirshfeld partitioning scheme (IGMH method).²⁵ Surfaces were visualized with VMD.²⁶

Further bonding characterization on extracted cations was performed by QTAIM (Quantum Theory of Atoms in Molecules),²⁷ as implemented in the AIMALL package²⁸ and natural bond orbital calculations with the NBO 7.0 program.²⁹ The donor-acceptor orbital plots were built with Chemcraft.³⁰

For mechanistic studies all stationary points were characterized via analytical frequency calculations as either minima (0 negative frequencies) or transition states (1 negative frequency). Transition states were further characterized via first IRC calculations and subsequent optimizations that showed then to link to the adjacent minima.

S5. Electronic Structure Analyses

S5.1 Experimental η^1 - σ -Bridgehead Cation

IGMH plots, QTAIM and NBO analyses of the experimental η^1 - σ -bridgehead 2^+ cation extracted from the fully optimised periodic-DFT structure of **[2][BAr^F₄]** are reported in this section.

S4.3.1 IGMH Plots

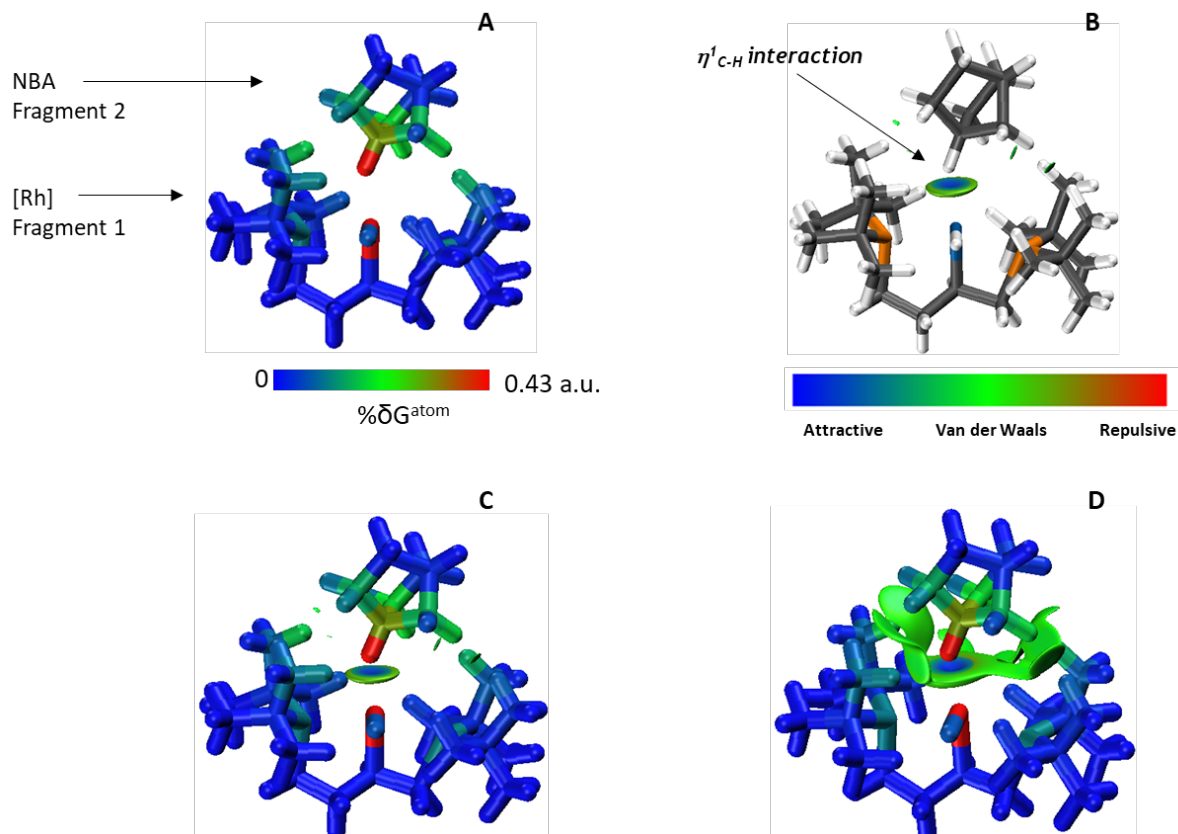


Figure S28: IGMH plots for η^1 - σ -bridgehead 2^+ cation. NBA and [Rh] are defined as separate fragments; relative atomic contributions coloured by $\% \delta G^{\text{atom}}$; $\text{sign}(\lambda_2)p$ -coloured isosurfaces are plotted with $\delta G^{\text{inter}} = 0.01$ a.u for **A** to **C**, and 0.003 a.u for **D**. **A:** The most important atoms interacting between both fragments are highlighted; **B:** Round blue disc located between bridgehead C-H and Rh metal centre consistent with an η^1 -C-H...Rh interaction; **C:** Both the interacting atoms and isosurfaces between fragments **1** and **2** are depicted; **D:** Isosurface value is 0.003 a.u to capture additional weak non-covalent interactions between NBA and the phosphine substituents.

S5.2 QTAIM Analysis

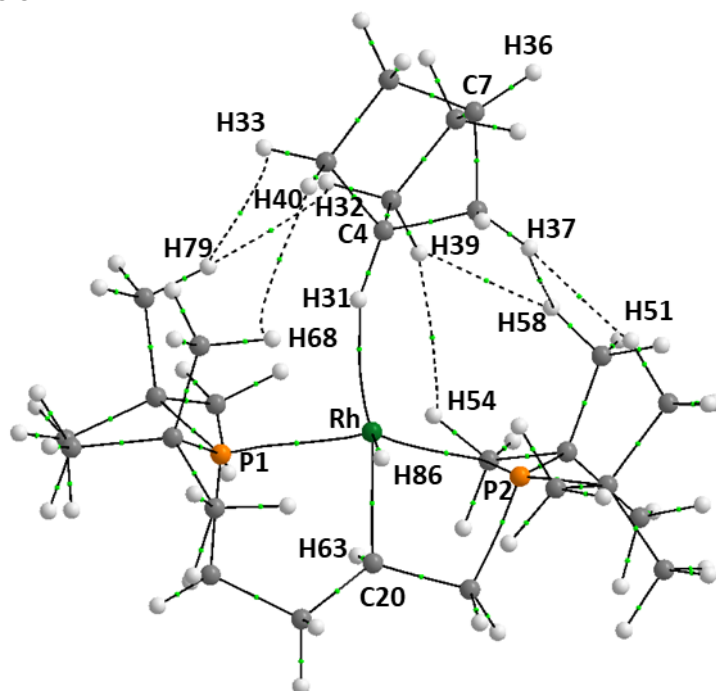


Figure S29: QTAIM molecular graph of η^1 - σ -bridgehead 2^+ cation. Note that the atom labelling scheme used here differs from that in the main paper.

Table S4: Selected QTAIM BCP parameters (a.u.) and bond distances; values in parenthesis refer to the cation extracted from the partially optimised SS structure.

<i>BCP</i>	<i>Distance(Å)</i>	ρ (e bohr ³)	$\nabla^2\rho$ (e bohr ⁵)	<i>H(r)</i>	<i>DI</i>
Rh...H31	2.080 (1.989)	0.0343 (0.0416)	+0.1032 (0.1241)	-0.0050 (-0.0073)	0.1868 (0.2149)
H40...H79	2.377 (2.104)	0.0056 (0.0093)	+0.0200 (0.0321)	+0.0012 (0.0016)	0.0248 (0.0132)
H39...H54	2.682 (2.564)	0.0031 (0.0039)	+0.0093 (0.0117)	+0.0006 (+0.0008)	0.0119 (0.0092)
H33...H79	2.312 (2.623)	0.0063 (-)	+0.0225 (-)	+0.0013 (-)	0.0153 (-)
H39...H58	2.156 (2.182)	0.0079 (0.0077)	+0.0268 (+0.0260)	+0.0014 (+0.0014)	0.0229 (0.0215)
H37...H58	2.413 (2.216)	0.0050 (0.0070)	+0.0169 (+0.0236)	+0.0011 (+0.0013)	0.0127(0.0192)
H37...H51	2.161 (2.098)	0.0076 (0.0093)	+0.0254 (0.0321)	+0.0013 (+0.0016)	0.0237 (0.0243)
H32...H68	2.389 (2.204)	0.0061 (0.0080)	+0.0223 (0.0278)	+0.0014 (+0.0015)	0.0209 (0.0127)
Rh-P2	2.309 (2.297)	0.0996 (0.1015)	+0.1205 (+0.1205)	-0.0392 (-0.0411)	0.8885 (0.8945)
Rh-P3	2.349 (2.328)	0.0907 (0.0947)	+0.1153 (+0.1165)	-0.0333 (-0.0362)	0.8031 (0.8176)
Rh-H86	1.520 (1.516)	0.1640 (0.1660)	+0.0378 (0.0314)	-0.0980 (-0.1006)	0.9888 (0.9892)
Rh-C20	2.063 (2.090)	0.1239 (0.1181)	+0.0837 (0.0822)	-0.0535 (-0.0488)	0.9382 (0.9156)
Rh-C4	3.071 (3.010)	-	-	-	0.0849
C4-H31	1.122 (1.115)	0.2502 (0.2521)	-0.7423 (-0.7523)	-0.2333 (-0.2375)	0.8294 (0.8217)
C7-H36	1.095 (1.093)	0.2761 (0.2767)	-0.9387 (-0.9435)	-0.2782 (-0.2795)	0.9350 (0.9368)

S5.3 NBO Analysis

The donor-acceptor interactions for σ -bonding (C–H to Rh-centred antibonding orbitals) and back-bonding (Rh to C–H antibonding orbitals) are reported in this section

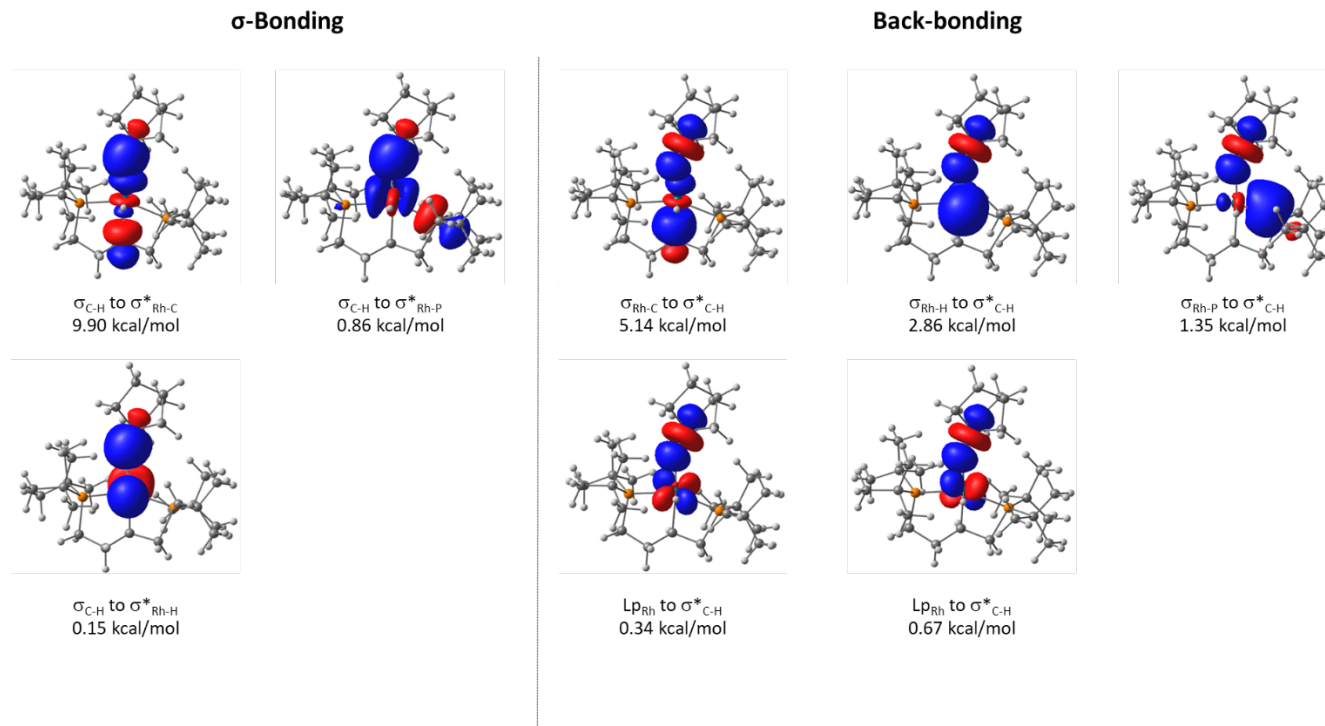
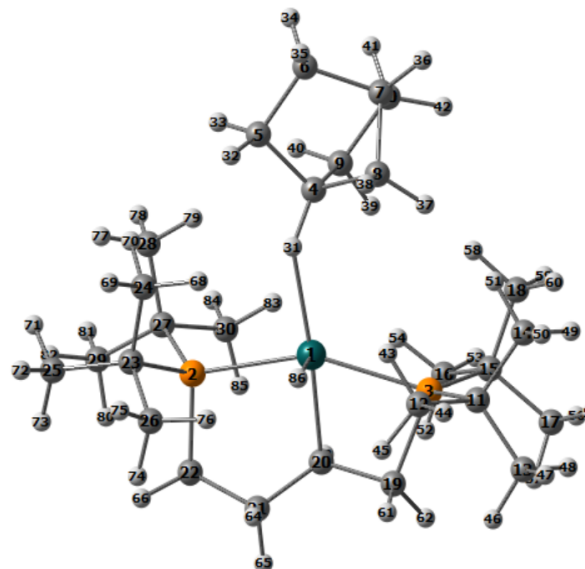


Figure S30: NBO donor-acceptor orbital overlaps with their associated 2nd order perturbation energies (E₂). Orbital plots and associated data are for the fully optimized structure; data for the partially optimized structure are given in Table S5.

Table S5: Selected NBO data for the experimental cation; values in parenthesis belong to cation extracted from partially optimised SS structure; figure shows the structure with atom labelling scheme employed.

<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>
33. LP (2) Rh1	135. BD*(1) C4-H31	0.34 (0.47)
34. LP (3) Rh1	135. BD*(1) C4-H31	0.67 (0.51)
36. BD (1) Rh1-P3	135. BD*(1) C4-H31	1.35 (1.69)
36. BD (1) Rh1-P3	142. BD*(1) C7-C8	0.10 (0.12)
36. BD (1) Rh1-P3	148. BD*(1) C9-H39	0.22 (0.13)
37. BD (1) Rh1-C20	132. BD*(1) C4-C5	0.24 (0.18)
37. BD (1) Rh1-C20	135. BD*(1) C4-H31	5.14 (6.56)
37. BD (1) Rh1-C20	142. BD*(1) C7-C8	0.06 (0.07)
37. BD (1) Rh1- C 20	148. BD*(1) C9-H39	0.24 (0.15)
38. BD (1) Rh1-H86	134. BD*(1) C4-C9	0.08 (0.06)
38. BD (1) Rh1-H86	135. BD*(1) C4-H31	2.86 (2.38)
48. BD (1) C4-H31	123. BD*(1) Rh1-P3	0.86 (0.93)
48. BD (1) C4-H31	124. BD*(1) Rh1-C20	9.90 (12.26)
48. BD (1) C4-H31	125. BD*(1) Rh1-H86	0.15 (0.36)



S5.4 Ion-Pair Interactions

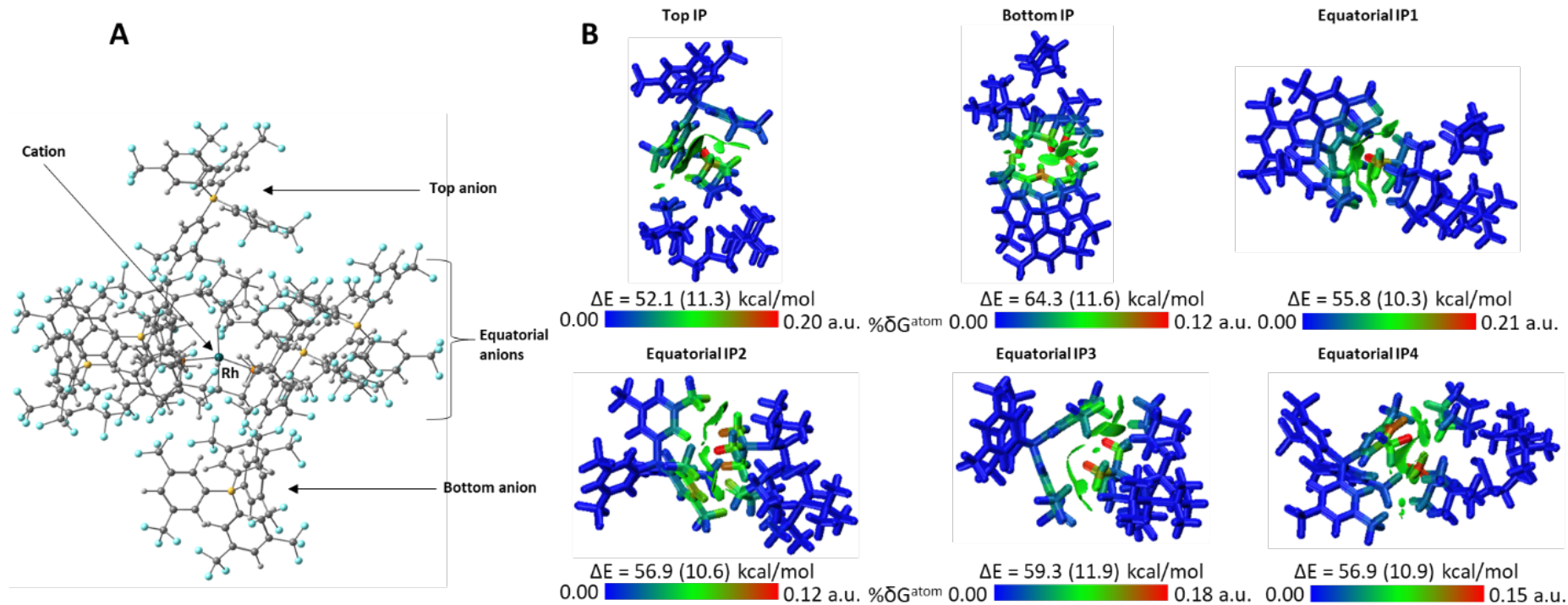


Figure S31: **A:** Packing diagram depicting the *pseudo*-octahedral arrangement of $[\text{BAr}^{\text{F}}_4]^-$ anions around the Rh cation in $2[\text{BAr}^{\text{F}}_4]$; **B:** IGMH plots for ion-pair interactions in η^1 - σ -bridgehead complex based on the partially optimised structure. Cations and anions are defined as separate fragments; $\text{sign}(\lambda_2)\rho$ -coloured isosurfaces are plotted with $\delta G^{\text{inter}} = 0.003$ a.u.; relative atomic contributions coloured by $\% \delta G^{\text{atom}}$. The ion-pair (IP) interaction energies are also indicated (kcal/mol) with the contribution from dispersion in brackets.

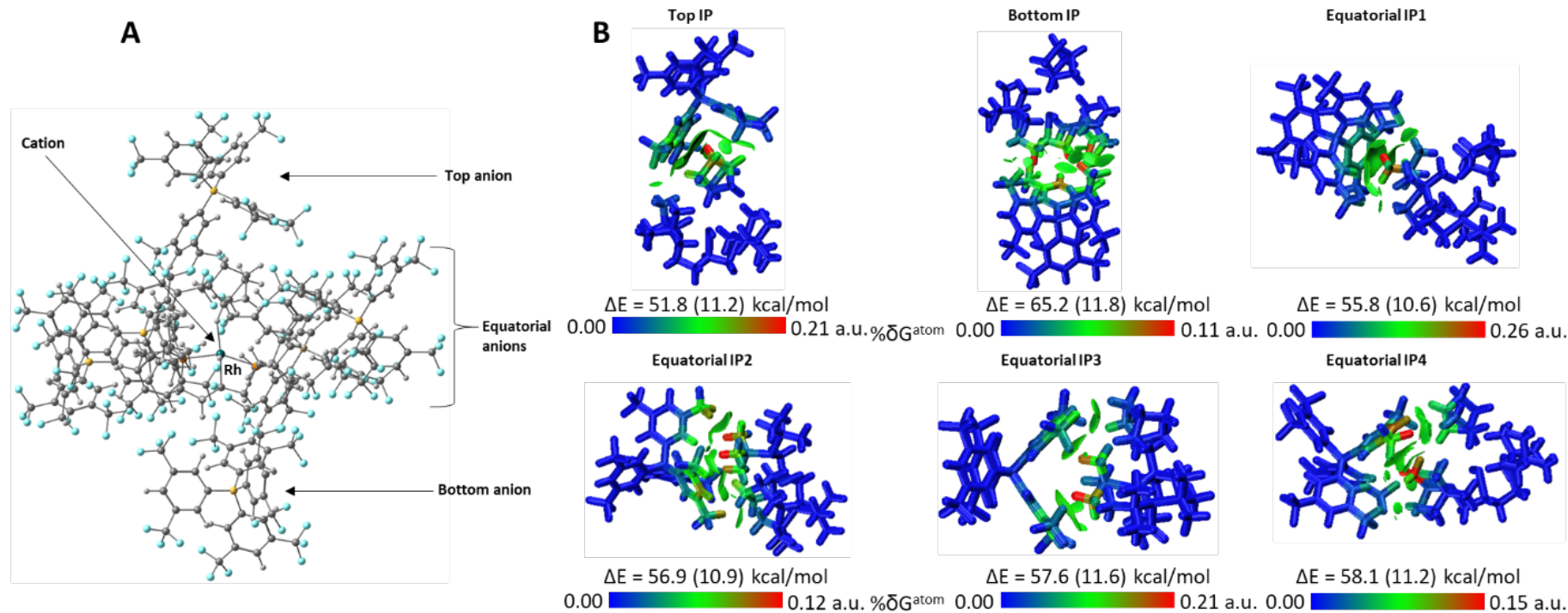


Figure S32: **A:** Packing diagram depicting the *pseudo*-octahedral arrangement of $[\text{BARF}_4]^-$ anions around the Rh cation in fully optimised $2[\text{BARF}_4]$; **B:** IGMH plots for ion-pair interactions in η^1 - σ -bridgehead complex based on the fully optimised structure. Cations and anions are defined as separate fragments; $\text{sign}(\lambda_2)\rho$ -coloured isosurfaces are plotted with $\delta G^{\text{inter}} = 0.003$ a.u.; relative atomic contributions coloured by % δG^{atom} . The ion-pair (IP) interaction energies are also indicated (kcal/mol) with the contribution from dispersion in brackets.

S5.5 η^1 - Isomers

S5.5.1. Sampling of Isomers and Conformers

To explore the different η^1 -isomers associated with different binding modes of the NBA ligand in **2**[BAr^F₄]⁻ and the different conformers accessible to each, conformational sampling was performed using the conformer-rotamer ensemble tool (CREST).³¹ CREST uses the GFN2-xTB method and meta-dynamic sampling approach to generate sets of different conformers and rank them according to their energies.³² Conformational searches were based on constrained conformational sampling which allows the NBA ligand to move over the coordination sphere while keeping all atoms of the [BAr^F₄]⁻ anion and the [Rh(PCP)]⁺ fragment fixed. To mimic the immediate solid state environment, the top ion-pair from the fully-optimised periodic-DFT structure was used as the reference structure for the conformational search (**Figure S33A**). CREST provided 13 unique conformers of 4 η^1 -isomers (bridgehead, endo, exo and methylene bridge, **conf1-13**, **Figure S33B**) within an energy window of 6.0 kcal/mol, which then used as a basis for input structures for periodic-DFT calculations.

Once generated, each conformation was placed within the unit cell of **2**[BAr^F₄]⁻ using a python script to replace a subset of the overall crystal structure (in this case one cation in the unit cell). The replacement was performed by specifying 3 or more equivalent reference atoms in the crystal and conformation structures. The centroids of these reference atoms are aligned with the origin. The Kabsch algorithm³³ was then applied to generate a rotation matrix with the lowest RMSE between the two sets of reference atoms. This allowed for the subset to be aligned within the crystal unit cell and then replacement of the specified atoms with those of the gas phase conformation. Code and further details can be found at <https://github.com/macgregor-group/ReplaceSubset>.

The periodic-DFT calculations for solid-state conformers showed most stable η^1 - σ -bridgehead structure (**conf1**) had an energy -0.1 kcal/mol lower than the experimental η^1 - σ -bridgehead structure (**Table S5**). The solid-state conformers for other η^1 - σ -structures have higher energies compared to experimental bridgehead structure, *i.e.* the endo (**conf4**), exo (**conf7**) and methylene bridge (**conf12**) conformers have energies 1.8 kcal/mol, 2.8 kcal/mol and 2.1 kcal/mol, respectively (**Table S5**). A combined XYZ file for periodic-DFT SS conformers is provided.

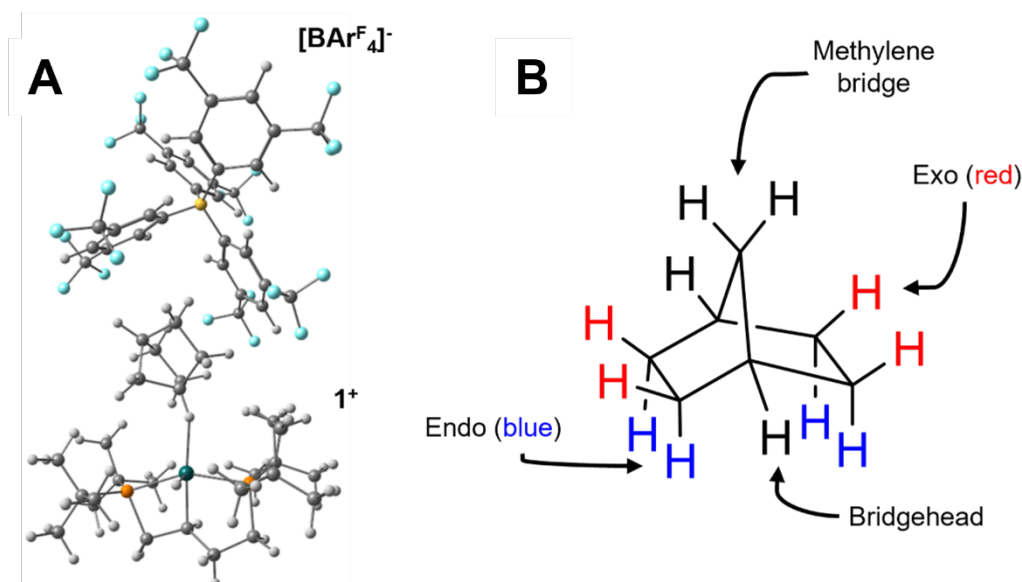


Figure S33: **A:** Top-ion pair used as reference structure for conformation sampling; **B:** NBA labelled to indicate each C-H bond that can engage in binding to the rhodium centre.

Table S5: Relative binding energies of solid-state η^1 -conformers and isomers in **2[BAR^F₄]**.

<i>Isomer</i>	<i>Conformer</i>	<i>Relative Energy (kcal/mol)</i>
Bridgehead	Experimental	0.0
	1	-0.1
	2	0.4
Endo	3	6.7
	4	1.8
	5	4.3
Exo	6	6.9
	7	2.8
	8	3.0
Methylene bridge	9	3.6
	10	5.2
	11	2.1
	12	9.4
	13	10.5

S5.6 Electronic structure analyses for most stable conformers of each η^1 -isomer

S5.6.1 NBO Analysis

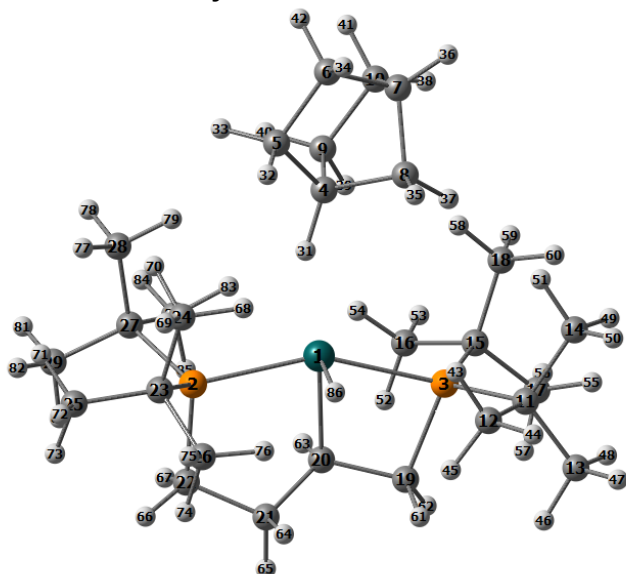


Figure S34: Structure with atom labelling of most stable η^1 - σ -bridgehead 1^+ conformer (**conf1**).

Table S6: Selected NBO data

<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>	<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>
33. LP(2) Rh1	135. BD*(1) C4-H31	0.35	48. BD(1) C4-H31	123. BD*(1) Rh1-P3	0.87
34. LP(3) Rh1	135. BD*(1) C4-H31	0.65	48. BD(1) C4-H31	124. BD*(1) Rh1-C20	9.79
35. LP(1) P2	135. BD*(1) C4-H31	0.59	48. BD(1) C4-H31	125. BD*(1) Rh1-H86	0.16
35. LP(1) P2	148. BD*(1) C9-H39	0.18			
36. BD(1) Rh1-P3	132. BD*(1) C4-C5	0.19			
36. BD(1) Rh1-P3	135. BD*(1) C4-H31	1.36			
36. BD(1) Rh1-P3	146. BD*(1) C4-H37	0.07			
36. BD(1) Rh1-P3	142. BD*(1) C7-C8	0.11			
36. BD(1) Rh1-P3	148. BD*(1) C9-H39	0.20			
37. BD(1) Rh1-C20	132. BD*(1) C4-C5	0.24			
37. BD(1) Rh1-C20	142. BD*(1) C7-C8	0.06			
37. BD(1) Rh1-C20	134. BD*(1) C4-H31	5.18			
37. BD(1) Rh1-C20	148. BD*(1) C9-H39	0.22			
38. BD(1) Rh1-H86	132. BD*(1) C4-C5	0.08			
38. BD(1) Rh1-H86	134. BD*(1) C4-C9	0.08			
38. BD(1) Rh1-H86	134. BD*(1) C4-H31	2.84			
38. BD(1) Rh1-H86	142. BD*(1) C7-C8	0.09			
38. BD(1) Rh1-H86	148. BD*(1) C9-H39	0.22			

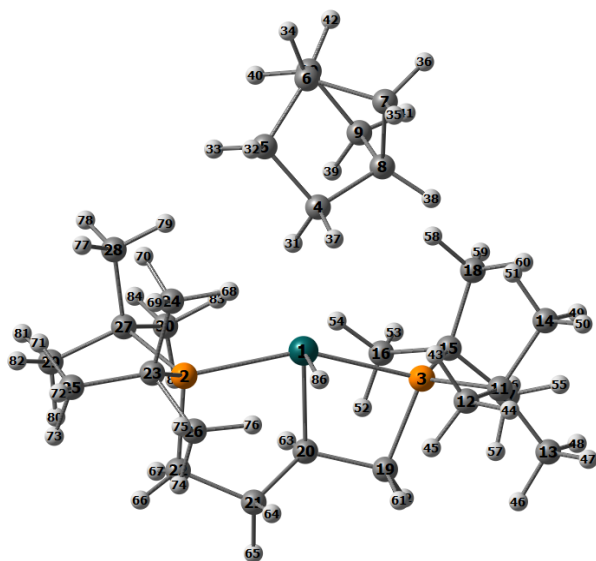


Figure S35: Structure with atom labelling of most stable η^1 - σ -endo 1^+ conformer (**conf4**).

Table S7: Selected NBO data.

<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>	<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>
32. LP(1) Rh1	134. BD*(1) C4-H31	1.43	47. BD(1) C4-H31	123. BD*(1) Rh1-P3	1.12
33. LP(2) Rh1	134. BD*(1) C4-H31	0.36	47. BD(1) C4-H31	124. BD*(1) Rh1-C20	10.82
34. LP(3) Rh1	134. BD*(1) C4-H31	0.14	47. BD(1) C4-H31	125. BD*(1) Rh1-H86	0.45
36. BD(1) Rh1-P3	132. BD*(1) C4-C5	0.22			
36. BD(1) Rh1-P3	134. BD*(1) C4-H31	2.30			
36. BD(1) Rh1-P3	135. BD*(1) C4-H37	0.06			
36. BD(1) Rh1-P3	142. BD*(1) C7-C8	0.09			
36. BD(1) Rh1-P3	148. BD*(1) C9-H39	0.10			
37. BD(1) Rh1-C20	132. BD*(1) C4-C5	0.25			
37. BD(1) Rh1-C20	133. BD*(1) C4-C8	0.10			
37. BD(1) Rh1-C20	134. BD*(1) C4-H31	5.88			
37. BD(1) Rh1-C20	135. BD*(1) C4-H37	0.13			
37. BD(1) Rh1-C20	148. BD*(1) C9-H39	0.14			
38. BD(1) Rh1-H86	132. BD*(1) C4-C5	0.14			
38. BD(1) Rh1-H86	133. BD*(1) C4-C8	0.16			
38. BD(1) Rh1-H86	134. BD*(1) C4-H31	3.31			
38. BD(1) Rh1-H86	135. BD*(1) C4-H37	0.36			
38. BD(1) Rh1-H86	148. BD*(1) C9-H39	0.11			

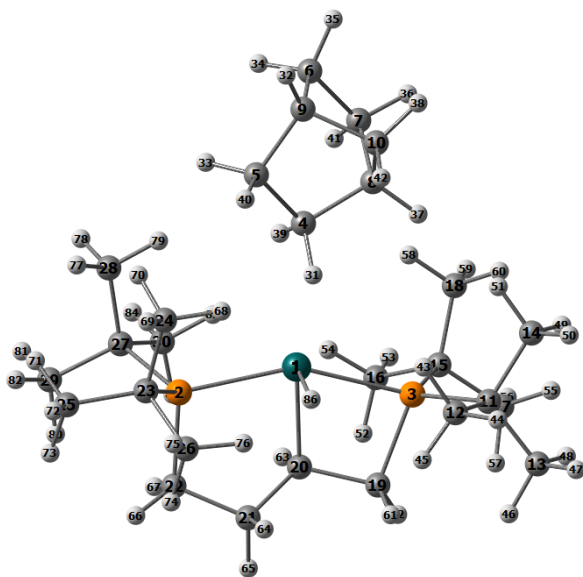


Figure S36: Structure with atom labelling of most stable η^1 - σ -exo 1^+ conformer (**conf7**).

Table S8: Selected NBO data.

<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>
32. LP(1) Rh1	134. BD*(1) C4-H31	2.05
33. LP(1) Rh1	135. BD*(1) C4-H39	0.25
35. LP(1) P2	132. BD*(1) C4-C5	0.09
35. LP(1) P2	134. BD*(1) C4-H31	0.11
35. LP(1) P2	135. BD*(1) C4-H39	0.26
36. LP(1) P3	133. BD*(1) C4-C8	0.11
35. LP(1) P3	135. BD*(1) C4-H39	0.41
35. LP(1) P3	147. BD*(1) C8-H37	0.07
37. BD(1) Rh1-C20	132. BD*(1) C4-C5	0.10
37. BD(1) Rh1-C20	133. BD*(1) C4-C8	0.06
37. BD(1) Rh1-C20	134. BD*(1) C4-H31	0.49
38. BD(1) Rh1-H86	134. BD*(1) C4-H31	0.67
47. BD(1) C4-H31	123. LV(1) Rh1	3.01
47. BD(1) C4-H31	124. BD*(1) Rh1-C20	8.28
47. BD(1) C4-H31	125. BD*(1) Rh1-H86	0.27

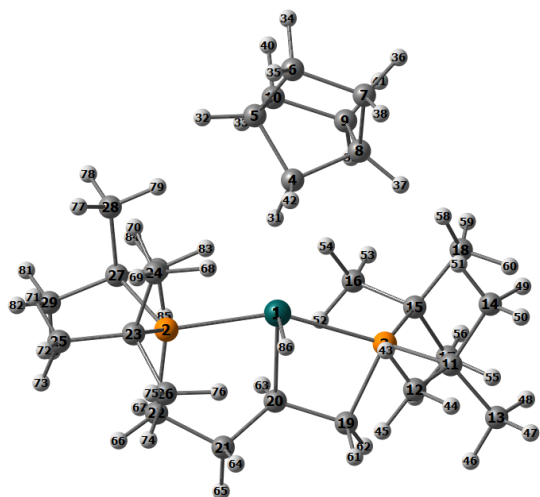


Figure S37: Structure with atom labelling of most stable η^1 - σ -methylene bridge **1⁺** conformer (**conf11**).

Table S9: Selected NBO data.

<i>Donor NBO</i>	<i>Acceptor NBO</i>	<i>E(2) kcal/mol</i>
32. LP(1) Rh1	134. BD*(1) C4-H31	0.97
33. LP(2) Rh1	134. BD*(1) C4-H31	0.27
34. LP(3) Rh1	134. BD*(1) C4-H31	0.11
35. LP(1) P2	134. BD*(1) C4-H31	0.12
35. LP(1) P2	135. BD*(1) C4-H42	0.08
36. LP(1) P3	135. BD*(1) C4-H31	0.35
37. BD(1) Rh1-C20	132. BD*(1) C4-C5	0.06
37. BD(1) Rh1-C20	134. BD*(1) C4-H31	1.95
38. BD(1) Rh1-H86	134. BD*(1) C4-H31	0.19
47. BD(1) C4-H31	123. LV(1) Rh1	4.98
47. BD(1) C4-H31	124. BD*(1) Rh1-C20	8.96

S5.6.2 QTAIM Analysis

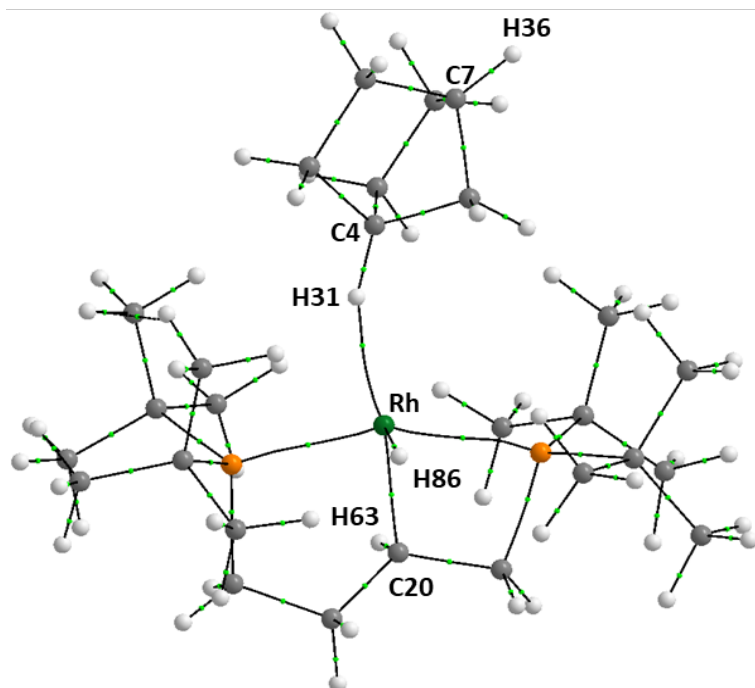


Figure S38: QTAIM molecular graph of most stable η^1 - σ -bridgehead 1^+ conformer (**conf1**).

Table S6: Selected QTAIM BCP parameters (a.u.) and bond distances.

BCP	Distance(Å)	ρ ($e \text{ bohr}^{-3}$)	$\nabla^2\rho$ ($e \text{ bohr}^{-5}$)	$H(r)$	DI
C4-H31	1.122	0.2502	-0.7426	-0.2333	0.8300
Rh...H31	2.084	0.0341	+0.1019	-0.0050	0.1856
Rh-C20	2.063	0.1239	+0.0835	-0.0535	0.9378
Rh-H86	1.520	0.1639	+0.0378	-0.0980	0.9887
Rh...C4	3.080	-	-	-	0.0839
C20-H63	1.103	0.2708	-0.8863	-0.2687	0.8936
C7-H36	1.095	0.2762	-0.9389	-0.2783	0.9367

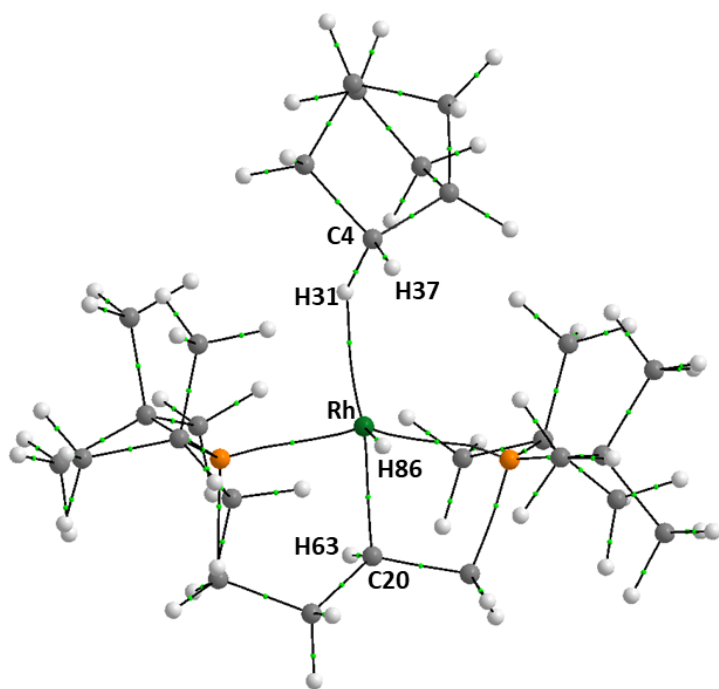


Figure S39: QTAIM molecular graph of most stable η^1 - σ -endo 1^+ conformer (**conf4**).

Table S7: Selected QTAIM BCP parameters (a.u.) and bond distances.

BCP	Distance(Å)	ρ (e bohr³)	$\nabla^2\rho$ (e bohr⁵)	$H(r)$	DI
C4-H31	1.125	0.2478	-0.7224	-0.2294	0.8330
Rh-H31	2.095	0.0347	+0.0998	-0.0051	0.1880
Rh-C20	2.063	0.1243	+0.0827	-0.0538	0.9394
Rh-H86	1.520	0.1640	+0.0365	-0.0980	0.9861
C20-H63	1.103	0.2710	-0.8880	-0.2691	0.8939
Rh-C4	2.994	-	-	-	0.1044
C4-H37	1.097	0.2751	-0.9258	-0.2763	0.9235

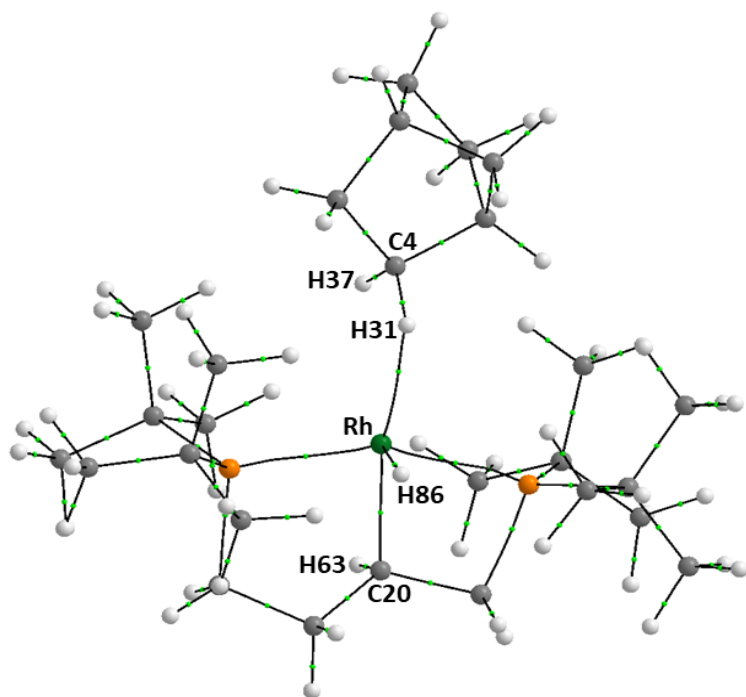


Figure S40: QTAIM molecular graph of most stable η^1 - σ -exo 1^+ conformer (**conf7**).

Table S8: Selected QTAIM BCP parameters (a.u.) and bond distances.

BCP	Distance(Å)	ρ (e bohr³)	$\nabla^2\rho$ (e bohr⁵)	$H(r)$	DI
C4-H31	1.124	0.2520	-0.7564	-0.2363	0.8427
Rh-H31	2.129	0.0336	+0.1074	-0.0037	0.1662
Rh-C20	2.070	0.1230	+0.0840	-0.0526	0.9327
Rh-H86	1.519	0.1640	+0.0387	-0.0981	0.9829
Rh-C4	2.812	–	–	–	0.1409
C20-H63	1.102	0.2716	-0.8917	-0.2702	0.8948
C4-H39	1.102	0.2685	-0.8718	-0.2651	0.9023

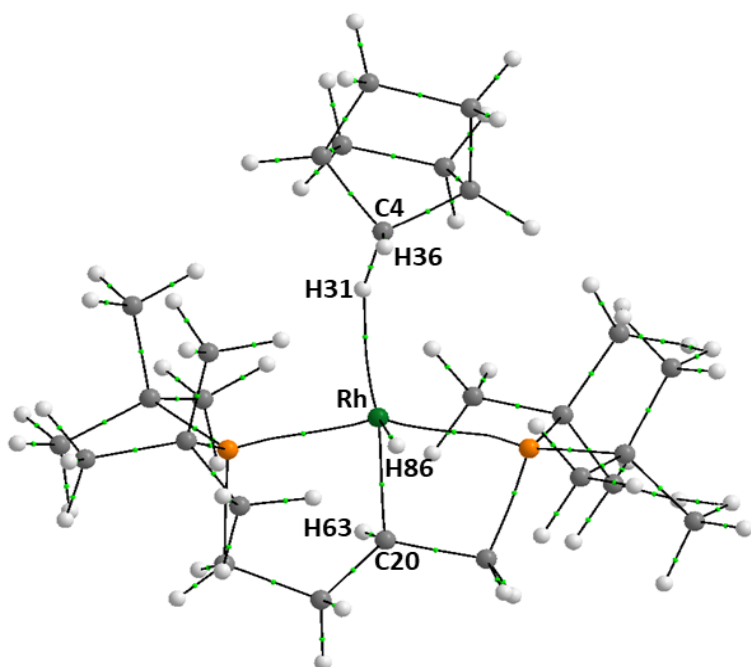


Figure S41: QTAIM molecular graph of most stable η^1 - σ -methylene bridge **1⁺** conformer (**conf11**).

Table S9: Selected QTAIM BCP parameters (a.u.) and bond distances.

BCP	Distance(Å)	ρ (e bohr³)	$\nabla^2\rho$ (e bohr⁵)	$H(r)$	DI
C4-H31	1.125	0.2470	-0.7177	-0.2282	0.8313
Rh-H31	2.081	0.0344	+0.0994	-0.0052	0.1937
Rh-C20	2.064	0.1239	+0.0825	-0.0535	0.9381
Rh-H86	1.520	0.1639	+0.0374	-0.0979	0.9883
Rh-C4	3.105	-	-	-	0.0882
C20-H63	1.104	0.2701	-0.8811	+0.2674	0.8961
C4-H42	1.096	0.2752	-0.9314	-0.2769	0.9242

S5.6.3 IGMH Analysis

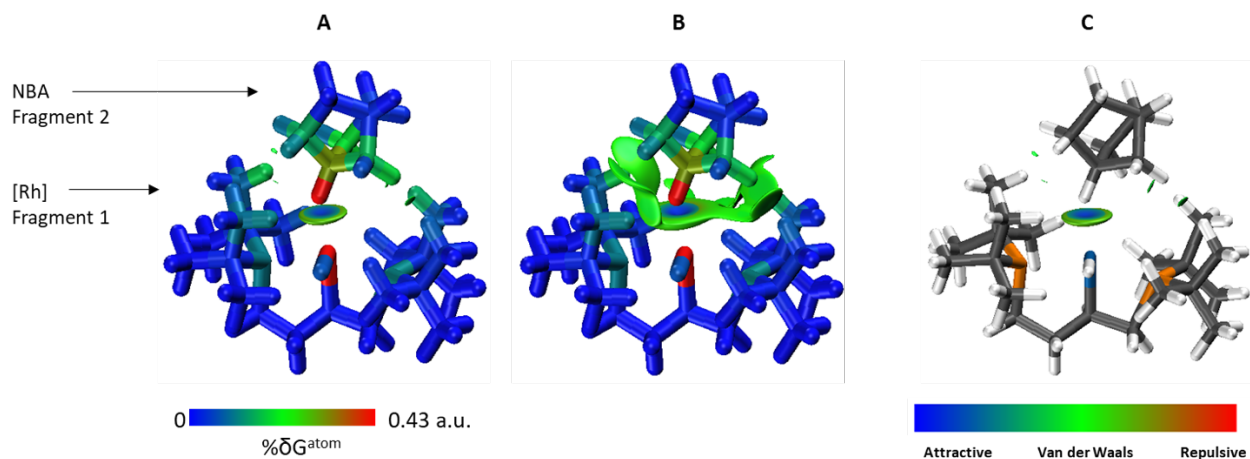


Figure S43: IGMH plots of most stable $\eta^1\text{-}\sigma$ -bridgehead 1^+ conformer (conf1).

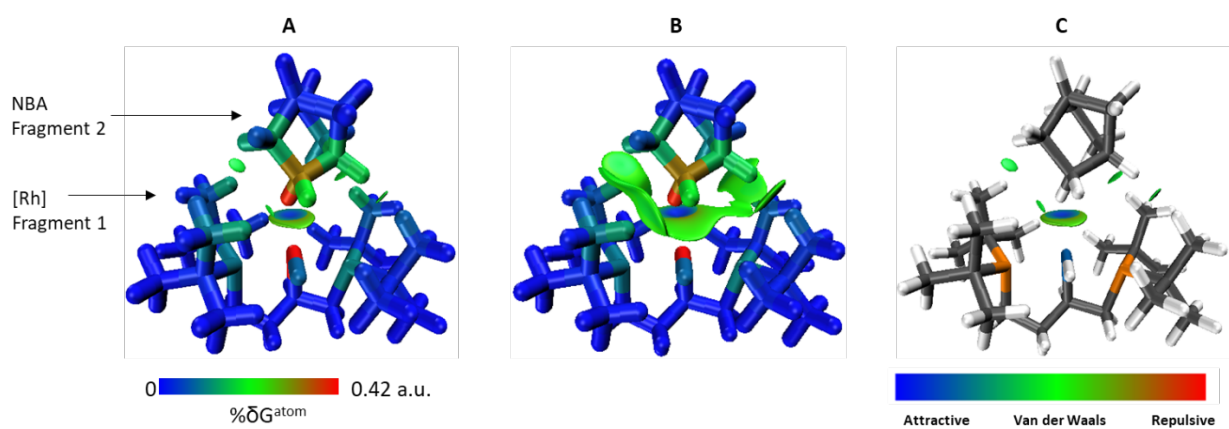


Figure S44: IGMH plots of most stable $\eta^1\text{-}\sigma$ -endo 1^+ conformer (conf4).

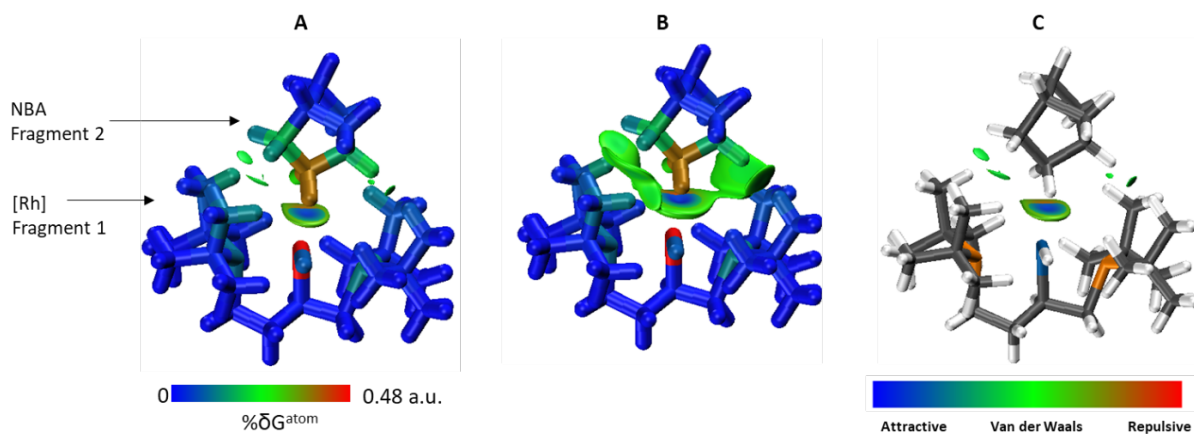


Figure S45: IGMH plots of most stable $\eta^1\text{-}\sigma$ -exo 1^+ conformer (conf7).

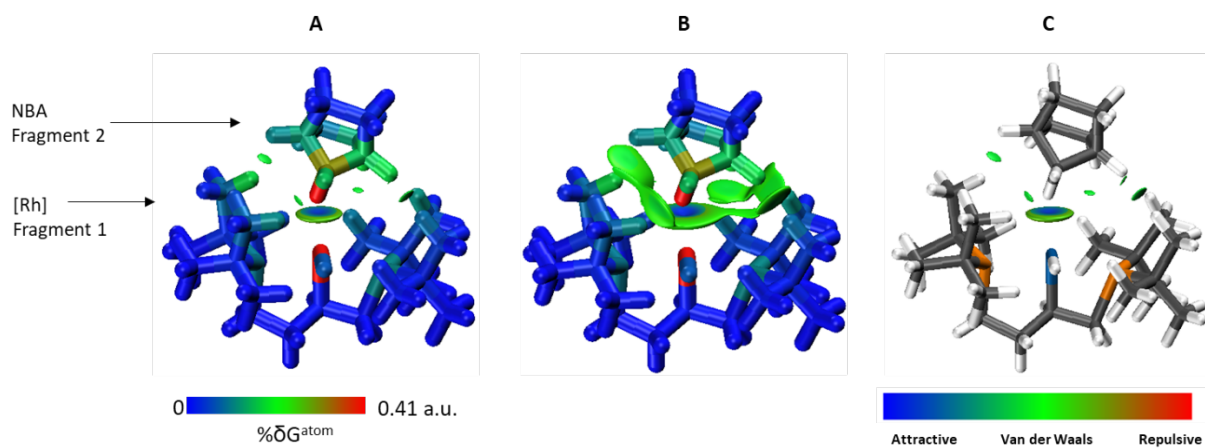


Figure S46: IGMH plots of most stable η^1 - σ -methylene bridge 1^+ conformer (**conf11**).

S6. Mechanistic Studies

S6.1 Thermodynamics of C-H Activation

Mechanistic studies employed the isolated cation model throughout. The thermodynamics of C-H activation in **1**⁺, **4**⁺ and **2b**⁺ to form **1b**⁺, **4b**⁺ and **2**⁺ respectively are summarised in Figure S47. The most stable form of **2**⁺ in the isolated cation model, **2**⁺_{endo,anti}, features the NBA ligand bound through an *endo*-C-H bond with the Rh-H^a and C-H^b bonds in an *anti* arrangement. The structure derived from the experimental structure, **2**⁺_{exp}, is 1.6 kcal/mol higher in energy. The most stable isomer of **2b**⁺ features an *exo*-bound NBA ligand in which the NBA methylene bridge and the C₄ backbone of the chelating phosphine are on the same side, thus **2b**⁺_{exo,syn}. See Figure S50 for alternative isomers of both **2**⁺ and **2b**⁺.

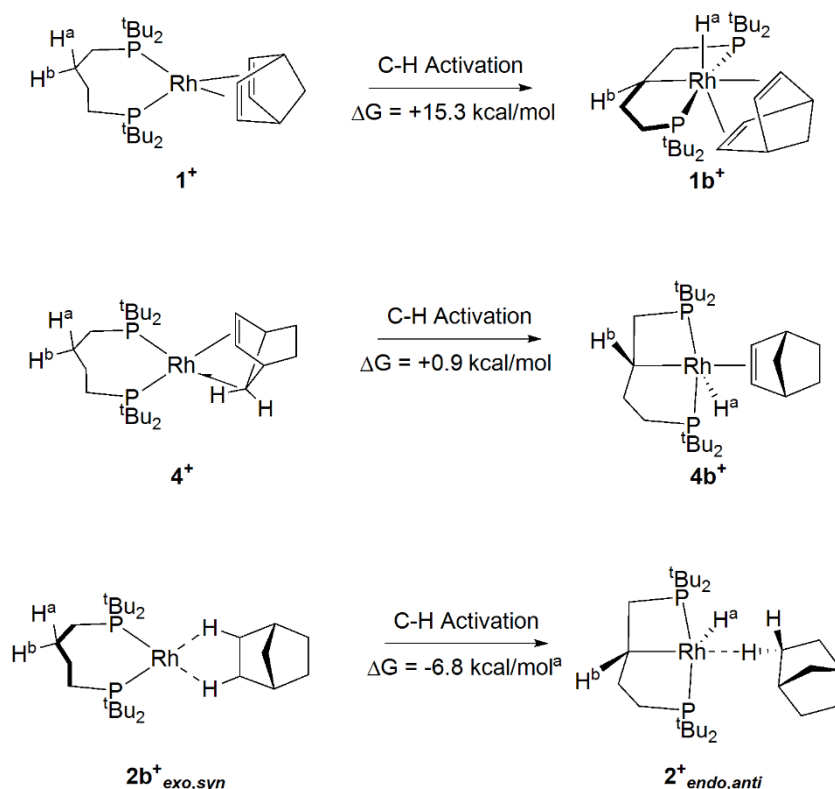


Figure S47. Computed thermodynamics (free energy, kcal/mol) for C-H activation in **1**⁺, **4**⁺ and **2b**⁺. ^athe geometry derived from the experimental structure, **2**⁺_{exp}, is 1.6 kcal/mol higher in energy than **2**⁺_{endo,anti}.

S6.2 Reactivity of 4^+ and $2b^+$

Reaction profiles were computed for the hydrogenation of 4^+ to give $2b^+$ as well as C-H activation in 4^+ and $2b^+$. In the following all free energies are quoted relative to 4^+ set to 0.0 kcal/mol. Hydrogenation of 4^+ was found to be kinetically and thermodynamically favoured over backbone C-H activation.

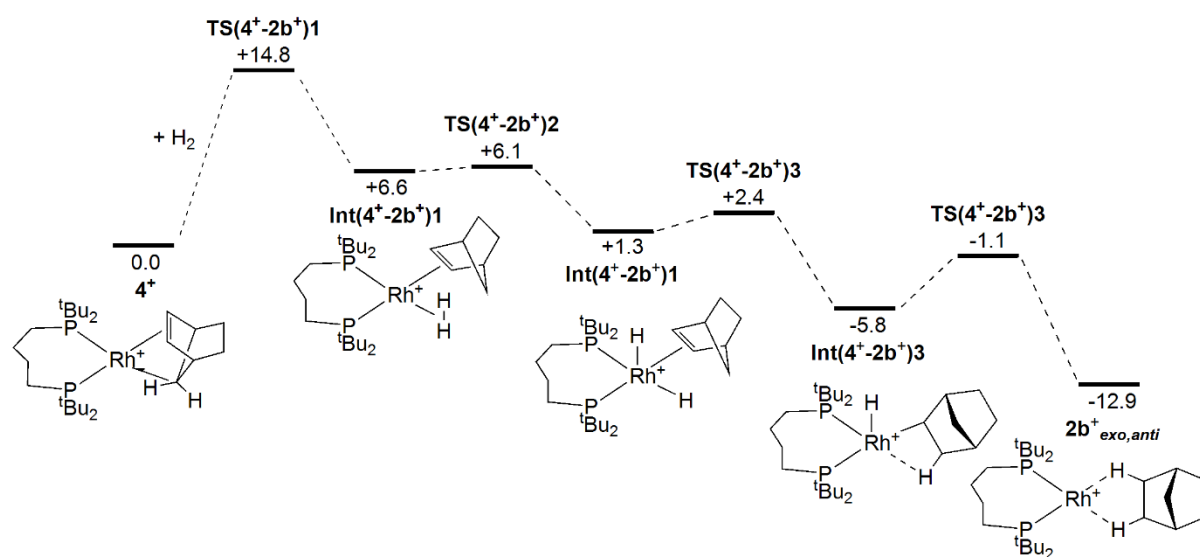


Figure S48. Computed free energy reaction profile (kcal/mol) for hydrogenation of 4^+ to form $2b^+$.

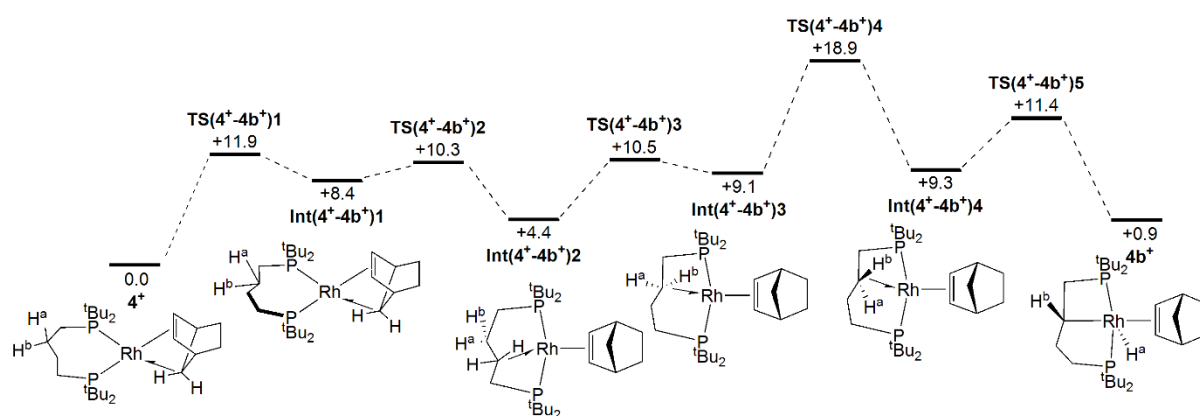


Figure S49. Computed free energy reaction profile (kcal/mol) for C-H activation in 4^+ to form $4b^+$.

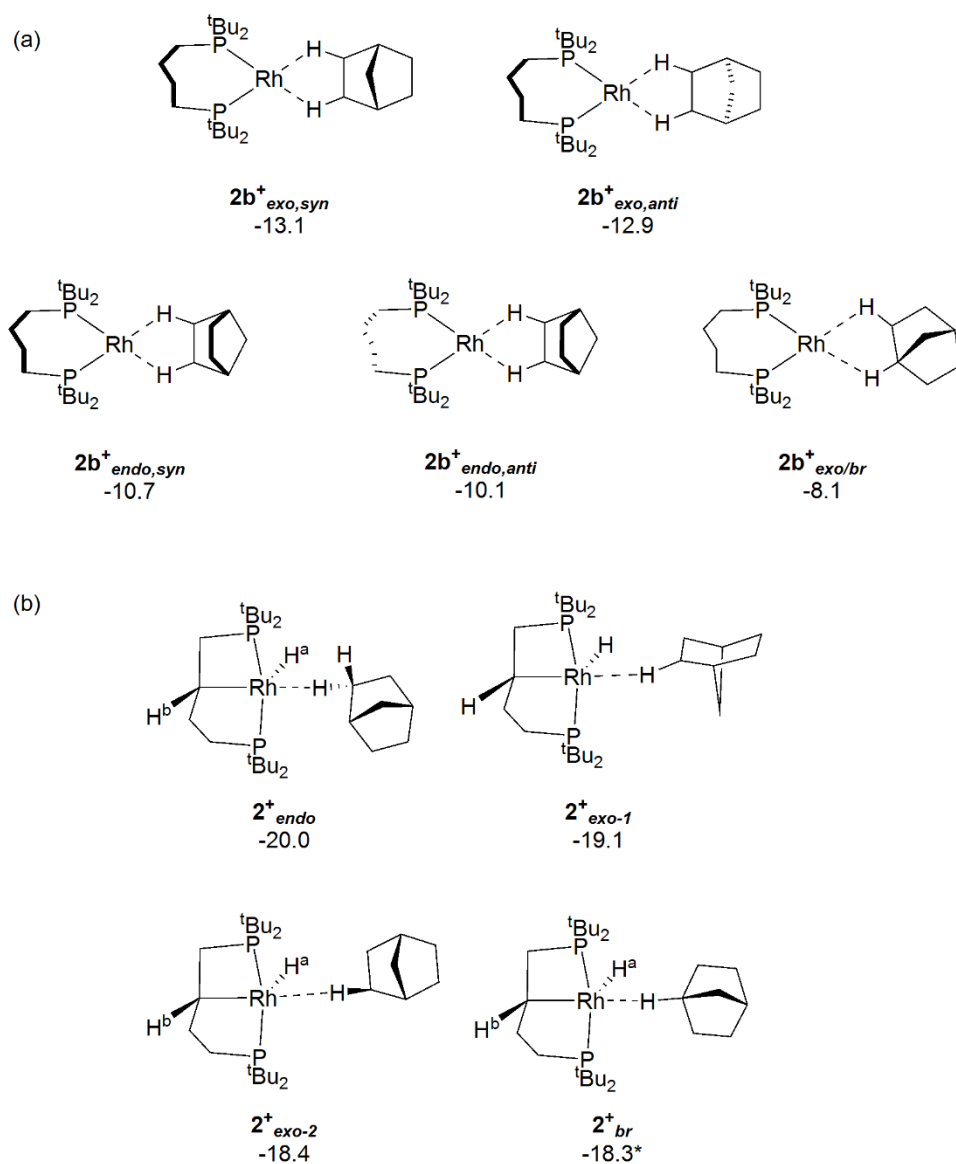


Figure S50. Isomers of (a) $2b^+$ and (b) 2^+ . * 2^+_{br} corresponds to the structure seen experimentally in the crystal structure of $2[BAR^F_4]$.

S7. Computed Structures

- Cartesian coordinates (Å) and energies (a.u.) for the computed structures.

(i) Figure 8

2b+

SCF(BP86/BS1)= -1184.75919219
G(298 K) = -1184.056797
SCF(BS2) = -1854.42636484
Lowest Frequencies = 30.1674cm⁻¹,
48.4401cm⁻¹

86

2b+

Rh	-0.03564	0.42565	0.21258
P	1.79399	-0.94322	0.01603
P	-1.70364	-1.12567	0.02535
C	-1.30623	3.70467	-0.42867
H	-2.30519	3.58190	-0.87315
C	-0.94429	2.61278	0.61486
H	-1.43067	2.75218	1.59214
C	-2.91483	-0.58603	-1.42081
C	1.68060	-2.82856	0.00884
H	2.71463	-3.19264	0.10557
H	1.19571	-3.04313	0.97753
C	-4.01630	-2.02298	1.55322
H	-3.89635	-3.02573	1.11278
H	-4.75030	-1.46516	0.95339
H	-4.45790	-2.16274	2.55587
C	2.82572	-0.47167	-1.56598
C	-2.67489	-1.28188	1.70490
C	-1.35099	-2.92453	-0.36789
H	-0.93887	-3.36669	0.55128
H	-2.32263	-3.41444	-0.53247
C	2.88121	-0.72850	1.64505
C	-0.10295	3.62750	-1.39301
H	-0.01411	2.64729	-1.89526
H	-0.10428	4.42667	-2.15108
C	1.97840	-0.83790	-2.80276
H	0.98174	-0.36948	-2.75372
H	1.85990	-1.92148	-2.93775
H	2.48693	-0.45353	-3.70459
C	-3.84562	0.55295	-0.96168
H	-3.29263	1.42748	-0.58326
H	-4.56432	0.23807	-0.19158
H	-4.43129	0.89982	-1.83108
C	0.47783	5.16198	0.37002
H	0.83538	5.26301	1.40770
H	0.87005	6.02336	-0.19343
C	4.17008	-1.21968	-1.60966
H	4.05048	-2.31243	-1.53459
H	4.86008	-0.88844	-0.81866
H	4.66283	-1.01407	-2.57633
C	-2.89605	0.11693	2.31429
H	-3.49102	0.78324	1.67343
H	-1.93034	0.60422	2.52943

H	-3.43816	0.00976	3.27025
C	3.06410	1.05043	-1.63627
H	3.63124	1.45253	-0.78681
H	2.11093	1.59650	-1.71886
H	3.64441	1.27061	-2.54963
C	-0.39086	-3.14336	-1.55295
H	-0.81949	-3.88479	-2.24853
H	-0.27609	-2.21608	-2.13461
C	0.99628	-3.62711	-1.11452
H	1.65968	-3.67938	-1.99384
H	0.91395	-4.66774	-0.74884
C	-2.04397	-0.05479	-2.58077
H	-1.43574	-0.84650	-3.04388
H	-1.36003	0.74228	-2.24212
H	-2.70224	0.35544	-3.36758
C	-1.07882	5.07348	0.26323
H	-1.48336	5.88251	-0.36553
H	-1.58466	5.13718	1.24036
H	4.51874	-1.59880	2.75220
C	-3.76764	-1.76114	-1.93809
H	-4.39134	-2.22052	-1.15716
H	-3.15345	-2.54686	-2.40478
H	-4.44974	-1.38235	-2.71943
C	0.95409	3.84044	-0.28771
H	2.00841	3.84487	-0.60126
C	-1.77233	-2.07027	2.67895
H	-0.76089	-1.63881	2.72820
H	-1.69651	-3.13876	2.42448
H	-2.20936	-2.01359	3.69120
C	0.60221	2.69190	0.69524
H	0.97291	2.84532	1.72048
H	1.37357	-1.72477	2.90952
C	1.88268	-0.75117	2.82117
H	1.10809	0.02865	2.71289
H	2.42869	-0.58262	3.76667
C	3.62658	0.61887	1.65308
H	2.96723	1.47890	1.46257
H	4.45479	0.64334	0.92910
H	4.06878	0.76873	2.65371
C	3.91697	-1.85277	1.86192
H	4.61718	-1.96861	1.02159
H	3.44897	-2.82725	2.06598
H	1.21488	1.77734	0.30764
H	-1.42659	1.62775	0.21326

TS (2b+-2+) 1

SCF(BP86/BS1)= -1184.70980189
G(298 K) = -1184.014664
SCF(BS2) = -1854.37712372
Lowest Frequencies = -194.6741cm⁻¹,
17.8873cm⁻¹

86

TS (2b+-2+) 1

Rh	-0.09525	-0.01613	-0.18338
P	-2.05226	-1.08131	-0.05038
P	2.29304	-0.82300	-0.05198
C	-1.90209	3.21866	0.06792
H	-2.62102	2.80480	0.79207

C -1.21211 4.48180 0.64492
 H -1.90607 5.13676 1.19283
 C 0.53316 3.08648 0.27286
 H 1.43037 2.48466 0.47085
 C 3.41812 -0.18288 -1.49435
 C 3.11968 -0.62466 1.68375
 C 2.31124 -2.69523 -0.34277
 H 3.14208 -3.13090 0.23559
 H 2.54680 -2.85571 -1.40769
 C -0.15583 -2.94391 -0.96179
 H 0.09161 -1.92522 -1.37653
 H -0.16798 -3.59658 -1.85206
 C -1.55319 -2.88480 -0.30503
 H -2.33209 -3.38324 -0.90301
 H -1.54201 -3.38169 0.67699
 C -0.05743 3.86580 1.46763
 H -0.39897 3.21166 2.28933
 H 0.63515 4.61900 1.87677
 C -0.68912 2.25816 -0.18989
 H -0.84651 1.36353 0.60041
 C -3.26368 -0.74941 -1.52315
 C -0.44567 5.18437 -0.50143
 H -0.08057 6.17114 -0.17415
 C -2.88168 -1.06076 1.69364
 C 0.96979 -3.36003 0.00047
 H 0.68584 -3.10068 1.03434
 H 1.08798 -4.45864 -0.02133
 C 0.74535 4.20905 -0.77878
 H 1.71784 4.69972 -0.60905
 C 3.78798 1.28973 -1.24118
 H 4.46989 1.40912 -0.38495
 H 4.30736 1.69104 -2.12919
 H 2.89688 1.91581 -1.06982
 C 2.35576 -1.57023 2.63358
 H 2.54950 -2.63383 2.42256
 H 2.68557 -1.37876 3.66980
 H 1.26771 -1.39110 2.59118
 C 2.89062 0.82028 2.16714
 H 1.81389 1.05736 2.20408
 H 3.29687 0.93195 3.18802
 H 3.39150 1.56636 1.53149
 C -1.72344 -1.20483 2.70472
 H -0.99263 -0.38523 2.60355
 H -2.13808 -1.18236 3.72810
 H -1.18227 -2.15884 2.59120
 C 4.61874 -0.96468 1.70777
 H 5.22028 -0.23045 1.15029
 H 4.97609 -0.95044 2.75271
 H 4.83296 -1.96810 1.30491
 C -3.86925 -2.23124 1.87675
 H -3.40672 -3.21551 1.70645
 H -4.22252 -2.22006 2.92303
 H -4.75489 -2.14889 1.23259
 C 2.52718 -0.26550 -2.75315
 H 1.60601 0.33327 -2.64141
 H 3.08792 0.12245 -3.62185
 H 2.23003 -1.30035 -2.99386
 C -3.60282 0.27448 1.93748
 H -4.46312 0.41845 1.26590
 H -3.98830 0.29143 2.97170
 H -2.92103 1.13226 1.82912

C 4.69614 -1.01325 -1.71846
 H 4.48340 -2.07297 -1.92866
 H 5.23055 -0.61262 -2.59813
 H 5.38782 -0.96541 -0.86655
 C -3.59510 0.74830 -1.62386
 H -2.69408 1.34251 -1.83072
 H -4.29418 0.90232 -2.46433
 H -4.07553 1.14602 -0.71811
 C -2.50193 -1.16623 -2.80081
 H -2.30696 -2.24875 -2.85216
 H -3.11785 -0.90476 -3.67888
 H -1.54023 -0.63272 -2.89151
 C -4.56369 -1.56377 -1.38964
 H -5.21216 -1.17870 -0.58791
 H -5.12923 -1.47644 -2.33425
 H -4.38995 -2.63763 -1.21481
 H -1.08167 5.34823 -1.38635
 H 0.75404 3.81848 -1.81045
 H -2.46120 3.42985 -0.85738
 H -0.62390 1.93485 -1.24957

Int (2b+-2+)
 SCF(BP86/BS1) = -1184.73591245
 G(298 K) = -1184.039118
 SCF(BS2) = -1854.40249011
 Lowest Frequencies = 27.6905cm⁻¹,
 29.3893cm⁻¹

86
 Int (2b+-2+)
 Rh -0.01960 -0.31867 -0.11394
 P -2.32465 -0.78432 -0.00891
 P 2.27030 -0.88507 -0.00529
 C -1.27789 2.90514 0.52939
 H -1.65567 2.65652 1.53489
 C -0.72076 4.34775 0.50869
 H -1.37247 5.07188 1.02018
 C 1.11965 3.09584 0.07217
 H 2.12528 2.67585 0.18821
 C 3.38531 -0.50944 -1.53991
 C 3.16046 -0.55139 1.68237
 C 2.12826 -2.77718 -0.04820
 H 2.93339 -3.23685 0.54639
 H 2.28924 -3.08605 -1.09484
 C -0.36831 -2.59543 -0.42849
 H -0.03381 -1.59046 -1.14347
 H -0.38827 -3.11321 -1.41174
 C -1.80442 -2.58478 0.14293
 H -2.48687 -3.30685 -0.33626
 H -1.76716 -2.81996 1.21788
 C 0.68189 4.13692 1.12527
 H 0.65230 3.73845 2.15451
 H 1.30568 5.04554 1.11294
 C -0.02216 2.04602 0.17565
 H 0.20275 1.31333 1.02186
 C -3.35302 -0.65430 -1.62866
 C -0.37664 4.72519 -0.95391
 H -0.16884 5.80355 -1.04056
 C -3.36690 -0.47335 1.58884
 C 0.73899 -3.23159 0.41745
 H 0.58279 -2.97353 1.47679

H	0.66603	-4.33439	0.34090
C	0.90682	3.87740	-1.24819
H	1.77608	4.52464	-1.44971
C	3.90217	0.93850	-1.48011
H	4.62235	1.09329	-0.66155
H	4.42732	1.17265	-2.42263
H	3.08142	1.66445	-1.37291
C	2.31794	-1.26698	2.76104
H	2.37650	-2.36395	2.68517
H	2.70598	-0.99022	3.75694
H	1.25669	-0.96386	2.71717
C	3.16687	0.95330	2.00359
H	2.14681	1.36160	2.07265
H	3.64691	1.10500	2.98628
H	3.73345	1.54466	1.26965
C	-2.33230	-0.28758	2.71951
H	-1.70318	0.60225	2.55780
H	-2.86309	-0.15952	3.67932
H	-1.66413	-1.15903	2.82516
C	4.60205	-1.08910	1.70682
H	5.27271	-0.50313	1.06006
H	4.99404	-1.01153	2.73641
H	4.67128	-2.14861	1.41259
C	-4.27725	-1.67428	1.91619
H	-3.71239	-2.60137	2.09934
H	-4.83387	-1.44952	2.84314
H	-5.01847	-1.87168	1.12898
C	2.44352	-0.65328	-2.75620
H	1.58609	0.03714	-2.69039
H	3.00640	-0.42366	-3.67802
H	2.04847	-1.67805	-2.86545
C	-4.22488	0.79823	1.45743
H	-5.04214	0.67654	0.73020
H	-4.69147	1.01386	2.43457
H	-3.63307	1.67986	1.17289
C	4.57159	-1.48114	-1.69510
H	4.25673	-2.53389	-1.76429
H	5.09977	-1.24214	-2.63501
H	5.30274	-1.39458	-0.88001
C	-3.51110	0.83915	-1.97770
H	-2.52855	1.32893	-2.08180
H	-4.03574	0.93229	-2.94471
H	-4.09911	1.39122	-1.22967
C	-2.51841	-1.32857	-2.73783
H	-2.41096	-2.41476	-2.58390
H	-3.03390	-1.18916	-3.70396
H	-1.51533	-0.87703	-2.82629
C	-4.72354	-1.34518	-1.52691
H	-5.39794	-0.84092	-0.81858
H	-5.21402	-1.31976	-2.51600
H	-4.63689	-2.40444	-1.23355
H	-1.20666	4.49846	-1.64361
H	0.79275	3.20632	-2.11714
H	-2.10207	2.75729	-0.18655
H	-0.13634	1.52843	-0.82683

TS (2b+-2+) 2
SCF (BP86/BS1) = -1184.71498079
G (298 K) = -1184.017648
SCF (BS2) = -1854.38089394

Lowest Frequencies = -650.9862cm-1, 26.8785cm-1

86
TS (2b+-2+) 2
Rh -0.03062 -0.17727 -0.14330
P -2.29162 -0.81767 -0.01963
P 2.24528 -0.91329 -0.02075
C -1.32180 3.02118 0.40112
H -1.76364 2.68309 1.35311
C -0.71300 4.43377 0.56900
H -1.37173 5.12674 1.11378
C 1.10830 3.16041 0.11482
H 2.08617 2.68310 0.25384
C 3.44708 -0.46863 -1.47052
C 3.03797 -0.72359 1.72826
C 2.12198 -2.84319 -0.24710
H 2.95701 -3.29946 0.30771
H 2.32521 -3.00940 -1.31770
C -0.37812 -2.69653 -0.52022
H 0.22645 -1.76250 -0.25034
H -0.37681 -2.77571 -1.61656
C -1.78761 -2.64980 0.08726
H -2.49120 -3.34490 -0.39876
H -1.74164 -2.90953 1.15661
C 0.63677 4.10033 1.24597
H 0.52454 3.59510 2.22142
H 1.29097 4.97821 1.37283
C -0.07429 2.15733 0.02756
H 0.07305 1.36076 0.86580
C -3.33818 -0.67379 -1.63016
C -0.25779 4.94895 -0.81965
H -0.00891 6.02120 -0.77470
C -3.33473 -0.55534 1.58570
C 0.77372 -3.51268 0.11482
H 0.63114 -3.54299 1.20744
H 0.76411 -4.55463 -0.25392
C 1.01423 4.08680 -1.12262
H 1.91650 4.71622 -1.19459
C 3.96836 0.96650 -1.28032
H 4.64055 1.05820 -0.41292
H 4.54824 1.25897 -2.17316
H 3.14663 1.69084 -1.17109
C 2.13625 -1.53490 2.68400
H 2.23143 -2.62126 2.52879
H 2.43855 -1.32776 3.72547
H 1.07432 -1.24957 2.57610
C 2.98251 0.75694 2.14807
H 1.94848 1.13705 2.15060
H 3.37549 0.85351 3.17537
H 3.59241 1.40551 1.50188
C -2.30157 -0.38297 2.71953
H -1.66363 0.50128 2.56037
H -2.83420 -0.25727 3.67876
H -1.63925 -1.25935 2.82129
C 4.48492 -1.23838 1.80700
H 5.18271 -0.60444 1.23865
H 4.81426 -1.22034 2.86096
H 4.58993 -2.27672 1.45310
C -4.24535 -1.75976 1.89573
H -3.68024 -2.68919 2.06637

H	-4.80214	-1.54893	2.82590	H	0.64483	3.57153	2.10451
H	-4.98656	-1.94662	1.10593	H	1.17125	5.12196	1.37078
C	2.56081	-0.51434	-2.73514	C	-0.06166	2.34130	-0.17152
H	1.69923	0.16979	-2.65076	H	0.26087	1.48707	0.49998
H	3.16217	-0.20993	-3.60975	C	-3.21014	-0.76929	-1.66591
H	2.17189	-1.52522	-2.94494	C	-0.61488	5.19644	-0.62496
C	-4.18899	0.72079	1.47082	H	-0.44881	6.27273	-0.45769
H	-5.01458	0.60743	0.75157	C	-3.43275	-0.63057	1.54696
H	-4.64316	0.93478	2.45419	C	0.82933	-3.30434	0.47924
H	-3.59438	1.60021	1.18256	H	0.71595	-3.17807	1.56994
C	4.63620	-1.43507	-1.63251	H	0.68390	-4.38305	0.26852
H	4.32472	-2.47682	-1.80350	C	0.67584	4.50652	-1.18202
H	5.21910	-1.12658	-2.51833	H	1.50268	5.22797	-1.28519
H	5.31853	-1.41713	-0.77149	C	3.65107	0.94073	-1.59259
C	-3.51697	0.82327	-1.95103	H	4.46017	1.13899	-0.87307
H	-2.54088	1.32505	-2.05613	H	4.03052	1.21497	-2.59254
H	-4.05245	0.92624	-2.91109	H	2.80614	1.60959	-1.36474
H	-4.10219	1.35683	-1.18796	C	2.64132	-1.28519	2.78540
C	-2.49624	-1.31239	-2.75522	H	2.78607	-2.37362	2.70131
H	-2.41111	-2.40591	-2.64656	H	3.11664	-0.96425	3.72850
H	-2.99169	-1.12197	-3.72319	H	1.56076	-1.07964	2.87422
H	-1.48308	-0.87573	-2.80458	C	3.11107	1.00278	1.88224
C	-4.69938	-1.38306	-1.53971	H	2.04866	1.27605	1.98704
H	-5.38078	-0.89643	-0.82568	H	3.61829	1.26313	2.82762
H	-5.18899	-1.35068	-2.52920	H	3.55136	1.62634	1.09062
H	-4.60168	-2.44525	-1.26067	C	-2.48891	-0.45379	2.75490
H	-1.04607	4.83044	-1.58132	H	-1.84482	0.43346	2.64510
H	0.93721	3.51861	-2.06547	H	-3.09556	-0.32562	3.66847
H	-2.10917	2.98015	-0.36826	H	-1.84088	-1.33253	2.91305
H	-0.14816	1.72308	-1.00634	C	4.77441	-0.87000	1.51431
2+ (anti, exo)				H	5.30315	-0.25293	0.77200
SCF(BP86/BS1)= -1184.76289339				H	5.25756	-0.69000	2.49061
G(298 K) = -1184.067901				H	4.93271	-1.93152	1.26279
SCF(BS2) = -1854.42735749				C	-4.35843	-1.83860	1.79261
Lowest Frequencies = 25.8867cm-1,				H	-3.79967	-2.76878	1.97966
29.8320cm-1				H	-4.96582	-1.63950	2.69299
86				H	-5.05460	-2.01682	0.96100
2+ (anti, exo)				C	2.15557	-0.73757	-2.70129
Rh	0.02891	-0.44039	-0.04202	H	1.28906	-0.06426	-2.55175
P	-2.29164	-0.91685	0.01853	H	2.58846	-0.49378	-3.68754
P	2.30615	-0.98077	0.03347	H	1.78468	-1.77481	-2.75324
C	-1.33773	3.02551	0.41633	C	-4.27434	0.64600	1.36590
H	-1.65450	2.52250	1.34513	H	-5.04613	0.53002	0.58966
C	-0.85396	4.46407	0.71854	H	-4.79891	0.86267	2.31286
H	-1.50672	5.00792	1.41786	H	-3.65750	1.52359	1.11999
C	1.01197	3.45875	-0.09133	C	4.44116	-1.43615	-1.89506
H	2.04849	3.09355	-0.12273	H	4.17931	-2.50426	-1.94937
C	3.22553	-0.53737	-1.60286	H	4.86163	-1.15686	-2.87743
C	3.28260	-0.50527	1.61776	H	5.24120	-1.31698	-1.15102
C	2.22994	-2.86761	0.02681	C	-3.41822	0.72389	-1.98912
H	3.03976	-3.30046	0.63487	H	-2.46169	1.27273	-1.99288
H	2.40014	-3.18941	-1.01379	H	-3.86178	0.81730	-2.99591
C	-0.23320	-2.48198	-0.25021	H	-4.09682	1.22284	-1.28293
H	0.01491	-0.62604	1.46490	C	-2.26494	-1.36683	-2.73021
H	-0.11369	-2.61223	-1.34643	H	-2.09664	-2.44681	-2.59368
C	-1.69535	-2.69970	0.16135	H	-2.71854	-1.22846	-3.72704
H	-2.25934	-3.43776	-0.43570	H	-1.28402	-0.85826	-2.74663
H	-1.76244	-2.99187	1.22220	C	-4.54705	-1.52833	-1.68268
C	0.59195	4.20026	1.19804	H	-5.29535	-1.06965	-1.01879
				H	-4.96390	-1.50670	-2.70523
				H	-4.42963	-2.58696	-1.39857

H -1.47754 5.10271 -1.30510
H 0.52412 4.04328 -2.17183
H -2.19036 3.00392 -0.28200
H -0.19741 1.97510 -1.20613

2+ (anti, endo)
SCF(BP86/BS1)= -1184.76424885
G(298 K) = -1184.070501
SCF(BS2) = -1854.42857998
Lowest Frequencies = 21.5282cm⁻¹,
28.4518cm⁻¹

86
2+ (anti, endo)
Rh 0.06673 -0.42244 -0.10397
P 2.35606 -0.86491 0.09686
P -2.23756 -0.94468 0.06394
C 1.01411 3.44351 -0.99648
H 1.31724 3.53931 -2.05257
C 0.24785 4.70175 -0.52194
H 0.70735 5.64479 -0.85364
C -1.30236 3.05834 -0.31095
H -2.24045 2.50605 -0.46443
C -3.35960 -0.48275 1.56509
C -3.18376 -1.06550 -1.60798
C -1.59169 -2.67486 0.45233
H -2.13029 -3.50049 -0.04488
H -1.66152 -2.82620 1.54190
C 0.94706 -3.14454 0.86895
H 0.81581 -2.86358 1.92824
H 0.83794 -4.24669 0.81847
C 2.33895 -2.73327 0.36796
H 3.15409 -3.04539 1.03965
H 2.53275 -3.19800 -0.61301
C -1.17504 4.41001 -1.05105
H -1.22334 4.31618 -2.14937
H -1.92412 5.14958 -0.72333
C -0.05227 2.30700 -0.82596
H -0.24574 1.78312 -1.77926
C 3.25468 -0.12396 1.62593
C 0.04244 4.60417 1.01069
H -0.32638 5.55961 1.41681
C 3.32352 -0.62894 -1.55306
C -0.13368 -2.47455 0.02105
H 0.05106 -0.32258 1.41070
H 0.00043 -2.75817 -1.04524
C -1.03531 3.47634 1.15554
H -1.95625 3.85868 1.62601
C -4.19585 0.77076 1.25179
H -4.95888 0.58263 0.48095
H -4.72984 1.07998 2.16727
H -3.57036 1.61909 0.93281
C -2.22417 -1.77300 -2.58925
H -2.01479 -2.81651 -2.30516
H -2.68792 -1.79171 -3.59084
H -1.26278 -1.23631 -2.68704
C -3.44905 0.35854 -2.13563
H -2.51319 0.93220 -2.23761
H -3.91143 0.29258 -3.13612
H -4.13480 0.93092 -1.49445
C 2.29951 -1.01541 -2.64545

H 1.41030 -0.35628 -2.61854
H 2.76071 -0.89965 -3.64212
H 1.95964 -2.06130 -2.56114
C -4.49399 -1.86240 -1.50257
H -5.25491 -1.33280 -0.90935
H -4.91383 -2.00586 -2.51402
H -4.34229 -2.86270 -1.06497
C 4.57124 -1.52260 -1.67254
H 4.33714 -2.59495 -1.58507
H 5.02365 -1.37101 -2.66860
H 5.33770 -1.27692 -0.92419
C -2.40487 -0.17484 2.73738
H -1.77025 0.70044 2.52723
H -3.00512 0.04782 3.63695
H -1.75093 -1.02809 2.98458
C 3.70858 0.84930 -1.73533
H 4.49066 1.16750 -1.02907
H 4.11101 0.99517 -2.75314
H 2.84140 1.51848 -1.62242
C -4.28611 -1.65218 1.95225
H -3.72865 -2.56353 2.21908
H -4.87073 -1.35850 2.84173
H -5.00255 -1.90728 1.15925
C 3.00811 1.39679 1.66369
H 1.93081 1.62928 1.69413
H 3.46714 1.81483 2.57662
H 3.45215 1.91918 0.80373
C 2.60966 -0.75760 2.87694
H 2.80691 -1.83812 2.95654
H 3.03775 -0.28036 3.77549
H 1.51843 -0.59565 2.90622
C 4.76346 -0.42853 1.61923
H 5.29178 0.09697 0.80931
H 5.20438 -0.08569 2.57163
H 4.97417 -1.50699 1.53178
H 0.98149 4.36781 1.53891
H -0.68493 2.62632 1.76754
H 1.92598 3.27028 -0.40312
H 0.30780 1.56686 -0.04786

(ii) Figure S47
H2
SCF(BP86/BS1) = -1.16466336022
G(298 K) = -1.166217
SCF(BS2) = -1.16590463844
Lowest Frequencies = 4368.4798cm-1, cm-1

2
H2
H 0.00000 0.00000 0.37505
H 0.00000 0.00000 -0.37505

1+
SCF(BP86/BS1) = -1182.33910565
G(298 K) = -1181.680250
SCF(BS2) = -1852.00252324
Lowest Frequencies = 22.7468cm-1, 41.4562cm-1

82
1+
Rh 0.01722 0.80087 -0.02698
P -1.92794 -0.71746 0.07714
P 1.90355 -0.75779 0.11328
C 1.44955 2.45793 -0.14214
H 2.50724 2.20699 -0.17684
C 0.71147 3.26872 -1.22970
H 1.28201 3.50725 -2.13617
C -0.52245 3.49979 0.66402
H -1.06994 3.94860 1.50242
C 2.93967 -0.71367 1.75492
C 3.07046 -0.61361 -1.47271
C 1.41470 -2.57071 0.04547
H 2.32515 -3.18273 -0.02151
H 0.96447 -2.79747 1.02426
C -0.90184 -3.45261 -0.59928
H -0.73084 -4.42742 -0.10517
H -1.55699 -3.67110 -1.45950
C -1.63544 -2.55907 0.40921
H -1.09438 -2.55454 1.37184
H -2.61858 -3.00362 0.61969
C 0.12828 4.43844 -0.38916
H 0.91216 5.09190 0.03138
H -0.61499 5.04225 -0.93793
C 0.66474 2.58824 1.02810
H 0.97647 2.38265 2.05572
C -2.89369 -0.33142 1.75992
C -0.53573 2.37974 -1.41277
H -0.87451 2.00092 -2.38109
C -3.10735 -0.71862 -1.47106
C 0.43353 -2.89803 -1.09980
H 0.22849 -1.99614 -1.70152
H 0.88919 -3.62668 -1.79116
C -1.31674 2.53623 -0.24232
H -2.38833 2.37407 -0.16742
C 3.59592 0.66054 1.99648
H 4.38309 0.89841 1.26980
H 4.06942 0.65006 2.99400
H 2.86412 1.48010 1.99743
C 2.19702 -0.08291 -2.63002

H 1.36859 -0.76445 -2.87791
H 2.82115 0.01905 -3.53602
H 1.76650 0.90310 -2.39717
C 4.25697 0.34912 -1.26790
H 3.95758 1.36763 -0.98263
H 4.79761 0.43651 -2.22693
H 4.97870 -0.02425 -0.52651
C -2.21532 -1.04825 -2.68966
H -1.34770 -0.36903 -2.75486
H -2.80901 -0.92217 -3.61223
H -1.84439 -2.08232 -2.68330
C 3.65604 -1.98368 -1.87257
H 4.25708 -2.44146 -1.07168
H 4.32816 -1.83359 -2.73565
H 2.88687 -2.70224 -2.19064
C -4.22940 -1.76453 -1.33687
H -3.85048 -2.78529 -1.17544
H -4.81599 -1.78256 -2.27231
H -4.92865 -1.51832 -0.52229
C 1.91979 -0.94679 2.89112
H 1.13184 -0.17614 2.88949
H 2.44270 -0.89085 3.86195
H 1.43766 -1.93625 2.84326
C -3.74334 0.66112 -1.73709
H -4.37608 1.01808 -0.91437
H -4.39043 0.57409 -2.62768
H -2.99368 1.43092 -1.96531
C 4.02390 -1.80754 1.79389
H 3.60953 -2.82300 1.70049
H 4.54447 -1.75971 2.76668
H 4.78763 -1.67002 1.01288
C -3.84791 0.87215 1.65692
H -3.35841 1.78723 1.29934
H -4.23341 1.09284 2.66806
H -4.72191 0.65989 1.02325
C -1.78366 -0.00438 2.77974
H -1.09906 -0.85390 2.93473
H -2.23989 0.23220 3.75777
H -1.18557 0.86572 2.45605
C -3.71980 -1.52342 2.29079
H -4.47542 -1.87783 1.57297
H -4.26387 -1.18649 3.19054
H -3.10042 -2.37762 2.59966

1b+
SCF(BP86/BS1) = -1182.31559341
G(298 K) = -1181.656104
SCF(BS2) = -1851.97876633
Lowest Frequencies = 38.0105cm-1, 55.5624cm-1

82
1b+
Rh 0.00482 0.29499 0.01028
P -2.28801 -0.45665 0.35905
P 2.30125 -0.47289 0.19994
C 3.01325 -1.56749 -1.24642
C 1.83325 -2.09471 -2.08540
C 3.78566 -2.79254 -0.71304
C 3.91588 -0.70617 -2.15153
C 3.74724 0.46494 1.12502

C 3.23654 0.89200 2.51968
 C 4.93863 -0.48863 1.35136
 C 4.23765 1.70314 0.34926
 C 1.62578 -1.59717 1.51478
 C 0.34054 -0.80468 1.83547
 C -0.77869 -1.73595 2.32567
 C -2.18345 -1.19832 2.08106
 C -2.69751 -1.94157 -0.85704
 C -2.40688 -1.48646 -2.30133
 C -4.14440 -2.46489 -0.77040
 C -1.78221 -3.13521 -0.51601
 C -3.90440 0.64701 0.54112
 C -4.41727 1.10519 -0.83679
 C -5.01843 -0.11298 1.30039
 C -3.57955 1.89321 1.39078
 H 1.22210 -1.28891 -2.51846
 H 2.24041 -2.69676 -2.91668
 H 1.17062 -2.75405 -1.50256
 H 3.16882 -3.41265 -0.04324
 H 4.06843 -3.42679 -1.57144
 H 4.71016 -2.53114 -0.18541
 H 4.85434 -0.41363 -1.65806
 H 4.19071 -1.29161 -3.04606
 H 3.40760 0.20812 -2.50091
 H 3.06295 0.02989 3.18123
 H 4.01357 1.51501 2.99540
 H 2.31184 1.48577 2.49482
 H 5.48695 -0.70934 0.42429
 H 5.65032 0.00630 2.03558
 H 4.64096 -1.43763 1.82536
 H 3.48425 2.49930 0.30028
 H 5.11542 2.12092 0.87257
 H 4.55262 1.46680 -0.67679
 H 1.36170 -2.54862 1.02218
 H 2.29831 -1.83096 2.35909
 H 0.53820 -0.01686 2.58319
 H -0.67291 -2.71355 1.83031
 H -0.64165 -1.93223 3.40767
 H -2.96452 -1.96313 2.22580
 H -2.40693 -0.36536 2.76946
 H -1.35251 -1.19491 -2.43017
 H -2.60825 -2.32612 -2.98936
 H -3.04750 -0.64808 -2.61705
 H -4.89450 -1.73357 -1.10147
 H -4.23169 -3.33780 -1.44096
 H -4.40425 -2.81282 0.24170
 H -2.05453 -3.60354 0.44265
 H -1.90055 -3.90211 -1.30137
 H -0.71730 -2.85878 -0.48440
 H -4.79141 0.27445 -1.45249
 H -5.26001 1.80381 -0.69188
 H -3.64569 1.63954 -1.41173
 H -4.73033 -0.34431 2.33720
 H -5.89838 0.55203 1.35546
 H -5.34646 -1.03841 0.81696
 H -3.00953 2.64290 0.83313
 H -4.53069 2.36736 1.68825
 H -3.03903 1.65264 2.32116
 H -0.05544 -1.09734 -0.66019
 C -1.08034 2.92617 -0.89538
 C -0.51276 2.58042 0.50345

C 0.85713 2.49703 0.34603
 C 1.15839 2.78003 -1.14202
 C 0.05690 3.83442 -1.44157
 C -0.81673 1.63856 -1.70921
 C 0.56422 1.54457 -1.85625
 H -2.10463 3.31702 -0.93014
 H -1.04593 2.64441 1.44950
 H 1.59407 2.50613 1.14402
 H 2.19761 3.02431 -1.39331
 H -0.04708 4.05813 -2.51653
 H 0.17967 4.76793 -0.86700
 H -1.56912 1.10828 -2.29016
 H 1.10282 0.92901 -2.57690

4+
 SCF(BP86/BS1)= -1183.55210170
 G(298 K) = -1182.870542
 SCF(BS2) = -1853.21715042
 Lowest Frequencies = 30.6379cm⁻¹,
 43.6301cm⁻¹

84
 4+
 Rh 0.03087 0.59427 0.12516
 P 1.71995 -0.93168 -0.00949
 P -1.90756 -0.85326 0.00229
 C 0.52599 3.33041 1.14604
 H 0.62735 3.23846 2.23719
 C 1.33908 2.33451 0.31725
 H 2.40617 2.19206 0.49493
 C -3.10233 -0.05928 -1.33930
 C 1.21618 -2.75373 -0.00732
 H 2.13171 -3.31225 0.23690
 H 0.56726 -2.83111 0.88271
 C -4.27316 -1.51698 1.58962
 H -4.35165 -2.46769 1.03797
 H -4.93078 -0.77820 1.10820
 H -4.67454 -1.69540 2.60304
 C 2.93188 -0.77600 -1.52416
 C -2.81763 -1.03102 1.70831
 C -1.78824 -2.63049 -0.59073
 H -1.52528 -3.24982 0.28008
 H -2.79542 -2.94964 -0.89600
 C 2.68845 -0.88321 1.72470
 C -0.87477 3.04722 0.55612
 H -1.26220 2.01410 0.81252
 H -1.67576 3.72668 0.89478
 C 2.05525 -0.78929 -2.79636
 H 1.27331 -0.01382 -2.76187
 H 1.56663 -1.75747 -2.96827
 H 2.69760 -0.59018 -3.67192
 C -3.76636 1.21330 -0.77988
 H -3.03356 1.95541 -0.43183
 H -4.46667 1.00164 0.04157
 H -4.34961 1.69032 -1.58707
 C 0.16158 4.69845 -0.84618
 H 0.87797 4.87774 -1.66284
 H -0.64558 5.44254 -0.94696
 C 3.91509 -1.96413 -1.53741
 H 3.41380 -2.94034 -1.61594
 H 4.56577 -1.97564 -0.64863

H	4.57319	-1.86659	-2.41865	C	4.25846	-2.19826	-1.40894
C	-2.76079	0.32202	2.44665	C	4.06539	0.27559	-1.89462
H	-3.27751	1.12808	1.90495	C	3.37482	-0.20766	1.61654
H	-1.71813	0.63573	2.62858	C	2.47335	-0.33834	2.86353
H	-3.25268	0.22007	3.43001	C	4.59601	-1.13244	1.77225
C	3.74750	0.53403	-1.52656	C	3.84474	1.25377	1.50828
H	4.49392	0.57878	-0.72473	C	1.63498	-2.42234	0.57780
H	3.12177	1.43337	-1.46810	C	0.21844	-1.96799	0.96640
H	4.29837	0.58612	-2.48201	C	-0.88198	-2.98817	0.68622
C	-0.75460	-2.82633	-1.71736	C	-2.23370	-2.36695	1.01833
H	-1.17374	-3.48275	-2.49896	C	-3.24540	-1.05679	-1.52697
H	-0.53259	-1.86543	-2.20912	C	-4.00432	0.17580	-2.05633
C	0.55165	-3.44396	-1.20912	C	-4.24316	-2.22451	-1.38485
H	1.26929	-3.53225	-2.04170	C	-2.16875	-1.44853	-2.56118
H	0.34850	-4.48362	-0.88931	C	-3.43731	0.31303	1.41092
C	-2.22609	0.32586	-2.55327	C	-3.98763	1.63006	0.82807
H	-1.86386	-0.55929	-3.09844	C	-4.62250	-0.52104	1.93590
H	-1.34731	0.91974	-2.25360	C	-2.46670	0.64298	2.56920
H	-2.83191	0.91929	-3.26133	H	1.57526	-0.47756	-2.81832
C	0.81750	4.75000	0.56986	H	2.80665	-1.51712	-3.57427
H	0.35283	5.52422	1.20217	H	1.66088	-2.21338	-2.41089
H	1.89858	4.95720	0.53525	H	3.74650	-3.12752	-1.11259
C	3.22883	-2.26500	2.15351	H	4.71429	-2.37934	-2.39815
H	3.93115	-2.69877	1.42401	H	5.07822	-2.01646	-0.70191
H	3.78850	-2.13037	3.09576	H	4.89455	0.47200	-1.19782
C	-4.20000	-1.02638	-1.82486	H	4.50839	0.15313	-2.89842
H	-4.84757	-1.39782	-1.01839	H	3.41456	1.16371	-1.92535
H	-3.78760	-1.88867	-2.37115	H	2.19029	-1.38069	3.07693
H	-4.84624	-0.48314	-2.53684	H	3.03074	0.03549	3.73989
C	-0.44283	3.25667	-0.92000	H	1.55286	0.26443	2.77884
H	-1.21435	3.12493	-1.69114	H	5.36460	-0.92980	1.01157
C	-2.02245	-2.05898	2.54325	H	5.05868	-0.94322	2.75703
H	-0.94159	-1.84374	2.54475	H	4.33509	-2.20201	1.73327
H	-2.17547	-3.09447	2.20223	H	3.00231	1.95827	1.52569
H	-2.36644	-2.01136	3.59105	H	4.48224	1.48221	2.38040
C	0.73911	2.29464	-0.97537	H	4.44490	1.44638	0.60747
H	1.26008	2.09285	-1.91542	H	1.60387	-3.04229	-0.33372
C	1.66029	-0.41103	2.77320	H	2.20522	-2.97676	1.34394
H	0.83903	-1.13374	2.89820	H	0.18547	-1.69076	2.03953
H	2.15916	-0.31290	3.75428	H	-0.84478	-3.31113	-0.37019
C	3.88314	0.08819	1.71865	H	-0.72331	-3.90124	1.29552
H	3.62387	1.10404	1.39337	H	-3.09462	-3.00449	0.77477
H	4.26316	0.16919	2.75232	H	-2.27843	-2.16039	2.10065
H	1.22176	0.56598	2.50372	H	-3.39391	1.09147	-2.07072
H	4.71525	-0.28046	1.10060	H	-4.31401	-0.02588	-3.09664
H	2.43358	-2.99637	2.35940	H	-4.91813	0.37845	-1.48060
				H	-4.98089	-2.06217	-0.58393
				H	-4.80416	-2.32317	-2.33056
				H	-3.74073	-3.18803	-1.20836
				H	-1.55989	-2.30704	-2.23325
				H	-2.66892	-1.74181	-3.50133
				H	-1.49414	-0.60771	-2.79074
				H	-4.88125	1.46576	0.21113
				H	-4.28991	2.28662	1.66272
				H	-3.25268	2.17742	0.22458
				H	-4.31476	-1.45110	2.43649
				H	-5.17577	0.08021	2.67910
				H	-5.33326	-0.77580	1.13419
				H	-1.63993	1.29203	2.23340
				H	-3.01536	1.18489	3.35941
				H	-2.03046	-0.25599	3.03525
4b+							
SCF(BP86/BS1)=	-1183.54805034						
G(298 K) =	-1182.870933						
SCF(BS2) =	-1853.21106099						
Lowest Frequencies =	19.4840cm ⁻¹ ,						
	28.3997cm ⁻¹						
84							
4b+							
Rh	-0.02005	-0.07458	0.01851				
P	-2.33896	-0.68791	0.16385				
P	2.28624	-0.74185	0.10343				
C	3.29134	-1.00307	-1.52700				
C	2.26266	-1.31670	-2.63468				

H	-0.04275	-0.87494	-1.25817
C	1.39725	2.86531	-0.48266
C	0.98491	4.20779	-1.17619
C	-0.49475	4.40273	-0.72044
C	-0.75360	3.14475	0.17296
C	0.62425	2.98097	0.84965
C	0.58815	1.78777	-1.19630
C	-0.74894	1.96711	-0.80678
H	2.48157	2.70623	-0.42802
H	1.62821	5.02791	-0.81813
H	-0.61451	5.32021	-0.12137
H	-1.61977	3.23883	0.84086
H	0.69485	2.06710	1.47402
H	0.91784	3.85055	1.45970
H	0.88400	1.41775	-2.18248
H	-1.59278	1.78206	-1.47502
H	-1.20351	4.46346	-1.56146
H	1.09747	4.15458	-2.27053

2b+ (exo, syn)

SCF(BP86/BS1)= -1184.75919219

G(298 K) = -1184.056797

SCF(BS2) = -1854.42636484

Lowest Frequencies = 30.1674cm⁻¹,

48.4401cm⁻¹

86

2b+ (exo, syn)

Rh	-0.03564	0.42565	0.21258
P	1.79399	-0.94322	0.01603
P	-1.70364	-1.12567	0.02535
C	-1.30623	3.70467	-0.42867
H	-2.30519	3.58190	-0.87315
C	-0.94429	2.61278	0.61486
H	-1.43067	2.75218	1.59214
C	-2.91483	-0.58603	-1.42081
C	1.68060	-2.82856	0.00884
H	2.71463	-3.19264	0.10557
H	1.19571	-3.04313	0.97753
C	-4.01630	-2.02298	1.55322
H	-3.89635	-3.02573	1.11278
H	-4.75030	-1.46516	0.95339
H	-4.45790	-2.16274	2.55587
C	2.82572	-0.47167	-1.56598
C	-2.67489	-1.28188	1.70490
C	-1.35099	-2.92453	-0.36789
H	-0.93887	-3.36669	0.55128
H	-2.32263	-3.41444	-0.53247
C	2.88121	-0.72850	1.64505
C	-0.10295	3.62750	-1.39301
H	-0.01411	2.64729	-1.89526
H	-0.10428	4.42667	-2.15108
C	1.97840	-0.83790	-2.80276
H	0.98174	-0.36948	-2.75372
H	1.85990	-1.92148	-2.93775
H	2.48693	-0.45353	-3.70459
C	-3.84562	0.55295	-0.96168
H	-3.29263	1.42748	-0.58326
H	-4.56432	0.23807	-0.19158
H	-4.43129	0.89982	-1.83108
C	0.47783	5.16198	0.37002

H	0.83538	5.26301	1.40770
H	0.87005	6.02336	-0.19343
C	4.17008	-1.21968	-1.60966
H	4.05048	-2.31243	-1.53459
H	4.86008	-0.88844	-0.81866
H	4.66283	-1.01407	-2.57633
C	-2.89605	0.11693	2.31429
H	-3.49102	0.78324	1.67343
H	-1.93034	0.60422	2.52943
H	-3.43816	0.00976	3.27025
C	3.06410	1.05043	-1.63627
H	3.63124	1.45253	-0.78681
H	2.11093	1.59650	-1.71886
H	3.64441	1.27061	-2.54963
C	-0.39086	-3.14336	-1.55295
H	-0.81949	-3.88479	-2.24853
H	-0.27609	-2.21608	-2.13461
C	0.99628	-3.62711	-1.11452
H	1.65968	-3.67938	-1.99384
H	0.91395	-4.66774	-0.74884
C	-2.04397	-0.05479	-2.58077
H	-1.43574	-0.84650	-3.04388
H	-1.36003	0.74228	-2.24212
H	-2.70224	0.35544	-3.36758
C	-1.07882	5.07348	0.26323
H	-1.48336	5.88251	-0.36553
H	-1.58466	5.13718	1.24036
H	4.51874	-1.59880	2.75220
C	-3.76764	-1.76114	-1.93809
H	-4.39134	-2.22052	-1.15716
H	-3.15345	-2.54686	-2.40478
H	-4.44974	-1.38235	-2.71943
C	0.95409	3.84044	-0.28771
H	2.00841	3.84487	-0.60126
C	-1.77233	-2.07027	2.67895
H	-0.76089	-1.63881	2.72820
H	-1.69651	-3.13876	2.42448
H	-2.20936	-2.01359	3.69120
C	0.60221	2.69190	0.69524
H	0.97291	2.84532	1.72048
H	1.37357	-1.72477	2.90952
C	1.88268	-0.75117	2.82117
H	1.10809	0.02865	2.71289
H	2.42869	-0.58262	3.76667
C	3.62658	0.61887	1.65308
H	2.96723	1.47890	1.46257
H	4.45479	0.64334	0.92910
H	4.06878	0.76873	2.65371
C	3.91697	-1.85277	1.86192
H	4.61718	-1.96861	1.02159
H	3.44897	-2.82725	2.06598
H	1.21488	1.77734	0.30764
H	-1.42659	1.62775	0.21326

2b+ (endo, syn)

SCF(BP86/BS1)= -1184.76424864

G(298 K) = -1184.070557

SCF(BS2) = -1854.42857842

Lowest Frequencies = 21.0190cm⁻¹,

28.4368cm⁻¹

86				H	-1.77131	0.70412	2.52552
2b+ (endo, syn)				H	-3.00605	0.05261	3.63611
Rh	0.06628	-0.42239	-0.10403	H	-1.75185	-1.02391	2.98475
P	2.35527	-0.86621	0.09719	C	3.70792	0.84596	-1.73676
P	-2.23840	-0.94328	0.06414	H	4.48991	1.16476	-1.03067
C	1.01493	3.44299	-1.00166	H	4.11058	0.99075	-2.75464
H	1.31483	3.53919	-2.05864	H	2.84081	1.51536	-1.62473
C	0.25095	4.70138	-0.52384	C	-4.28691	-1.64944	1.95302
H	0.70983	5.64436	-0.85656	H	-3.72931	-2.56027	2.22129
C	-1.29938	3.05867	-0.30854	H	-4.87204	-1.35481	2.84184
H	-2.23831	2.50696	-0.45896	H	-5.00289	-1.90579	1.15999
C	-3.36060	-0.48020	1.56481	C	3.00852	1.39643	1.66232
C	-3.18446	-1.06433	-1.60781	H	1.93135	1.62937	1.69354
C	-1.59342	-2.67356	0.45350	H	3.46850	1.81498	2.57455
H	-2.13237	-3.49923	-0.04327	H	3.45201	1.91799	0.80157
H	-1.66347	-2.82420	1.54315	C	2.60906	-0.75684	2.87713
C	0.94496	-3.14433	0.87100	H	2.80589	-1.83737	2.95763
H	0.81376	-2.86239	1.93004	H	3.03732	-0.27904	3.77530
H	0.83511	-4.24646	0.82144	H	1.51790	-0.59443	2.90626
C	2.33715	-2.73434	0.36985	C	4.76297	-0.42979	1.61906
H	3.15205	-3.04633	1.04190	H	5.29153	0.09507	0.80888
H	2.53082	-3.20000	-0.61070	H	5.20409	-0.08670	2.57128
C	-1.17392	4.41073	-1.04825	H	4.97319	-1.50838	1.53211
H	-1.22605	4.31760	-2.14644	H	0.99146	4.36595	1.53431
H	-1.92144	5.15051	-0.71749	H	-0.67488	2.62495	1.76744
C	-0.05158	2.30700	-0.82845	H	1.92854	3.26894	-0.41126
H	-0.24859	1.78402	-1.78148	H	0.31095	1.56587	-0.05237
C	3.25435	-0.12445	1.62562				
C	0.05071	4.60301	1.00942				
H	-0.31632	5.55837	1.41734				
C	3.32264	-0.63206	-1.55307				
C	-0.13520	-2.47433	0.02240				
H	0.05043	-0.32128	1.41056				
H	-0.00097	-2.75870	-1.04366				
C	-1.02703	3.47558	1.15728				
H	-1.94615	3.85799	1.63123				
C	-4.19720	0.77278	1.25027				
H	-4.96060	0.58346	0.48009				
H	-4.73073	1.08319	2.16561				
H	-3.57205	1.62076	0.92969				
C	-2.22486	-1.77221	-2.58880				
H	-2.01562	-2.81567	-2.30436				
H	-2.68851	-1.79119	-3.59043				
H	-1.26340	-1.23565	-2.68666				
C	-3.44954	0.35964	-2.13577				
H	-2.51371	0.93344	-2.23718				
H	-3.91126	0.29353	-3.13656				
H	-4.13578	0.93199	-1.49509				
C	2.29844	-1.01933	-2.64500				
H	1.40929	-0.36010	-2.61851				
H	2.75952	-0.90441	-3.64183				
H	1.95847	-2.06512	-2.55981				
C	-4.49479	-1.86104	-1.50223				
H	-4.91471	-2.00463	-2.51362				
H	-4.34317	-2.86129	-1.06446				
H	-5.25561	-1.33125	-0.90904				
C	4.57019	-1.52601	-1.67189				
H	4.33601	-2.59822	-1.58287				
H	5.02220	-1.37582	-2.66835				
H	5.33699	-1.27939	-0.92421				
C	-2.40587	-0.17095	2.73672				

(iii) Figure S48

4+

SCF(BP86/BS1)= -1183.55210176
G(298 K) = -1182.870537
SCF(BS2) = -1853.21714915
Lowest Frequencies = 30.6907cm⁻¹,
43.6070cm⁻¹

84

4+

Rh	0.03093	0.59411	0.12518
P	1.71948	-0.93223	-0.00967
P	-1.90795	-0.85272	0.00203
C	0.52825	3.33021	1.14634
H	0.63019	3.23823	2.23744
C	1.34011	2.33368	0.31711
H	2.40722	2.19054	0.49416
C	-3.10270	-0.05754	-1.33893
C	1.21506	-2.75411	-0.00807
H	2.13033	-3.31306	0.23619
H	0.56593	-2.83153	0.88181
C	-4.27352	-1.51622	1.58967
H	-4.35262	-2.46664	1.03761
H	-4.93093	-0.77691	1.10878
H	-4.67471	-1.69491	2.60313
C	2.93174	-0.77677	-1.52413
C	-2.81773	-1.03103	1.70817
C	-1.78928	-2.62966	-0.59203
H	-1.52679	-3.24963	0.27846
H	-2.79650	-2.94821	-0.89776
C	2.68760	-0.88436	1.72476
C	-0.87309	3.04814	0.55728
H	-1.26109	2.01540	0.81408
H	-1.67329	3.72837	0.89628
C	2.05533	-0.78978	-2.79651
H	1.27339	-0.01431	-2.76197
H	1.56673	-1.75790	-2.96878
H	2.69783	-0.59045	-3.67190
C	-3.76569	1.21523	-0.77873
H	-3.03226	1.95664	-0.43051
H	-4.46591	1.00366	0.04282
H	-4.34883	1.69306	-1.58551
C	0.16372	4.69845	-0.84572
H	0.87976	4.87717	-1.66282
H	-0.64294	5.44314	-0.94605
C	3.91470	-1.96508	-1.53720
H	3.41324	-2.94120	-1.61565
H	4.56535	-1.97663	-0.64840
H	4.57285	-1.86777	-2.41844
C	-2.76002	0.32160	2.44720
H	-3.27643	1.12821	1.90602
H	-1.71717	0.63469	2.62907
H	-3.25177	0.21941	3.43061
C	3.74754	0.53315	-1.52651
H	4.49304	0.57852	-0.72387
H	3.12175	1.43255	-1.46954
H	4.29949	0.58447	-2.48139
C	-0.75540	-2.82524	-1.71850
H	-1.17455	-3.48105	-2.50060
H	-0.53287	-1.86413	-2.20963

C	0.55046	-3.44367	-1.21020
H	1.26823	-3.53206	-2.04266
H	0.34672	-4.48333	-0.89077
C	-2.22658	0.32753	-2.55300
H	-1.86492	-0.55764	-3.09851
H	-1.34743	0.92091	-2.25339
H	-2.83229	0.92146	-3.26074
C	0.82054	4.74954	0.56993
H	0.35684	5.52415	1.20248
H	1.90175	4.95592	0.53465
H	3.78650	-2.13238	3.09599
C	-4.20108	-1.02375	-1.82454
H	-4.84855	-1.39528	-1.01804
H	-3.78938	-1.88598	-2.37147
H	-4.84731	-0.47978	-2.53600
C	-0.44183	3.25712	-0.91912
H	-1.21389	3.12593	-1.68981
C	-2.02285	-2.05982	2.54236
H	-0.94186	-1.84521	2.54364
H	-2.17654	-3.09506	2.20086
H	-2.36647	-2.01254	3.59029
C	0.73943	2.29430	-0.97523
H	1.25983	2.09238	-1.91558
H	0.83788	-1.13380	2.89808
C	1.65960	-0.41162	2.77317
H	1.22172	0.56568	2.50372
H	2.15848	-0.31384	3.75428
C	3.88283	0.08638	1.71897
H	3.62395	1.10257	1.39438
H	4.71460	-0.28232	1.10051
H	4.26314	0.16658	2.75260
C	3.22707	-2.26652	2.15351
H	3.92944	-2.70051	1.42417
H	2.43139	-2.99749	2.35895

TS(4+-2b+) 1

SCF(BP86/BS1)= -1184.70817528
G(298 K) = -1184.014586
SCF(BS2) = -1854.37303843
Lowest Frequencies = -266.3539cm⁻¹,
23.6067cm⁻¹

86

TS(4+-2b+) 1

Rh	-0.06312	0.54101	-0.35235
P	-1.39297	-1.27781	0.05878
P	2.17886	-0.35545	0.10094
C	-1.70192	3.14561	-1.31724
H	-1.81269	3.12178	-2.41127
C	-1.84115	1.80232	-0.59181
H	-2.75997	1.23180	-0.74516
C	3.04089	1.01632	1.18027
C	-0.40345	-2.86720	0.32810
H	-1.09322	-3.69183	0.10051
H	0.33033	-2.84517	-0.49643
C	4.55602	-1.60169	-1.07025
H	4.31416	-2.58826	-0.64716
H	5.22266	-1.08114	-0.36968
H	5.13136	-1.78435	-1.99487
C	-2.68171	-1.25963	1.53546
C	3.29999	-0.78192	-1.43520

C 2.42168 -1.89049 1.16142
 H 2.52954 -2.74448 0.47191
 H 3.39878 -1.78159 1.65836
 C -2.31379 -1.77257 -1.64653
 C -0.37016 3.68896 -0.75934
 H 0.51871 3.14869 -1.12054
 H -0.21923 4.76032 -0.96955
 C -1.91450 -0.93632 2.83800
 H -1.26409 -0.05377 2.73651
 H -1.29633 -1.77329 3.18644
 H -2.64812 -0.72410 3.63484
 C 2.83105 2.39046 0.51955
 H 1.76065 2.62356 0.42420
 H 3.29794 2.47384 -0.47157
 H 3.27395 3.17323 1.16088
 C -2.05720 4.26167 0.83084
 H -2.69900 3.91731 1.65777
 H -1.80472 5.31642 1.02836
 C -3.33691 -2.65330 1.65143
 H -2.61035 -3.46821 1.78637
 H -3.97245 -2.89012 0.78444
 H -3.99193 -2.65447 2.54044
 C 3.73588 0.49076 -2.18442
 H 4.48868 1.06804 -1.62702
 H 2.89123 1.15842 -2.42037
 H 4.19595 0.20048 -3.14521
 C -3.80908 -0.21425 1.37993
 H -4.44460 -0.38552 0.50405
 H -3.44225 0.81855 1.34455
 H -4.45950 -0.29550 2.26854
 C 1.30135 -2.17126 2.17596
 H 1.74381 -2.56065 3.10928
 H 0.78153 -1.23921 2.44660
 C 0.29016 -3.19490 1.65854
 H -0.46432 -3.40142 2.43514
 H 0.81294 -4.15797 1.50257
 C 2.31992 1.02480 2.54592
 H 2.52255 0.11763 3.13576
 H 1.22839 1.13518 2.42705
 H 2.68628 1.88408 3.13510
 C -2.71525 4.07944 -0.57615
 H -2.80299 5.04162 -1.10654
 H -3.72355 3.63824 -0.52406
 H -3.03781 -3.48288 -2.73625
 C 4.54367 0.77791 1.40306
 H 5.13174 0.89798 0.48124
 H 4.76648 -0.21100 1.83491
 H 4.91368 1.52998 2.12269
 C -0.73358 3.42363 0.72078
 H 0.01824 3.66590 1.48569
 C 2.41380 -1.62786 -2.37169
 H 1.54974 -1.05331 -2.73849
 H 2.04358 -2.54699 -1.88537
 H 3.00419 -1.94407 -3.24970
 C -1.24986 1.98493 0.69725
 H -1.63449 1.56610 1.63036
 H -0.41346 -1.63840 -2.75635
 C -1.43878 -1.24091 -2.79591
 H -1.39448 -0.14117 -2.79507
 H -1.87801 -1.56095 -3.75782
 C -3.72204 -1.16411 -1.78324

H -3.74506 -0.07274 -1.65571
 H -4.44879 -1.62055 -1.09531
 H -4.08004 -1.36971 -2.80761
 C -2.45422 -3.30210 -1.81659
 H -2.99989 -3.78659 -0.99243
 H -1.48742 -3.80925 -1.95197
 H 0.17249 1.18841 -2.26672
 H 0.88638 1.38484 -2.50528

Int(4+-2b+)1

SCF(BP86/BS1)= -1184.72468794

G(298 K) = -1184.027873

SCF(BS2) = -1854.38927882

Lowest Frequencies = 22.3010cm⁻¹,
41.8064cm⁻¹

86

Int(4+-2b+)1

Rh 0.02717 0.59901 -0.24874
 P -1.40991 -1.39770 0.02890
 P 2.23601 -0.31011 0.03186
 C -1.98229 3.13963 -1.17885
 H -2.20553 3.06791 -2.25283
 C -1.85669 1.81973 -0.41419
 H -2.69753 1.12796 -0.44701
 C 3.19527 0.76907 1.34535
 C -0.45854 -3.03307 0.05507
 H -1.18661 -3.82911 -0.15562
 H 0.18150 -2.95759 -0.84268
 C 4.47329 -1.29709 -1.56112
 H 4.22661 -2.34256 -1.32133
 H 5.21931 -0.94407 -0.83632
 H 4.95814 -1.30220 -2.55306
 C -2.61426 -1.50643 1.55381
 C 3.22464 -0.39383 -1.63422
 C 2.44103 -2.05114 0.70317
 H 2.37891 -2.72369 -0.16901
 H 3.47226 -2.14213 1.07970
 C -2.38188 -1.66586 -1.68033
 C -0.71732 3.92117 -0.76761
 H 0.21608 3.56675 -1.22846
 H -0.80502 4.99857 -0.98017
 C -1.75921 -1.31450 2.82695
 H -1.15146 -0.39510 2.78055
 H -1.08978 -2.16069 3.02912
 H -2.43452 -1.22203 3.69551
 C 3.04370 2.27795 1.06280
 H 2.00373 2.61616 1.20130
 H 3.38088 2.57411 0.05896
 H 3.66037 2.83377 1.79083
 C -2.28943 4.23997 0.98867
 H -2.77740 3.82058 1.88286
 H -2.18733 5.32546 1.14703
 C -3.32178 -2.87422 1.59379
 H -2.61831 -3.72062 1.62379
 H -3.99999 -3.01613 0.73780
 H -3.93783 -2.93214 2.50838
 C 3.63785 1.01074 -2.11186
 H 4.42046 1.45703 -1.48017
 H 2.78676 1.70980 -2.16338
 H 4.05157 0.93147 -3.13244

C	-3.67794	-0.38728	1.55631
H	-4.35974	-0.42828	0.69865
H	-3.23416	0.61698	1.60268
H	-4.29445	-0.50930	2.46431
C	1.40775	-2.45513	1.77426
H	1.93038	-2.88928	2.64361
H	0.87815	-1.56635	2.15192
C	0.37787	-3.46679	1.26751
H	-0.28969	-3.75648	2.09644
H	0.90019	-4.39797	0.97710
C	2.55280	0.48413	2.71998
H	2.75201	-0.53679	3.07891
H	1.46174	0.64969	2.70072
H	2.98324	1.17934	3.46206
C	-3.05385	3.91943	-0.33739
H	-3.34838	4.84163	-0.86405
H	-3.96698	3.32522	-0.17332
H	-3.19219	-3.20230	-2.95774
C	4.69390	0.41775	1.40209
H	5.23638	0.74735	0.50332
H	4.88037	-0.65795	1.54903
H	5.14651	0.94017	2.26319
C	-0.86322	3.61537	0.74071
H	-0.08283	3.98845	1.41969
C	2.23500	-0.98973	-2.65614
H	1.36204	-0.33240	-2.79834
H	1.87186	-1.98781	-2.35557
H	2.73937	-1.10684	-3.63158
C	-1.16582	2.12216	0.78609
H	-1.34938	1.64488	1.75636
H	-0.52112	-1.57455	-2.85109
C	-1.47945	-1.04006	-2.76277
H	-1.26603	0.02433	-2.55526
H	-1.98327	-1.10688	-3.74388
C	-3.76608	-0.98955	-1.71867
H	-3.74574	0.08612	-1.49724
H	-4.48881	-1.47800	-1.04808
H	-4.16272	-1.09093	-2.74433
C	-2.60257	-3.15475	-2.02559
H	-3.17481	-3.69655	-1.25628
H	-1.66582	-3.69738	-2.21845
H	0.71056	1.70723	-1.20867
H	1.03732	1.87856	-0.32255

TS(4+-2b+) 2

SCF(BP86/BS1) = -1184.72429217

G(298 K) = -1184.029159

SCF(BS2) = -1854.38841827

Lowest Frequencies = -321.5858cm-
1, 23.4894cm-1

86

TS(4+-2b+) 2

Rh -0.05358 0.62401 0.12382

P 1.45002 -1.40283 -0.00168

P -2.24343 -0.33661 -0.00028

C 1.94418 3.14838 1.12345

H 2.17877 3.03270 2.19112

C 1.83772 1.86362 0.30185

H 2.67532 1.16820 0.30568

C -3.27668 0.61181 -1.35499

C	0.52814	-3.05378	0.08195
H	1.27406	-3.83071	0.30211
H	-0.08143	-2.94640	0.99748
C	-4.39347	-1.24288	1.74394
H	-4.13590	-2.29758	1.56300
H	-5.17484	-0.95104	1.02947
H	-4.83727	-1.19036	2.75352
C	2.61278	-1.56451	-1.55234
C	-3.16069	-0.31583	1.70630
C	-2.41005	-2.13027	-0.52794
H	-2.28987	-2.72831	0.39105
H	-3.44957	-2.28814	-0.85656
C	2.47206	-1.56587	1.68843
C	0.65767	3.91657	0.75649
H	-0.26243	3.50705	1.19955
H	0.71692	4.98420	1.02144
C	1.71708	-1.45175	-2.80703
H	1.09747	-0.53832	-2.78892
H	1.05540	-2.31653	-2.94633
H	2.36438	-1.39318	-3.69967
C	-3.17062	2.14178	-1.18955
H	-2.14696	2.50326	-1.38076
H	-3.48983	2.50051	-0.20073
H	-3.82593	2.61954	-1.93893
C	2.21008	4.35132	-0.99537
H	2.69925	3.98423	-1.91153
H	2.08412	5.44048	-1.10222
C	3.35615	-2.91281	-1.55145
H	2.67399	-3.77661	-1.51928
H	4.06209	-2.99676	-0.71035
H	3.94659	-2.99990	-2.48058
C	-3.58032	1.11366	2.09444
H	-4.40274	1.49409	1.47017
H	-2.74232	1.82864	2.04485
H	-3.94074	1.10807	3.13795
C	3.63830	-0.41397	-1.63862
H	4.34685	-0.39190	-0.80203
H	3.15553	0.57097	-1.71557
H	4.23079	-0.55439	-2.55988
C	-1.39927	-2.57633	-1.60460
H	-1.93840	-3.05574	-2.43931
H	-0.88989	-1.70064	-2.03770
C	-0.34385	-3.55281	-1.07987
H	0.29998	-3.87690	-1.91495
H	-0.84768	-4.47307	-0.72853
C	-2.66616	0.24491	-2.72492
H	-2.83829	-0.80644	-3.00017
H	-1.58156	0.44840	-2.75493
H	-3.14322	0.86729	-3.50220
C	2.99243	3.98682	0.30831
H	3.27211	4.88974	0.87486
H	3.91626	3.41992	0.11093
H	3.35248	-3.02258	3.01340
C	-4.76329	0.20865	-1.33542
H	-5.28923	0.59425	-0.44912
H	-4.91721	-0.88084	-1.38790
H	-5.25890	0.64406	-2.22079
C	0.80094	3.68508	-0.76540
H	0.00484	4.06742	-1.42043
C	-2.12405	-0.82295	2.72950
H	-1.25655	-0.14670	2.79149

H -1.75758 -1.83545 2.48719
H -2.59167 -0.87629 3.72848
C 1.12685 2.20043 -0.87132
H 1.28780 1.74623 -1.85800
H 0.63513 -1.44227 2.89414
C 1.58695 -0.90453 2.76359
H 1.35783 0.14704 2.51820
H 2.11246 -0.92807 3.73516
C 3.84200 -0.85984 1.65444
H 3.79174 0.20351 1.38295
H 4.55605 -1.36435 0.98637
H 4.26994 -0.90369 2.67153
C 2.73444 -3.03122 2.09866
H 3.29413 -3.59821 1.33829
H 1.81526 -3.58209 2.34556
H -0.69834 1.63669 1.12465
H -1.04299 1.85585 0.05900

Int(4+-2b+) 2
SCF(BP86/BS1) = -1184.73481166
G(298 K) = -1184.038073
SCF(BS2) = -1854.39764296
Lowest Frequencies = 22.5341cm⁻¹,
42.6442cm⁻¹

86

Int(4+-2b+) 2
Rh -0.05013 0.52361 -0.29753
P 1.59057 -1.25075 0.13368
P -2.14505 -0.51404 0.13311
C 1.97393 3.08617 0.44254
H 2.72133 2.76024 1.17877
C 1.56922 2.06774 -0.63134
H 2.33678 1.64889 -1.28506
C -3.34417 -0.19657 -1.37135
C 0.86377 -2.81413 0.92200
H 1.71076 -3.40305 1.30214
H 0.34819 -2.41301 1.81367
C -4.13912 -0.74638 2.23629
H -3.87226 -1.79816 2.42082
H -4.96905 -0.72157 1.51879
H -4.52046 -0.34073 3.18941
C 2.52994 -1.85239 -1.46452
C -2.92795 0.10597 1.79700
C -2.22032 -2.38017 0.35354
H -1.99405 -2.57183 1.41596
H -3.26906 -2.68545 0.20873
C 2.87515 -0.81398 1.55615
C 0.61222 3.56546 0.99128
H 0.06383 2.79877 1.56374
H 0.69784 4.47946 1.60012
C 1.47435 -2.33880 -2.48202
H 0.69565 -1.57621 -2.66189
H 0.98665 -3.27695 -2.18817
H 1.97561 -2.52318 -3.44858
C -3.32852 1.28581 -1.79642
H -2.34526 1.59383 -2.18459
H -3.60703 1.97394 -0.98560
H -4.06019 1.42250 -2.61202
C 1.04382 4.85426 -0.97490
H 1.03533 4.88227 -2.07621

H 0.80168 5.86832 -0.61920
C 3.51581 -2.99313 -1.15698
H 3.03882 -3.83600 -0.63161
H 4.37313 -2.65018 -0.55811
H 3.92082 -3.38753 -2.10593
C -3.34658 1.58312 1.68735
H -4.22668 1.71889 1.04036
H -2.52986 2.22084 1.30997
H -3.62133 1.95407 2.69026
C 3.27274 -0.68707 -2.15129
H 4.02277 -0.19842 -1.51772
H 2.56846 0.07605 -2.51971
H 3.80118 -1.08648 -3.03486
C -1.26933 -3.17877 -0.55857
H -1.82907 -4.00022 -1.03822
H -0.90825 -2.54272 -1.37958
C -0.06300 -3.78108 0.16753
H 0.52993 -4.37114 -0.55202
H -0.42506 -4.51524 0.91205
C -2.80497 -1.03234 -2.55311
H -2.92224 -2.11534 -2.39826
H -1.74076 -0.82120 -2.76155
H -3.37345 -0.76836 -3.46204
C 2.39904 4.34739 -0.38326
H 2.85048 5.09827 0.28539
H 3.14390 4.10510 -1.15794
H 4.28892 -1.69377 2.93009
C -4.79726 -0.61649 -1.08230
H -5.29506 0.06808 -0.37913
H -4.88363 -1.64386 -0.69449
H -5.36946 -0.58168 -2.02603
C 0.00229 3.83402 -0.40152
H -1.04429 4.16957 -0.44218
C -1.83952 -0.02501 2.88470
H -1.00685 0.67938 2.72674
H -1.41943 -1.04278 2.95026
H -2.28537 0.20850 3.86725
C 0.32246 2.53676 -1.13824
H 0.02353 2.42135 -2.19114
H 1.22407 -0.57923 3.00966
C 2.09141 -0.01954 2.62230
H 1.73736 0.94874 2.23727
H 2.75712 0.18394 3.47992
C 4.02637 0.05842 1.02250
H 3.67457 0.90830 0.42336
H 4.74271 -0.52488 0.42385
H 4.58666 0.46792 1.88171
C 3.49528 -2.04806 2.24933
H 3.96410 -2.75384 1.54815
H 2.77182 -2.59734 2.87041
H -0.02195 0.85691 1.16319
H -1.20347 1.60835 -0.38330

TS(4+-2b+) 3
SCF(BP86/BS1) = -1184.73481066
G(298 K) = -1184.036434
SCF(BS2) = -1854.39765188
Lowest Frequencies = -34.9499cm⁻¹,
35.8649cm⁻¹

86

TS (4+-2b+) 3
 Rh -0.04609 0.51888 -0.30242
 P 1.59560 -1.24563 0.13575
 P -2.13940 -0.52270 0.13453
 C 1.96134 3.09321 0.42684
 H 2.71915 2.76791 1.15255
 C 1.54880 2.07687 -0.64657
 H 2.31128 1.67206 -1.31549
 C -3.34301 -0.21727 -1.36885
 C 0.87532 -2.80676 0.93390
 H 1.72494 -3.39027 1.31661
 H 0.35943 -2.40181 1.82365
 C -4.13208 -0.74372 2.24183
 H -3.86566 -1.79504 2.42968
 H -4.96394 -0.72095 1.52656
 H -4.51054 -0.33410 3.19441
 C 2.53148 -1.84945 -1.46340
 C -2.92126 0.10577 1.79604
 C -2.21186 -2.38768 0.36672
 H -1.98540 -2.57282 1.43026
 H -3.26016 -2.69535 0.22360
 C 2.88311 -0.79738 1.55117
 C 0.60396 3.56232 0.99498
 H 0.06651 2.78972 1.56996
 H 0.69222 4.47324 1.60803
 C 1.47466 -2.34607 -2.47461
 H 0.69137 -1.58839 -2.65525
 H 0.99294 -3.28525 -2.17426
 H 1.97334 -2.53257 -3.44208
 C -3.32640 1.26154 -1.80600
 H -2.34462 1.56341 -2.20270
 H -3.59823 1.95713 -0.99922
 H -4.06224 1.39379 -2.61856
 C 1.00488 4.86338 -0.96994
 H 0.98275 4.89614 -2.07095
 H 0.76197 5.87465 -0.60696
 C 3.52447 -2.98370 -1.15479
 H 3.05381 -3.82656 -0.62369
 H 4.38253 -2.63378 -0.56104
 H 3.92751 -3.38031 -2.10365
 C -3.33957 1.58240 1.67828
 H -4.21941 1.71492 1.03025
 H -2.52250 2.21775 1.29763
 H -3.61448 1.95912 2.67900
 C 3.26506 -0.68271 -2.15757
 H 4.01563 -0.18827 -1.52924
 H 2.55509 0.07586 -2.52440
 H 3.79097 -1.08230 -3.04257
 C -1.25991 -3.19075 -0.54053
 H -1.81766 -4.01904 -1.01068
 H -0.90434 -2.56108 -1.36875
 C -0.04899 -3.78208 0.18712
 H 0.54511 -4.37422 -0.52979
 H -0.40613 -4.51301 0.93719
 C -2.80810 -1.06313 -2.54533
 H -2.92606 -2.14474 -2.38138
 H -1.74429 -0.85476 -2.75840
 H -3.37889 -0.80596 -3.45477
 C 2.36973 4.36082 -0.39704
 H 2.82496 5.11085 0.27001
 H 3.10659 4.12663 -1.18179

H 4.30791 -1.66502 2.92147
 C -4.79584 -0.63314 -1.07290
 H -5.29132 0.05789 -0.37443
 H -4.88211 -1.65704 -0.67600
 H -5.37025 -0.60592 -2.01555
 C -0.02442 3.83580 -0.38847
 H -1.07290 4.16699 -0.41421
 C -1.83210 -0.01921 2.88378
 H -0.99912 0.68378 2.72123
 H -1.41244 -1.03676 2.95516
 H -2.27711 0.22038 3.86524
 C 0.29181 2.54344 -1.13641
 H -0.01372 2.43820 -2.18836
 H 1.23692 -0.56509 3.01076
 C 2.09991 -0.00275 2.61754
 H 1.73969 0.96223 2.23006
 H 2.76821 0.20735 3.47153
 C 4.02679 0.07917 1.00833
 H 3.66691 0.92237 0.40443
 H 4.74507 -0.50327 0.41118
 H 4.58708 0.49823 1.86294
 C 3.51240 -2.02565 2.24627
 H 3.98061 -2.73230 1.54559
 H 2.79449 -2.57549 2.87329
 H -0.01829 0.85403 1.15779
 H -1.19322 1.61256 -0.40376

Int (4+-2b+) 3
 SCF(BP86/BS1) = -1184.74823110
 G(298 K) = -1184.048942
 SCF(BS2) = -1854.41159348
 Lowest Frequencies = 24.4478cm⁻¹,
 42.9841cm⁻¹

86
 Int (4+-2b+) 3
 Rh 0.07341 0.43365 -0.32347
 P 1.57366 -1.24618 0.15869
 P -2.11517 -0.53441 0.15031
 C 1.94340 3.03402 0.27683
 H 2.75637 2.63719 0.89957
 C 1.35336 2.05975 -0.76015
 H 2.01826 1.85101 -1.61101
 C -3.34303 -0.27112 -1.34323
 C 0.81996 -2.73292 1.05396
 H 1.66500 -3.28898 1.48575
 H 0.30323 -2.25367 1.90500
 C -4.12678 -0.49755 2.27893
 H -3.94592 -1.56198 2.49412
 H -4.97173 -0.42594 1.58342
 H -4.44553 -0.02910 3.22672
 C 2.39740 -1.90187 -1.47773
 C -2.86030 0.22839 1.77775
 C -2.28886 -2.37740 0.50100
 H -2.09589 -2.51612 1.57827
 H -3.34757 -2.64320 0.34666
 C 2.93991 -0.77264 1.48298
 C 0.69112 3.54436 1.02531
 H 0.16486 2.76273 1.60035
 H 0.90449 4.39502 1.69224
 C 1.27283 -2.40055 -2.41100

H 0.49479 -1.63182 -2.56451
 H 0.79247 -3.32047 -2.05465
 H 1.71012 -2.62307 -3.40015
 C -3.16216 1.14578 -1.92379
 H -2.16720 1.27147 -2.38065
 H -3.30789 1.94427 -1.18074
 H -3.90532 1.30221 -2.72530
 C 0.96466 4.93952 -0.90658
 H 0.81675 5.02836 -1.99505
 H 0.84667 5.94761 -0.47866
 C 3.37840 -3.05229 -1.18953
 H 2.92195 -3.86310 -0.59935
 H 4.28308 -2.70574 -0.66774
 H 3.70614 -3.49096 -2.14878
 C -3.16310 1.72327 1.56752
 H -4.01160 1.88678 0.88554
 H -2.28871 2.27169 1.17811
 H -3.43236 2.18051 2.53592
 C 3.11813 -0.76739 -2.23430
 H 3.93938 -0.30861 -1.67174
 H 2.41644 0.02614 -2.53463
 H 3.54845 -1.19048 -3.15896
 C -1.36132 -3.27638 -0.33853
 H -1.92411 -4.16813 -0.66600
 H -1.06862 -2.75616 -1.26078
 C -0.10425 -3.76755 0.38851
 H 0.48530 -4.39227 -0.30493
 H -0.41555 -4.45479 1.19805
 C -2.94458 -1.27862 -2.44311
 H -3.16553 -2.32080 -2.16670
 H -1.87536 -1.20469 -2.70822
 H -3.52296 -1.05371 -3.35653
 C 2.34374 4.31334 -0.52149
 H 2.92400 4.99378 0.12340
 H 2.96967 4.07763 -1.39728
 H 4.45951 -1.63000 2.75315
 C -4.82412 -0.49030 -0.98839
 H -5.22273 0.30903 -0.34582
 H -5.00861 -1.45981 -0.49857
 H -5.41835 -0.48240 -1.91938
 C -0.05766 3.96761 -0.25472
 H -1.07011 4.38079 -0.12979
 C -1.78013 0.09132 2.87377
 H -0.88924 0.70305 2.65882
 H -1.45265 -0.95144 3.02288
 H -2.19672 0.44128 3.83451
 C 0.00470 2.66769 -1.09414
 H -0.23481 2.78183 -2.16414
 H 1.39516 -0.49929 3.04465
 C 2.23858 0.04515 2.58826
 H 1.87119 1.01421 2.21834
 H 2.96634 0.25076 3.39307
 C 4.04375 0.08392 0.83606
 H 3.63954 0.88100 0.19753
 H 4.73992 -0.52675 0.24075
 H 4.63816 0.56176 1.63475
 C 3.60538 -1.99522 2.15680
 H 4.00268 -2.73050 1.44242
 H 2.93271 -2.51269 2.85756
 H 0.19016 0.71472 1.14720
 H -0.89287 2.00247 -0.69363

TS (4+-2b+) 4

SCF(BP86/BS1)= -1184.73849733

G(298 K) = -1184.039511

SCF(BS2) = -1854.40378372

Lowest Frequencies = -534.7074cm-1, 27.9278cm-1

86

TS (4+-2b+) 4

Rh 0.06094 0.47952 -0.21859

P 1.70634 -1.09230 0.12521

P -1.94753 -0.85159 0.13759

C 1.37162 3.48290 0.26787

H 2.27698 3.29337 0.86359

C 0.96883 2.35133 -0.70296

H 1.65380 2.20152 -1.54738

C -3.24826 -0.72294 -1.30819

C 1.22584 -2.74188 0.91661

H 2.16841 -3.18826 1.26636

H 0.68755 -2.41924 1.82539

C -3.81215 -1.12628 2.38171

H -3.45571 -2.15098 2.56745

H -4.70798 -1.18181 1.74979

H -4.12716 -0.71603 3.35749

C 2.59993 -1.48632 -1.55853

C -2.71353 -0.21067 1.80540

C -1.86943 -2.70651 0.44328

H -1.60213 -2.84086 1.50483

H -2.89572 -3.09462 0.33850

C 3.01324 -0.51527 1.48151

C 0.06194 3.71940 1.05348

H -0.24778 2.84864 1.65827

H 0.09858 4.61211 1.69780

C 1.57235 -2.13126 -2.51276

H 0.66511 -1.51105 -2.60503

H 1.28516 -3.14778 -2.21347

H 2.02784 -2.20551 -3.51596

C -3.27831 0.71201 -1.86917

H -2.32908 0.96750 -2.36620

H -3.49567 1.47580 -1.10696

H -4.07160 0.77902 -2.63417

C -0.04758 5.08058 -0.92180

H -0.26064 5.11112 -2.00256

H -0.35897 6.04950 -0.50053

C 3.78925 -2.44292 -1.36040

H 3.51238 -3.35868 -0.81332

H 4.62979 -1.96169 -0.83827

H 4.16196 -2.75607 -2.35170

C -3.26623 1.21575 1.63003

H -4.15547 1.24835 0.98217

H -2.50858 1.90633 1.22468

H -3.56915 1.60792 2.61684

C 3.06893 -0.18546 -2.24056

H 3.77159 0.40482 -1.63969

H 2.20914 0.44984 -2.50343

H 3.58254 -0.45296 -3.18071

C -0.88685 -3.46313 -0.47103

H -1.36624 -4.38936 -0.83261

H -0.67434 -2.86802 -1.36954

C 0.43576 -3.84777 0.19859

H	1.08410	-4.33987	-0.54658	C	-2.48610	-1.27291	1.75885
H	0.23517	-4.62188	0.96329	C	-0.65369	-3.15290	0.40412
C	-2.78097	-1.65614	-2.44552	H	-0.25104	-3.16571	1.42792
H	-2.85429	-2.72150	-2.18000	H	-1.48369	-3.87534	0.39387
H	-1.74636	-1.43994	-2.76192	C	2.82921	0.47567	1.61165
H	-3.43215	-1.49441	-3.32258	C	-1.06595	3.60266	1.12170
C	1.45002	4.77433	-0.59866	H	-0.77702	2.71420	1.71135
H	1.90857	5.58878	-0.01482	H	-1.31241	4.42984	1.80609
H	2.06624	4.63176	-1.50124	C	2.43715	-1.33008	-2.53090
H	4.70424	-1.20308	2.63446	H	1.36021	-1.14757	-2.67707
C	-4.66782	-1.13557	-0.87887	H	2.59198	-2.38583	-2.27086
H	-5.12533	-0.40987	-0.19010	H	2.93993	-1.15803	-3.49904
H	-4.70141	-2.13222	-0.41043	C	-3.74544	-0.73680	-1.39535
H	-5.31025	-1.18093	-1.77596	H	-3.44421	0.31852	-1.30652
C	-0.80390	3.92838	-0.20719	H	-4.45634	-0.96491	-0.58807
H	-1.87779	4.11184	-0.05198	H	-4.29528	-0.83275	-2.34810
C	-1.53694	-0.16627	2.80377	C	-2.23659	4.63988	-0.70828
H	-0.73018	0.48957	2.43752	H	-2.66267	4.50077	-1.71522
H	-1.10690	-1.16567	2.98788	H	-2.87460	5.36870	-0.18367
H	-1.89662	0.21754	3.77496	C	4.50989	-0.70003	-1.24019
C	-0.48773	2.64802	-1.02214	H	4.64379	-1.68909	-0.77320
H	-0.73712	2.69771	-2.09307	H	5.01538	0.05269	-0.61644
H	1.50605	-0.69200	3.09758	H	5.03907	-0.72568	-2.20917
C	2.21975	0.03879	2.68474	C	-3.09405	0.14099	1.84188
H	1.65934	0.95517	2.43654	H	-3.76412	0.37856	1.00337
H	2.93225	0.29470	3.48867	H	-2.30314	0.90711	1.89087
C	3.91465	0.60022	0.92070	H	-3.68970	0.21989	2.76833
H	3.34441	1.39349	0.41386	C	2.90518	1.05586	-2.09447
H	4.66896	0.20988	0.22070	H	3.23520	1.85984	-1.42332
H	4.46187	1.06969	1.75695	H	1.86774	1.25597	-2.40579
C	3.91484	-1.65536	2.00944	H	3.53507	1.10578	-2.99999
H	4.41848	-2.22484	1.21652	C	0.44035	-3.52407	-0.61498
H	3.37054	-2.35979	2.65657	H	0.23910	-4.52600	-1.03074
H	1.10044	1.22563	0.64384	H	0.42155	-2.83234	-1.47106
H	-1.21504	1.81932	-0.61403	C	1.84650	-3.51821	-0.00558
2b+ (exo)				H	2.58819	-3.71956	-0.79604
SCF(BP86/BS1)= -1184.75905413				C	1.93493	-4.36527	0.70022
G(298 K) = -1184.056382				C	-1.68896	-1.36426	-2.66959
SCF(BS2) = -1854.42625173				H	-0.87930	-2.09275	-2.82895
Lowest Frequencies = 33.2327cm ⁻¹ ,				H	-1.22901	-0.36332	-2.59099
47.9961cm ⁻¹				H	-2.33322	-1.38904	-3.56688
86				C	-0.74451	5.10390	-0.73196
2b+ (exo)				H	-0.61731	6.06978	-0.21785
Rh	-0.11366	0.40173	-0.19665	H	-0.34398	5.22343	-1.75177
P	1.96989	-0.50352	0.13468	H	4.51296	0.43229	2.96358
P	-1.40340	-1.45305	0.15155	C	-3.05841	-3.14734	-1.55229
C	-0.01526	3.98639	0.05827	H	-3.64945	-3.47357	-0.68344
H	0.98186	4.27110	0.42582	H	-2.24209	-3.86860	-1.71286
C	-0.01380	2.72459	-0.84661	H	-3.71766	-3.20847	-2.43603
H	0.35944	2.90840	-1.86534	C	-2.18156	3.31385	0.09378
C	-2.54273	-1.70022	-1.42609	H	-3.15193	2.98408	0.49309
C	2.24795	-2.25706	0.77929	C	-1.53150	-1.43376	2.96205
H	3.32146	-2.32581	1.01238	H	-0.66115	-0.76549	2.87490
H	1.72990	-2.23614	1.75451	H	-1.17840	-2.46807	3.09517
C	-3.59562	-2.33789	1.84730	H	-2.07332	-1.16071	3.88437
H	-3.20131	-3.36468	1.78612	C	-1.49384	2.26318	-0.82020
H	-4.36925	-2.21596	1.07490	H	-1.93706	2.18197	-1.82472
H	-4.09863	-2.24442	2.82605	H	1.47787	-0.39655	3.12165
C	3.03054	-0.35766	-1.49006	C	1.76098	0.58952	2.71865
				H	0.84582	1.08210	2.34634
				H	2.16738	1.18038	3.55895

C	3.24318	1.89271	1.17584
H	2.41716	2.45707	0.71601
H	4.09620	1.88807	0.48075
H	3.55765	2.45871	2.07029
C	4.06812	-0.23207	2.20203
H	4.85012	-0.43866	1.45729
H	3.81454	-1.17190	2.71459
H	-1.74095	1.23779	-0.31787
H	0.78484	2.01241	-0.38489

(iv) Figure S49

4+

SCF(BP86/BS1)= -1183.55210170
G(298 K) = -1182.870542
SCF(BS2) = -1853.21715042
Lowest Frequencies = 30.6379cm⁻¹,
43.6301cm⁻¹

84

4+

Rh	0.03087	0.59427	0.12516
P	1.71995	-0.93168	-0.00949
P	-1.90756	-0.85326	0.00229
C	0.52599	3.33041	1.14604
H	0.62735	3.23846	2.23719
C	1.33908	2.33451	0.31725
H	2.40617	2.19206	0.49493
C	-3.10233	-0.05928	-1.33930
C	1.21618	-2.75373	-0.00732
H	2.13171	-3.31225	0.23690
H	0.56726	-2.83111	0.88271
C	-4.27316	-1.51698	1.58962
H	-4.35165	-2.46769	1.03797
H	-4.93078	-0.77820	1.10820
H	-4.67454	-1.69540	2.60304
C	2.93188	-0.77600	-1.52416
C	-2.81763	-1.03102	1.70831
C	-1.78824	-2.63049	-0.59073
H	-1.52528	-3.24982	0.28008
H	-2.79542	-2.94964	-0.89600
C	2.68845	-0.88321	1.72470
C	-0.87477	3.04722	0.55612
H	-1.26220	2.01410	0.81252
H	-1.67576	3.72668	0.89478
C	2.05525	-0.78929	-2.79636
H	1.27331	-0.01382	-2.76187
H	1.56663	-1.75747	-2.96827
H	2.69760	-0.59018	-3.67192
C	-3.76636	1.21330	-0.77988
H	-3.03356	1.95541	-0.43183
H	-4.46667	1.00164	0.04157
H	-4.34961	1.69032	-1.58707
C	0.16158	4.69845	-0.84618
H	0.87797	4.87774	-1.66284
H	-0.64558	5.44254	-0.94696
C	3.91509	-1.96413	-1.53741
H	3.41380	-2.94034	-1.61594
H	4.56577	-1.97564	-0.64863
H	4.57319	-1.86659	-2.41865
C	-2.76079	0.32202	2.44665
H	-3.27751	1.12808	1.90495
H	-1.71813	0.63573	2.62858
H	-3.25268	0.22007	3.43001
C	3.74750	0.53403	-1.52656
H	4.49392	0.57878	-0.72473
H	3.12177	1.43337	-1.46810
H	4.29837	0.58612	-2.48201
C	-0.75460	-2.82633	-1.71736
H	-1.17374	-3.48275	-2.49896
H	-0.53259	-1.86543	-2.20912

C	0.55165	-3.44396	-1.20912
H	1.26929	-3.53225	-2.04170
H	0.34850	-4.48362	-0.88931
C	-2.22609	0.32586	-2.55327
H	-1.86386	-0.55929	-3.09844
H	-1.34731	0.91974	-2.25360
H	-2.83191	0.91929	-3.26133
C	0.81750	4.75000	0.56986
H	0.35283	5.52422	1.20217
H	1.89858	4.95720	0.53525
C	3.22883	-2.26500	2.15351
H	3.93115	-2.69877	1.42401
H	3.78850	-2.13037	3.09576
C	-4.20000	-1.02638	-1.82486
H	-4.84757	-1.39782	-1.01839
H	-3.78760	-1.88867	-2.37115
H	-4.84624	-0.48314	-2.53684
C	-0.44283	3.25667	-0.92000
H	-1.21435	3.12493	-1.69114
C	-2.02245	-2.05898	2.54325
H	-0.94159	-1.84374	2.54475
H	-2.17547	-3.09447	2.20223
H	-2.36644	-2.01136	3.59105
C	0.73911	2.29464	-0.97537
H	1.26008	2.09285	-1.91542
C	1.66029	-0.41103	2.77320
H	0.83903	-1.13374	2.89820
H	2.15916	-0.31290	3.75428
C	3.88314	0.08819	1.71865
H	3.62387	1.10404	1.39337
H	4.26316	0.16919	2.75232
H	1.22176	0.56598	2.50372
H	4.71525	-0.28046	1.10060
H	2.43358	-2.99637	2.35940

TS(4+-4b+) 1

SCF(BP86/BS1)= -1183.53288882
G(298 K) = -1182.851093
SCF(BS2) = -1853.19845614
Lowest Frequencies = -131.9789cm⁻¹,
27.2428cm⁻¹

84

TS(4+-4b+) 1

Rh	-0.00930	0.58417	0.00716
P	-1.78476	-0.86986	-0.11303
P	1.87882	-0.93213	-0.10123
C	0.38431	3.37422	-0.90355
H	0.90328	3.31129	-1.86988
C	-0.83721	2.47993	-0.73529
H	-1.60326	2.42916	-1.51035
C	2.96850	-0.65178	1.51736
C	-1.66962	-2.64014	-0.78724
H	-2.54868	-3.10756	-0.31199
H	-1.94812	-2.51511	-1.84294
C	4.20531	-1.23141	-1.79262
H	4.10226	-2.32409	-1.70693
H	4.90662	-0.88809	-1.01615
H	4.67744	-1.02666	-2.76978
C	-2.58570	-1.16776	1.66092
C	2.85762	-0.48884	-1.72550

C 1.87298 -2.81023 -0.24958
 H 2.00265 -3.03434 -1.31897
 H 2.78822 -3.16561 0.24165
 C -3.16517 -0.25065 -1.37621
 C 1.17311 2.94846 0.35523
 H 1.51969 1.86997 0.34006
 H 2.09402 3.52653 0.54317
 C -1.69230 -2.16585 2.41830
 H -0.65902 -1.79826 2.50838
 H -1.68439 -3.16380 1.95410
 H -2.08828 -2.28856 3.44169
 C 3.81724 0.63136 1.44087
 H 3.22706 1.53480 1.23817
 H 4.61833 0.55927 0.68978
 H 4.30429 0.78448 2.41999
 C -0.30625 4.70866 1.03751
 H -1.33453 4.97033 1.33183
 H 0.37592 5.36514 1.60219
 C -4.00746 -1.75610 1.57975
 H -4.06408 -2.68558 0.99128
 H -4.74055 -1.04073 1.18051
 H -4.33049 -2.01029 2.60485
 C 3.09344 1.02589 -1.86522
 H 3.69258 1.45534 -1.05106
 H 2.13947 1.56940 -1.92983
 H 3.63992 1.21086 -2.80664
 C -2.63220 0.13614 2.47398
 H -3.29885 0.88822 2.02564
 H -1.62755 0.57129 2.59186
 H -3.02863 -0.08877 3.47973
 C 0.64884 -3.56958 0.26747
 H 0.30727 -3.16930 1.23162
 H 0.97650 -4.60326 0.47638
 C -0.48908 -3.64172 -0.76694
 H -0.02051 -3.62895 -1.76676
 H -0.95988 -4.63699 -0.69162
 C 1.95542 -0.52662 2.67493
 H 1.39021 -1.46169 2.82074
 H 1.22670 0.28594 2.50226
 H 2.49355 -0.31785 3.61696
 C -0.06284 4.81822 -0.50086
 H 0.74087 5.53582 -0.73399
 H -0.95785 5.13362 -1.05934
 C -4.26083 -1.29209 -1.71479
 H -4.87992 -1.57151 -0.85340
 H -3.87431 -2.21058 -2.17827
 C 3.92287 -1.82411 1.82228
 H 4.61618 -2.04321 0.99495
 H 3.38998 -2.74851 2.09364
 H 4.53873 -1.54902 2.69626
 C 0.01369 3.21073 1.34279
 H 0.20040 2.97870 2.40128
 C 1.93942 -0.91167 -2.89590
 H 0.95298 -0.42201 -2.82147
 H 1.78225 -1.99949 -2.96315
 H 2.40703 -0.59697 -3.84527
 C -1.07326 2.38426 0.65966
 H -2.05590 2.25902 1.11400
 C -2.40855 0.06077 -2.68887
 H -2.05737 -0.86078 -3.18295
 H -1.52946 0.70358 -2.53665

H -3.09557 0.56059 -3.39425
 C -3.89148 0.99561 -0.83166
 H -3.22446 1.81374 -0.54181
 H -4.52402 0.75037 0.03532
 H -4.56324 1.38459 -1.61704
 H -4.93295 -0.82642 -2.45708

Int(4+-4b+)1

SCF(BP86/BS1)= -1183.53858030

G(298 K) = -1182.857569

SCF(BS2) = -1853.20318044

Lowest Frequencies = 30.7932cm⁻¹,
36.3589cm⁻¹

84

Int(4+-4b+)1

Rh -0.06231 0.51737 0.00011

P -1.87485 -0.92579 -0.11144

P 2.03865 -0.87197 -0.09625

C 0.22482 3.30037 -0.90694

H 0.76310 3.26474 -1.86408

C -0.94753 2.33994 -0.76008

H -1.69749 2.25818 -1.54816

C 3.04449 -0.59698 1.57235

C -1.62271 -2.66523 -0.83935

H -2.01323 -3.39156 -0.10773

H -2.28987 -2.71391 -1.70948

C 4.49314 -0.90903 -1.62693

H 4.48692 -2.00645 -1.53374

H 5.11860 -0.49620 -0.82061

H 4.99432 -0.66782 -2.58112

C -2.57803 -1.29583 1.67904

C 3.08069 -0.29510 -1.63803

C 2.11234 -2.75436 -0.29285

H 2.51881 -2.96831 -1.29373

H 2.83570 -3.15363 0.42908

C -3.31695 -0.33093 -1.31411

C 1.01232 2.91492 0.36610

H 1.41505 1.85569 0.35793

H 1.90190 3.53598 0.56757

C -1.55148 -2.18253 2.40896

H -0.55509 -1.71727 2.42097

H -1.47285 -3.19279 1.97910

H -1.87467 -2.30542 3.45759

C 3.72149 0.78527 1.62750

H 3.02268 1.61832 1.47260

H 4.54709 0.87763 0.90607

H 4.15558 0.91941 2.63392

C -0.56809 4.59812 1.02026

H -1.61374 4.80554 1.29660

H 0.06835 5.29156 1.59415

C -3.92824 -2.03513 1.62402

H -3.91608 -2.91892 0.96708

H -4.75053 -1.37556 1.31070

H -4.16957 -2.39027 2.64150

C 3.18464 1.23826 -1.72349

H 3.67170 1.69662 -0.85220

H 2.19331 1.69476 -1.85703

H 3.78729 1.50084 -2.61060

C -2.74221 -0.00401 2.49813

H -3.46541 0.69474 2.05102

H	-1.77935	0.51309	2.63129	H	-4.56811	-2.42049	1.04947
H	-3.12626	-0.26949	3.49871	H	-5.23097	-0.77256	1.24503
C	0.74230	-3.40490	-0.13095	H	-4.79914	-1.73108	2.67176
H	0.31493	-3.10321	0.83747	C	3.28819	-0.41707	-1.54458
H	0.86128	-4.50138	-0.07709	C	-3.07253	-0.90832	1.65196
C	-0.21017	-3.03013	-1.28164	C	-2.15012	-2.46306	-0.80683
H	0.20058	-2.17973	-1.85295	H	-2.47437	-3.20270	-0.05724
H	-0.27346	-3.86737	-1.99905	H	-2.85020	-2.54369	-1.65091
C	1.99172	-0.68924	2.69548	C	2.97919	-0.92273	1.65338
H	1.52915	-1.68927	2.73591	C	-0.61549	3.12508	-0.73232
H	1.18743	0.05806	2.56807	H	-1.00159	2.26058	-1.30338
H	2.47575	-0.51315	3.67286	H	-1.09688	4.04017	-1.11528
C	-0.30606	4.71779	-0.51468	C	2.35633	-0.20198	-2.75728
H	0.46065	5.47792	-0.73746	H	1.64125	0.61956	-2.57604
H	-1.20819	4.98309	-1.08781	H	1.78334	-1.10915	-3.01490
C	-4.43117	-1.37966	-1.55749	H	2.96489	0.05846	-3.64133
H	-5.07387	-1.53670	-0.68267	C	-3.95962	1.48596	-0.87524
H	-4.07132	-2.36046	-1.89999	H	-3.10399	2.10569	-0.56897
C	4.13196	-1.66304	1.82489	H	-4.66329	1.42468	-0.03056
H	4.84168	-1.76611	0.99110	H	-4.47992	2.01698	-1.69174
H	3.71283	-2.65473	2.05389	C	1.16734	4.40832	0.21894
H	4.71250	-1.36012	2.71367	H	2.17300	4.39067	0.67027
C	-0.17496	3.12091	1.33459	H	1.07551	5.35322	-0.34133
H	0.00770	2.90087	2.39641	C	4.26403	-1.57693	-1.84802
C	2.30316	-0.76305	-2.88814	H	3.76491	-2.52971	-2.07507
H	1.27408	-0.36312	-2.89093	H	4.98715	-1.74998	-1.03955
H	2.25469	-1.85813	-2.99094	H	4.84234	-1.30174	-2.74744
H	2.81623	-0.37941	-3.78744	C	-3.06199	0.46440	2.35272
C	-1.20555	2.23437	0.63802	H	-3.69600	1.20701	1.84687
H	-2.19347	2.08115	1.07192	H	-2.03949	0.86751	2.42195
C	-2.61460	-0.07828	-2.66949	H	-3.44812	0.34836	3.38071
H	-2.29747	-1.02260	-3.14260	C	4.12320	0.85621	-1.31141
H	-1.72203	0.55828	-2.58175	H	4.77750	0.77619	-0.42954
H	-3.32513	0.40625	-3.36200	H	3.50644	1.76001	-1.21978
C	-4.02850	0.93327	-0.79304	H	4.78127	1.00362	-2.18562
H	-3.36551	1.78643	-0.61909	C	-0.71076	-2.73315	-1.26891
H	-4.58029	0.73030	0.13819	H	-0.33801	-1.82804	-1.80333
H	-4.77473	1.24991	-1.54295	H	-0.69071	-3.53776	-2.02677
H	-5.07448	-0.98630	-2.36429	C	0.24593	-3.08662	-0.11683
				H	-0.10076	-2.61837	0.81790
				H	0.21799	-4.17742	0.05603
				C	-2.72916	0.21541	-2.67936
				H	-2.43700	-0.76719	-3.08643
				H	-1.81109	0.81429	-2.55586
				H	-3.35291	0.71120	-3.44387
				C	0.02608	4.25644	1.27897
				H	-0.66071	5.11841	1.26520
				H	0.40465	4.15611	2.30869
				C	4.27271	-1.75678	1.55944
				H	5.06473	-1.22755	1.00843
				H	4.13180	-2.74825	1.10240
				C	-4.80492	-0.73985	-1.65365
				H	-5.46225	-0.82853	-0.77894
				H	-4.58965	-1.75437	-2.02404
				H	-5.38141	-0.23076	-2.44630
				C	0.92566	3.19397	-0.72940
				H	1.42054	3.26605	-1.70937
				C	-2.13826	-1.84562	2.44294
				H	-1.10148	-1.47020	2.44216
				H	-2.14005	-2.87902	2.06139
				H	-2.47895	-1.88675	3.49236

TS (4+-4b+) 2
SCF (BP86/BS1) = -1183.53391938
G (298 K) = -1182.854206
SCF (BS2) = -1853.19895227
Lowest Frequencies = -74.2934cm⁻¹,
28.0806cm⁻¹

84
TS (4+-4b+) 2
Rh 0.07375 0.24629 -0.22064
P 2.07541 -0.82581 -0.06687
P -2.29399 -0.71069 -0.10422
C -0.74298 2.97319 0.80556
H -1.75439 2.87615 1.22421
C 0.23014 1.83478 1.10306
H 0.39460 1.53137 2.14513
C -3.53733 0.08896 -1.36723
C 1.68495 -2.65742 -0.41363
H 1.91137 -2.83879 -1.47570
H 2.41656 -3.24138 0.16722
C -4.49577 -1.49098 1.63736

C 1.28722 1.97057 0.11836
H 2.33413 1.85460 0.39931
C 1.97880 -1.59909 2.61361
H 1.75314 -2.64007 2.33487
H 1.03185 -1.03748 2.66496
H 2.41689 -1.62027 3.62662
C 3.34238 0.46125 2.22610
H 2.45815 1.07945 2.43239
H 4.03015 1.02712 1.58008
H 3.86002 0.30629 3.18892
H 4.64797 -1.92589 2.58397

Int(4+-4b+) 2
SCF(BP86/BS1) = -1183.54318001
G(298 K) = -1182.862804
SCF(BS2) = -1853.20898672
Lowest Frequencies = 29.9846cm⁻¹,
37.8439cm⁻¹

84
Int(4+-4b+) 2
Rh 0.03425 0.00641 -0.15095
P 2.28444 -0.65303 -0.15986
P -2.26894 -0.65048 -0.10720
C -1.32074 2.80927 0.59121
H -2.40540 2.66570 0.68109
C -0.43575 1.68350 1.12910
H -0.56237 1.33582 2.16163
C -3.52418 -0.11048 -1.48118
C 2.17101 -2.35614 -0.99711
H 2.35294 -2.18303 -2.07103
H 2.99463 -2.99125 -0.63245
C -4.10359 -2.18230 1.53889
H -3.67179 -3.10278 1.11464
H -5.00584 -1.93008 0.96666
H -4.42578 -2.42149 2.56770
C 3.55507 0.25740 -1.30767
C -3.09093 -1.02171 1.60137
C -1.71651 -2.35147 -0.69924
H -1.60791 -2.99563 0.18635
H -2.47035 -2.82375 -1.34885
C 3.03556 -1.06737 1.58391
C -0.74868 3.01897 -0.83074
H -0.90910 2.15408 -1.49713
H -1.11517 3.94061 -1.31185
C 2.72806 0.69322 -2.53719
H 1.86763 1.31941 -2.25482
H 2.34317 -0.16975 -3.10695
H 3.37401 1.27080 -3.22165
C -3.97551 1.34736 -1.27518
H -3.13403 2.05062 -1.32976
H -4.49907 1.49977 -0.31978
H -4.68258 1.61374 -2.08036
C 0.61517 4.31184 0.65606
H 1.43841 4.30595 1.38907
H 0.66515 5.27048 0.11445
C 4.71270 -0.64851 -1.77878
H 4.36852 -1.54160 -2.32165
H 5.36524 -0.97375 -0.95748
H 5.33755 -0.06994 -2.48180
C -3.77748 0.24669 2.14043

H -4.65873 0.52604 1.54280
H -3.09272 1.10796 2.17871
H -4.13041 0.05622 3.16899
C 4.14682 1.49815 -0.61111
H 4.77983 1.23136 0.24932
H 3.37687 2.20576 -0.27386
H 4.79074 2.03425 -1.33015
C -0.33856 -2.19664 -1.39822
H -0.03143 -1.08066 -1.58998
H -0.44279 -2.41806 -2.47743
C 0.80808 -3.02667 -0.80522
H 0.61588 -3.19781 0.26498
H 0.82227 -4.02338 -1.28441
C -2.73952 -0.20259 -2.80827
H -2.50845 -1.24220 -3.09106
H -1.79677 0.36974 -2.77177
H -3.35876 0.22151 -3.61759
C -0.78791 4.09383 1.30993
H -1.46308 4.94133 1.10870
H -0.73808 3.96687 2.40330
C 4.48542 -1.57504 1.48727
H 5.18808 -0.78221 1.19010
H 4.59904 -2.42210 0.79218
C -4.76279 -1.02184 -1.54772
H -5.45059 -0.84101 -0.70827
H -4.51549 -2.09527 -1.57125
H -5.31796 -0.79558 -2.47512
C 0.71487 3.12547 -0.35855
H 1.48252 3.25565 -1.13431
C -1.93810 -1.42335 2.54701
H -1.16478 -0.64430 2.61860
H -1.44525 -2.35880 2.23460
H -2.35104 -1.59585 3.55643
C 0.84991 1.90074 0.54709
H 1.76647 1.78349 1.12389
C 2.14616 -2.16834 2.19927
H 2.26091 -3.13750 1.68936
H 1.08139 -1.87897 2.18960
H 2.44615 -2.31967 3.25102
C 2.98137 0.15623 2.51896
H 1.94402 0.46588 2.72238
H 3.54678 1.01981 2.13624
H 3.43368 -0.12275 3.48681
H 4.80047 -1.93091 2.48414

TS(4+-4b+) 3
SCF(BP86/BS1) = -1183.53363198
G(298 K) = -1182.853598
SCF(BS2) = -1853.19892148
Lowest Frequencies = -139.7254cm⁻¹,
29.2493cm⁻¹

84
TS(4+-4b+) 3
Rh 0.07961 -0.03863 0.01610
P 2.31127 -0.64761 -0.14548
P -2.28097 -0.66037 -0.13541
C -1.20660 2.80305 0.74054
H -2.27456 2.66243 0.95130
C -0.26724 1.68843 1.19888
H -0.27714 1.37336 2.25146

C -3.52181 0.08019 -1.44135
 C 1.91958 -2.36519 -0.83306
 H 2.02129 -2.34037 -1.92919
 H 2.67332 -3.07633 -0.45935
 C -4.30641 -2.04170 1.46030
 H -4.06907 -2.96279 0.90474
 H -5.18501 -1.57638 0.99313
 H -4.60313 -2.34554 2.47967
 C 3.43005 0.14189 -1.50673
 C -3.11275 -1.07412 1.56206
 C -1.98780 -2.38335 -0.90445
 H -2.14188 -3.14248 -0.12008
 H -2.77063 -2.54948 -1.65862
 C 3.24245 -1.01503 1.51017
 C -0.78951 3.00678 -0.73594
 H -1.01041 2.13607 -1.37275
 H -1.21407 3.92076 -1.18251
 C 2.45703 0.52107 -2.64467
 H 1.65980 1.19658 -2.29809
 H 1.97695 -0.36508 -3.09316
 H 3.02199 1.02633 -3.44768
 C -3.95958 1.51023 -1.07575
 H -3.11697 2.20792 -1.01492
 H -4.51791 1.54932 -0.12886
 H -4.63705 1.87965 -1.86564
 C 0.72238 4.31346 0.58452
 H 1.62095 4.31331 1.22325
 H 0.70965 5.26966 0.03655
 C 4.48077 -0.84887 -2.05019
 H 4.03459 -1.77350 -2.44717
 H 5.23757 -1.12337 -1.30312
 H 5.01025 -0.36350 -2.88890
 C -3.55386 0.22895 2.25377
 H -4.38729 0.72036 1.72973
 H -2.72441 0.94644 2.34454
 H -3.90522 -0.00574 3.27383
 C 4.14449 1.40293 -0.98432
 H 4.87631 1.17030 -0.19506
 H 3.44521 2.16125 -0.60364
 H 4.70415 1.86294 -1.81738
 C -0.58649 -2.54141 -1.52081
 H -0.33987 -1.64524 -2.12721
 H -0.57784 -3.39358 -2.22428
 C 0.47792 -2.76159 -0.43062
 H 0.18309 -2.18575 0.49125
 H 0.43900 -3.81128 -0.08904
 C -2.72628 0.11389 -2.76617
 H -2.52284 -0.89367 -3.16282
 H -1.76378 0.64189 -2.66118
 H -3.32210 0.64720 -3.52719
 C -0.59929 4.09457 1.38952
 H -1.29768 4.93683 1.25798
 H -0.42997 3.97527 2.47168
 C 4.63309 -1.62695 1.26540
 H 5.33625 -0.90134 0.82937
 H 4.60144 -2.51743 0.61693
 C -4.79398 -0.77141 -1.62625
 H -5.48692 -0.66236 -0.77967
 H -4.60151 -1.84485 -1.77672
 H -5.32353 -0.41106 -2.52576
 C 0.71260 3.12211 -0.42849

H 1.39237 3.24789 -1.28344
 C -1.99824 -1.72735 2.40883
 H -1.10597 -1.08079 2.47383
 H -1.68455 -2.70753 2.01287
 H -2.37783 -1.89789 3.43158
 C 0.94738 1.90340 0.46119
 H 1.92233 1.81793 0.94349
 C 2.36594 -2.00927 2.30099
 H 2.28806 -2.99420 1.81429
 H 1.34933 -1.61289 2.46227
 H 2.82555 -2.17233 3.29131
 C 3.37540 0.27316 2.34662
 H 2.39035 0.66995 2.63945
 H 3.94138 1.06518 1.83276
 H 3.92074 0.03482 3.27650
 H 5.05505 -1.94590 2.23470

Int(4+-4b+) 3

SCF(BP86/BS1)= -1183.53574314

G(298 K) = -1182.855166

SCF(BS2) = -1853.20168818

Lowest Frequencies = 23.1435cm⁻¹,
41.3923cm⁻¹

84

Int(4+-4b+) 3

Rh -0.07259 -0.09245 -0.15220
 P -2.33496 -0.63916 0.13870
 P 2.26450 -0.68992 0.11165
 C 1.23978 2.89307 -0.48947
 H 2.33250 2.80849 -0.48308
 C 0.47097 1.74966 -1.14437
 H 0.71559 1.45136 -2.17167
 C 3.36837 -0.00504 1.56694
 C -1.83420 -2.27366 0.91644
 H -1.77611 -2.11573 2.00453
 H -2.57263 -3.07236 0.73997
 C 4.40494 -1.92757 -1.46243
 H 4.06901 -2.92489 -1.13895
 H 5.22014 -1.60827 -0.80000
 H 4.83395 -2.04611 -2.47306
 C -3.39719 0.21125 1.50177
 C 3.25854 -0.89951 -1.53883
 C 2.05968 -2.50250 0.67645
 H 2.14871 -3.12791 -0.22769
 H 2.90624 -2.76769 1.32710
 C -3.34434 -1.12207 -1.43625
 C 0.52074 3.02233 0.87293
 H 0.65287 2.13551 1.51613
 H 0.79517 3.93590 1.42488
 C -2.38702 0.68562 2.56932
 H -1.60928 1.33845 2.14851
 H -1.88220 -0.16052 3.06469
 H -2.92941 1.24428 3.35221
 C 3.67069 1.49718 1.43070
 H 2.76559 2.10971 1.50825
 H 4.19045 1.74589 0.49417
 H 4.33745 1.79187 2.26015
 C -0.74789 4.31098 -0.70169
 H -1.49707 4.29691 -1.50990
 H -0.89285 5.24556 -0.13572

C 4.66101 -0.79774 1.76486
H 5.36678 -0.39851 1.02066
H 4.64710 -1.89537 1.67707
H 5.07358 -0.56041 2.76139
C -1.05549 3.12806 0.31604
H -1.94311 3.13751 0.96300
C 2.36159 -1.09814 -2.66290
H 1.48869 -0.42556 -2.69396
H 1.98449 -2.12966 -2.55737
H 2.88365 -1.04175 -3.63425
C -0.94439 1.99052 -0.69900
H -1.75431 1.84333 -1.41647
C -2.40886 -2.12369 -2.30611
H -2.29561 -3.11267 -1.83345
H -1.40965 -1.69123 -2.48975
H -2.89069 -2.28830 -3.28557
C -3.55265 0.09478 -2.31309
H -2.61143 0.51743 -2.69845
H -4.09467 0.87771 -1.76232
H -4.16934 -0.17962 -3.18679
H -5.07737 -2.23759 -2.07284

Int (4+-4b+) 4
SCF(BP86/BS1)= -1183.53449397
G(298 K) = -1182.854764
SCF(BS2) = -1853.20044075
Lowest Frequencies = 16.9285cm-1,
47.6303cm-1

84

Int (4+-4b+) 4
Rh -0.04882 -0.01831 -0.05591
P -2.33686 -0.68963 0.10708
P 2.27324 -0.72047 0.06401
C 1.18262 3.01092 -0.22764
H 2.27045 2.96201 -0.09643
C 0.53284 1.87200 -1.01565
H 0.88976 1.63223 -2.02357
C 3.31149 -0.21730 1.62368
C -1.79638 -2.37660 0.79911
H -1.96140 -2.38951 1.88802
H -2.30872 -3.24686 0.35921
C 4.45036 -1.68836 -1.63691
H 4.10069 -2.72763 -1.54227
H 5.22599 -1.51490 -0.87935
H 4.93560 -1.60376 -2.62525
C -3.50777 0.03990 1.45284
C 3.30533 -0.65571 -1.57430
C 2.11702 -2.62462 0.29798
H 2.14352 -3.02770 -0.72715
H 3.02455 -2.98257 0.80748
C -3.23878 -1.12720 -1.54740
C 0.31555 3.04553 1.05172
H 0.41478 2.13469 1.66800
H 0.48891 3.94280 1.66777
C -2.56811 0.51650 2.58162
H -1.83939 1.26100 2.22889
H -2.00491 -0.31870 3.03152
H -3.17467 0.97151 3.38434
C 3.46795 1.30949 1.71309
H 2.49516 1.81143 1.79016

H 4.01797 1.73204 0.85964
H 4.04180 1.55219 2.62474
C -0.82589 4.36429 -0.59328
H -1.47866 4.36346 -1.48122
H -1.07274 5.26309 -0.00501
C -4.48692 -1.00619 2.02098
H -3.97377 -1.87231 2.46704
H -5.20231 -1.37603 1.27428
H -5.07181 -0.53029 2.82773
C 3.89116 0.75590 -1.76580
H 4.69773 0.96543 -1.04622
H 3.13201 1.54590 -1.67620
H 4.33146 0.82800 -2.77564
C -4.29648 1.23086 0.87673
H -5.07439 0.90479 0.16903
H -3.64854 1.96140 0.36947
H -4.80800 1.75625 1.70194
C 0.83383 -3.12606 0.98371
H 0.90143 -3.06837 2.08280
H 0.66032 -4.18553 0.72233
C -0.31088 -2.25872 0.44902
H -0.00555 -1.26093 1.08740
H -0.19723 -2.24201 -0.65307
C 2.48362 -0.69127 2.83820
H 2.45610 -1.78844 2.92715
H 1.44865 -0.30744 2.80117
H 2.94939 -0.30404 3.76119
C 0.69377 4.31154 -0.94807
H 1.23156 5.18592 -0.54693
H 0.88267 4.27923 -2.03310
C -4.55060 -1.88803 -1.28254
H -5.32611 -1.23922 -0.84824
H -4.41304 -2.75991 -0.62256
C 4.70691 -0.86690 1.65947
H 5.38256 -0.43347 0.90660
H 4.68873 -1.95990 1.52500
H 5.15816 -0.67185 2.64834
C -1.02249 3.08541 0.28663
H -1.94029 3.09420 0.88999
C 2.30093 -0.96661 -2.70649
H 1.44939 -0.26945 -2.71600
H 1.89382 -1.98952 -2.63516
H 2.82132 -0.89278 -3.67752
C -0.85247 1.93520 -0.70576
H -1.62560 1.76098 -1.45662
C -2.27550 -2.01773 -2.36117
H -2.09374 -2.99627 -1.88792
H -1.30661 -1.51760 -2.53181
H -2.72953 -2.21647 -3.34761
C -3.52353 0.14364 -2.37281
H -2.59304 0.61159 -2.72990
H -4.11151 0.89575 -1.82748
H -4.10379 -0.14178 -3.26765
H -4.94349 -2.26419 -2.24352

TS (4+-4b+) 5
SCF(BP86/BS1)= -1183.52741765
G(298 K) = -1182.851084
SCF(BS2) = -1853.19369221
Lowest Frequencies = -669.5621cm-1,
21.5340cm-1

84
 TS (4+-4b+) 5
 Rh 0.05652 -0.03350 0.02333
 P 2.33770 -0.69526 -0.12837
 P -2.24669 -0.72787 -0.07310
 C -1.19140 3.03854 0.24026
 H -2.27363 2.99073 0.07125
 C -0.57147 1.89203 1.03555
 H -0.98207 1.60367 2.00732
 C -3.33727 -0.20087 -1.59298
 C 1.78101 -2.22074 -1.09218
 H 2.25191 -2.30835 -2.08318
 H 1.99598 -3.14512 -0.53271
 C -4.34870 -1.79174 1.65888
 H -3.95599 -2.81383 1.54746
 H -5.14583 -1.64546 0.91831
 H -4.81763 -1.73715 2.65715
 C 3.60858 0.17245 -1.28692
 C -3.24780 -0.71181 1.58623
 C -2.03947 -2.60066 -0.34524
 H -1.98891 -3.00980 0.67682
 H -2.95453 -3.00863 -0.80162
 C 3.09885 -1.35145 1.52221
 C -0.27634 3.07746 -1.00428
 H -0.36127 2.17118 -1.63309
 H -0.42138 3.97594 -1.62558
 C 2.75757 0.72716 -2.45054
 H 1.96416 1.40579 -2.10453
 H 2.28395 -0.08046 -3.03397
 H 3.41347 1.28545 -3.14127
 C -3.51785 1.32486 -1.64810
 H -2.55398 1.84077 -1.75344
 H -4.03988 1.72553 -0.76718
 H -4.12790 1.57745 -2.53321
 C 0.80252 4.38557 0.69172
 H 1.42211 4.37916 1.60272
 H 1.07248 5.28604 0.11634
 C 4.65735 -0.80056 -1.86043
 H 4.20572 -1.64936 -2.39738
 H 5.33697 -1.19900 -1.09561
 H 5.27413 -0.25079 -2.59315
 C -3.88786 0.67268 1.80382
 H -4.72540 0.84942 1.11135
 H -3.16936 1.49761 1.69402
 H -4.29904 0.72177 2.82720
 C 4.31952 1.31618 -0.53970
 H 5.03842 0.93433 0.20218
 H 3.61687 1.98934 -0.02676
 H 4.89237 1.92046 -1.26457
 C -0.76606 -3.01492 -1.11362
 H -1.01166 -3.31408 -2.14746
 H -0.32875 -3.90574 -0.62946
 C 0.28310 -1.88798 -1.15505
 H 0.08628 -1.23631 -2.02652
 H 0.09754 -1.58459 0.29711
 C -2.55972 -0.63389 -2.85358
 H -2.44079 -1.72603 -2.92976
 H -1.56549 -0.15915 -2.90115
 H -3.12126 -0.30648 -3.74590
 C -0.72814 4.33403 0.98782

H -1.24900 5.21171 0.57189
 H -0.95972 4.29362 2.06402
 C 4.43299 -2.07844 1.27968
 H 5.23597 -1.38484 0.98795
 H 4.35209 -2.86511 0.51177
 C -4.72101 -0.87614 -1.58660
 H -5.37283 -0.47511 -0.79617
 H -4.67371 -1.97132 -1.47995
 H -5.21718 -0.66722 -2.55085
 C 1.03178 3.10957 -0.18530
 H 1.97310 3.12225 -0.75019
 C -2.21570 -0.99944 2.69993
 H -1.38760 -0.27529 2.70739
 H -1.77357 -2.00572 2.60746
 H -2.72523 -0.95702 3.67854
 C 0.81864 1.94927 0.78841
 H 1.56603 1.73341 1.55453
 C 2.08145 -2.32674 2.15174
 H 1.93751 -3.24292 1.55689
 H 1.10037 -1.84766 2.30784
 H 2.46517 -2.64160 3.13791
 C 3.29508 -0.17402 2.49810
 H 2.32985 0.27148 2.78636
 H 3.94515 0.61741 2.09700
 H 3.76903 -0.55273 3.42054
 H 4.75081 -2.56547 2.21828

4b+
 SCF(BP86/BS1) = -1183.54691524
 G(298 K) = -1182.870913
 SCF(BS2) = -1853.21024071
 Lowest Frequencies = 21.0526cm⁻¹,
 28.9746cm⁻¹

84
 4b+
 Rh 0.07369 -0.05282 -0.03897
 P 2.34539 -0.70851 -0.15879
 P -2.24861 -0.78149 -0.12525
 C -1.26206 2.98446 0.45188
 H -2.35138 2.89791 0.35947
 C -0.54314 1.84555 1.17047
 H -0.88084 1.48114 2.14485
 C -3.30722 -0.13816 -1.62914
 C 1.80572 -2.22889 -1.08477
 H 2.24558 -2.28824 -2.09218
 H 2.06160 -3.16045 -0.55588
 C -4.44730 -1.82046 1.50032
 H -4.14738 -2.86376 1.32037
 H -5.20756 -1.54674 0.75676
 H -4.93658 -1.79830 2.48995
 C 3.53212 0.23144 -1.35239
 C -3.25831 -0.83729 1.53291
 C -2.05513 -2.61834 -0.56096
 H -2.67516 -3.23490 0.10432
 H -2.45308 -2.75410 -1.57815
 C 3.18261 -1.30155 1.47682
 C -0.44037 3.07610 -0.85386
 H -0.54383 2.17789 -1.49588
 H -0.66372 3.97089 -1.45689
 C 2.60202 0.76091 -2.46712

H	1.81387	1.42198	-2.07294
H	2.11948	-0.05812	-3.02687
H	3.19767	1.34350	-3.19165
C	-3.68004	1.34748	-1.48981
H	-2.79277	1.99283	-1.46328
H	-4.29324	1.55402	-0.60155
H	-4.27412	1.64401	-2.37216
C	0.70768	4.40159	0.78070
H	1.39050	4.40369	1.64515
H	0.90334	5.32017	0.20373
C	4.59481	-0.68651	-1.98650
H	4.15590	-1.55270	-2.50597
H	5.32858	-1.05740	-1.25857
H	5.14973	-0.10511	-2.74396
C	-3.79408	0.55507	1.91581
H	-4.65109	0.84836	1.29068
H	-3.03129	1.34178	1.84894
H	-4.15310	0.52486	2.95953
C	4.22136	1.40061	-0.62540
H	4.97637	1.04807	0.09469
H	3.50857	2.04609	-0.09161
H	4.74866	2.02696	-1.36615
C	-0.58097	-3.01414	-0.51325
H	-0.42573	-3.95281	-1.08442
H	-0.27663	-3.23151	0.52594
C	0.29613	-1.90327	-1.08012
H	-0.02922	-1.64511	-2.10707
H	0.12100	-0.83370	1.25321
C	-2.39872	-0.28100	-2.87108
H	-2.14156	-1.32595	-3.10583
H	-1.45966	0.28950	-2.76187
H	-2.93038	0.12662	-3.74851
C	-0.79501	4.28841	1.18273
H	-1.37547	5.15144	0.81803
H	-0.94857	4.22422	2.27144
C	4.56932	-1.90392	1.18494
H	5.29653	-1.14129	0.86852
H	4.52945	-2.69380	0.41719
C	-4.59742	-0.95698	-1.83150
H	-5.35548	-0.71798	-1.07108
H	-4.43675	-2.04607	-1.83034
H	-5.03189	-0.69311	-2.81202
C	0.92123	3.14668	-0.12987
H	1.81905	3.20191	-0.76030
C	-2.25337	-1.32410	2.60029
H	-1.43179	-0.60708	2.75452
H	-1.81409	-2.30319	2.34307
H	-2.78018	-1.44423	3.56318
C	0.81392	1.96063	0.82912
H	1.62837	1.72676	1.51601
C	2.28905	-2.38275	2.11817
H	2.22960	-3.30348	1.51819
H	1.26354	-2.02110	2.30486
H	2.72323	-2.65774	3.09509
C	3.30103	-0.12330	2.46297
H	2.30905	0.22832	2.78901
H	3.86116	0.72930	2.05058
H	3.83935	-0.46477	3.36431
H	4.96145	-2.36238	2.10963

(v) Figure S50

2b_exo,syn

SCF(BP86/BS1)= -1184.75919219
G(298 K) = -1184.056797
SCF(BS2) = -1854.42636484
Lowest Frequencies = 30.1674cm⁻¹,
48.4401cm⁻¹

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2b_exo,syn

Rh	-0.03564	0.42565	0.21258
P	1.79399	-0.94322	0.01603
P	-1.70364	-1.12567	0.02535
C	-1.30623	3.70467	-0.42867
H	-2.30519	3.58190	-0.87315
C	-0.94429	2.61278	0.61486
H	-1.43067	2.75218	1.59214
C	-2.91483	-0.58603	-1.42081
C	1.68060	-2.82856	0.00884
H	2.71463	-3.19264	0.10557
H	1.19571	-3.04313	0.97753
C	-4.01630	-2.02298	1.55322
H	-3.89635	-3.02573	1.11278
H	-4.75030	-1.46516	0.95339
H	-4.45790	-2.16274	2.55587
C	2.82572	-0.47167	-1.56598
C	-2.67489	-1.28188	1.70490
C	-1.35099	-2.92453	-0.36789
H	-0.93887	-3.36669	0.55128
H	-2.32263	-3.41444	-0.53247
C	2.88121	-0.72850	1.64505
C	-0.10295	3.62750	-1.39301
H	-0.01411	2.64729	-1.89526
H	-0.10428	4.42667	-2.15108
C	1.97840	-0.83790	-2.80276
H	0.98174	-0.36948	-2.75372
H	1.85990	-1.92148	-2.93775
H	2.48693	-0.45353	-3.70459
C	-3.84562	0.55295	-0.96168
H	-3.29263	1.42748	-0.58326
H	-4.56432	0.23807	-0.19158
H	-4.43129	0.89982	-1.83108
C	0.47783	5.16198	0.37002
H	0.83538	5.26301	1.40770
H	0.87005	6.02336	-0.19343
C	4.17008	-1.21968	-1.60966
H	4.05048	-2.31243	-1.53459
H	4.86008	-0.88844	-0.81866
H	4.66283	-1.01407	-2.57633
C	-2.89605	0.11693	2.31429
H	-3.49102	0.78324	1.67343
H	-1.93034	0.60422	2.52943
H	-3.43816	0.00976	3.27025
C	3.06410	1.05043	-1.63627
H	3.63124	1.45253	-0.78681
H	2.11093	1.59650	-1.71886
H	3.64441	1.27061	-2.54963
C	-0.39086	-3.14336	-1.55295
H	-0.81949	-3.88479	-2.24853
H	-0.27609	-2.21608	-2.13461

C	0.99628	-3.62711	-1.11452
H	1.65968	-3.67938	-1.99384
H	0.91395	-4.66774	-0.74884
C	-2.04397	-0.05479	-2.58077
H	-1.43574	-0.84650	-3.04388
H	-1.36003	0.74228	-2.24212
H	-2.70224	0.35544	-3.36758
C	-1.07882	5.07348	0.26323
H	-1.48336	5.88251	-0.36553
H	-1.58466	5.13718	1.24036
H	4.51874	-1.59880	2.75220
C	-3.76764	-1.76114	-1.93809
H	-4.39134	-2.22052	-1.15716
H	-3.15345	-2.54686	-2.40478
H	-4.44974	-1.38235	-2.71943
C	0.95409	3.84044	-0.28771
H	2.00841	3.84487	-0.60126
C	-1.77233	-2.07027	2.67895
H	-0.76089	-1.63881	2.72820
H	-1.69651	-3.13876	2.42448
H	-2.20936	-2.01359	3.69120
C	0.60221	2.69190	0.69524
H	0.97291	2.84532	1.72048
H	1.37357	-1.72477	2.90952
C	1.88268	-0.75117	2.82117
H	1.10809	0.02865	2.71289
H	2.42869	-0.58262	3.76667
C	3.62658	0.61887	1.65308
H	2.96723	1.47890	1.46257
H	4.45479	0.64334	0.92910
H	4.06878	0.76873	2.65371
C	3.91697	-1.85277	1.86192
H	4.61718	-1.96861	1.02159
H	3.44897	-2.82725	2.06598
H	1.21488	1.77734	0.30764
H	-1.42659	1.62775	0.21326

2b_exo,anti

SCF(BP86/BS1)= -1184.75905413
G(298 K) = -1184.056382
SCF(BS2) = -1854.42625173
Lowest Frequencies = 33.2327cm⁻¹,
47.9961cm⁻¹

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2b_exo,anti

Rh	-0.11366	0.40173	-0.19665
P	1.96989	-0.50352	0.13468
P	-1.40340	-1.45305	0.15155
C	-0.01526	3.98639	0.05827
H	0.98186	4.27110	0.42582
C	-0.01380	2.72459	-0.84661
H	0.35944	2.90840	-1.86534
C	-2.54273	-1.70022	-1.42609
C	2.24795	-2.25706	0.77929
H	3.32146	-2.32581	1.01238
H	1.72990	-2.23614	1.75451
C	-3.59562	-2.33789	1.84730
H	-3.20131	-3.36468	1.78612
H	-4.36925	-2.21596	1.07490
H	-4.09863	-2.24442	2.82605

C 3.03054 -0.35766 -1.49006
 C -2.48610 -1.27291 1.75885
 C -0.65369 -3.15290 0.40412
 H -0.25104 -3.16571 1.42792
 H -1.48369 -3.87534 0.39387
 C 2.82921 0.47567 1.61165
 C -1.06595 3.60266 1.12170
 H -0.77702 2.71420 1.71135
 H -1.31241 4.42984 1.80609
 C 2.43715 -1.33008 -2.53090
 H 1.36021 -1.14757 -2.67707
 H 2.59198 -2.38583 -2.27086
 H 2.93993 -1.15803 -3.49904
 C -3.74544 -0.73680 -1.39535
 H -3.44421 0.31852 -1.30652
 H -4.45634 -0.96491 -0.58807
 H -4.29528 -0.83275 -2.34810
 C -2.23659 4.63988 -0.70828
 H -2.66267 4.50077 -1.71522
 H -2.87460 5.36870 -0.18367
 C 4.50989 -0.70003 -1.24019
 H 4.64379 -1.68909 -0.77320
 H 5.01538 0.05269 -0.61644
 H 5.03907 -0.72568 -2.20917
 C -3.09405 0.14099 1.84188
 H -3.76412 0.37856 1.00337
 H -2.30314 0.90711 1.89087
 H -3.68970 0.21989 2.76833
 C 2.90518 1.05586 -2.09447
 H 3.23520 1.85984 -1.42332
 H 1.86774 1.25597 -2.40579
 H 3.53507 1.10578 -2.99999
 C 0.44035 -3.52407 -0.61498
 H 0.23910 -4.52600 -1.03074
 H 0.42155 -2.83234 -1.47106
 C 1.84650 -3.51821 -0.00558
 H 2.58819 -3.71956 -0.79604
 H 1.93493 -4.36527 0.70022
 C -1.68896 -1.36426 -2.66959
 H -0.87930 -2.09275 -2.82895
 H -1.22901 -0.36332 -2.59099
 H -2.33322 -1.38904 -3.56688
 C -0.74451 5.10390 -0.73196
 H -0.61731 6.06978 -0.21785
 H -0.34398 5.22343 -1.75177
 H 4.51296 0.43229 2.96358
 C -3.05841 -3.14734 -1.55229
 H -3.64945 -3.47357 -0.68344
 H -2.24209 -3.86860 -1.71286
 H -3.71766 -3.20847 -2.43603
 C -2.18156 3.31385 0.09378
 H -3.15193 2.98408 0.49309
 C -1.53150 -1.43376 2.96205
 H -0.66115 -0.76549 2.87490
 H -1.17840 -2.46807 3.09517
 H -2.07332 -1.16071 3.88437
 C -1.49384 2.26318 -0.82020
 H -1.93706 2.18197 -1.82472
 H 1.47787 -0.39655 3.12165
 C 1.76098 0.58952 2.71865
 H 0.84582 1.08210 2.34634

H 2.16738 1.18038 3.55895
 C 3.24318 1.89271 1.17584
 H 2.41716 2.45707 0.71601
 H 4.09620 1.88807 0.48075
 H 3.55765 2.45871 2.07029
 C 4.06812 -0.23207 2.20203
 H 4.85012 -0.43866 1.45729
 H 3.81454 -1.17190 2.71459
 H -1.74095 1.23779 -0.31787
 H 0.78484 2.01241 -0.38489

2b+ endo, syn

SCF(BP86/BS1)= -1184.75558857

G(298 K) = -1184.053057

SCF(BS2) = -1854.42255105

Lowest Frequencies = 25.2349cm⁻¹,
37.6566cm⁻¹

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2b+ endo, syn

Rh 0.06514 0.44693 -0.27143
 P -1.89128 -0.70064 0.01239
 P 1.54836 -1.27054 0.01113
 C -0.41098 4.08187 -0.06021
 H -1.39469 4.57341 -0.08596
 C -0.37265 2.75687 -0.86649
 H -0.99849 1.99066 -0.26583
 C 2.81631 -0.72950 1.40931
 C -1.95205 -2.58295 0.13555
 H -3.01105 -2.85938 0.02247
 H -1.45545 -2.90397 -0.79720
 C 3.75723 -2.51667 -1.42410
 H 3.55254 -3.45599 -0.88600
 H 4.54604 -1.97116 -0.88563
 H 4.17192 -2.79439 -2.40938
 C -2.89175 -0.05284 1.55538
 C 2.48723 -1.67413 -1.64566
 C 1.03054 -2.98522 0.56640
 H 0.58673 -3.48097 -0.30944
 H 1.95592 -3.53681 0.79082
 C -2.93388 -0.48521 -1.64809
 C 0.75955 4.83689 -0.73810
 H 0.61161 4.99405 -1.81967
 H 0.98202 5.80683 -0.26504
 C -2.02633 -0.32326 2.80464
 H -1.02094 0.11515 2.69282
 H -1.92475 -1.39252 3.03438
 H -2.50831 0.15038 3.67804
 C 3.83774 0.28335 0.85604
 H 3.36234 1.16457 0.39773
 H 4.52445 -0.16031 0.12061
 H 4.45444 0.65449 1.69341
 C 1.68110 3.66748 1.13286
 H 2.07944 2.72646 1.54267
 H 2.24437 4.49019 1.60148
 C -4.24838 -0.77005 1.68334
 H -4.15144 -1.86656 1.71906
 H -4.93803 -0.50558 0.86707
 H -4.72901 -0.45691 2.62693
 C 2.83025 -0.36572 -2.38408
 H 3.47955 0.30590 -1.80418

H	1.91091	0.17906	-2.65449	H	-1.17341	1.92152	-0.30223
H	3.36231	-0.61089	-3.32000	C	-2.96958	-0.73216	-1.42424
C	-3.11976	1.47059	1.49729	C	1.28088	-2.80752	0.91700
H	-3.74251	1.79515	0.65502	H	2.25880	-3.22181	1.20504
H	-2.16862	2.02363	1.46883	H	0.77216	-2.54928	1.86285
H	-3.63799	1.77686	2.42295	C	-4.21041	-0.90508	1.84426
C	0.05062	-3.00149	1.75430	H	-4.17474	-2.00580	1.82851
H	0.38973	-3.73141	2.50894	H	-4.88700	-0.56679	1.04567
H	0.04421	-2.02413	2.26023	H	-4.67105	-0.61213	2.80427
C	-1.38150	-3.35516	1.33658	C	2.69800	-1.45868	-1.43135
H	-2.05440	-3.24990	2.20424	C	-2.81268	-0.26320	1.75394
H	-1.42090	-4.42634	1.06391	C	-1.73218	-2.68901	0.48677
C	1.99800	-0.04414	2.52689	H	-1.39184	-2.81437	1.52544
H	1.37072	-0.75930	3.08070	H	-2.76574	-3.06469	0.45921
H	1.33413	0.73985	2.12132	C	2.77418	-0.39446	1.60747
H	2.69042	0.41584	3.25474	C	0.33667	4.82065	-1.15401
C	0.14390	3.82640	1.36465	H	0.18866	4.83615	-2.24684
H	-0.08325	4.67566	2.02759	H	0.48378	5.85377	-0.80021
H	-0.29809	2.92469	1.82287	C	1.80057	-2.19467	-2.44831
H	-4.63580	-1.26241	-2.72451	H	0.87164	-1.63272	-2.63716
C	3.57332	-1.92698	2.01671	H	1.54714	-3.21787	-2.14078
H	4.15314	-2.49601	1.27544	H	2.34568	-2.27092	-3.40573
H	2.90113	-2.62023	2.54574	C	-3.77393	0.58227	-1.44050
H	4.28873	-1.54316	2.76525	H	-3.13514	1.47398	-1.35183
C	1.81136	3.74991	-0.40277	H	-4.53977	0.62331	-0.65223
H	2.83460	3.92668	-0.76614	H	-4.30108	0.65830	-2.40781
C	1.50893	-2.46573	-2.54054	C	1.31962	3.92820	0.84445
H	0.53690	-1.95587	-2.62328	H	1.74014	3.04170	1.34569
H	1.34661	-3.49715	-2.19148	H	1.85558	4.80762	1.23517
H	1.93547	-2.53591	-3.55637	C	3.93567	-2.31521	-1.10855
C	1.14938	2.49754	-1.04954	H	3.68010	-3.25575	-0.59484
H	1.59503	1.57218	-0.52401	H	4.67393	-1.77273	-0.49873
H	-1.51527	-1.69429	-2.82478	H	4.43570	-2.58873	-2.05444
C	-1.92911	-0.67310	-2.80335	C	-2.93114	1.27148	1.78712
H	-1.08460	0.03492	-2.72690	H	-3.47291	1.69100	0.92811
H	-2.44650	-0.51129	-3.76597	H	-1.93450	1.73685	1.83572
C	-3.55266	0.92117	-1.74899	H	-3.47904	1.56914	2.69833
H	-2.83273	1.72737	-1.54651	C	3.12748	-0.14198	-2.11013
H	-4.41538	1.04324	-1.07705	H	3.72364	0.52044	-1.46970
H	-3.92447	1.06746	-2.77838	H	2.25170	0.41347	-2.47888
C	-4.06719	-1.52029	-1.81367	H	3.74745	-0.39178	-2.98900
H	-4.78215	-1.52127	-0.97744	C	-0.82080	-3.46676	-0.47977
H	-3.69128	-2.54438	-1.95623	H	-1.34686	-4.36494	-0.84570
H	1.41877	2.38461	-2.10951	H	-0.59821	-2.86302	-1.37288
H	-0.88077	2.84748	-1.83859	C	0.49585	-3.90125	0.17333

2b+ endo,anti

SCF(BP86/BS1)= -1184.75504933

G(298 K) = -1184.051969

SCF(BS2) = -1854.42214145

Lowest Frequencies = 28.5230cm⁻¹,
46.6514cm⁻¹

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2b+ endo,anti

Rh 0.01001 0.44043 -0.23935

P 1.63773 -1.11274 0.16604

P -1.83126 -0.84112 0.17440

C -0.78252 4.07139 -0.38797

H -1.79967 4.48044 -0.47823

C -0.64104 2.65706 -1.01671

H	-1.17341	1.92152	-0.30223	H	-1.17341	1.92152	-0.30223
C	-2.96958	-0.73216	-1.42424	C	-2.96958	-0.73216	-1.42424
C	1.28088	-2.80752	0.91700	C	1.28088	-2.80752	0.91700
H	2.25880	-3.22181	1.20504	H	2.25880	-3.22181	1.20504
H	0.77216	-2.54928	1.86285	H	0.77216	-2.54928	1.86285
C	-4.21041	-0.90508	1.84426	C	-4.21041	-0.90508	1.84426
H	-4.17474	-2.00580	1.82851	H	-4.17474	-2.00580	1.82851
H	-4.88700	-0.56679	1.04567	H	-4.88700	-0.56679	1.04567
H	-4.67105	-0.61213	2.80427	H	-4.67105	-0.61213	2.80427
C	2.69800	-1.45868	-1.43135	C	2.69800	-1.45868	-1.43135
C	-2.81268	-0.26320	1.75394	C	-2.81268	-0.26320	1.75394
C	-1.73218	-2.68901	0.48677	C	-1.73218	-2.68901	0.48677
H	-1.39184	-2.81437	1.52544	H	-1.39184	-2.81437	1.52544
H	-2.76574	-3.06469	0.45921	H	-2.76574	-3.06469	0.45921
C	2.77418	-0.39446	1.60747	C	2.77418	-0.39446	1.60747
C	0.33667	4.82065	-1.15401	C	0.33667	4.82065	-1.15401
H	0.18866	4.83615	-2.24684	H	0.18866	4.83615	-2.24684
H	0.48378	5.85377	-0.80021	H	0.48378	5.85377	-0.80021
C	1.80057	-2.19467	-2.44831	C	1.80057	-2.19467	-2.44831
H	0.87164	-1.63272	-2.63716	H	0.87164	-1.63272	-2.63716
H	1.54714	-3.21787	-2.14078	H	1.54714	-3.21787	-2.14078
H	2.34568	-2.27092	-3.40573	H	2.34568	-2.27092	-3.40573
C	-3.77393	0.58227	-1.44050	C	-3.77393	0.58227	-1.44050
H	-3.13514	1.47398	-1.35183	H	-3.13514	1.47398	-1.35183
H	-4.53977	0.62331	-0.65223	H	-4.53977	0.62331	-0.65223
H	-4.30108	0.65830	-2.40781	H	-4.30108	0.65830	-2.40781
C	1.31962	3.92820	0.84445	C	1.31962	3.92820	0.84445
H	1.74014	3.04170	1.34569	H	1.74014	3.04170	1.34569
H	1.85558	4.80762	1.23517	H	1.85558	4.80762	1.23517
C	3.93567	-2.31521	-1.10855	C	3.93567	-2.31521	-1.10855
H	3.68010	-3.25575	-0.59484	H	3.68010	-3.25575	-0.59484
H	4.67393	-1.77273	-0.49873	H	4.67393	-1.77273	-0.49873
H	4.43570	-2.58873	-2.05444	H	4.43570	-2.58873	-2.05444
C	-2.93114	1.27148	1.78712	C	-2.93114	1.27148	1.78712
H	-3.47291	1.69100	0.92811	H	-3.47291	1.69100	0.92811
H	-1.93450	1.73685	1.83572	H	-1.93450	1.73685	1.83572
H	-3.47904	1.56914	2.69833	H	-3.47904	1.56914	2.69833
C	3.12748	-0.14198	-2.11013	C	3.12748	-0.14198	-2.11013
H	3.72364	0.52044	-1.46970	H	3.72364	0.52044	-1.46970
H	2.25170	0.41347	-2.47888	H	2.25170	0.41347	-2.47888
H	3.74745	-0.39178	-2.98900	H	3.74745	-0.39178	-2.98900
C	-0.82080	-3.46676	-0.47977	C	-0.82080	-3.46676	-0.47977
H	-1.34686	-4.36494	-0.84570	H	-1.34686	-4.36494	-0.84570
H	-0.59821	-2.86302	-1.37288	H	-0.59821	-2.86302	-1.37288
C	0.49585	-3.90125	0.17333	C	0.49585	-3.90125	0.17333
H	1.14181	-4.37985	-0.58118	H	1.14181	-4.37985	-0.58118
H	0.28167	-4.69118	0.91739	H	0.28167	-4.69118	0.91739
C	-2.03711	-0.74678	-2.65623	C	-2.03711	-0.74678	-2.65623
H	-1.51876	-1.71070	-2.77419	H	-1.51876	-1.71070	-2.77419
H	-1.26583	0.04139	-2.59503	H	-1.26583	0.04139	-2.59503
H	-2.64058	-0.58453	-3.56751	H	-2.64058	-0.58453	-3.56751
C	-0.22313	4.05809	1.05466	C	-0.22313	4.05809	1.05466
H	-0.48396	4.99452	1.57231	H	-0.48396	4.99452	1.57231
H	-0.63350	3.23004	1.65430	H	-0.63350	3.23004	1.65430
H	4.30819	-0.93432	3.02705	H	4.30819	-0.93432	3.02705
C	-3.94591	-1.92056	-1.52909	C	-3.94591	-1.92056	-1.52909
H	-4.62120	-2.00425	-0.66451	H	-4.62120	-2.00425	-0.66451
H	-3.42375	-2.88068	-1.66255	H	-3.42375	-2.88068	-1.66255
H	-4.57827	-1.77364	-2.42241	H	-4.57827	-1.77364	-2.42241
C	1.46040	3.85893	-0.69289	C	1.46040	3.85893	-0.69289
H	2.47254	4.06880	-1.06942	H	2.47254	4.06880	-1.06942

C -1.97514 -0.68515 2.98099
H -0.93493 -0.33473 2.89531
H -1.97446 -1.77318 3.14948
H -2.41099 -0.22344 3.88413
C 0.89549 2.50326 -1.20398
H 1.42584 1.67327 -0.60343
H 1.19424 -0.60980 3.12877
C 1.80211 0.18058 2.65902
H 1.11159 0.91917 2.21353
H 2.38056 0.66882 3.46377
C 3.68620 0.73367 1.09143
H 3.14248 1.50831 0.52956
H 4.50410 0.35357 0.46096
H 4.15241 1.23434 1.95826
C 3.66315 -1.45269 2.29589
H 4.32784 -1.98495 1.59994
H 3.07963 -2.19414 2.86157
H 1.15723 2.31855 -2.25598
H -1.17062 2.58031 -1.97826

2b+ exo,br
SCF(BP86/BS1)= -1184.74893084
G(298 K) = -1184.048308
SCF(BS2) = -1854.41656061
Lowest Frequencies = 18.3168cm⁻¹,
26.5610cm⁻¹

86

2b+ exo,br
Rh 0.14183 0.38347 -0.09702
P -2.05113 -0.17638 0.03334
P 1.10278 -1.66709 0.03250
C 0.44137 4.21933 0.04142
H -0.32226 4.30182 0.83286
C 1.86067 4.33747 0.64671
H 1.96534 5.16882 1.35901
C 1.82143 2.22434 -0.13697
H 1.96262 1.09173 -0.14054
C 2.34168 -1.80877 -1.49233
C 2.06965 -1.84223 1.71194
C 0.23820 -3.32762 -0.17720
H 1.03889 -4.06193 0.01281
H 0.02152 -3.38865 -1.25797
C -2.34568 -3.18933 0.07281
H -2.34795 -3.21142 -1.02803
H -3.14515 -3.88655 0.38189
C -2.76148 -1.81852 0.62375
H -3.84934 -1.69375 0.49105
H -2.58508 -1.81397 1.71368
C 2.04964 2.91843 1.22524
H 1.29551 2.64927 1.98361
H 3.05650 2.73417 1.63352
C 0.45897 2.78560 -0.59636
H -0.45625 2.23191 -0.18437
C -2.92021 0.13781 -1.67784
C 2.90155 4.35834 -0.50421
H 3.89465 4.64595 -0.12518
C -2.84015 0.97527 1.42539
C -1.02014 -3.74866 0.59447
H -0.93337 -3.54339 1.67268
H -1.06687 -4.84911 0.50782

C 2.91311 2.87991 -1.02433
H 3.89069 2.40224 -0.84887
C 3.58244 -0.91622 -1.30652
H 4.23356 -1.25818 -0.48816
H 4.18180 -0.95214 -2.23321
H 3.32998 0.13983 -1.13599
C 1.02802 -2.12409 2.81559
H 0.64945 -3.15593 2.77874
H 1.50892 -1.99226 3.80091
H 0.17748 -1.42436 2.76267
C 2.75218 -0.50257 2.04842
H 2.00299 0.29698 2.16600
H 3.28881 -0.60615 3.00812
H 3.48803 -0.18710 1.29410
C -1.86250 0.91422 2.61879
H -0.85192 1.25718 2.33403
H -2.24101 1.55585 3.43466
H -1.76390 -0.10676 3.02387
C 3.11019 -2.97605 1.69671
H 3.95125 -2.77285 1.01730
H 3.53228 -3.08032 2.71205
H 2.67342 -3.95251 1.43203
C -4.23233 0.50207 1.90070
H -4.20540 -0.47396 2.40607
H -4.60523 1.23138 2.64123
H -4.97446 0.45655 1.09072
C 1.54925 -1.31605 -2.72220
H 1.18931 -0.28097 -2.58580
H 2.20075 -1.35217 -3.61373
H 0.67228 -1.95049 -2.93323
C -2.97327 2.43632 0.95784
H -3.71916 2.56084 0.15896
H -3.30933 3.04890 1.81291
H -2.02361 2.87067 0.61374
C 2.82625 -3.25127 -1.76060
H 2.01488 -3.92748 -2.06609
H 3.54336 -3.21840 -2.59965
H 3.35125 -3.69918 -0.90483
C -2.33453 1.41352 -2.31419
H -1.25286 1.29457 -2.49285
H -2.82269 1.58266 -3.29019
H -2.49341 2.31638 -1.70627
C -2.56698 -1.04903 -2.59869
H -3.12748 -1.95894 -2.33938
H -2.83803 -0.78764 -3.63679
H -1.48761 -1.27167 -2.58167
C -4.45101 0.25268 -1.56922
H -4.77418 1.15253 -1.02544
H -4.87225 0.32147 -2.58792
H -4.91102 -0.62852 -1.09356
H 2.62935 5.07913 -1.29169
H 2.68480 2.78957 -2.09840
H 0.22379 4.99106 -0.71343
H 0.35123 2.80177 -1.69043

2+ endo
SCF(BP86/BS1)= -1184.76424864
G(298 K) = -1184.070557
SCF(BS2) = -1854.42857842
Lowest Frequencies = 21.0190cm⁻¹,
28.4368cm⁻¹

86
 2+ endo
 Rh 0.06628 -0.42239 -0.10403
 P 2.35527 -0.86621 0.09719
 P -2.23840 -0.94328 0.06414
 C 1.01493 3.44299 -1.00166
 H 1.31483 3.53919 -2.05864
 C 0.25095 4.70138 -0.52384
 H 0.70983 5.64436 -0.85656
 C -1.29938 3.05867 -0.30854
 H -2.23831 2.50696 -0.45896
 C -3.36060 -0.48020 1.56481
 C -3.18446 -1.06433 -1.60781
 C -1.59342 -2.67356 0.45350
 H -2.13237 -3.49923 -0.04327
 H -1.66347 -2.82420 1.54315
 C 0.94496 -3.14433 0.87100
 H 0.81376 -2.86239 1.93004
 H 0.83511 -4.24646 0.82144
 C 2.33715 -2.73434 0.36985
 H 3.15205 -3.04633 1.04190
 H 2.53082 -3.20000 -0.61070
 C -1.17392 4.41073 -1.04825
 H -1.22605 4.31760 -2.14644
 H -1.92144 5.15051 -0.71749
 C -0.05158 2.30700 -0.82845
 H -0.24859 1.78402 -1.78148
 C 3.25435 -0.12445 1.62562
 C 0.05071 4.60301 1.00942
 H -0.31632 5.55837 1.41734
 C 3.32264 -0.63206 -1.55307
 C -0.13520 -2.47433 0.02240
 H 0.05043 -0.32128 1.41056
 H -0.00097 -2.75870 -1.04366
 C -1.02703 3.47558 1.15728
 H -1.94615 3.85799 1.63123
 C -4.19720 0.77278 1.25027
 H -4.96060 0.58346 0.48009
 H -4.73073 1.08319 2.16561
 H -3.57205 1.62076 0.92969
 C -2.22486 -1.77221 -2.58880
 H -2.01562 -2.81567 -2.30436
 H -2.68851 -1.79119 -3.59043
 H -1.26340 -1.23565 -2.68666
 C -3.44954 0.35964 -2.13577
 H -2.51371 0.93344 -2.23718
 H -3.91126 0.29353 -3.13656
 H -4.13578 0.93199 -1.49509
 C 2.29844 -1.01933 -2.64500
 H 1.40929 -0.36010 -2.61851
 H 2.75952 -0.90441 -3.64183
 H 1.95847 -2.06512 -2.55981
 C -4.49479 -1.86104 -1.50223
 H -4.91471 -2.00463 -2.51362
 H -4.34317 -2.86129 -1.06446
 H -5.25561 -1.33125 -0.90904
 C 4.57019 -1.52601 -1.67189
 H 4.33601 -2.59822 -1.58287
 H 5.02220 -1.37582 -2.66835
 H 5.33699 -1.27939 -0.92421

C -2.40587 -0.17095 2.73672
 H -1.77131 0.70412 2.52552
 H -3.00605 0.05261 3.63611
 H -1.75185 -1.02391 2.98475
 C 3.70792 0.84596 -1.73676
 H 4.48991 1.16476 -1.03067
 H 4.11058 0.99075 -2.75464
 H 2.84081 1.51536 -1.62473
 C -4.28691 -1.64944 1.95302
 H -3.72931 -2.56027 2.22129
 H -4.87204 -1.35481 2.84184
 H -5.00289 -1.90579 1.15999
 C 3.00852 1.39643 1.66232
 H 1.93135 1.62937 1.69354
 H 3.46850 1.81498 2.57455
 H 3.45201 1.91799 0.80157
 C 2.60906 -0.75684 2.87713
 H 2.80589 -1.83737 2.95763
 H 3.03732 -0.27904 3.77530
 H 1.51790 -0.59443 2.90626
 C 4.76297 -0.42979 1.61906
 H 5.29153 0.09507 0.80888
 H 5.20409 -0.08670 2.57128
 H 4.97319 -1.50838 1.53211
 H 0.99146 4.36595 1.53431
 H -0.67488 2.62495 1.76744
 H 1.92854 3.26894 -0.41126
 H 0.31095 1.56587 -0.05237

2+ exo-1
 SCF(BP86/BS1)= -1184.76272688
 G(298 K) = -1184.068947
 Lowest Frequencies = 24.6635cm⁻¹,
 29.7584cm⁻¹

86
 2+ exo-1
 C -0.00343 5.24018 0.28481
 C -1.00666 4.17870 0.80115
 C -0.22783 2.86604 1.07269
 C 0.14232 2.37726 -0.36285
 C -0.50459 3.44296 -1.28825
 C 0.34054 4.73538 -1.15737
 C -1.77416 3.81837 -0.49224
 Rh 0.05292 -0.44817 0.06363
 P -2.20983 -1.08376 0.02159
 C -3.28360 -0.68367 1.56954
 C -4.34983 -1.75490 1.86086
 C -0.09090 -2.41615 0.67159
 C -1.52822 -2.82088 0.30448
 P 2.37005 -0.83711 0.07026
 C 3.30060 0.00684 1.53403
 C 2.26721 0.01191 2.68451
 C 1.04250 -3.29505 0.14341
 C 2.40336 -2.67627 0.49687
 C 3.29036 -0.67661 -1.60985
 C 2.99353 0.71305 -2.20680
 C 2.70307 -1.74958 -2.55126
 C 4.80699 -0.89864 -1.47215
 C -3.17246 -1.01709 -1.64341
 C -2.38203 -1.83269 -2.68594

C -3.20219 0.46027 -2.08670
 C -4.59933 -1.58241 -1.53397
 C -3.93766 0.69954 1.39923
 C -2.28637 -0.63175 2.74856
 C 4.56505 -0.75127 1.97966
 C 3.65831 1.46165 1.17895
 H -1.61664 4.51293 1.65401
 H 0.65929 3.02783 1.70826
 H -2.06036 -3.40475 1.07421
 H -1.55986 -3.38463 -0.64020
 H 5.04814 -1.86239 -0.99439
 H 5.29781 -0.09456 -0.90332
 H 5.26190 -0.90984 -2.47814
 H 3.25031 -3.18280 0.00763
 H 2.56978 -2.74637 1.58466
 H -2.47658 2.97663 -0.36721
 H -2.31911 4.67219 -0.92727
 H -1.48867 0.11536 2.58630
 H -1.81566 -1.60921 2.94317
 H -2.82679 -0.34108 3.66639
 H 2.78099 2.03393 0.83833
 H 4.43928 1.52504 0.40603
 H 4.05106 1.96530 2.07970
 H 1.41703 4.54354 -1.30205
 H 0.03662 5.46894 -1.92175
 H -3.91632 -2.76208 1.96755
 H -5.13189 -1.79665 1.09107
 H -4.84373 -1.51323 2.81866
 H 3.38169 1.53467 -1.58629
 H 1.91077 0.86456 -2.34685
 H 3.47584 0.79167 -3.19680
 H -4.70654 0.70554 0.61115
 H -3.19548 1.48153 1.16891
 H -4.43655 0.98281 2.34249
 H 0.96633 -4.31125 0.58040
 H 0.94050 -3.41471 -0.94890
 H 0.01013 -2.29892 1.77283
 H 0.09513 -0.87084 -1.39521
 H 1.94869 -1.00360 2.97443
 H 1.36715 0.59873 2.42194
 H 2.71366 0.48198 3.57856
 H -0.47369 6.23624 0.25581
 H 0.88430 5.31920 0.93386
 H -5.24672 -0.96320 -0.89479
 H -4.61085 -2.61589 -1.15170
 H 5.34087 -0.77143 1.20155
 H 4.35502 -1.78887 2.28241
 H 4.99464 -0.23955 2.85913
 H -0.65203 3.10406 -2.32563
 H 1.60824 -1.65637 -2.65268
 H 2.93994 -2.77514 -2.22756
 H 3.13921 -1.61505 -3.55632
 H 1.22204 2.29128 -0.54162
 H -2.42803 -2.91676 -2.49830
 H -1.32285 -1.52849 -2.74015
 H -2.82716 -1.65538 -3.68020
 H -2.18421 0.86408 -2.21098
 H -3.74251 1.10459 -1.37707
 H -3.71815 0.53598 -3.05981
 H -5.05597 -1.59684 -2.53918
 H -0.87347 2.13440 1.59223

H -0.34859 1.38664 -0.61577

2+ exo-2

SCF(BP86/BS1) = -1184.76289339

G(298 K) = -1184.067901

SCF(BS2) = -1854.42735749

Lowest Frequencies = 25.8867cm⁻¹,
29.8320cm⁻¹

86

2+ exo-2

Rh 0.02891 -0.44039 -0.04202

P -2.29164 -0.91685 0.01853

P 2.30615 -0.98077 0.03347

C -1.33773 3.02551 0.41633

H -1.65450 2.52250 1.34513

C -0.85396 4.46407 0.71854

H -1.50672 5.00792 1.41786

C 1.01197 3.45875 -0.09133

H 2.04849 3.09355 -0.12273

C 3.22553 -0.53737 -1.60286

C 3.28260 -0.50527 1.61776

C 2.22994 -2.86761 0.02681

H 3.03976 -3.30046 0.63487

H 2.40014 -3.18941 -1.01379

C -0.23320 -2.48198 -0.25021

H 0.01491 -0.62604 1.46490

H -0.11369 -2.61223 -1.34643

C -1.69535 -2.69970 0.16135

H -2.25934 -3.43776 -0.43570

H -1.76244 -2.99187 1.22220

C 0.59195 4.20026 1.19804

H 0.64483 3.57153 2.10451

H 1.17125 5.12196 1.37078

C -0.06166 2.34130 -0.17152

H 0.26087 1.48707 0.49998

C -3.21014 -0.76929 -1.66591

C -0.61488 5.19644 -0.62496

H -0.44881 6.27273 -0.45769

C -3.43275 -0.63057 1.54696

C 0.82933 -3.30434 0.47924

H 0.71595 -3.17807 1.56994

H 0.68390 -4.38305 0.26852

C 0.67584 4.50652 -1.18202

H 1.50268 5.22797 -1.28519

C 3.65107 0.94073 -1.59259

H 4.46017 1.13899 -0.87307

H 4.03052 1.21497 -2.59254

H 2.80614 1.60959 -1.36474

C 2.64132 -1.28519 2.78540

H 2.78607 -2.37362 2.70131

H 3.11664 -0.96425 3.72850

H 1.56076 -1.07964 2.87422

C 3.11107 1.00278 1.88224

H 2.04866 1.27605 1.98704

H 3.61829 1.26313 2.82762

H 3.55136 1.62634 1.09062

C -2.48891 -0.45379 2.75490

H -1.84482 0.43346 2.64510

H -3.09556 -0.32562 3.66847

H -1.84088 -1.33253 2.91305

C	4.77441	-0.87000	1.51431
H	5.30315	-0.25293	0.77200
H	5.25756	-0.69000	2.49061
H	4.93271	-1.93152	1.26279
C	-4.35843	-1.83860	1.79261
H	-3.79967	-2.76878	1.97966
H	-4.96582	-1.63950	2.69299
H	-5.05460	-2.01682	0.96100
C	2.15557	-0.73757	-2.70129
H	1.28906	-0.06426	-2.55175
H	2.58846	-0.49378	-3.68754
H	1.78468	-1.77481	-2.75324
C	-4.27434	0.64600	1.36590
H	-5.04613	0.53002	0.58966
H	-4.79891	0.86267	2.31286
H	-3.65750	1.52359	1.11999
C	4.44116	-1.43615	-1.89506
H	4.17931	-2.50426	-1.94937
H	4.86163	-1.15686	-2.87743
H	5.24120	-1.31698	-1.15102
C	-3.41822	0.72389	-1.98912
H	-2.46169	1.27273	-1.99288
H	-3.86178	0.81730	-2.99591
H	-4.09682	1.22284	-1.28293
C	-2.26494	-1.36683	-2.73021
H	-2.09664	-2.44681	-2.59368
H	-2.71854	-1.22846	-3.72704
H	-1.28402	-0.85826	-2.74663
C	-4.54705	-1.52833	-1.68268
H	-5.29535	-1.06965	-1.01879
H	-4.96390	-1.50670	-2.70523
H	-4.42963	-2.58696	-1.39857
H	-1.47754	5.10271	-1.30510
H	0.52412	4.04328	-2.17183
H	-2.19036	3.00392	-0.28200
H	-0.19741	1.97510	-1.20613

2+ br

SCF(BP86/BS1)= -1184.76313842
 G(298 K) = -1184.068351
 SCF(BS2) = -1854.42705258
 Lowest Frequencies = 23.3169cm⁻¹,
 34.1962cm⁻¹

86

2+ br

Rh	-0.07957	-0.36933	0.06154
P	-2.37359	-0.82773	0.08533
P	2.22636	-0.94142	0.00945
C	3.26266	-1.00658	-1.61899
C	2.24248	-1.00905	-2.77654
C	4.12485	-2.28185	-1.69343
C	4.15768	0.24023	-1.74012
C	3.28103	-0.57801	1.58149
C	2.36393	-0.88034	2.78663
C	4.54246	-1.45418	1.66014
C	3.65753	0.91580	1.62224
C	1.55080	-2.68924	0.24039
C	0.12057	-2.33625	0.66314
C	-0.99665	-3.24715	0.15451
C	-2.36872	-2.66344	0.51898

C	-3.29560	-0.68837	-1.59568
C	-3.02184	0.70419	-2.19548
C	-4.80853	-0.93368	-1.45526
C	-2.69332	-1.75499	-2.53477
C	-3.31751	0.00567	1.54259
C	-3.68321	1.45341	1.16995
C	-4.57517	-0.76379	1.98706
C	-2.29047	0.02444	2.69853
H	1.64169	-0.08543	-2.79310
H	2.78829	-1.08048	-3.73377
H	1.55474	-1.87051	-2.72819
H	3.52227	-3.20288	-1.66031
H	4.66728	-2.28497	-2.65518
H	4.87634	-2.33415	-0.89355
H	4.97495	0.24136	-1.00278
H	4.62532	0.24552	-2.74022
H	3.58657	1.17629	-1.63821
H	2.10070	-1.94706	2.86519
H	2.89315	-0.60440	3.71524
H	1.43032	-0.28989	2.75641
H	5.28491	-1.18197	0.89452
H	5.02326	-1.30804	2.64366
H	4.31668	-2.52865	1.56239
H	2.76527	1.56068	1.59335
H	4.18885	1.12647	2.56698
H	4.32260	1.21229	0.79900
H	1.55415	-3.18597	-0.74349
H	2.11754	-3.32054	0.94721
H	0.04706	-2.23123	1.76654
H	-0.90527	-3.37084	-0.93834
H	-0.88562	-4.25797	0.59623
H	-3.20770	-3.18933	0.03644
H	-2.52611	-2.73291	1.60818
H	-1.94261	0.86728	-2.34720
H	-3.51511	0.77674	-3.18052
H	-3.40790	1.52256	-1.57062
H	-5.31148	-0.13358	-0.89154
H	-5.26319	-0.95809	-2.46107
H	-5.03462	-1.89821	-0.97173
H	-2.91570	-2.78316	-2.20884
H	-3.13204	-1.62862	-3.53976
H	-1.59998	-1.64615	-2.63776
H	-4.48908	1.50087	0.42162
H	-4.04310	1.98108	2.07061
H	-2.81561	2.00983	0.78141
H	-4.35342	-1.79704	2.29679
H	-5.01337	-0.25178	2.86209
H	-5.34818	-0.79763	1.20684
H	-1.39389	0.61695	2.43969
H	-2.74676	0.49407	3.58777
H	-1.96556	-0.98737	2.99411
H	-0.12650	-0.82682	-1.38417
C	0.01965	2.53452	-0.42005
C	-0.94555	3.57156	-1.04728
C	-0.11710	4.89870	-0.96186
C	1.22092	4.44501	-0.32560
C	1.39022	3.03144	-0.92873
C	0.11367	2.80389	1.10236
C	0.97580	4.11104	1.16646
H	-0.25984	1.48558	-0.72939
H	-1.17536	3.30989	-2.09324

H	-1.90392	3.63018	-0.50568
H	-0.61894	5.67137	-0.35743
H	0.04923	5.32376	-1.96472
H	2.05458	5.14349	-0.49157
H	2.23841	2.47623	-0.49749
H	1.47260	3.02554	-2.02883
H	0.61573	1.96993	1.63049
H	-0.87911	2.92889	1.56419
H	0.46191	4.92706	1.69905
H	1.93119	3.93082	1.68763

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