

Supporting Information

Cleavage of N–H Bond of Ammonia via Metal–Ligand Cooperation Enables Rational Design of a Conceptually New Noyori–Ikariya Catalyst

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1. Experimental Details

1.1. General Procedures, Instrumentation. Unless otherwise stated, all manipulations were carried out under argon using standard Schlenk or glovebox techniques. Solvents were distilled under argon over appropriate drying agent and stored over freshly activated 4 Å molecular sieves. CD₂Cl₂ (ISOTEC, CIL) for the VT NMR experiments with water sensible complex **4**¹ was distilled under argon from CaH₂ and used immediately. Commercially available deuterated solvents were used for routine NMR measurements after distillation. All NMR experiments were carried out on a JEOL ECX-400 instrument equipped with a field-gradient probe. Assignments of the signals in the spectra were carried out with the use of routine 1D and 2D correlation techniques. The ¹H (399.78 MHz) and ¹³C (100.5 MHz) NMR spectra were calibrated by using the residual solvent signal relative to TMS, and the ¹⁹F (376.2 MHz) spectra were calibrated relative to CFC₃ in ppm (δ). Full assignment of peaks are provided in Table S1 and are based on DFT NMR GIAO computed chemicals shifts, *vide infra*. ³¹P (161.8 MHz) chemical shifts were referenced to external 85% H₃PO₄. High-resolution electrospray ionization mass spectrometry (HRESI-MS) analysis was performed for selected compounds in positive ion mode on JEOL JMS-T100CS spectrometer. The compounds were dissolved in methanol and immediately analyzed in the presence of internal polyethylene glycol (PEG). Statistical accuracy (reproducibility of the data) was ± 0.009. Metallacycles **6**, **7**, and **10** feature remarkable stabilities in the HRESI-MS spectra towards fragmentation and mostly protonated M–H⁺ (or less-intensive M–Na⁺, M–K⁺) peaks are observed. HRESI-MS spectra of corresponding protonated derivatives [6H]⁺X[–], [7H]⁺BF₄[–], [10H]⁺X[–] (X = BF₄, OTf) and **17** are almost identical to the neutral precursors **6**, **7**, and **10**; the difference being the absence of the ions M–Na⁺ and M–K⁺ for the initially protonated ionic complexes. Elemental analyses were performed on a Perkin-Elmer 2400II CHN analyzer, ATR-IR spectra (neat) were measured on JASCO FT/IR-6100 spectrometer with a resolution of 2 cm^{–1}. Peak assignment is performed based on the DFT computed frequencies, *vide infra*. Complexes [RuCl₂(η⁶-*p*-cymene)]₂,² [RuCl₂(η⁶-hmb)]₂,² [Cp*IrCl₂]₂,³ [Ru{(S,S)-*p*-TsNCH(Ph)CH(Ph)NH}(η⁶-*p*-cymene)] **1**,⁴ [Ru{(S,S)-N(SO₂CF₃)CH(Ph)CH(Ph)NH}(η⁶-hmb)] **2**⁵ were prepared according to literature procedures. The complex [Cp*Ir{(S,S)-N(SO₂CF₃)CH(Ph)CH(Ph)NH}] **3** was prepared similarly to **5**.⁶ Pentafluorophenylsulfonyl chloride (TCI) and triethylamine were distilled under Ar prior to use. ^tBuOK was sublimed prior to use. Tetrafluoroboric acid diethyl ether complex was purchased from Sigma-Aldrich, and TfOH and (S)-(+)-1,1'-binaphthyl-2,2'-diyl hydrogenphosphate (BNPH) were purchased from TCI. (S,S)-DPEN where DPEN = H₂NCH(Ph)CH(Ph)NH₂, was generously donated by Takasago International Corporation. HPLC analysis was performed by using a Chiralcel OD column (hexane/iPrOH = 95/5, flow rate 1.0 mL/min, 30 °C, UV = 254 nm; retention time for 1-phenylethanol: 7.9 min (S), 8.9 (R); retention time for 1-indanol: 8.3 min (R), 9.2 (S)) or a Chiralcel OB column (hexane/iPrOH = 98/2, flow rate 1.0 mL/min, 35 °C, UV = 220 nm; retention time for the 1-phenyl-1,2-ethanediol: 30.1 min (R), 41.5 (S)).

1.2. Synthesis. (S,S)-FsDPEN, where FsDPEN = NH(SO₂C₆F₅)CH(Ph)CH(Ph)NH₂.⁷ Under argon, a dry CH₂Cl₂ solution (50 mL) of pentafluorophenylsulfonyl chloride (2.970 mL, 20.0 mmol) was added in a dropwise-manner over 3 h to a mixture of (S,S)-DPEN (4245 mg, 20.0 mmol) and triethylamine (2.945 mL, 19.2 mmol) in dry CH₂Cl₂ (120 mL) at 0 °C.

After the reaction mixture was stirred overnight, the solution was washed with water (40 mL $\times$ 2) and saturated NaCl solution (40 mL), then dried with Na₂SO₄. After filtration, the solvent was removed under reduced pressure to give a white solid. After recrystallization from hot ethyl acetate, the compound was washed with pentane and dried under vacuum. Yield: 5574 mg (63%). Elem. Anal. (%): Calc. C, 54.30; H, 3.42; N, 6.33; Found C, 54.25; H, 3.38; N, 6.33. ¹H NMR (CD₂Cl₂, 25 °C): 3.34 (br, 3H), 4.36 (d, ³J_{HH} = 4 Hz, 1H), 4.64 (d, ³J_{HH} = 4 Hz, 1H), 7.15–7.70 (m, 10H); ¹⁹F NMR (CD₂Cl₂, 25 °C): –136.1 (m, *o*-F, 2F), –148.4 (m, *p*-F, 1F), –160.2 (m, *m*-F, 2F); ¹³C{¹H} NMR (CD₂Cl₂, 25 °C): 59.4 (s, 1C, Ph^FSO₂NHCH₂CH₂NH₂), 63.7 (s, 1C, Ph^FSO₂NHCH₂CH₂NH₂), 116.1 (t, 1C_{ipso}, Ph^F), 126.3 (s, 2C), 126.6 (s, 2C), 127.6 (s, 1C), 128.0 (s, 1C), 128.4 (s, 2C), 128.7 (s, 2C), 137.5 (td, ¹J_{C-F} = 260 Hz), 139.1 (s, 1C_{ipso}), 141.1 (s, 1C_{ipso}), 143.4 (td, ¹J_{C-F} = 260 Hz), 143.9 (dd, ¹J_{C-F} = 260 Hz).

[Ru{(S,S)-C₆F₅SO₂NCH(Ph)CH(Ph)NH}{η⁶-hmb}] 4. Dry dichloromethane (10 mL) was added to a mixture of **8** (300 mg, 0.41 mmol) and ^tBuOK (1.2 equiv.; 55 mg) under argon. Immediate change of the color to violet was observed. The mixture was stirred for 5 min at room temperature and the solvent was evaporated. The product was extracted with dry diethyl ether (5 $\times$ 20 mL) and filtered through Celite on a coarse porosity frit. The yield after solvent evaporation was 274 mg (95%), giving violet powder. The compound changes color to brown upon standing in air in the solid state and immediately in wet solutions, but is stable indefinitely under dry argon. Elem. Anal. (%): Calc. C: 54.62; H: 4.44; N: 3.98; Found C: 54.25; H 4.48; N: 3.97. ¹H NMR (CD₂Cl₂, 25 °C): 2.35 (s, 18H), 3.86 (d, ³J_{H_CNH} = 4 Hz, 1H), 3.90 (s, 1H), 5.98 (d, ³J_{H_NCH} = 4 Hz, 1H), 6.97–7.12 (m, 5H), 7.17–7.30 (m, 3H), 7.42–7.44 (m, 2H); ¹⁹F NMR (CD₂Cl₂, 25 °C): –135.7 (virtual td, J_{F-F} = 4 Hz, J_{F-F} = 23 Hz, *o*-F, 2F), –153.8 (tt, ³J_{F-F} = 20 Hz, ⁴J_{F-F} = 4 Hz, *p*-F, 1F), –162.1 (m, *m*-F, 2F).

[Cp*Ir{(S,S)-C₆F₅SO₂NCHPhCHPhNH}] 5. Method A: A mixture of [Cp*IrCl₂]₂ (500 mg, 0.628 mmol), (S,S)-FsDPEN (555 mg, 1.255 mmol), and powdered potassium hydroxide (500 mg, 8.9 mmol) in dichloromethane (10 mL) was stirred at room temperature under argon for 20 min. Water (10 mL) was then added to the reaction and the obtained two-phase mixture was stirred for 30 min. The water was removed via a syringe and the organic phase was washed with an additional 5 mL of water three times. After addition of CaH₂ to the organic phase, extensive gas evolution was observed. Additional CaH₂ was added until gas evolution ceased. An additional 10 mL of dichloromethane was added to the deep purple colored organic phase, which was then was filtered through a WhatmanTM filter then Celite, and finally dried in vacuo. Yield: 858 mg (89%), red-purple powder. The product contains ~0.3% of (*R*)-Cp*Ir[κ³(*N,N',O*)-(S,S)-OC₆F₄SO₂NCH(Ph)CH(Ph)NH₂].¹ Elem. Anal. (%): Calc. C: 46.93; H 3.65; N: 3.65; Found C: 46.22; H: 3.55; N: 3.50. HRESI-MS, *m/z*: 769.1521 (calc. 769.1499, [M–H⁺]). ¹H NMR (CD₂Cl₂, 25 °C): 1.95 (s, 15H, Cp*), 4.04 (s, 1H), 4.06 (d, ³J_{H_CNH} = 5 Hz, 1H), 5.39 (1H, NH, d, ³J_{H_NCH} = 5 Hz), 7.04–7.60 (10H); ¹⁹F NMR (CD₂Cl₂, 25 °C): –135.4 (virtual td, J_{F-F} = 4 Hz, J_{F-F} = 23 Hz, *o*-F, 2F), –152.9 (tt, ³J_{F-F} = 20 Hz, ⁴J_{F-F} = 4 Hz, *p*-F, 1F), –161.7 (m, *m*-F, 2F); ¹³C{¹H} NMR (CD₂Cl₂, 25 °C): 10.1 (s, 5C, C₅Me₅), 72.9 (s, 1C, RSO₂NCH₂CH₂NH), 79.2 (s, 1C, RSO₂NCH₂CH₂NH), 86.0 (s, 5C, C₅Me₅), 117.7 (low intensity t, C_{ipso}, 1C) 126.0 (s, 2C), 126.5 (s, 1C), 126.7 (s, 1C), 127.1 (2C), 127.6 (4C), 137.0 (td, ¹J_{C-F} = 255Hz, *m*-C, 2C), 141.7 (td, ¹J_{C-F} = 255Hz, *p*-C, 1C) 143.9 (dd, ¹J_{C-F} = 255Hz, *o*-C, 2C), 144.7 (C_{ipso}, s, 1C), 147.2 (C_{ipso}, s, 1C).

Method B: A KOH (129 mg, 2.30 mmol) solution in 5 mL of water was added to $[\text{Cp}^*\text{IrCl}\{\kappa^2(N,N')\text{-(S,S)-FsNCHPhCHPhNH}_2\}]^6$ (1.385 g, 1.72 mmol) in CH_2Cl_2 (40 mL) at room temperature. After stirring for 15 min, the red-purple organic layer was washed with water (3 mL $\times$ 3), dried over Na_2SO_4 , and further dried with CaH_2 . After filtration, the resulting anhydrous solution was evaporated to dryness to afford a red-purple solid **5** (1.197 g, 1.56 mmol 91%). Elem. Anal. (%): Calc.: C, 43.66; H, 3.55; N, 3.29; Found: C, 43.71; H, 3.39; N, 3.37%.

[(S)-Ru $\{\kappa^3(N,N',N'')\text{-(S,S)-NHC}_6\text{F}_4\text{SO}_2\text{dpn}\}(\eta^6\text{-hmb})]$ **6. **Method A:** To a mixture of $[\text{RuCl}_2(\eta^6\text{-hmb})]_2$ (200 mg, 0.30 mmol), (S,S)-FsDPEN (265 mg, 0.60 mmol) and powdered potassium hydroxide (240 mg, 4.3 mmol) was added freshly distilled dichloromethane (10 mL) at room temperature. Argon was then removed by freeze-pump-thaw and replaced with ammonia atmosphere (connected with a balloon in series with a KOH drying column). This procedure was repeated two times. The system was stirred for 3 h at room temperature. An additional 5 mL of dichloromethane was added to homogenize the system. ^{19}F NMR analysis of the mixture revealed 100% yield of the desired compound. The resulting yellow suspension was washed with water, and organic phase was filtered then evaporated. Yield after two recrystallizations from hot hexane–dichloromethane is 85%, yellow product. Elem. Anal. (%): Calc. C: 54.85; H 4.75; N: 6.00; Found C: 54.78; H: 4.94; N: 6.07. HRESI-MS, m/z : 702.1446 (calc. 702.1359, $[\text{M}-\text{H}^+]$). ^1H NMR (CD_2Cl_2 , 25 °C): 2.11 (s, 18H), 2.54 (m, 1H), 3.32 (d, $^4J_{\text{H-F}} = 5$ Hz, 1H), 3.44 (m, 1H), 3.66 (d, $^2J_{\text{H-H}} = 10$ Hz, 1H), 3.74 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H), 6.74 (m, 2H), 6.94 (m, 2H), 7.03–7.21 (m, 6H); ^{19}F NMR (376.2 MHz, CD_2Cl_2 , r.t., δ/ppm): –142.6 (m, 1F), –160.7 (m, 1F), –166.3 (m, 1F), –185.2 (m, 1F); $^{13}\text{C}\{^1\text{H}\}$ NMR selected (CD_2Cl_2 , 25 °C): 15.4 (C_6Me_6 , 6C), 69.1 (s, 1C, $\text{RSO}_2\text{NCH}_2\text{CH}_2\text{NH}_2$), 70.7 (s, 1C, $\text{RSO}_2\text{NCH}_2\text{CH}_2\text{NH}_2$), 92.6 (C_6Me_6 , 6C), 107.4 (d, 1C, $^2J_{\text{C-F}} = 15\text{Hz}$, CSO_2 , Ph^{F}), 126.3 (s, 1C), 127.0 (s, 2C), 127.4 (s, 2C), 127.7 (s, 2C), 128.7 (s, 3C), 138.3 (dd, $^1J_{\text{C-F}} = 235\text{Hz}$, $^2J_{\text{C-F}} = 10$ Hz, 1C, Ph^{F}), 140.2 (m, overlapped, 1C, Ph^{F}), 141.4 (md, Ph^{F} , $^1J_{\text{C-F}} = 245$ Hz), 138.9 (C_{ipso} , s, $\text{RSO}_2\text{NCH}_2(\text{Ph})\text{CH}_2(\text{Ph})\text{NH}_2$, 1C), 143.8 (C_{ipso} , s, $\text{RSO}_2\text{NCH}_2(\text{Ph})\text{CH}_2(\text{Ph})\text{NH}_2$, 1C), 146.7 (md, $^1J_{\text{C-F}} = 245$ Hz, 1C, Ph^{F}). IR (neat/ cm^{-1}): 3150 $\nu^{\text{s}}(\text{NH}_2)$, 3229 $\nu^{\text{as}}(\text{NH}_2)$ and 3276 ν_{NH} .**

Method B: 100 mg of the complex **8** (*vide infra*) and powdered KOH (5 equiv.) were stirred in dry dichloromethane (8 mL) under ammonia atmosphere over 3 h. The solution than was filtered through a WhatmanTM syringe filter and Celite, then dried under high vacuum. Two recrystallizations from hot 1,2-dichloroethane–diethyl ether afforded yellow crystals (total yield 95%).

[(S)-Cp*Ir $\{\kappa^3(N,N',N'')\text{-(S,S)-NHC}_6\text{F}_4\text{SO}_2\text{dpn}\}]$ **7. **Method A:** To a mixture of $[\text{Cp}^*\text{IrCl}_2]_2$ (200 mg, 0.25 mmol), (S,S)-FsDPEN (222 mg, 0.50 mmol), and powdered KOH (280 mg, 5 mmol) was added dry dichloromethane (10 mL), followed by stirring of the suspension for 20 min. During this time the initial yellow color of the solution turned to red then a deep purple. Argon was removed by freeze-pump-thaw cycles and replaced by ammonia atmosphere (connected with balloon by passing through KOH pellets). This procedure was repeated two times. The system was stirred for 48 h at room temperature. At the end of this time, the color was changed to brown. The reaction progress was monitored continuously by ^{19}F NMR. An additional 15 mL of dichloromethane was added to**

homogenize the system. ^{19}F NMR analysis of the mixture revealed > 99% yield of the desired compound. Less than 0.5 % of the S_{R} -diastereomer⁸ was detected. The following operation was performed under air. The solution was separated from KOH/salts using a 20-mL syringe and filtration through a WhatmanTM syringe filter to afford clear solution from which solvent was then evaporated. Analytically pure yellow complex **7** was obtained in 84% yield (321 mg) after two recrystallizations from hot diethyl ether–dichloromethane. Using an alternative procedure, diethyl ether (ca. 15 mL) was layered on the red dichloromethane solution obtained after above-mentioned filtration. In ca. 0.5–2 hrs, yellow crystals formed on the Schlenk wall. After two days the crystals were separated and dried to afford 219 mg of the desired product. Additional recrystallization of the solid from the mother liquor from hot diethyl ether–1,2-dichloroethane afforded an additionally 123 mg of the product. Total yield: 342 mg (89%). Elem. Anal. (%): Calc. for $7 \cdot 0.5\text{CH}_2\text{ClCH}_2\text{Cl}$, C: 45.72; H 3.96; N: 5.16; Found C: 45.36; H: 3.75; N: 5.20. HRESI-MS, m/z : 766.1697 (calc. 766.1702, $[\text{M}-\text{H}^+]$). ^1H NMR (CD_2Cl_2 , 25 °C): 1.68 (s, 15H), 3.42 (d, $^4J_{\text{H-F}} = 4$ Hz, 1H), 3.60 (m, 2H), 4.23 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H, CH), 4.29 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H, CH), 6.79 (d, 2H), 6.87 (m, 2H), 7.06–7.20 (m, 6H); ^{19}F NMR (376.2 MHz, CD_2Cl_2 , r.t., δ/ppm): –142.0 (m, 1F), –160.1 (m, 1F), –165.4 (m, 1F), –184.1 (m, 1F); $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 25 °C): 8.6 (C_5Me_5 , 5C), 70.3 (s, 1C, $\text{RSO}_2\text{NCH}_2\text{CH}_2\text{NH}_2$), 73.1 (s, 1C, $\text{RSO}_2\text{NCH}_2\text{CH}_2\text{NH}_2$), 85.8 (C_5Me_5 , 5C), 108.5 (d, $^2J_{\text{C-F}} = 14$ Hz, 1C), 126.4 (s), 127.2 (s), 127.6 (s), 128.3 (dd, $^1J_{\text{C-F}} = 245$ Hz, 1C), 128.7 (s), 128.8 (s), 138.4 (dd, $^1J_{\text{C-F}} = 230$ Hz, $^2J_{\text{C-F}} = 10$ Hz, 1C), 138.3 (C_{ipso} , s), 141.5 (vtd, $J_{\text{C-F}} = 247$ Hz, $J_{\text{C-F}} = 15$ Hz, $J_{\text{C-F}} = 6$ Hz, 1C), 142.1 (vdd, $^1J_{\text{C-F}} = 11$ Hz, 1C), 143.6 (C_{ipso} , s), 146.6 (md, $^1J_{\text{C-F}} = 242$ Hz, 1C). IR (neat/ cm^{-1}): 3136 $\nu^{\text{s}}(\text{NH}_2)$, 3216 $\nu^{\text{as}}(\text{NH}_2)$ and 3275 ν_{NH} .

Method B: A solution of $[\text{Cp}^*\text{IrCl}_2]_2$ (300 mg, 0.376 mmol), (*S,S*)-FsDPEN (332 mg, 0.75 mmol) and NaNH_2 (75 mg, 1.93 mmol) in THF (30 mL) was stirred under reflux for 16 days. The resulting orange solution was then evaporated and dissolved in CH_2Cl_2 , then purified by flash-column chromatography on a short pad of neutral alumina eluted with 2-propanol under air. The resulting crude yellow solid was washed with Et_2O and dried under reduced pressure to give a pure yellow powder (484 mg, 84%).

$[(R)\text{-RuCl}_2\{(\text{S,S})\text{-C}_6\text{F}_5\text{SO}_2\text{NCH}(\text{Ph})\text{CH}(\text{Ph})\text{NH}_2\}(\eta^6\text{-hmb})]$ **8.** A red-colored suspension of $[\text{RuCl}_2(\eta^6\text{-hmb})]_2$ (250 mg, 0.37 mmol), (*S,S*)-FsDPEN (330 mg, 0.75 mmol) and NEt_3 (205 μL , 1.50 mmol) was stirred for 30 h at room temperature in commercial 2-propanol (30 mL) which was degassed by sparging with argon. After removal of solvent under vacuum, all subsequent manipulations were performed under air. The brick-colored compound was dissolved in dichloromethane (ca. 20 mL) and water (ca. 20 mL) was added. The two-phase system was stirred for 3 min, the organic phase was separated and solvent was removed under vacuum. Recrystallization from hot methanol afforded red crystals, which were dried under argon. X-Ray and NMR (CDCl_3) analysis showed that these crystals contained lattice methanol (up to 2 equiv.), which was removed by drying under dynamic vacuum. The yield of pure red crystals was 356 mg (85%). Elem. Anal. (%): Calc., C: 51.93; H 4.36; N: 3.78; Found C: 52.28; H: 4.67; N: 3.63. HRESI-MS, m/z : major 705.1124 (calc. 705.1156, cation $\text{C}_{32}\text{H}_{32}\text{F}_5\text{N}_2\text{O}_2\text{RuS}^+$). ^1H NMR (CDCl_3 , 25 °C): 2.26 (s, 18H), 3.66 (m, 2H), 3.87 (m, 1H), 4.17 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H), 6.88 (m, 7H), 7.18 (m, 3H); ^{19}F NMR (CDCl_3 , 25 °C): –134.2 (virtual td, $J_{\text{F-F}} = 5$ Hz, $J_{\text{F-F}} = 22$ Hz, *o*-F, 2F), –153.4 (tt, $^3J_{\text{F-F}} = 15$ Hz, $^4J_{\text{F-F}} = 8$ Hz, *p*-F, 1F), –163.1 (m, *m*-F, 2F). ^1H NMR (acetone- d_6 , 25 °C): 2.29 (s, 18H), 3.59 (vt, $J = 12$ Hz, 1H),

3.83 (dt, $J = 11$ Hz, $J = 2$ Hz, 1H), 4.10 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H), 5.29 (d, $J_{\text{H-H}} = 10$ Hz, 1H), 6.91 (m, 7H), 7.16 (m, 3H); ^{19}F NMR (acetone- d_6 , 25 °C): -135.2 (virtual td, $J_{\text{F-F}} = 5$ Hz, $J_{\text{F-F}} = 22$ Hz, $o\text{-F}$, 2F), -157.4 (tt, $^3J_{\text{F-F}} = 15$ Hz, $^4J_{\text{F-F}} = 8$ Hz, $p\text{-F}$, 1F), -165.6 (m, $m\text{-F}$, 2F). IR (neat/ cm^{-1}): 3033 $\nu^{\text{s}}(\text{NH}_2)$, 3058 $\nu^{\text{as}}(\text{NH}_2)$.

[(*R*)-RuCl $\{\eta^6\text{-}p\text{-cymene}\}$ [(*S,S*)-C $_6$ F $_5$ SO $_2$ NCH(Ph)CH(Ph)NH $_2$)] 9. To a premixed solution of [RuCl $_2(\eta^6\text{-}p\text{-cymene})$] $_2$ (383 mg, 0.625 mmol) and (*S,S*)-FsDPEN (554 mg, 1.25 mmol) in 2-propanol (50 mL) was added NEt $_3$ (0.35 mL, 2.5 mmol), and the resulting mixture was stirred at room temperature for 3 h. After evaporation of the orange suspension, the crude material was dissolved in CH $_2$ Cl $_2$ and washed with water (30 mL), then evaporated under reduced pressure to give an orange solid. Recrystallization from hot-methanol afforded orange crystals of **11** (541 mg, 0.76 mmol, 61% yield) suitable for X-ray diffraction analysis. Elem. Anal. (%): Calc.: C, 50.60; H, 3.96; N, 3.93; Found: C, 50.50; H, 3.84; N, 3.94%. ^1H NMR (399.8 MHz, CD $_2$ Cl $_2$, r.t., δ/ppm): 1.36, 1.38 (each d, $^3J_{\text{HH}} = 6.0$ Hz, $^3J_{\text{HH}} = 5.8$ Hz, each 3H; CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 2.36 (s, 3H; CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 3.08 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 1H; CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 3.64 (dd, $^3J_{\text{HH}} = 10$ Hz, $^3J_{\text{HH}} = 13$ Hz, 1H; FsNCHPhCHPhNH $_2$), 3.74 (td, $^3J_{\text{HH}} = 11$ Hz, $^4J_{\text{HH}} = 2\sim 4$ Hz, 1H; FsNCHPhCHPhNH $_2$), 3.96 (d, $^3J_{\text{HH}} = 11$ Hz, 1H; FsNCHPhCHPhNH $_2$), 5.33 (br d, $^3J_{\text{HH}} = 8.5$ Hz, 1H; FsNCHPhCHPhNH $_2$), 5.61 (t, $^3J_{\text{HH}} = 5.4$ Hz, $^3J_{\text{HH}} = 5.5$ Hz, 2H; CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 5.69, 5.73 (each d, $^3J_{\text{HH}} = 5.8$ Hz, $^3J_{\text{HH}} = 5.5$ Hz, each 1H; CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 6.72–6.74, 6.80–6.87, 7.07–7.11 (each m, 2H, 5H, 3H; FsNCH(C $_6$ H $_5$)CH(C $_6$ H $_5$)NH); ^{19}F NMR (376.2 MHz, CD $_2$ Cl $_2$, r.t., δ/ppm): -162.6 (dd, $^3J_{\text{FF}} = 26$ Hz, $^3J_{\text{FF}} = 17$ Hz, 2F; $m\text{-F}$), -153.2 (dd, $^3J_{\text{FF}} = 26$ Hz, $^3J_{\text{FF}} = 17$ Hz, 1F; $p\text{-F}$), -135.4 (d, $^3J_{\text{FF}} = 26$ Hz, 2F; $o\text{-F}$); $^{13}\text{C}\{^1\text{H}\}$ NMR (100.5 MHz, CD $_2$ Cl $_2$, r.t., δ/ppm): 18.3, 22.2, 30.4 (CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 68.4, 71.3 (FsNCHPhCHPhNH $_2$), 78.7, 79.8, 83.3, 84.7, 94.8, 106.3 (CH $_3$ C $_6$ H $_4$ CH(CH $_3$) $_2$), 126.8, 127.0, 127.4, 127.9, 128.2, 138.8. IR (neat/ cm^{-1}): 3228 $\nu^{\text{s}}(\text{NH}_2)$, 3281 $\nu^{\text{as}}(\text{NH}_2)$.

[(*S*)-Ru $\{\kappa^3(N,N',N'')\text{-(}S,S\text{)-NHC}_6\text{F}_4\text{SO}_2\text{dpn}\}$ ($\eta^6\text{-}p\text{-cymene}$)] 10. Prepared similarly to the complex **6**. Isolated yields were typically 85–89%. Elem. Anal. (%): Calc. C: 53.56; H 4.35; N: 6.25; Found C: 52.80; H: 3.74; N: 6.22. ^1H NMR (CD $_2$ Cl $_2$, 25 °C): 1.22 (d, $^2J_{\text{H-H}} = 7$ Hz, 3H), 1.27 (d, $^2J_{\text{H-H}} = 7$ Hz, 3H), 2.08 (s, 3H), 2.43 (dt, 1H, NH), 2.73 (sept, 1H), 3.21 (d, $J_{\text{H-F}} = 5$ Hz, 1H, NH), 3.42 (vt, 1H, CH), 3.63 (d, $^3J_{\text{H-H}} = 10$ Hz, 1H, CH), 5.04 (d, $^3J_{\text{H-H}} = 7$ Hz, 1H, CH $_{\text{ar}}$), 5.11 (d, $^3J_{\text{H-H}} = 7$ Hz, 1H, CH $_{\text{ar}}$), 5.25 (d, $^3J_{\text{H-H}} = 7$ Hz, 1H, CH $_{\text{ar}}$), 5.37 (d, $^3J_{\text{H-H}} = 7$ Hz, 1H, CH $_{\text{ar}}$), 5.44 (vd, $^2J_{\text{H-H}} = 8$ Hz, 1H, NH), 6.64 (vd, 2H), 6.78 (vd, 2H), 6.98–7.17 (m, 6H); ^{19}F NMR (376.2 MHz, CD $_2$ Cl $_2$, r.t., δ/ppm): -142.2 (m, 1F), -160.6 (m, 1F), -166.2 (m, 1F), -184.2 (m, 1F); $^{13}\text{C}\{^1\text{H}\}$ NMR (CD $_2$ Cl $_2$, 25 °C): 18.0 (s), 22.4 (s), 22.7 (s), 30.5 (s), 69.9 (s), 72.0 (s), 82.5 (s), 82.9 (s), 83.2 (s), 84.6 (s), 98.0 (s), 104.1 (s), 107.7 (d, $^2J_{\text{C-F}} = 8$ Hz, 1C), 126.1 (s), 127.2 (s), 127.4 (s), 127.7 (s), 127.7 (dd, $^1J_{\text{C-F}} = 245$ Hz, 1C), 128.2 (s), 128.3 (s), 138.6 (dd, $^1J_{\text{C-F}} = 230$ Hz, $^2J_{\text{C-F}} = 10$ Hz, 1C), 138.8 (C $_{\text{ipso}}$, s), 141.4 (vtd, $^1J_{\text{C-F}} = 245$ Hz, 1C), 144.4 (d, $^2J_{\text{C-F}} = 12$ Hz, 1C), 144.8 (C $_{\text{ipso}}$, s), 146.4 (md, $^1J_{\text{C-F}} = 230$ Hz, 1C). IR (neat/ cm^{-1}): 3250 $\nu^{\text{s}}(\text{NH}_2)$, 3315 $\nu^{\text{as}}(\text{NH}_2)$ and 3349 ν_{NH} .

Method B: A premixed solution of [RuCl $_2(\eta^6\text{-}p\text{-cymene})$] $_2$ (521 mg, 0.851 mmol), (*S,S*)-FsDPEN (752 mg, 1.701 mmol), and NaNH $_2$ (293 mg, 7.5 mmol) in THF (65 mL) was stirred at room temperature for 38 h. The resulting solution was then evaporated, dissolved in CH $_2$ Cl $_2$, and washed with water. After evaporating the solvent, the resulting crude solid was

washed with Et₂O 3 times which afforded a brown powder. Recrystallization from hot methanol gave a small amount of orange crystals suitable for single X-ray crystallography. Yield: 803 mg (70%). Elem. Anal. (%): Calc.: C, 53.56; H, 4.35; N, 6.25; Found: C, 53.95; H, 4.47; N, 6.27.

[(S)-Cp*Ir{ κ^3 (N,N',N'')-(S,S)-N(CH₃)C₆F₄SO₂dpen}] 11. To a mixture of [Cp*IrCl₂]₂ (200 mg, 0.25 mmol), (S,S)-FsDPEN (222 mg, 0.50 mmol), and powdered KOH (280 mg, 5 mmol) was added dry THF (10 mL). The suspension was stirred for 20 min, during which the initial yellow color of the solution turned to red then deep purple. Addition of 10 mL of MeNH₂ (2.0 M in THF) followed by stirring for 7 days gave a yellow precipitate and clear red solution. Analysis of the red solution by ¹⁹F NMR reveals >70% of the desired compound plus additional identified products. The yellow precipitate was collected by filtration and dissolved in dichloromethane. The isolated yellow-green solution was then filtered through a WhatmanTM syringe filter to afford 278 mg (71% yield) of the crude product with a purity of ~ 95%. No further purification was performed. The compound is sparingly soluble in CH₂Cl₂, THF, toluene, MeOH, and acetone. ¹⁹F NMR (376.2 MHz, CD₃OD, r.t., δ /ppm): -140.1 (m, 1F), -160.0 (m, 1F), -160.7 (m, 1F), -182.9 (m, 1F). HRESI-MS, m/Z: 780.1857 (calc. 780.1859, [M-H⁺]). IR (neat/cm⁻¹): 3133 ν^s (NH₂), 3208 ν^{as} (NH₂).

[Ru[(S,S)-C₆F₅SO₂NCH(Ph)CH(Ph)NH](η^6 -*p*-cymene)] 12. A mixture of [RuCl₂(η^6 -*p*-cymene)]₂ (123 mg, 0.20 mmol) and (S,S)-FsDPEN (177 mg, 0.40 mmol) and ^tBuOK (147 mg, 1.31 mmol) in dry CH₂Cl₂ solution (10 mL) was stirred at room temperature for 15 min under argon. The solvent was removed under reduced pressure. After extraction with toluene (15 mL) followed by evaporation of the solvent afforded a purple solid of **12** (141 mg, 52%). ¹H NMR (CD₂Cl₂, 25 °C): 1.31, 1.38 (each d, ³J_{HH} = 7 Hz, ³J_{HH} = 7 Hz, each 3H, CH₃C₆H₄CH(CH₃)₂), 2.39 (s, 3H, CH₃C₆H₄CH(CH₃)₂), 2.84 (sept, ³J_{HH} = 7 Hz, 1H, CH₃C₆H₄CH(CH₃)₂), 3.95 (d, ³J_{HH} = 5 Hz, 1H, FsNCHPhCHPhNH), 4.10 (s, 1H, FsNCHPhCHPhNH), 5.50, 5.61, 5.67, 5.82 (each d, ³J_{HH} = 6 Hz, 4H, CH₃C₆H₄CH(CH₃)₂), 7.02-7.39 (m, 10H, FsNCH(C₆H₅)CH(C₆H₅)NH); ¹⁹F NMR (CD₂Cl₂, 25 °C): -134.3 (vdt, ³J_{FF} = 22 Hz, ⁴J_{FF} = 4-6 Hz, 2F, *o*-F), -152.4 (vtt, ³J_{FF} = 20 Hz, ³J_{FF} = 21 Hz, ⁴J_{FF} = 4-6 Hz, 1F, *p*-F), -161.0 (m, 2F, *m*-F).

Typical procedure for the reactions between 6, 7, and 10 with acids HA (A = BF₄, OTf, Cl, (S)-BNPA) in dichloromethane. In aerobic atmosphere, a solution of 1.1 equiv. of Et₂O·HBF₄ (22 μ L) in CH₂Cl₂ (5 mL) was added to a 100 mg (0.143 mmol) solution of complex **6** in CH₂Cl₂ (10 mL). The color turned slightly yellow upon addition. After 5 min of stirring, the solvent was evaporated. The obtained yellow residue was washed three times with diethyl ether (~ 30 mL) and dried under high vacuum overnight. The compounds [6H]⁺X⁻, [7H]⁺BF₄⁻, [10H]⁺X⁻ (X = BF₄, OTf), **15** and **17** were characterized by HRESI-MS and NMR-spectroscopies (¹H, ¹⁹F, ¹³C). The microanalysis (C, H, N) was also performed in several cases. For complexes [6H]⁺X⁻, [7H]⁺BF₄⁻, [10H]⁺X⁻ (X = BF₄, OTf) and **17**, the analysis was typically underestimated, possibly due to difficulties in achieving complete combustion of the samples due to their ionic nature. No attempts were done to perform the analysis in the presence of V₂O₅ as complexes were sufficiently pure based on spectroscopies and were prepared from analytically pure precursors.

[(S)-Ru{ $\kappa^3(N,N',N'')$ -(S,S)-N(H)₂C₆F₄SO₂dpen}(η^6 -hmb)]⁺BF₄[−] [6H]⁺BF₄[−]]. Yield: 110 mg (97%). ¹H NMR (CD₂Cl₂, 25 °C): 2.21 (s, 18H), 3.46 (m, 1H), 3.50 (m, 1H), 3.75 (t, ^{av}J_{H-H} = 12 Hz, 1H), 4.30 (d, ²J_{H-H} = 12 Hz, 1H), 5.25 (d, ²J_{H-H} = 9 Hz, 1H), 5.74 (d, ²J_{H-H} = 9 Hz, 1H), 6.68 (m, 2H), 6.93 (m, 2H), 7.12–7.26 (m, 6H); ¹⁹F NMR (376.2 MHz, CD₂Cl₂, r.t., δ /ppm): −137.4 (m, 1F), −142.7 (m, 1F), −148.8 (s, 4F), −149.6 (m, 1F), −155.4 (m, 1F); ¹³C{¹H} NMR selected (CD₂Cl₂, 25 °C): 15.3 (s, C₆Me₆, 18C), 70.0 (s, CH, 1C), 72.1 (s, CH, 1C), 93.7 (s, C₆Me₆, 6C), 136.8 (s, C_{ipso}, 1C), 140.4 (s, C_{ipso}, 1C), others (s) 126.9, 127.5, 127.6, 127.9, 129.0, 129.2.

[(S)-Cp*Ir{ $\kappa^3(N,N',N'')$ -(S,S)-N(H)₂C₆F₄SO₂dpen}]⁺BF₄[−] [7H]⁺BF₄[−]. Elem. Anal. (%): Calc., C: 42.01; H 4.23; N: 4.90; Found C: 41.35; H: 3.24; N: 4.83. ¹H NMR (CD₂Cl₂, 25 °C): 1.69 (s, 15H, Cp*), 3.65 (vt, CH, 1H), 4.26 (d, ³J_{H-H} = 10Hz, 1H, CH), 4.72 (vt, NH, 1H), 4.79 (vt, NH, 1H), 6.05 (br, NH, 2H), 6.78 (vd, 2H), 6.93 (2H), 7.16–7.28 (m, 4H); ¹⁹F NMR (376.2 MHz, CD₂Cl₂, r.t., δ /ppm): −135.7 (m, 1F), −144.9 (m, 1F), −148.5 (s, 4F), −149.4 (m, 1F), −155.2 (m, 1F); ¹³C{¹H} NMR selected (CD₂Cl₂, 25 °C): 8.4 (s, C₅Me₅, 15C), 70.5 (s, CH, 1C), 73.7 (s, CH, 1C), 88.1 (s, C₅Me₅, 5C), 136.2 (s, C_{ipso}, 1C), 140.6 (s, C_{ipso}, 1C), others (s) 126.9, 127.2, 127.6, 128.2, 129.0, 129.3.

[(S)-Ru{ $\kappa^3(N,N',N'')$ -(S,S)-N(H)₂C₆F₄SO₂dpen}(η^6 -*p*-cymene)]⁺BF₄[−] [10H]⁺BF₄[−]. ¹H NMR (CD₂Cl₂, 25 °C): 1.33 (d, ²J_{H-H} = 7 Hz, 3H), 1.39 (d, ²J_{H-H} = 7 Hz, 3H), 2.22 (s, 3H), 2.96 (sept, 1H), 3.44 (vt, 1H, NH), 3.72 (vt, CH, 1H), 3.99 (d, ³J_{H-H} = 10 Hz, 1H, CH), 5.19 (br, 1H, NH), 5.33 (d, ³J_{H-H} = 7 Hz, 1H, CH_{ar}), 5.60 (d, ³J_{H-H} = 7 Hz, 1H, CH_{ar}), 5.66 (d, ³J_{H-H} = 7 Hz, 1H, CH_{ar}), 5.67 (1H, NH), 5.91 (d, ³J_{H-H} = 7Hz, 1H, CH_{ar}), 6.17 (br, 1H, NH), 6.80 (vd, 2H), 6.99 (2H), 7.16 (m, 6H); ¹⁹F NMR (CD₂Cl₂, 25 °C): −133.7 (m, 2F), −146.1 (dd, ³J_{FF} = 17 Hz, ⁴J_{FF} = 10 Hz, 1F), −146.7 (s, 4F), −148.7 (ddd, ³J_{FF} = 21 Hz, ³J_{FF} = 6-7 Hz, 1F), −153.6 (dd, ³J_{FF} = 21 Hz, ³J_{FF} = 22 Hz, 1F).

[(S)-Ru{ $\kappa^3(N,N',N'')$ -(S,S)-N(H)₂C₆F₄SO₂dpen}(η^6 -hmb)]⁺OTf[−] [6H]⁺OTf[−]. Complex **6 (15 mg, 21.4 μmol) was dissolved in 2 mL of dichloromethane in common atmosphere. To the obtained solution was added 1 mL of the dichloromethane stock-solution containing 1 equiv. of TfOH. The stock solution was prepared via dissolution of 19 μL of TfOH (10 equiv., 0.214 mmol) in 10 mL of dichloromethane. The mixture was stirred 5 min, then evaporated to dryness, yielding a greenish crystalline material. ¹H NMR (CD₂Cl₂, 25 °C): 2.19 (s, 18H), 3.45 (m, 1H), 3.81 (d, ²J_{H-H} = 11 Hz, 1H), 4.28 (d, ^{av}J_{H-H} = 11 Hz, 1H), 4.37 (t, ^{av}J_{H-H} = 12 Hz, 1H), 5.61 (brs, 2H), 6.82 (vd, ^{av}J_{H-H} = 8 Hz, 2H), 6.94 (m, 2H), 7.09–7.27 (m, 6H); ¹⁹F NMR (CD₂Cl₂, 25 °C): −133.7 (m, 1F), −143.4 (br, 1F), −147.5 (m, 4F), −148.2 (m, 1F), −154.0 (br, 1F); ¹³C{¹H} NMR selected (CD₂Cl₂, 25 °C): 15.4 (s, C₆Me₆, 18C), 69.7 (s, CH, 1C), 72.4 (s, CH, 1C), 93.8 (s, C₆Me₆, 6C), others (s) 127.2, 127.3, 127.9, 128.9, 129.2, 136.8, 141.3.**

[(S)-Ru{ $\kappa^3(N,N',N'')$ -(S,S)-N(H)₂C₆F₄SO₂dpen}(η^6 -*p*-cymene)]⁺OTf[−] [10H]⁺ OTf[−]. For selected characterization see Tables S1–S2 and Figure S9.

[(R)-RuCl{(S,S)-N(SO₂-*o*-C₆F₄NH₂)CH(Ph)CH(Ph)NH₂}(η^6 -*p*-cymene)] **15. To a premixed CH₂Cl₂ solution (10 mL) of **10** (135 mg, 0.20 mmol), HCl in Et₂O solution (0.24 mL, 0.24 mmol) was added followed by stirring at room temperature for 2 h. The solvent was then removed under vacuum and the resulting orange powder was washed with *n*-hexane (2 × 3 mL). Recrystallization from hot 1,2-dimethoxyethane afforded orange crystals of **15**. Elem.**

Anal. (%): Calc. C, 50.81; H, 4.26; N, 5.93; Found: C, 51.13; H, 4.28; N, 5.84. ^1H NMR (CD_2Cl_2 , 25 °C): 1.37, 1.40 (each d, $^3J_{\text{HH}} = 7$ Hz, 3H), 2.42 (s, 3H), 3.08 (sept, $^3J_{\text{HH}} = 7$ Hz, 1H), 3.75 (overlapped, 2H), 3.94 (m, 1H), 4.94 (s, 2H), 5.02 (br, 1H), 5.56, 5.59, 5.68 (each d, $^3J_{\text{HH}} = 7$ Hz), 6.78–7.17 (m, 10H); ^{19}F NMR (CD_2Cl_2 , 25 °C): –133.4 (dt, 1F, $^3J_{\text{FF}} = 25$ Hz, $^4J_{\text{FF}} = 6$, 7 Hz), –156.9 (td, 1F, $^3J_{\text{FF}} = 22$, 20 Hz, $^4J_{\text{FF}} = 6$, 8 Hz), –163.3 (dt, 1F, $^3J_{\text{FF}} = 20$ Hz, $^4J_{\text{FF}} = 6$, 9 Hz), –177.4 (m, 1F); $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 25 °C): 18.4, 22.0, 22.6, 30.7, 67.9, 71.8, 78.6, 79.5, 83.2, 85.0, 95.1, 105.8, 127.0, 127.1, 128.5, 128.7, 138.0, 138.6.

Complex 17. $^{31}\text{P}\{^1\text{H}\}$ NMR (CD_2Cl_2 , 25°C): 5.0 (isomer **A**), 11.2 (isomer **B**). ^{19}F NMR for isomer **A** (376.2 MHz, CD_2Cl_2 , r.t., δ/ppm): –134.6 (m, 1F), –149.9 (m, 1F), –152.8 (m, 1F), –155.1 (m, 1F); for isomer **B** (376.2 MHz, CD_2Cl_2 , r.t., δ/ppm): –138.6 (m, 1F), –158.1 (m, 1F), –164.4 (m, 1F), –178.5 (m, 1F).

1.3. Computational studies. The reactions between complexes **1–3** with ammonia were studied under DFT $^9/\omega\text{B97X-D}^{10}/\text{def2-TZVP/SMD}(\text{dichloromethane})^{11}$ level of theory with Gaussian 09 code (revision E.01). 12 All other computational studies were performed at the B3LYP $^{13}/\text{SDD}(\text{Ru,Ir})/6\text{-}31\text{G}^*(\text{C,H,N,O,S,F,P})/\text{C-PCM}^{14}(\text{dichloromethane})$ level of theory with Gaussian 09 code (revision C.01) 15 by using supercomputer TSUBAME-2 (TokyoTech). 16 Although hybrid B3LYP functional is twenty five years old and does not account for dispersion as $\omega\text{B97X-D}$ does in particular, the results can be used to understand the trend. Frequency calculations were carried out for all optimized geometries in order to verify their nature as local minima, under the harmonic approximations, and for the identification of all transition states (one imaginary frequency in the Hessian Matrix). The Gibbs free energies, G , were calculated under standard-state conditions of 1 atm (as default for the continuum model) and then corrected to 1 M (standard-state in solution) by adding 0.00301 Hartree. The intrinsic reaction coordinate (IRC) 17 calculations were carried out in both directions starting from the located transition states. DFT NMR GIAO 18 approach was used to compute the ^{19}F chemical shifts, reported here relative to the calculated chemical shift value of CFCl_3 under the same level of theory. Calculated and experimental ^{19}F NMR chemical shifts for the isolated $\kappa^3[\text{N},\text{N}',\text{N}'']$ metallacycles described in this paper are compared in Table S1. Molecular graphics images were produced using the UCSF Chimera package 19 or Chemcraft graphical program. 20

1.4. X-Ray diffraction studies. Diffraction experiments were performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å). Single crystals suitable for X-ray analyses were mounted on glass fibers. Intensity data were corrected for Lorentz-polarization effects and for absorption. Details of crystal and data collection parameters for the complexes **7**· $\text{CH}_2\text{ClCH}_2\text{Cl}$, **8**, **9**, **10**, and **15** are summarized in Table S3. For the complexes **6** and **8**, original measurements were performed on its (*R,R*)-FsDPEN enantiomer. For the sake of clarity, Figure 3 and Figure S1 contains the mirror inversion of the original structure. Structure solution and refinements were performed with the CrystalStructure program package. 21 The heavy-atom positions were determined by a direct method program (SIR92 22) and the remaining non-hydrogen atoms were found by subsequent Fourier syntheses and refined by full-matrix least-squares techniques against F^2 using the SHELXL-2014/7 program. 23 The amido NH hydrogen atom in **7**· $\text{CH}_2\text{ClCH}_2\text{Cl}$ was found in the difference Fourier map, while the rest hydrogen atoms were placed at calculated

positions; these hydrogen atoms were included in the refinements with a riding model. In the data set for **8**, **9**, and **15**, the PLATON SQUEEZE procedure²⁴ was used to deal with heavily disordered co-crystallizing solvent. The solid-state structures of the compounds **6**·CH₂Cl₂, [10H]⁺BF₄[−], and **11** have also been determined by X-ray crystallography, although the crystal qualities did not allow a satisfactory data refinement. Nevertheless, the structural determinations were sufficient to establish the chemical connectivities and molecular geometries. Details for these preliminary crystallographic studies can be found in CCDC 1880465–1880467. Table S4 contains additional information.

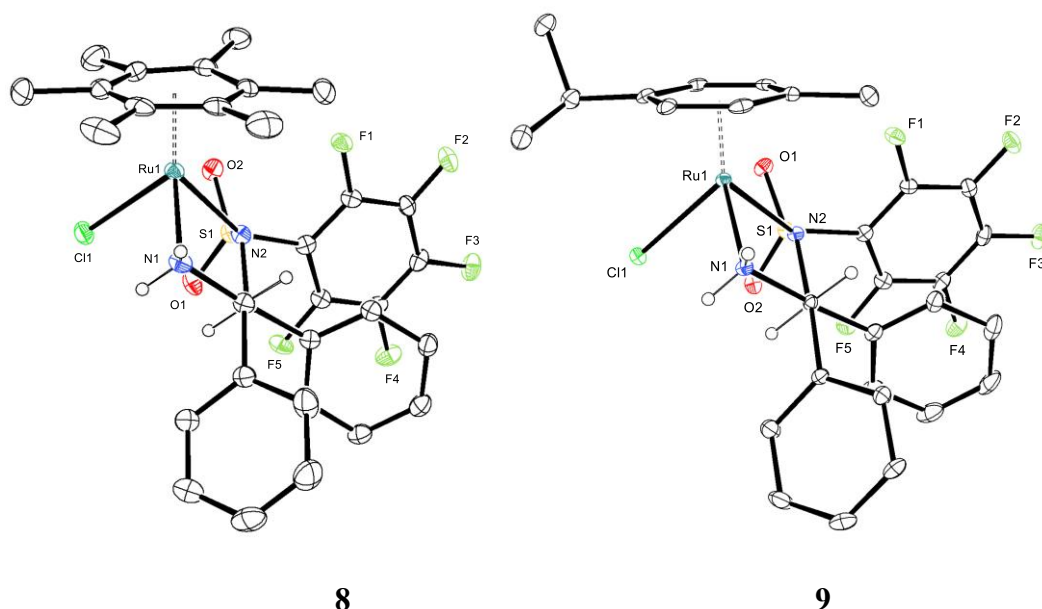


Figure S1. X-ray structures (30% level of thermal ellipsoids) of the compounds **8** and **9**. Non-critical H-atoms are omitted. Selected bond distances (Å) for **8**: Ru1–N1 = 2.113(3), Ru1–N2 = 2.198(3), Ru1–Cl1 = 2.4141(11), Ru1–CNT^{hmb} = 1.685(2); for **9**:²¹ Ru1–N1 = 2.126(3)/2.110(3), Ru1–N2 = 2.150(3)/2.168(3), Ru1–Cl1 = 2.4362(9)/2.4042(8), Ru1–CNT^{cym} = 1.661(1)/1.662(1).

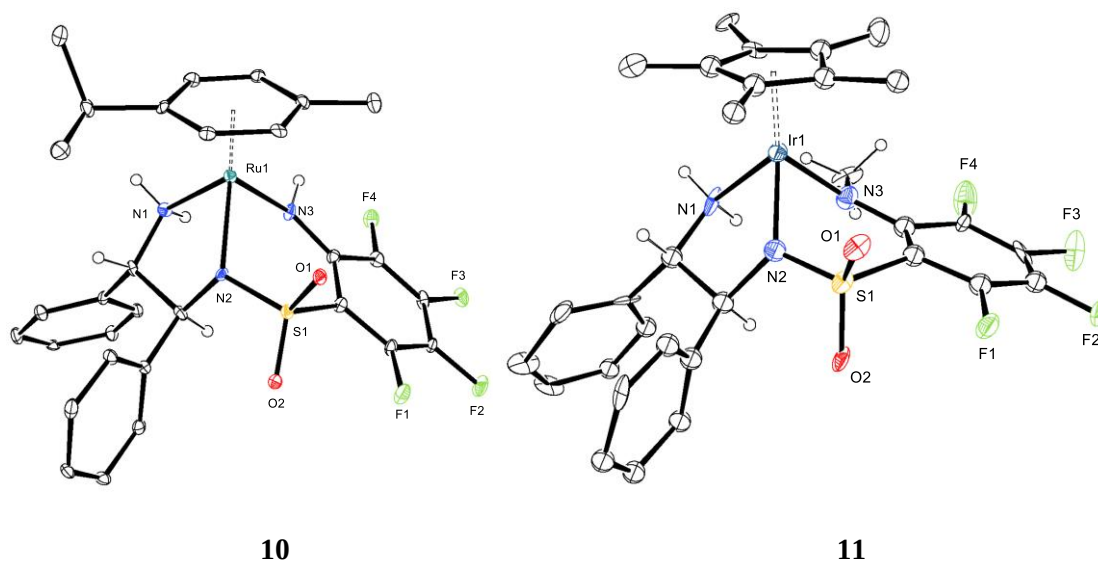
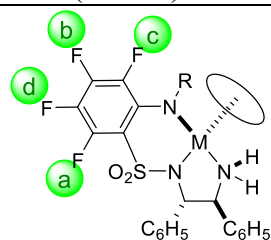


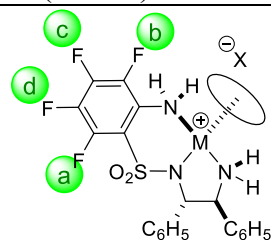
Figure S2. X-ray structures (30% level of thermal ellipsoids) of the compounds **10** and **11**. Non-critical H-atoms are omitted. Selected bond distances (Å) for **10**: Ru1–N1 = 2.116(5), Ru1–N2 = 2.109(6), Ru1–N3 = 2.090(5), Ru1–CNT^{hmb} = 1.682(3).

Table S1. Experimental (376.2 MHz, 25 °C, CD₂Cl₂) and calculated (DFT-GIAO) ¹⁹F NMR chemical shifts for the isolated $\kappa^3[N,N',N'']$ metallacycles described in this paper.^a

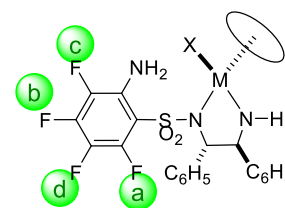
cmpd	δ /ppm				
	F _a	F _b	F _c	F _d	others
6	-142.6 (-153.1)	-160.7 (-172.2)	-166.3 (-184.2)	-185.2 (-201.6)	
10	-142.2	-160.6	-166.2	-184.2	
7	-142.0 (-149.2)	-160.1 (-171.5)	-165.4 (-181.6)	-184.1 (-197.7)	
11^b	-140.1	-160.0	-160.7	-182.9	
15	-138.2 (-141.6)	-158.1 (-166.4)	-164.4 (-177.5)	-178.5 (-187.8)	
[6H]⁺BF₄⁻	-137.4	-142.7	-149.6	-155.4	-148.8 (4F)
[6H]⁺OTf⁻	-136.2	-143.5	-150.5	-155.3	-78.6 (3F)
[10H]⁺BF₄⁻	-134.8 (-140.3)	-147.3 (-156.5)	-149.9 (-160.5)	-154.7 (-165.1)	-147.8 (4F)
[10H]⁺OTf^{-c}	-134.5	-147.3	-150.6	-154.9	-78.6 (3F)
[7H]⁺BF₄⁻	-135.7	-144.9	-149.4	-155.2	-148.5 (4F)
17	17_A^d -134.6 (-140.8)	-149.9 (-156.8)	-152.8 (-158.2)	-155.1 (-166.1)	
	17_B^d -138.6 (-144.5)	-158.1 (-166.0)	-164.4 (-177.2)	-178.5 (-187.3)	



6: Ru(hmb), R = H
10: Ru(*p*-cymene), R = H
7: Cp*Ir, R = H
11: Cp*Ir, R = CH₃



[6H]⁺X⁻, X = BF₄, TfO
[10H]⁺X⁻, X = BF₄, TfO
[7H]⁺BF₄⁻
17_A: Ru(*p*-cymene), X = (S)-BNPA



15: Ru(*p*-cymene), X = Cl
17_B: Ru(*p*-cymene), X = (S)-BNPA

^aCalculated values are presented in brackets. Experimental peak splittings and measured values of *J* are not reported. ^bIn CD₃OD at 25 °C. ^c*In situ*.

^dCoordination isomer (see text).

Table S2. Physical, microanalytical and selected IR data for the organometallic complexes described in this paper.

cmpd	color	M_w , g·mol ⁻¹	HRESI-MS, m/z ^a	anal. % found (calc.)			IR, cm ⁻¹		
				C	H	N	$\nu^s(\text{NH}_2)$	$\nu^{as}(\text{NH}_2)$	$\nu(\text{NH})$
4	violet	703.73	n/a (705.1156)	54.25 (54.62)	4.48 (4.44)	3.97 (3.98)			
5	prune	767.83	769.1521 ^b (769.1499)	46.22 (46.93)	3.55 (3.65)	3.50 (3.65)			
6	yellow	700.75	702.1446 ^b (702.1359)	54.78 (54.85)	4.94 (4.75)	6.07 (6.00)	3150	3229	3276
10	yellow	672.70	674.0295 (674.1046)	53.95 (53.56)	4.23 (4.35)	6.27 (6.25)	3250	3315	3349
7	yellow	764.85	766.1697 ^b (766.1702)	45.36 (45.72) ^e	3.75 (3.96) ^e	5.20 (5.16) ^e	3136	3216	3275
8	red	740.19	705.1124 ^b (705.1156) ^c	52.28 (51.92)	4.67 (4.36)	3.63 (3.78)	3033	3058	
9	red	712.14	676.9836 (677.0843) ^d	50.50 (50.60)	3.84 (3.96)	3.94 (3.93)	3228	3281	
11	yellow	778.88	780.1857 ^b (780.1859)	n/a	n/a	n/a	3133	3208	
15	orange	709.16	n/a	51.13 (50.81)	4.28 (4.26)	5.84 (5.93)			
[6H]⁺BF₄⁻	yellow	788.56	702.0383 (702.1359)	u/e ^f	u/e ^f	u/e ^f			
[6H]⁺OTf⁻	greenish	834.83	702.1446 (702.1359)	u/e ^f	u/e ^f	u/e ^f			
[10H]⁺BF₄⁻	yellow	760.51	674.0522 (674.1046)	u/e ^f	u/e ^f	u/e ^f			
[7H]⁺BF₄⁻	red	857.71	766.1031 (766.1702)	41.35 (42.01)	3.24 (4.23)	4.83 (4.90)			
17	yellow	1022.90	674.0657 (674.1046)	u/e ^f	u/e ^f	u/e ^f			

^aCalculated values for the protonated [M-H]⁺ in parentheses; for the ionic complexes the values are for the cation; only major peak position is shown.²⁶ ^bRelative to internal standard (PEG). ^cMajor peak observed for the cation C₃₂H₃₂F₅N₂O₂RuS⁺. ^dMajor peak observed for the cation C₃₀H₂₈F₅N₂O₂RuS⁺. ^eCalculated for C₃₀H₃₀F₄IrN₃O₂S·0.5CH₂ClCH₂Cl. ^fMicroanalysis was underestimated possibly due the difficulty to fully burn samples due to their ionic nature.

Table S3. X-ray crystallographic data for **7**·C₂H₄Cl₂, (*R,R*)-**8**, **9**, **10**, and **15**

	7 ·CH ₂ ClCH ₂ Cl	(<i>R,R</i>)- 8	9	10	15
formula	C ₃₂ H ₃₄ Cl ₂ F ₄ Ir- N ₃ O ₂ S	C ₃₂ H ₃₂ ClF ₅ N ₂ - O ₂ RuS	C ₃₀ H ₂₈ ClF ₅ N ₂ O ₂ - RuS	C ₃₀ H ₂₉ F ₄ N ₃ O ₂ - RuS	C ₃₀ H ₃₀ ClF ₄ N ₃ O ₂ - RuS
fw	863.82	740.19	712.14	672.70	709.16
crystal syst	tetragonal	trigonal	orthorhombic	orthorhombic	orthorhombic
space group	<i>P</i> 4 ₁	<i>P</i> 3 ₂ 21	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	12.3048(11)	14.9367(7)	15.605(3)	17.110(3)	15.499(3)
<i>b</i> (Å)	12.3048(11)	14.9367(7)	16.467(3)	20.318(3)	16.632(4)
<i>c</i> (Å)	21.8820(19)	27.3869(17)	25.342(4)	7.9383(13)	25.507(5)
α (deg)	90	90	90	90	90
β (deg)	90	90	90	90	90
γ (deg)	90	120	90	90	90
<i>V</i> (Å ³)	3313.1(5)	5291.5(5)	6511.8(16)	2759.7(8)	6575(2)
<i>Z</i>	4	6	8	4	8
<i>T</i> (K)	93	123	93	93	93
<i>D</i> _{calc} (g/cm ³)	1.732	1.394	1.453	1.619	1.433
μ (mm ⁻¹)	4.322	0.635	0.685	0.705	0.674
no. of reflns collected	27342	42852	69879	22907	54251
no. of independent	6985	8110	14875	6284	15025
no. of variables	414	403	759	374	759
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0248	0.0369	0.0282	0.0558	0.0996
w <i>R</i> 2 (all data)	0.0474	0.0767	0.0602	0.1060	0.2259
GOF	0.987	1.074	1.095	1.072	1.050

Table S4. X-ray crystallographic data for (R,R) -**6**·(CH₂Cl₂)_{0.25}, [**10H**]⁺BF₄⁻·(CH₂Cl₂)_{0.33}, and **11**.

	(R, R) - 6 ·(CH ₂ Cl ₂) _{0.25}	[10H] ⁺ BF ₄ ⁻ ·(CH ₂ Cl ₂) _{0.33}	11
formula	C _{32.25} H _{33.5} Cl _{0.5} F ₄ N ₃ O ₂ RuS	C _{30.33} H _{30.67} BCl _{0.67} F ₈ N ₃ O ₂ RuS	C ₃₁ H ₃₂ F ₄ IrN ₃ O ₂ S
fw	721.99	788.91	778.89
crystal syst	monoclinic	monoclinic	orthorhombic
space group	$P2_1$	$P2_1$	$P2_12_12_1$
a (Å)	11.900(11)	14.887(9)	12.538(3)
b (Å)	25.06(2)	14.256(8)	22.036(5)
c (Å)	22.06(2)	26.602(17)	22.528(5)
α (deg)	90	90	90
β (deg)	104.679(15)	105.943(10)	90
γ (deg)	90	90	90
V (Å ³)	6364(10)	5428(6)	6224(3)
Z	8	6	8
T (K)	93	93	93
D_{calc} (g/cm ³)	1.507	1.448	1.662
μ (mm ⁻¹)	0.658	0.612	4.425
no. of reflns collected	34253	37452	51518
no. of independent reflns	21010	22271	14148
no. of variables	1468	1146	769
$R1$ [$I > 2\sigma(I)$]	0.1472	0.1596	0.1230
w $R2$ (all data)	0.3596	0.3928	0.3351
GOF	1.640	1.423	1.023

2. Reactions of complexes 1–4 with ammonia in dichloromethane- d_2 .

2.1. Reaction of complex 1 with ammonia in dichloromethane- d_2 .

Replacement of argon atmosphere with ammonia gas via three freeze-pump-thaw cycles in a 2×10^{-2} M violet solution of **1** in CD_2Cl_2 at room temperature did not result in any visible color change of the reaction mixture. The amount of ammonia present in solution ~ 120 equiv. (δ 0.40 ppm, t, $^1J_{\text{H-N}} = 42$ Hz), was determined from the relative peak integration of the ^1H NMR spectrum, Figure S1. Weak high field shift ~ 0.02 ppm of all resonances was detected, whereas several selected peaks slightly broadened, the most notable being the C–H proton of the five-membered NN ring at 5.91 ppm, that lost a $^3J_{\text{HCNH}}$ coupling (initially 5 Hz) with the N–H proton at 6.98 ppm as shown in Figure S3.

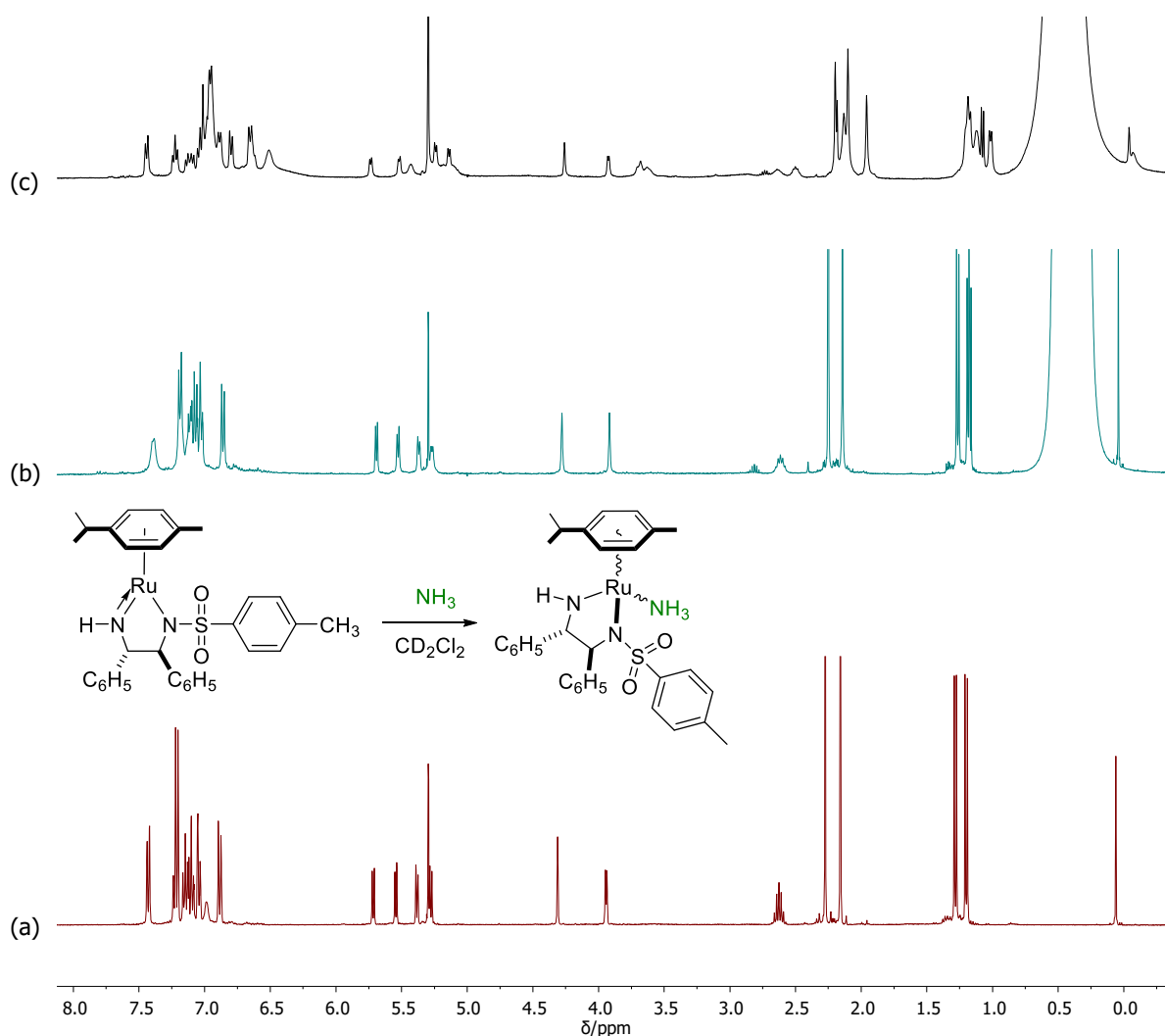


Figure S3. ^1H NMR spectrum of complex **1** (a) and **1** in the presence of ~ 120 equiv. NH_3 CD_2Cl_2 at 25 °C (b) and ~ 255 equiv. at -80 °C (c). The amount of the ammonia is calculated from the relative integration.

Decreasing the temperature resulted in further reversible broadening of the ^1H signals. Decoalescence of several resonances occurred at $-60\text{ }^\circ\text{C}$. At $-80\text{ }^\circ\text{C}$, ammonia was present in solution at ~ 255 equiv., and two Ru complexes in a 1:1 ratio were clearly observed, the starting **1** and the reaction product, most probably the adduct of the 16e amido complex and ammonia, $[\text{Ru}(\text{NH}_3)\{(\text{S,S})\text{-TsNCH(Ph)CH(Ph)NH}\}(\eta^6\text{-p-cymene})]$ **1a**. Under these conditions the equilibrium constant, $K = 0.2\text{ M}^{-1}$. The identity of **1a** was not possible to confirm directly from the ^1H or further by 2D $^1\text{H}\text{-}^1\text{H}$ gCOSY analysis because of the resonances broadening at $-80\text{ }^\circ\text{C}$. Formulation of **1a**, however, is suggested by the DFT analysis, see text. The color of this solution was between violet and prune at $-80\text{ }^\circ\text{C}$, and turned back reversibly to violet on heating. The spectra at room temperature were fully recovered consistent with the equilibrium.

2.2. Reaction of complex **2** with ammonia in dichloromethane- d_2 .

The same reaction was studied with structurally and electronically modified Ru complex **2**.⁵ Contrary to **1**, after replacing argon atmosphere with ammonia via one freeze-pump-thaw cycle at ambient temperature the $1.5 \times 10^{-2}\text{ M}$ violet solution of **2** in CD_2Cl_2 changed the color on yellow after several minutes on stirring.²⁷ The ^1H , ^{19}F and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra revealed $\sim 75\%$ conversion of the starting material to the ammonia adduct complex $[(R)\text{-Ru}(\text{NH}_3)\{(\text{S,S})\text{-TfNCH(Ph)CH(Ph)NH}\}(\eta^6\text{-hmb})]$ **2a** as shown in Scheme 2 and Figures S4–S6. “Free” ammonia was present in ~ 68 equiv. at $0\text{ }^\circ\text{C}$, as determined from the ^1H NMR spectrum. Identity of **2a** was confirmed from the 2D $^1\text{H}\text{-}^1\text{H}$ gCOSY, signal integration and further supported by the continuum dichloromethane reaction field DFT NMR GIAO chemical shift calculations as shown in Figures S7. At $0\text{ }^\circ\text{C}$, the signal of N–H proton of the five membered NN ring, which resonates at 1.82 ppm (overlapped with the protons of the hmb), gives a cross-peak in the 2D $^1\text{H}\text{-}^1\text{H}$ gCOSY with the signal at 3.65 ppm due to the C–H proton of the five membered NN ring (resonates as a virtual quadruplet). In turn, a cross-peak between this C–H proton and the second C–H proton of the five-membered NN ring at ppm (singlet), is observed in the 2D spectrum as shown in Figure S5. The singlet resonance of coordinated ammonia resonates at 1.92 ppm in the ^1H NMR spectrum. Notably, the rotation of $\eta^6\text{-hmb}$ ring is hindered in both ^1H and $^{13}\text{C}\{^1\text{H}\}$ spectra of **2a** at $0\text{ }^\circ\text{C}$: multiple resonances were observed in the range δ 1.73–1.83 ppm (m, 18H) for the CH_3 protons of the $\eta^6\text{-hmb}$ ligand in the ^1H spectrum, whereas two sets of six signals were observed in $^{13}\text{C}\{^1\text{H}\}$ spectrum of **2a** in the characteristic position of the $\eta^6\text{-hmb}$ ring (see Figures S6 and S7). In the ^{19}F NMR a singlet peak at δ -77.1 ppm appeared.

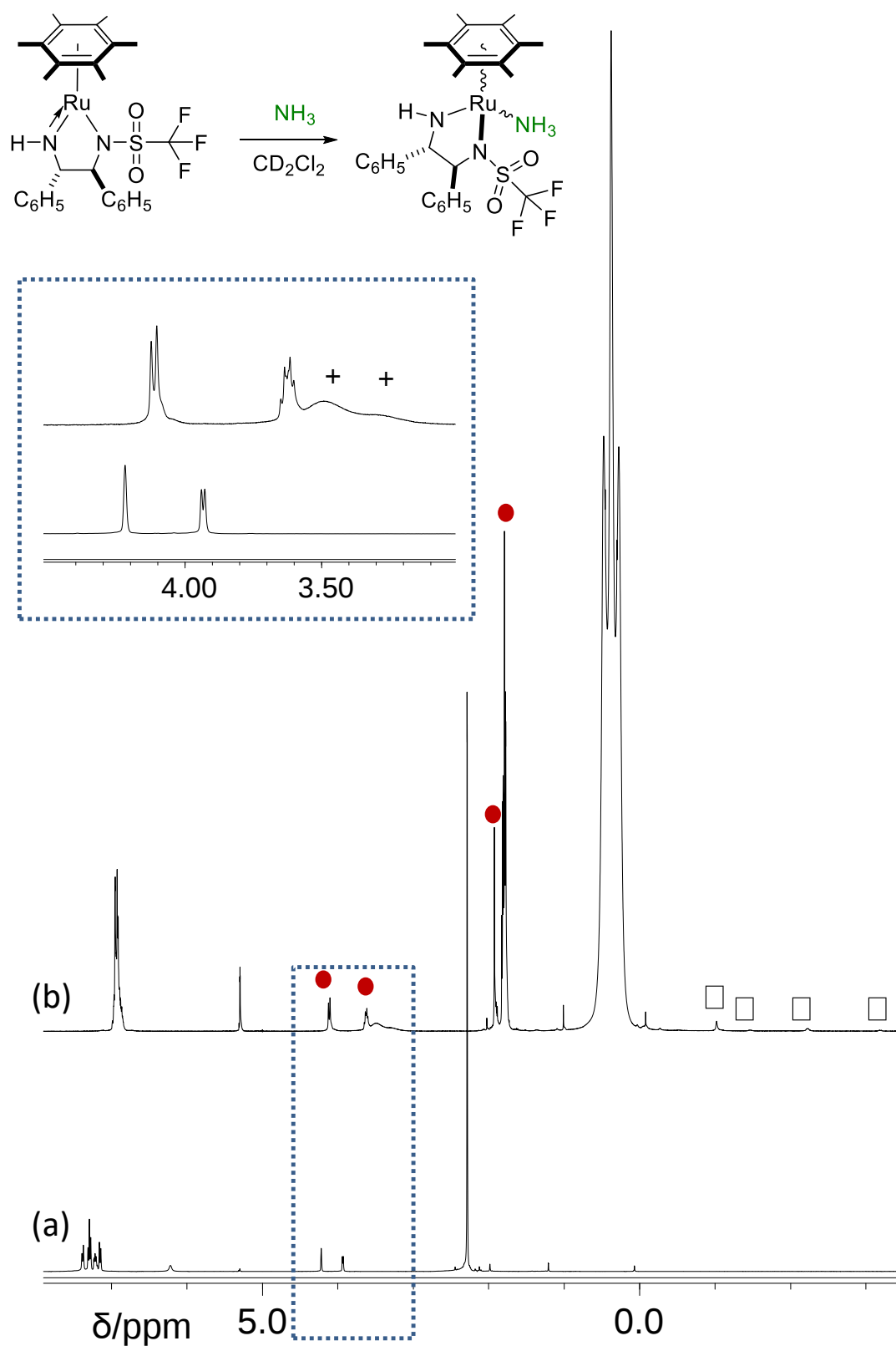


Figure S4. ^1H NMR spectrum of complex **2** (a) and **2** in the presence of *ca.* 68 equiv. NH_3 (b), CD_2Cl_2 , 0°C . The red dots assigned to the ammine complex **2a** based on 2D ^1H - ^1H gCOSY (Figure S4) and DFT NMR GIAO chemical shift calculations (Figure S6). The symbol “+” corresponds to the fast exchange (NMR timescale) of **2** with water traces, as determined by

separate experiments. The overall broad resonance “+” significantly shifted to a low field on decreasing the temperature. It was not possible to avoid some small water amount in ammonia gas, even if the gas was passed through KOH pallets. The symbol “□” corresponds to the unidentified reaction products. Presumably these peaks are due to the sample decomposition, which was observed further on standing at 25 °C.

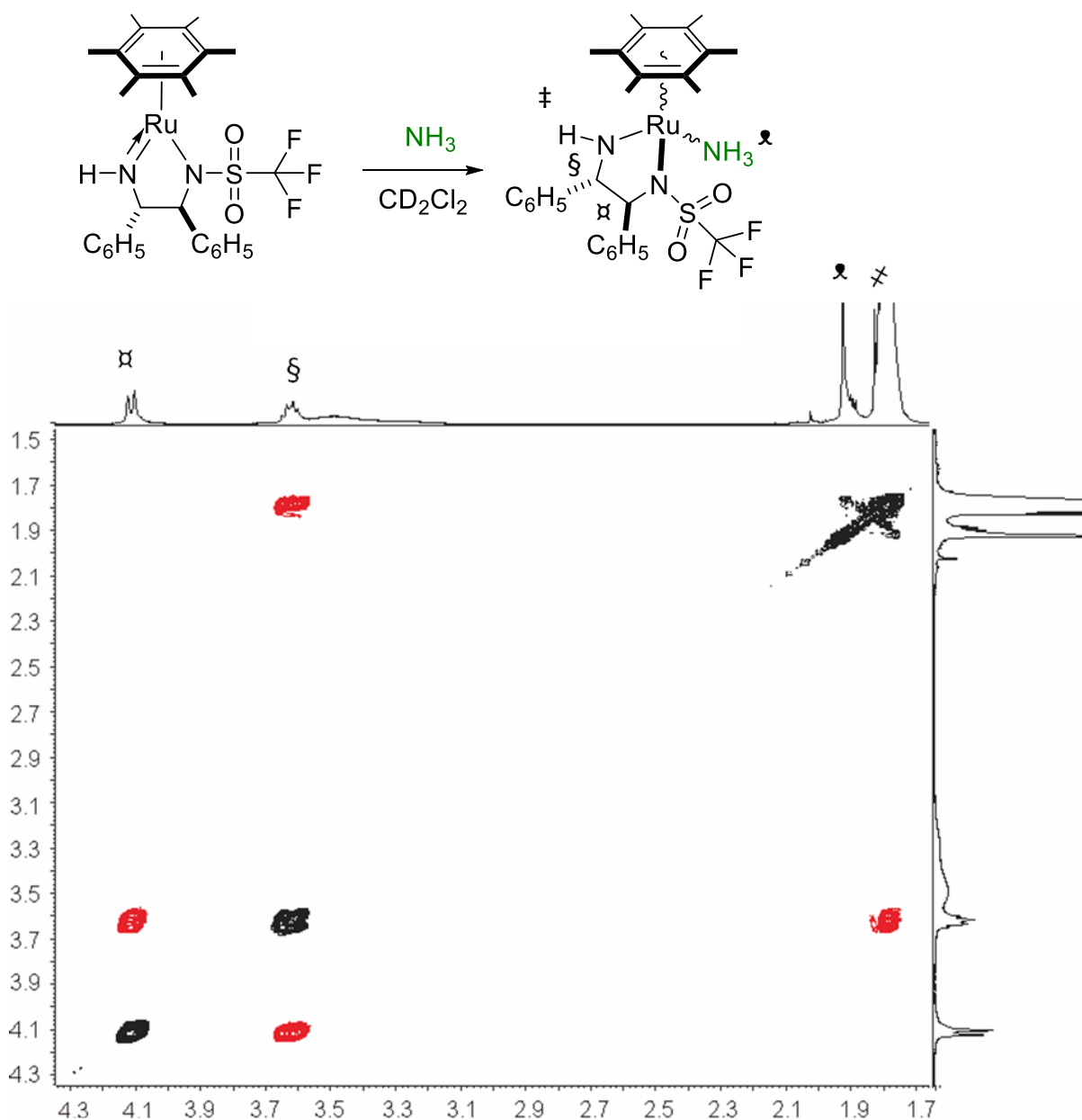


Figure S5. Plot of the 2D ^1H - ^1H gCOSY spectrum of complex 2 in the presence of *ca.* 68 equiv. NH_3 (spectrum b in Figure S3), CD_2Cl_2 , 0 °C. Peak assignment is presented.

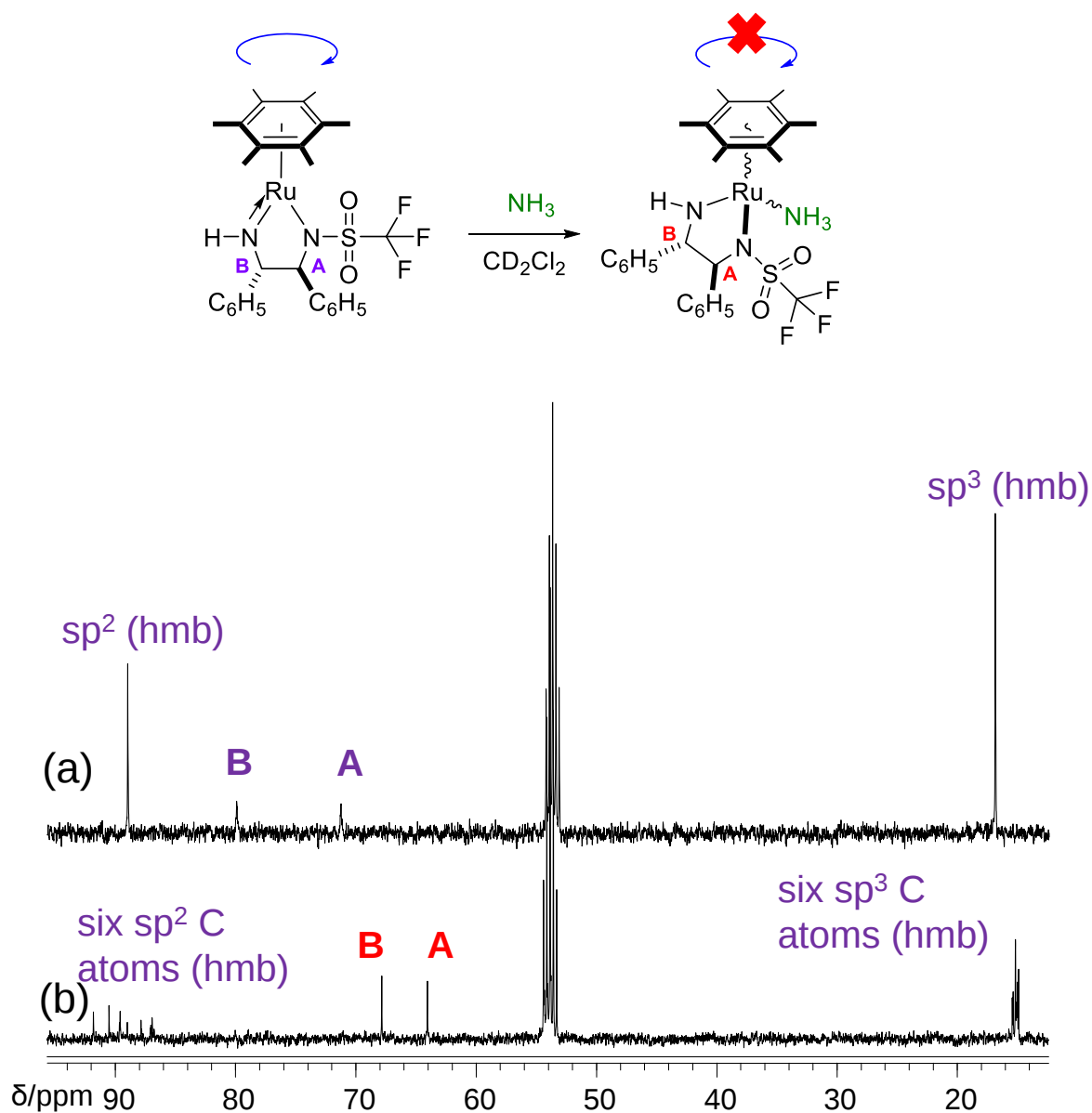


Figure S6. ¹³C{¹H} NMR spectrum of complex 2 (a) and 2 in the presence of *ca.* 68 equiv. NH₃ (b), CD₂Cl₂, 0 °C. Peak assignment (five membered NN ring) is done based on DFT NMR GIAO Chemical shift calculations (Figure S7).

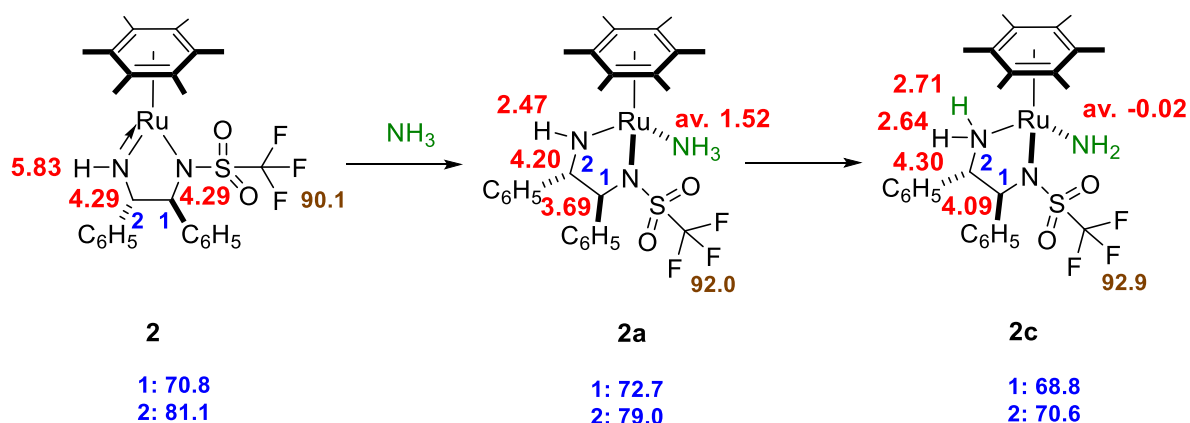


Figure S7. DFT GIAO ^1H , ^{19}F and ^{13}C Chemical shift values (ppm) in continuum CH_2Cl_2 at 298 K computed at the DFT/B3LYP/SDD(Ru,Ir)/6-31G*(C,H,N,O,S,F,P) level of theory (relative to TMS). Abbreviation for the putative Ru– NH_2 complex is **2c**.

2.3. Reaction of complex 3 with ammonia in dichloromethane- d_2 .

The Ir complex **3** reacted in a similar fashion to **1**: replacing argon atmosphere by ammonia via a freeze-pump-thaw cycle at ambient temperature of the 1.5×10^{-2} M prune solution of **3** in CD_2Cl_2 did not result in any visible color change. At -60°C , the ammonia was present at ~ 45 equiv. and, in addition to **3** (90%), the ammine Ir complex $[\text{Cp}^*\text{Ir}(\text{NH}_3)\{(\text{S,S})\text{-TfNCH}(\text{Ph})\text{CH}(\text{Ph})\text{NH}\}]$ **3a** was observed in 10% amount ($K_{213\text{K}} = 0.15 \text{ M}^{-1}$). The formulation of **3a** was consistent with the 2D ^1H – ^1H gCOSY spectrum, see Figure S8. No high field ^1H NMR peaks were observed.

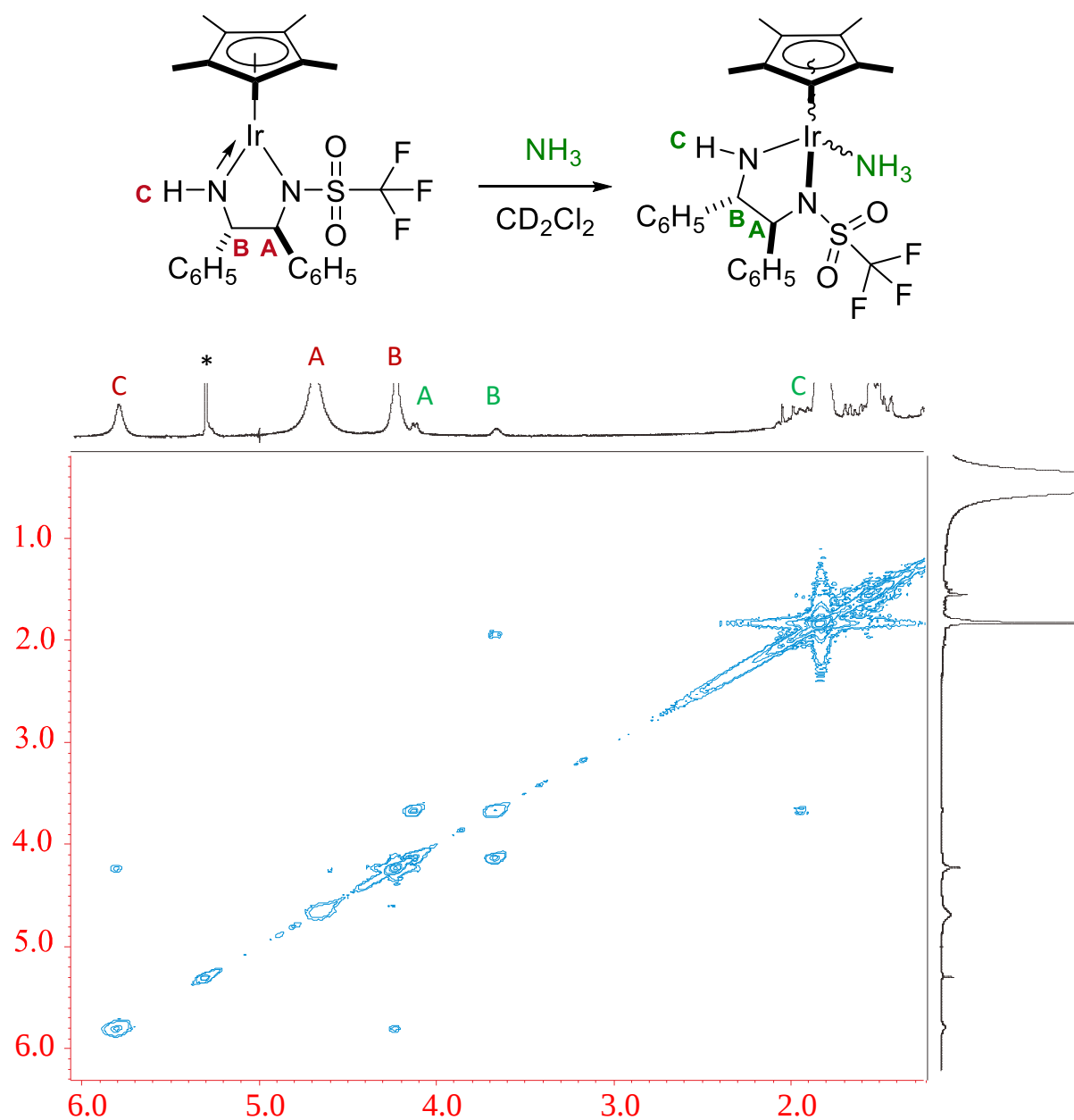


Figure S8. Plot of the 2D ^1H - ^1H gCOSY spectrum of complex **3** in the presence of *ca.* 45 equiv NH_3 , CD_2Cl_2 , -60°C . Peak assignment is presented.

2.4. VT NMR Reaction of complex 4 with ammonia in dichloromethane- d_2 .

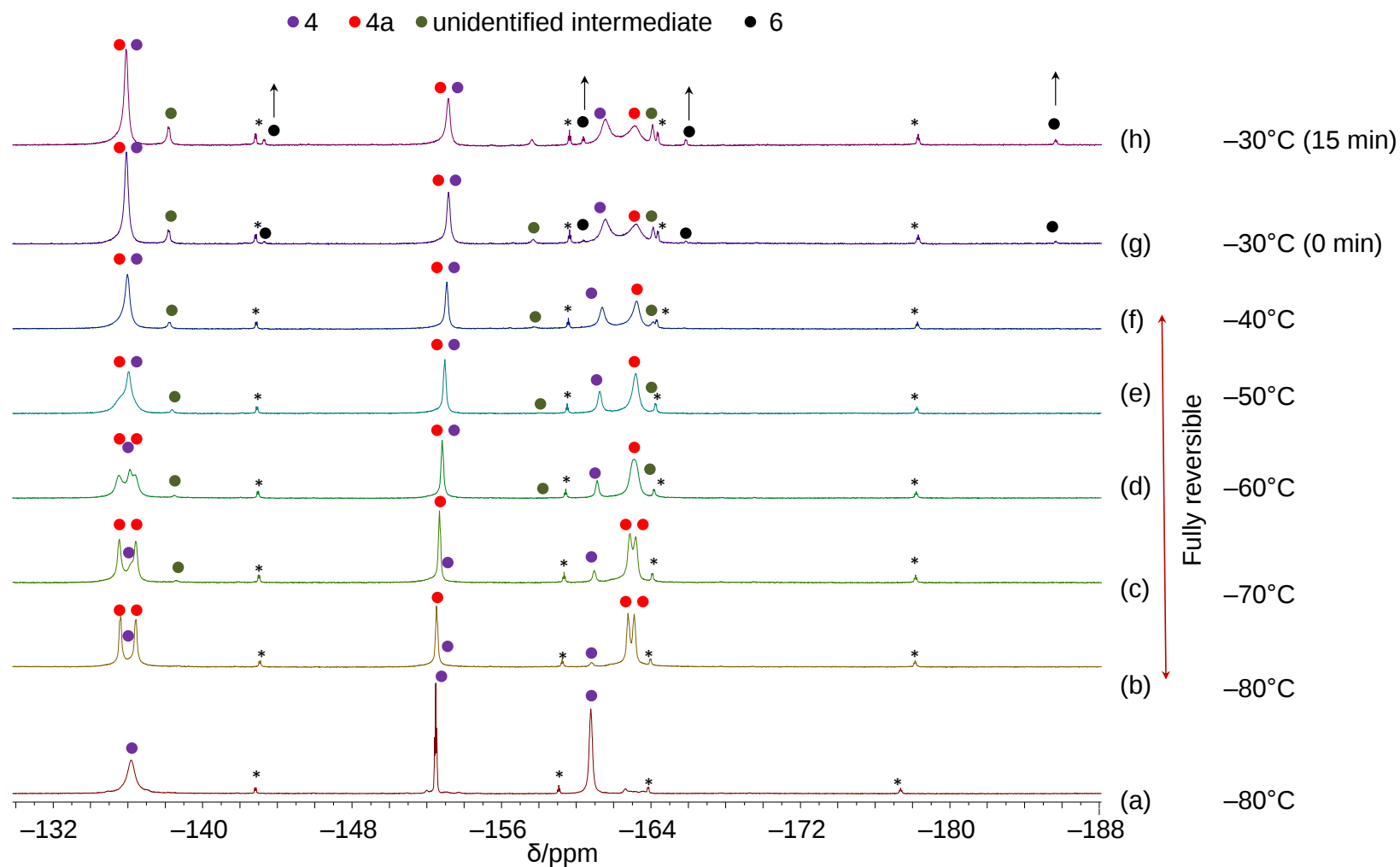


Figure S9. ^{19}F NMR (376.2 MHz; CD_2Cl_2): (a) spectrum of **4** at $-80\text{ }^\circ\text{C}$; (b) replacement of argon atmosphere in (a) with dry ammonia via a freeze-pump-thaw cycle at $-80\text{ }^\circ\text{C}$; (c-f) same as (b) at different temperatures (spectra are fully reversible); (g) the same as (b) $-30\text{ }^\circ\text{C}$ immediately after warming; (h) the same as (g) in 15 min. “*” is Ru oxometallacycle, by-product of the synthesis present at $\sim 5\%$ level.¹

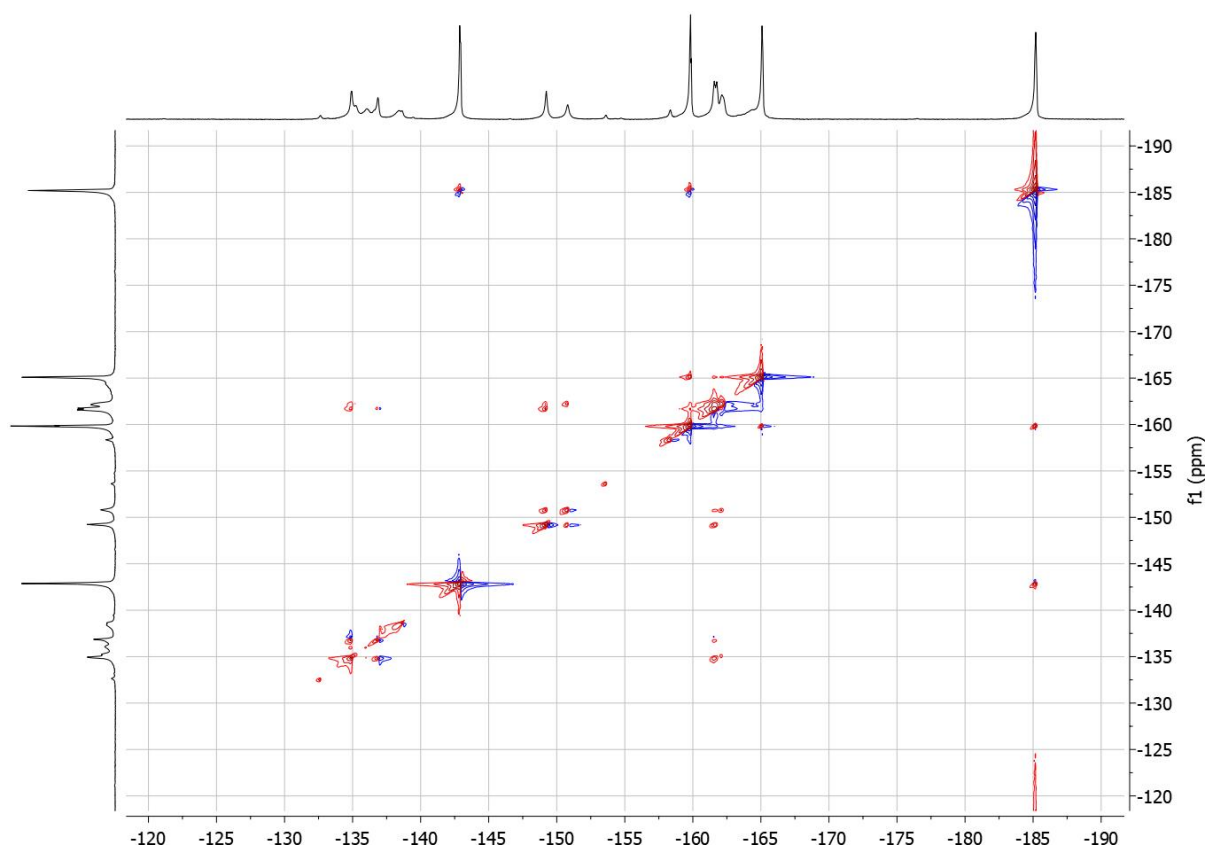


Figure S10. ^{19}F - ^{19}F phase-sensitive 2D NOESY spectrum of spectrum (d) in Figure 5.

3. Free Energy Profiles for the reaction of Ru complex 4 or Ir complex 5 with one molecule of NH₃.

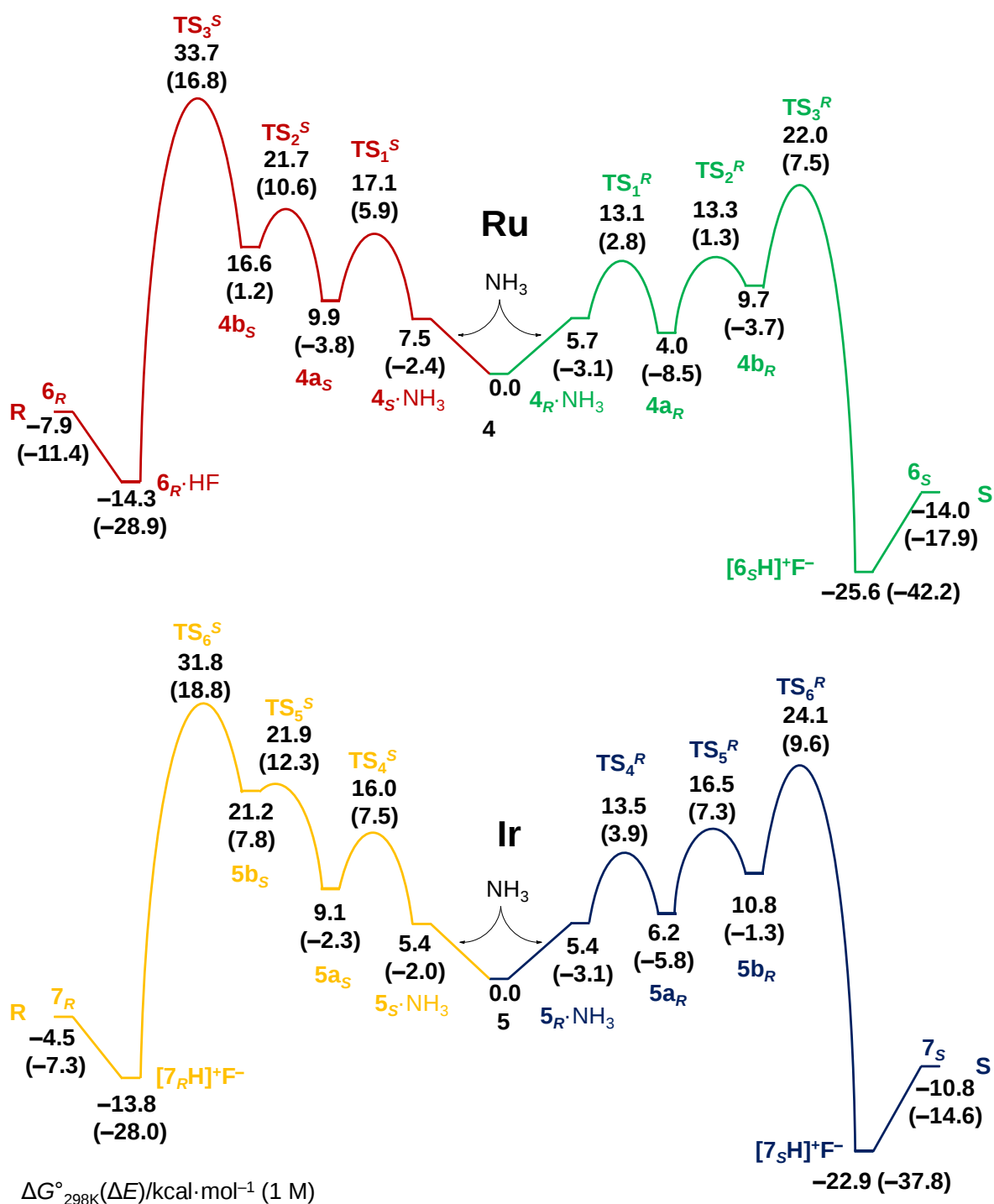


Figure S11. Free Energy Profiles for the reaction of Ru complex 4 or Ir complex 5 with one molecule of NH₃ computed at the B3LYP/SDD(Ru)/6-31G*(C,H,N,O,S,F)/C-PCM(CH₂Cl₂) level of theory.

4. NMR spectra/charts for selected complexes.

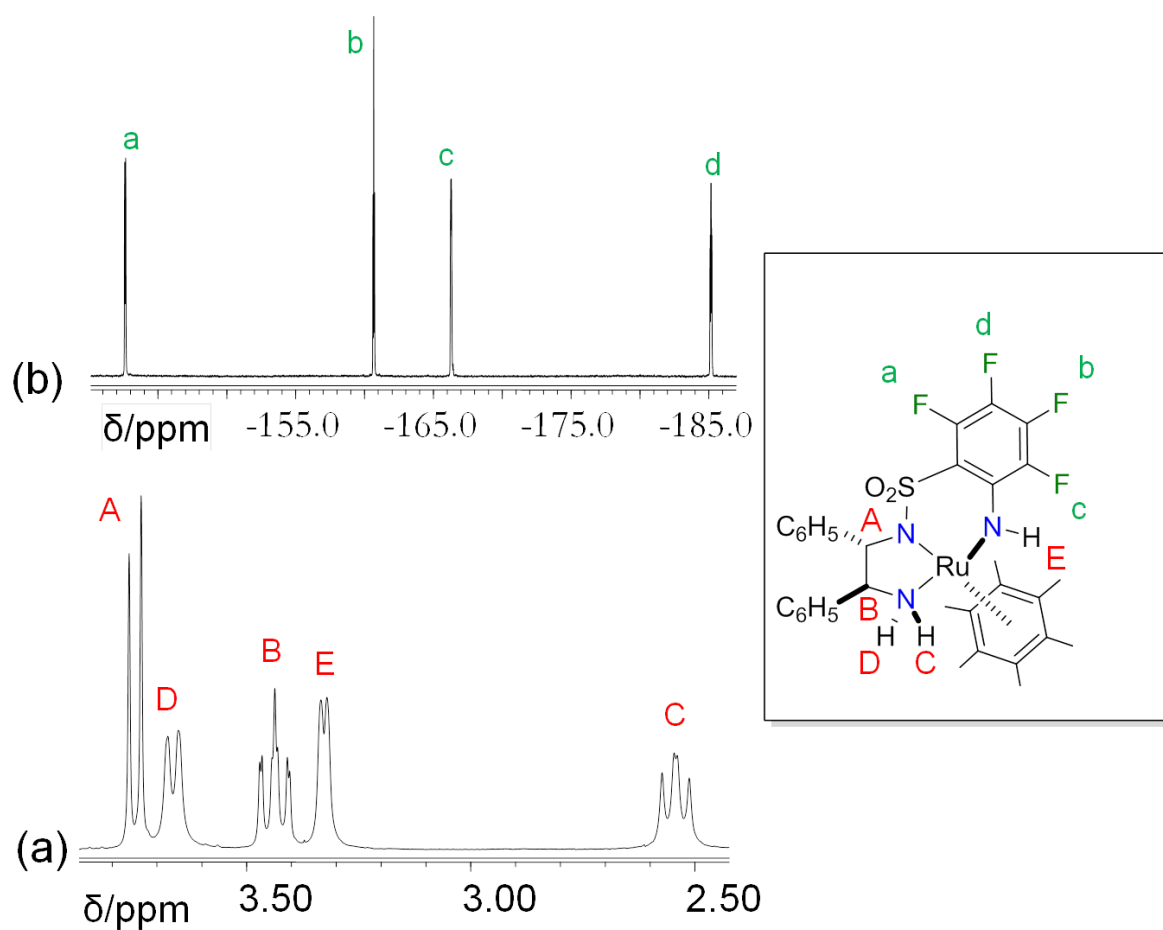


Figure S12. Section plot of the ^1H NMR (399.78 MHz, 25 °C) spectrum of **6** in CD_2Cl_2 (a). Routine assignment is done based on Karplus equation²⁸ using the experimental values of coupling constants J . ^{19}F NMR (376.2 MHz, 25 °C) spectrum of **6** in CD_2Cl_2 (b). Assignment is done based on the NMR GIAO DFT/B3LYP/SDD(Ru)/6-31G*(C,H,N,O,S,F)/C-PCM(CH_2Cl_2) calculated ^{19}F chemical shifts.

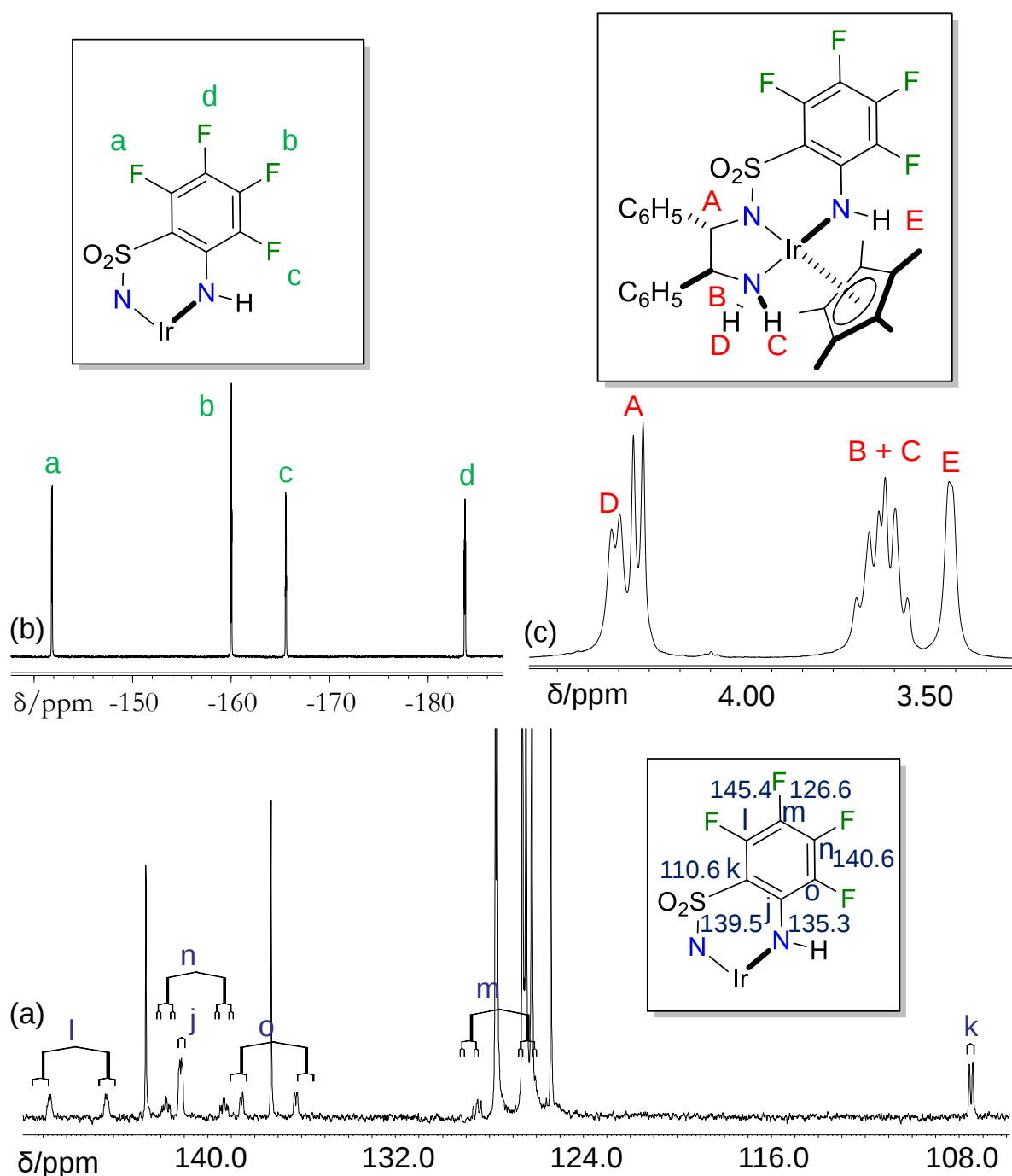


Figure S13. Section plot of the $^{13}\text{C}\{^1\text{H}\}$ NMR (100.5 MHz, 25 °C) spectrum of 7 in CD_2Cl_2 (a); ^{19}F NMR (376.2 MHz, 25 °C) spectrum of 7 in CD_2Cl_2 (b); ^1H NMR (399.78 MHz, 25 °C) spectrum of 7 in CD_2Cl_2 (c). For (a) and (b) assignment is done based on the NMR GIAO DFT/B3LYP/SDD(Ru)/6-31G*(C,H,N,O,S,F)/C-PCM(CH_2Cl_2) calculated ^{13}C and ^{19}F chemical shifts relative to TMS and CFCl_3 , correspondingly (^{13}C shifts' values are presented on the picture; for the ^{19}F see Table 2). Assignment of (c) is routine and done based on Karplus equation using the experimental values of coupling constants J.

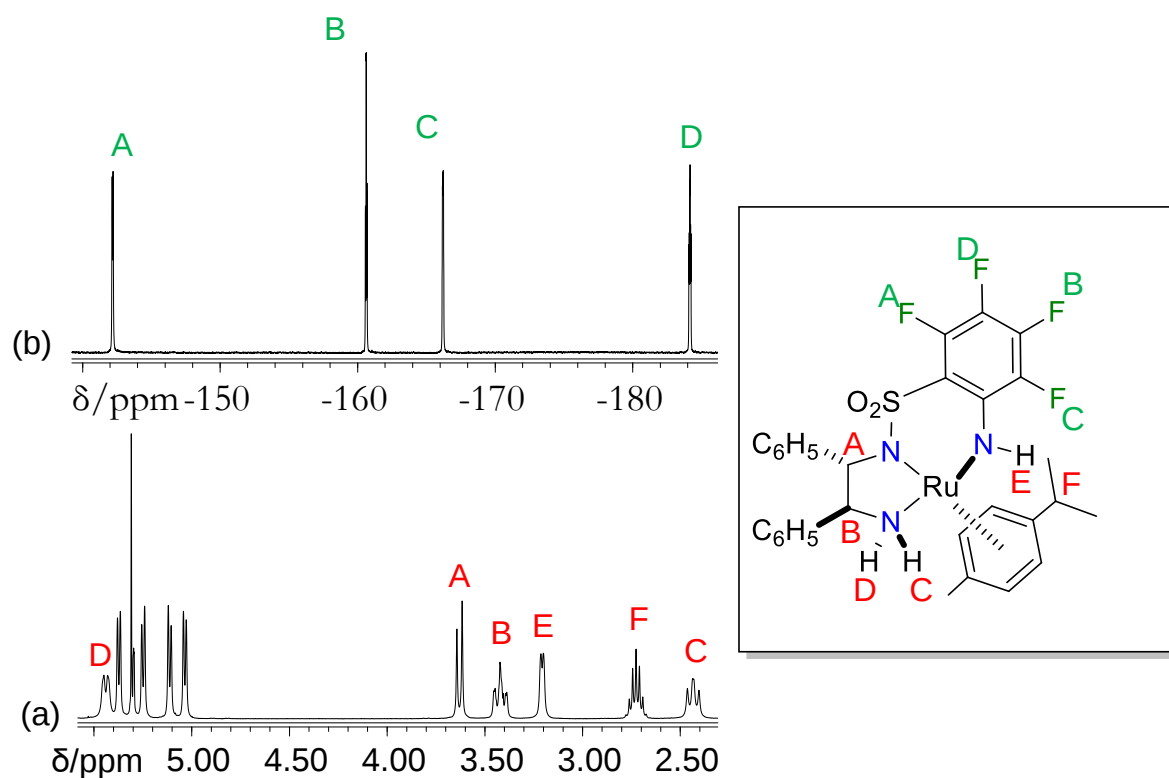


Figure S14. Section plot of the ^1H NMR (399.78 MHz, 25 °C) spectrum of **10** in CD_2Cl_2 (a). Routine assignment is done based on Karplus equation²⁸ using the experimental values of coupling constants J . ^{19}F NMR (376.2 MHz, 25 °C) spectrum of **10** in CD_2Cl_2 (b). Assignment is done similarly as in **6** (vide supra).

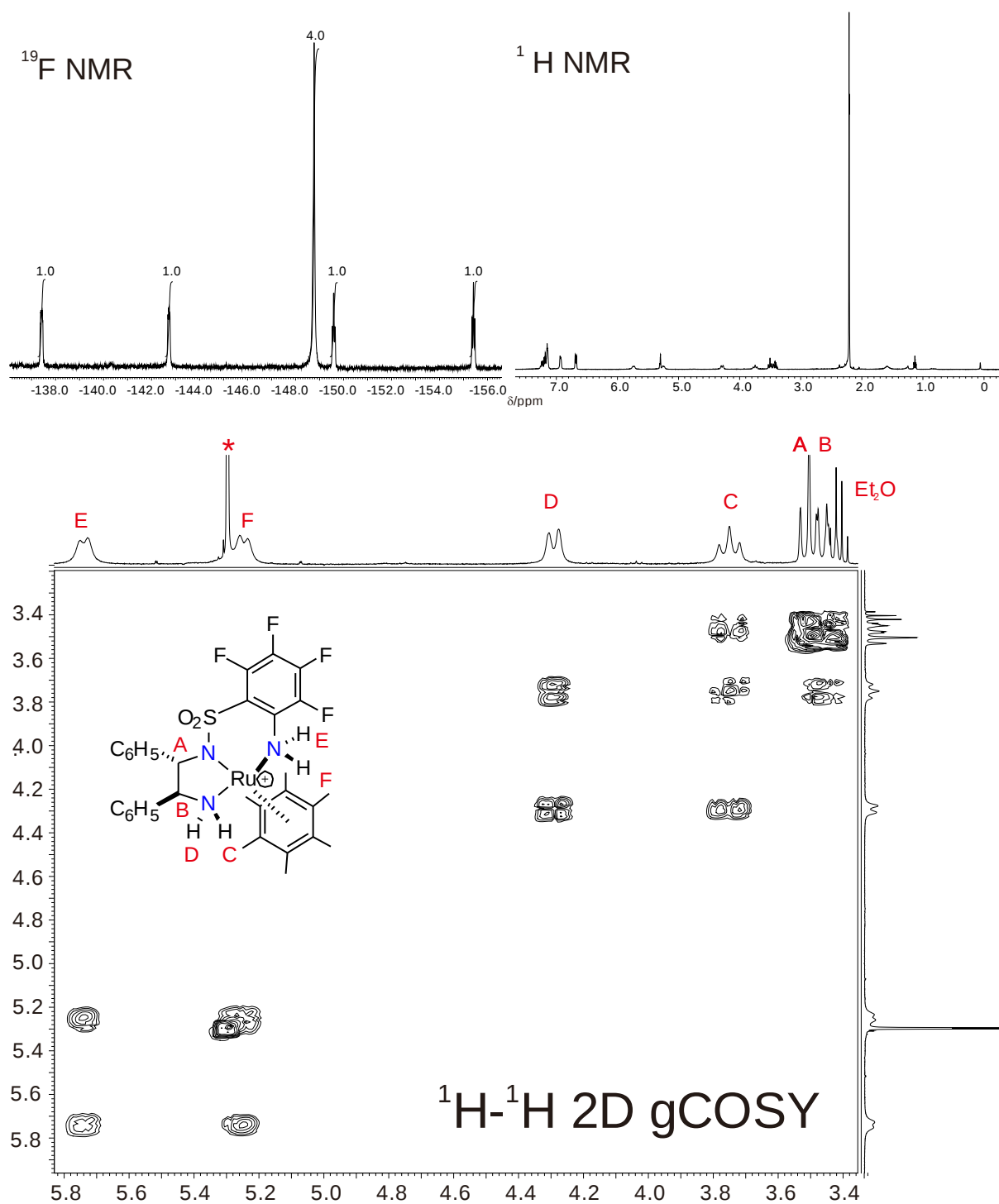


Figure S15. Section plots of the ^{19}F (376.2 MHz, 25 °C), ^1H (399.78 MHz, 25 °C) and ^1H - ^1H gCOSY NMR spectra of the complex $[\text{6H}]^+\text{BF}_4^-$ in CD_2Cl_2 .

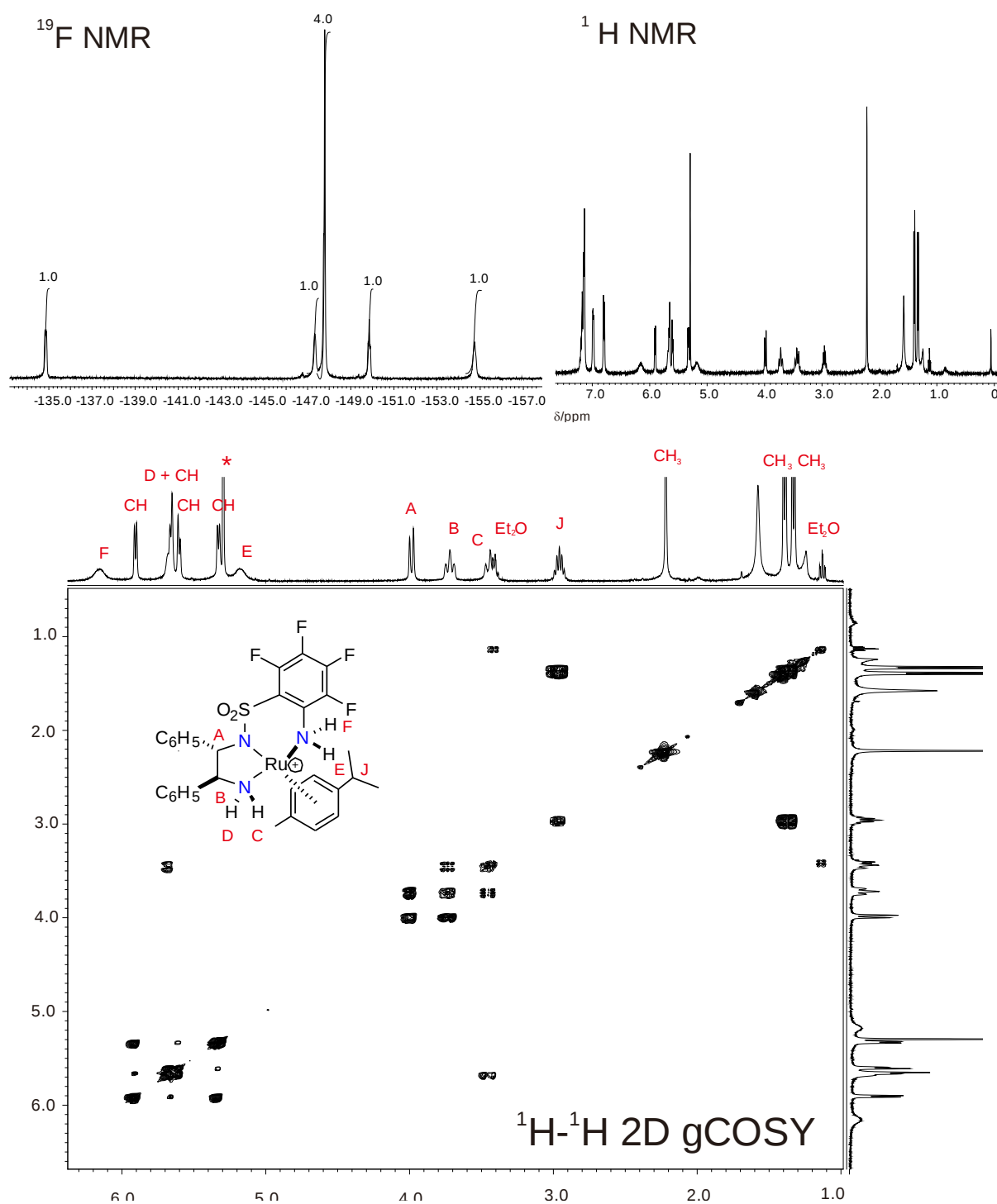


Figure S16. Section plots of the ^{19}F (376.2 MHz, 25 °C), ^1H (399.78 MHz, 25 °C) and ^1H - ^1H gCOSY NMR spectra of the complex $[\mathbf{10H}]^+\text{BF}_4^-$ in CD_2Cl_2 .

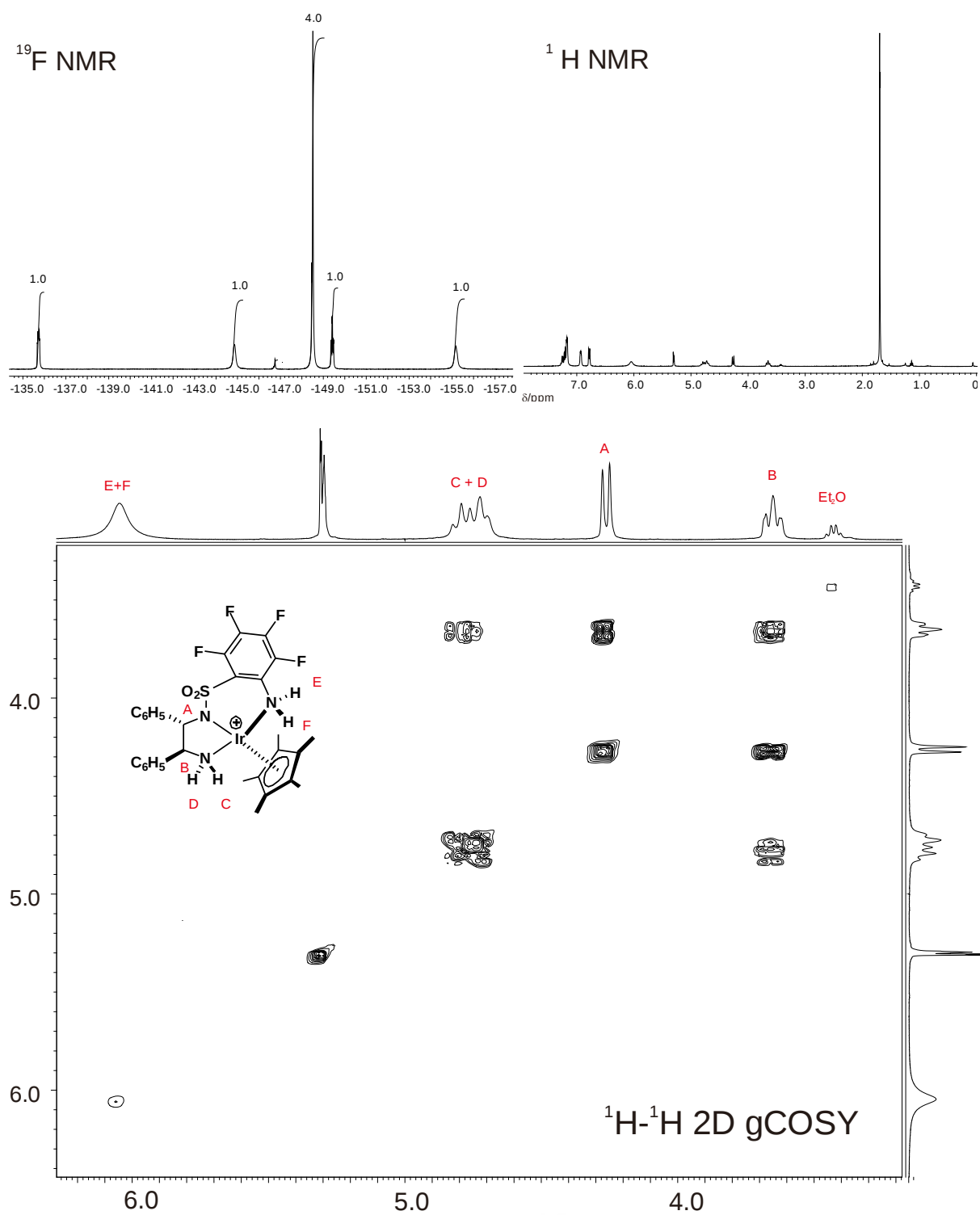


Figure S17. Section plots of the ^{19}F (376.2 MHz, 25 °C), ^1H (399.78 MHz, 25 °C) and ^1H - ^1H gCOSY NMR spectra of the complex $[7\text{H}]^+\text{BF}_4^-$ in CD_2Cl_2 .



Figure S18. ^1H NMR (399.78 MHz, 25 °C) spectrum of $[\mathbf{6H}]^+\text{OTf}^-$ in CD_2Cl_2 .

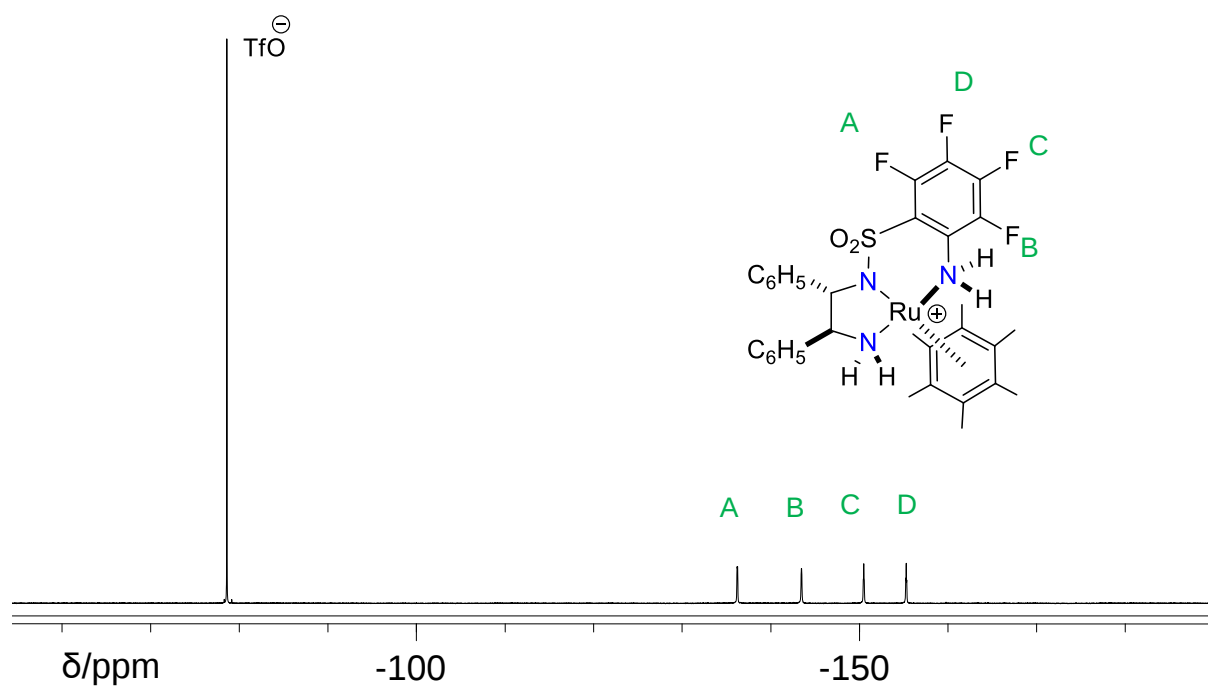


Figure S19. ^{19}F NMR (376.2 MHz, 25 °C) spectrum of $[\mathbf{6H}]^+\text{OTf}^-$ in CD_2Cl_2 .

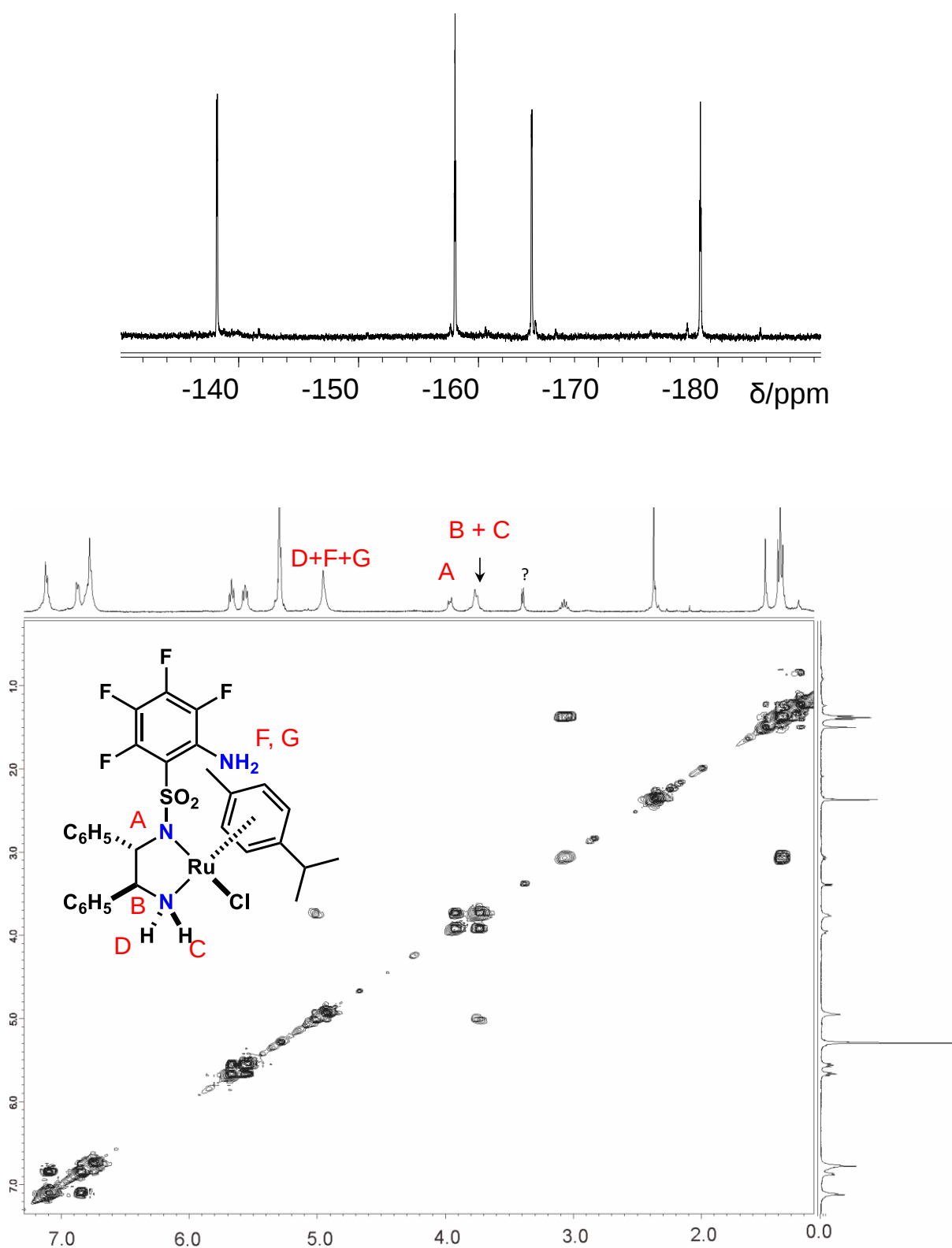


Figure S20. Section plots of the ¹⁹F (376.2 MHz, 25 °C) and ¹H-¹H gCOSY (399.78 MHz, 25 °C) NMR spectra of the complex **15** in CD₂Cl₂.

5. ^{19}F (376.2 MHz, 25 °C) NMR monitoring (selected region) of the reaction between the complex **15** and ca. 1.5 equiv AgOTf in CD_2Cl_2 .

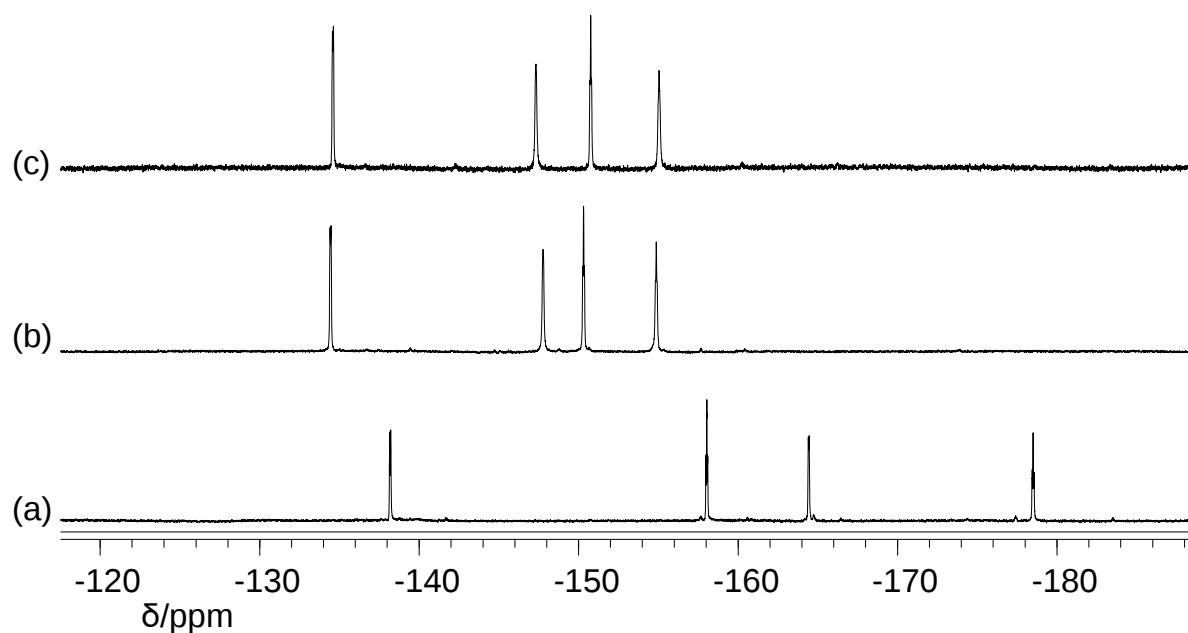


Figure S21. ^{19}F (376.2 MHz, 25 °C) NMR monitoring (selected region) of the reaction between the complex **15** and ca. 1.5 equiv AgOTf in CD_2Cl_2 : starting material (a); starting material in the presence of ca. 1.5 equiv AgOTf in 12 h after mixing the reagents (b); complex $[\mathbf{10H}]^+\text{OTf}^-$ generated in situ by the addition of ca. 1 equiv of TfOH to the **10** (c).

6. Cartesian Coordinates for all optimized geometries.

Cartesian Coordinates for all optimized geometries under ω B97X-D/def2-TZVP/SMD(dichloromethane) level.

NH₃

7	0.000000000	0.000000000	0.114298000
1	0.000000000	0.939028000	-0.266696000
1	-0.813222000	-0.469514000	-0.266696000
1	0.813222000	-0.469514000	-0.266696000

Complex 1

7	1.228361000	0.705053000	1.761413000
1	1.817565000	0.805802000	2.576943000
6	-0.272516000	1.700435000	0.181283000
1	-0.295110000	2.506652000	-0.552106000
6	0.873908000	1.976486000	1.170636000
1	0.487315000	2.653156000	1.940709000
6	2.745165000	-2.132367000	1.014095000
6	1.981024000	-2.277435000	2.189240000
6	2.191729000	-2.426508000	-0.267540000
6	0.064228000	-2.939310000	0.831772000
6	0.857730000	-2.878396000	-0.320368000
6	3.014634000	-2.312497000	-1.529751000
1	2.314514000	-2.390797000	-2.362365000
7	0.067688000	0.438614000	-0.483900000
16	-0.516716000	0.221120000	-1.950656000
8	-0.520628000	1.463567000	-2.686688000
8	0.147239000	-0.905144000	-2.554524000
6	-1.621671000	1.707691000	0.889425000
6	-2.333711000	2.901843000	0.943769000
6	-2.174298000	0.582019000	1.490454000
6	-3.565641000	2.974080000	1.577824000
1	-1.923712000	3.786120000	0.467140000
6	-3.404842000	0.647312000	2.126089000
1	-1.643235000	-0.360214000	1.443649000
6	-4.107758000	1.843416000	2.171489000
1	-4.107135000	3.912294000	1.598422000
1	-3.821625000	-0.244119000	2.579960000
1	-5.073147000	1.892226000	2.660340000
6	2.038046000	2.697948000	0.499254000
6	1.876678000	4.027479000	0.112058000
6	3.256128000	2.081127000	0.252675000
6	2.899455000	4.716233000	-0.518198000
1	0.933427000	4.527783000	0.305530000
6	4.285812000	2.766700000	-0.380973000
1	3.397811000	1.051380000	0.551544000
6	4.111726000	4.084718000	-0.770608000
1	2.752574000	5.748104000	-0.814091000
1	5.226092000	2.263307000	-0.573070000
1	4.912924000	4.619561000	-1.265895000
6	0.609409000	-2.615569000	2.108194000
6	-0.254569000	-2.637401000	3.330162000
1	0.107579000	-1.933475000	4.078819000
1	-1.285826000	-2.386099000	3.081910000
1	-0.246775000	-3.638612000	3.768805000
44	0.989260000	-0.938075000	0.808223000
6	-2.224827000	-0.236702000	-1.758283000
6	-3.214256000	0.734625000	-1.817944000
6	-2.560369000	-1.546303000	-1.451005000
6	-4.528498000	0.395398000	-1.548269000
1	-2.953190000	1.754334000	-2.066366000
6	-3.879723000	-1.876041000	-1.184243000
1	-1.795070000	-2.310115000	-1.423022000
6	-4.882502000	-0.910846000	-1.217717000

1	-5.294460000	1.161444000	-1.590793000
1	-4.134318000	-2.902804000	-0.947303000
6	-6.305938000	-1.254278000	-0.886525000
1	-6.463092000	-2.333096000	-0.873617000
1	-6.572782000	-0.863460000	0.099209000
1	-6.996141000	-0.813417000	-1.608067000
6	3.992066000	-3.487395000	-1.601667000
1	4.542101000	-3.464545000	-2.544560000
1	4.718936000	-3.441086000	-0.786044000
1	3.469886000	-4.444385000	-1.536087000
6	3.738136000	-0.977186000	-1.661200000
1	3.029738000	-0.148537000	-1.652785000
1	4.458466000	-0.824392000	-0.853627000
1	4.289031000	-0.946179000	-2.603411000
1	2.402577000	-1.988207000	3.142876000
1	3.757433000	-1.757741000	1.085894000
1	0.403277000	-3.031481000	-1.288104000
1	-0.989356000	-3.170727000	0.750588000

Complex (R)-1a_i

7	1.468278000	1.757194000	-0.021424000
1	2.025530000	2.308100000	0.624490000
1	2.076341000	1.108775000	-2.075351000
6	-0.744960000	0.948194000	-0.498823000
1	-0.684576000	1.323198000	-1.526385000
6	0.081690000	1.904088000	0.376146000
1	-0.090657000	1.594822000	1.420964000
6	4.065679000	-0.908053000	0.384790000
6	3.750957000	0.061439000	1.352966000
6	3.233226000	-2.067339000	0.282183000
6	1.761933000	-1.208063000	2.059123000
6	2.103340000	-2.200327000	1.089027000
6	5.256199000	-0.776665000	-0.537198000
1	4.967469000	-1.239124000	-1.486160000
6	0.528987000	-1.350343000	2.893643000
1	0.725597000	-2.009159000	3.743404000
1	0.203664000	-0.383989000	3.279525000
1	-0.284673000	-1.783902000	2.312854000
7	-0.093437000	-0.371128000	-0.407101000
16	-0.587988000	-1.459364000	-1.459812000
8	-0.892344000	-0.872688000	-2.751695000
8	0.344032000	-2.562615000	-1.469051000
6	-2.199569000	0.964752000	-0.079602000
6	-3.151296000	1.587731000	-0.875837000
6	-2.604944000	0.396872000	1.124186000
6	-4.483098000	1.638815000	-0.486065000
1	-2.846765000	2.031923000	-1.816935000
6	-3.932545000	0.438485000	1.515933000
1	-1.872886000	-0.103411000	1.745978000
6	-4.878483000	1.060665000	0.710252000
1	-5.212621000	2.125502000	-1.122297000
1	-4.233873000	-0.021109000	2.449820000
1	-5.917991000	1.090203000	1.013681000
6	-0.416829000	3.330139000	0.247057000
6	-1.139011000	3.926280000	1.274667000
6	-0.189410000	4.062433000	-0.915835000
6	-1.629128000	5.219560000	1.147439000
1	-1.327157000	3.366438000	2.184361000
6	-0.676771000	5.353217000	-1.049263000
1	0.378337000	3.611180000	-1.720609000
6	-1.400481000	5.937248000	-0.016890000
1	-2.190952000	5.665710000	1.959409000
1	-0.493169000	5.906815000	-1.962636000
1	-1.781551000	6.946021000	-0.120482000

6	2.599205000	-0.088735000	2.177861000
44	1.999647000	-0.234090000	0.102632000
7	2.277005000	0.112345000	-2.012036000
1	1.614820000	-0.384666000	-2.599013000
1	3.204665000	-0.062995000	-2.381021000
6	-2.118071000	-2.130236000	-0.849103000
6	-3.325581000	-1.807813000	-1.443930000
6	-2.091070000	-2.964483000	0.259673000
6	-4.507036000	-2.298629000	-0.910415000
1	-3.341765000	-1.163804000	-2.312189000
6	-3.274866000	-3.452721000	0.782694000
1	-1.144677000	-3.229999000	0.713524000
6	-4.503097000	-3.118721000	0.213285000
1	-5.449777000	-2.033161000	-1.374924000
1	-3.247490000	-4.103354000	1.649457000
6	-5.789623000	-3.600973000	0.818458000
1	-5.653020000	-4.547898000	1.342207000
1	-6.163838000	-2.872886000	1.543990000
1	-6.561160000	-3.732358000	0.058716000
6	6.426818000	-1.581375000	0.032194000
1	6.153720000	-2.626949000	0.187528000
1	7.277333000	-1.550291000	-0.651729000
1	6.746522000	-1.166963000	0.991824000
6	5.665828000	0.664641000	-0.816267000
1	4.817572000	1.270098000	-1.142682000
1	6.097271000	1.136946000	0.069033000
1	6.423983000	0.687833000	-1.600915000
1	2.326234000	0.707818000	2.858170000
1	4.336061000	0.966969000	1.426013000
1	3.435531000	-2.803034000	-0.484624000
1	1.426896000	-3.026486000	0.919967000

Complex (R)-1a_s

7	1.391333000	0.628410000	1.430136000
1	1.275310000	0.116480000	2.295491000
1	1.294814000	1.405234000	-1.760528000
6	-0.932657000	0.865050000	0.588516000
1	-1.526162000	1.630315000	0.087476000
6	0.265313000	1.542782000	1.297311000
1	-0.079305000	1.805826000	2.304169000
6	3.669182000	-1.497793000	-0.093055000
6	3.020745000	-1.837116000	1.108171000
6	3.037722000	-1.898728000	-1.311521000
6	1.157576000	-2.881286000	-0.103794000
6	1.822536000	-2.584493000	-1.326056000
6	4.975115000	-0.739376000	-0.150598000
1	4.947604000	-0.151608000	-1.073603000
6	-0.167335000	-3.572717000	-0.128904000
1	-0.008463000	-4.652439000	-0.194185000
1	-0.742820000	-3.368024000	0.772652000
1	-0.739169000	-3.255915000	-0.999360000
7	-0.419559000	-0.117967000	-0.384542000
16	-1.112518000	-0.096554000	-1.803864000
8	-0.919454000	1.154969000	-2.521613000
8	-0.737031000	1.279062000	-2.544788000
6	-1.858783000	0.224702000	1.603422000
6	-3.061515000	0.841725000	1.929565000
6	-1.534251000	-0.970857000	2.235907000
6	-3.926692000	0.275948000	2.855595000
1	-3.334606000	1.768002000	1.435898000
6	-2.392866000	-1.540040000	3.164129000
1	-0.606997000	-1.463858000	1.979863000
6	-3.596061000	-0.920190000	3.475788000
1	-4.866051000	0.765557000	3.083687000
1	-2.125309000	-2.474849000	3.643004000
1	-4.271927000	-1.368447000	4.193887000

6	0.709724000	2.876087000	0.690286000
6	0.134554000	3.485802000	-0.418376000
6	1.773092000	3.533100000	1.313684000
6	0.616529000	4.698902000	-0.900963000
1	-0.672853000	3.006719000	-0.954444000
6	2.250938000	4.744482000	0.844774000
1	2.236382000	3.069000000	2.176048000
6	1.674706000	5.334523000	-0.274577000
1	0.158456000	5.141720000	-1.777539000
1	3.075632000	5.231255000	1.352096000
1	2.048302000	6.279371000	-0.650207000
6	1.778920000	-2.530951000	1.112029000
44	1.631268000	-0.726835000	-0.096893000
7	2.118814000	1.027142000	-1.299452000
1	2.799345000	0.814514000	-2.019658000
1	2.504483000	1.760440000	-0.714328000
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6	-3.373524000	-1.351279000	-0.895952000
6	-5.039093000	0.797605000	-1.413917000
1	-3.283557000	1.774707000	-2.181920000
6	-4.716178000	-1.421111000	-0.582193000
1	-2.720385000	-2.185167000	-0.675524000
6	-5.571142000	-0.345403000	-0.830388000
1	-5.684383000	1.644357000	-1.617367000
1	-5.110955000	-2.320980000	-0.124262000
1	1.332526000	-2.800719000	-2.263345000
1	1.281644000	-2.738157000	2.049925000
1	3.422251000	-1.488909000	2.050213000
1	3.478752000	-1.589190000	-2.251463000
6	-7.022679000	-0.430870000	-0.457301000
1	-7.559805000	0.475650000	-0.736614000
1	-7.503049000	-1.279084000	-0.950182000
1	-7.134901000	-0.575957000	0.619922000
6	6.139738000	-1.725650000	-0.257220000
1	7.085457000	-1.190703000	-0.366718000
1	6.201271000	-2.343678000	0.642527000
1	6.023214000	-2.389511000	-1.116466000
6	5.173215000	0.226854000	1.011072000
1	6.058290000	0.840962000	0.834785000
1	4.311419000	0.886564000	1.130119000
1	5.327009000	-0.304107000	1.953549000

Complex (R)-1b_s

7	1.368199000	1.885699000	0.111887000
1	1.877899000	2.503021000	0.734346000
1	1.580865000	2.154944000	-0.849603000
6	-0.773695000	0.937657000	-0.520155000
1	-0.704828000	1.328964000	-1.541724000
6	-0.069192000	1.947050000	0.399140000
1	-0.194618000	1.610419000	1.430165000
6	4.107604000	-0.829047000	0.321931000
6	3.830829000	0.117675000	1.322983000
6	3.229989000	-1.949117000	0.196139000
6	1.853484000	-1.145904000	2.088994000
6	2.124009000	-2.081464000	1.049930000
6	5.282446000	-0.700309000	-0.618426000
1	4.969126000	-1.139380000	-1.569698000
6	0.654509000	-1.303653000	2.970619000
1	0.847678000	-2.047000000	3.748168000
1	0.398968000	-0.362555000	3.458691000
1	-0.207179000	-1.640576000	2.393370000
7	-0.054934000	-0.342893000	-0.421223000
16	-0.513311000	-1.454252000	-1.473464000
8	-0.877471000	-0.877974000	-2.752176000
8	0.460625000	-2.517875000	-1.494989000

6	-2.241386000	0.879732000	-0.143072000
6	-3.202453000	1.432123000	-0.977551000
6	-2.643619000	0.310517000	1.060706000
6	-4.544794000	1.414350000	-0.622389000
1	-2.897837000	1.874774000	-1.919075000
6	-3.980935000	0.283657000	1.417037000
1	-1.900923000	-0.135550000	1.711444000
6	-4.938027000	0.837011000	0.574727000
1	-5.283441000	1.846472000	-1.286626000
1	-4.281147000	-0.176076000	2.351058000
1	-5.985193000	0.813069000	0.850804000
6	-0.645532000	3.338800000	0.271326000
6	-1.374570000	3.889032000	1.318674000
6	-0.486933000	4.077918000	-0.898089000
6	-1.939186000	5.151597000	1.203939000
1	-1.510530000	3.318194000	2.230262000
6	-1.046295000	5.340733000	-1.014912000
1	0.070616000	3.664956000	-1.731397000
6	-1.775865000	5.880903000	0.035866000
1	-2.508196000	5.564176000	2.028075000
1	-0.916109000	5.903322000	-1.931291000
1	-2.215256000	6.866440000	-0.057299000
6	2.707624000	-0.039903000	2.189374000
44	2.040383000	-0.129788000	0.106665000
7	2.342413000	0.414101000	-1.884057000
1	1.551343000	0.093825000	-2.435100000
1	3.135095000	-0.081679000	-2.278672000
6	-1.997519000	-2.197769000	-0.828288000
6	-3.221927000	-1.990270000	-1.438037000
6	-1.915051000	-2.981428000	0.314634000
6	-4.366801000	-2.548362000	-0.888939000
1	-3.280957000	-1.383055000	-2.330706000
6	-3.061739000	-3.534413000	0.854491000
1	-0.954684000	-3.153966000	0.784172000
6	-4.308480000	-3.318600000	0.267264000
1	-5.323848000	-2.373803000	-1.367120000
1	-2.991251000	-4.144200000	1.748196000
1	2.481237000	0.742091000	2.903625000
1	4.433540000	1.010817000	1.405612000
1	3.374310000	-2.658739000	-0.606293000
1	1.416836000	-2.877792000	0.863579000
6	6.447057000	-1.535808000	-0.081456000
1	7.286324000	-1.508023000	-0.779316000
1	6.790824000	-1.144308000	0.879652000
1	6.157560000	-2.578973000	0.060462000
6	5.709717000	0.738765000	-0.880338000
1	6.464374000	0.760627000	-1.668545000
1	4.864620000	1.351002000	-1.200087000
1	6.152605000	1.194735000	0.008352000
6	-5.557372000	-3.874217000	0.888375000
1	-6.335080000	-4.035150000	0.140905000
1	-5.362492000	-4.820085000	1.395709000
1	-5.954470000	-3.177341000	1.632176000

Complex (R)-1b₈

7	1.744652000	1.230334000	0.986563000
1	2.312581000	1.164955000	1.822236000
1	2.281170000	1.728297000	0.276024000
6	-0.727157000	1.083600000	0.829028000
1	-1.533912000	1.774289000	0.575773000
6	0.476497000	1.945037000	1.289551000
1	0.415473000	2.051732000	2.370345000
6	3.411865000	-1.789163000	-0.355445000
6	3.031896000	-1.715156000	0.997345000
6	2.426042000	-2.244888000	-1.283263000
6	0.794189000	-2.590226000	0.527776000
6	1.141539000	-2.601189000	-0.859239000

6	4.787295000	-1.398656000	-0.842777000
1	4.676360000	-1.099314000	-1.888734000
6	-0.569711000	-3.026995000	0.957647000
1	-0.713775000	-4.080340000	0.705023000
1	-0.707131000	-2.904330000	2.029902000
1	-1.340502000	-2.452527000	0.447130000
7	-0.343531000	0.317880000	-0.364057000
16	-1.155515000	0.579674000	-1.699821000
8	-1.492611000	1.973842000	-1.883522000
8	-0.472725000	-0.080754000	-2.787456000
6	-1.264954000	0.190866000	1.947176000
6	-2.590950000	-0.233371000	1.890736000
6	-0.503822000	-0.210793000	3.040284000
6	-3.133128000	-1.043960000	2.875025000
1	-3.213393000	0.077925000	1.062480000
6	-1.041516000	-1.016133000	4.035410000
1	0.529671000	0.094432000	3.132796000
6	-2.358220000	-1.440936000	3.955930000
1	-4.167657000	-1.357132000	2.800960000
1	-0.423750000	-1.313685000	4.874403000
1	-2.778883000	-2.069587000	4.731157000
6	0.419268000	3.350570000	0.731288000
6	-0.231334000	4.328664000	1.480609000
6	0.940970000	3.697904000	-0.509599000
6	-0.360430000	5.624098000	1.003978000
1	-0.642675000	4.071213000	2.450852000
6	0.818507000	4.995809000	-0.985531000
1	1.441583000	2.949999000	-1.114004000
6	0.167417000	5.962750000	-0.234212000
1	-0.868033000	6.370588000	1.602957000
1	1.229058000	5.248388000	-1.955822000
1	0.072628000	6.974405000	-0.609616000
6	1.751789000	-2.153528000	1.443167000
44	1.602416000	-0.589463000	-0.165303000
7	2.287295000	0.784547000	-1.576878000
1	1.544954000	0.903521000	-2.259622000
1	3.040845000	0.361421000	-2.110120000
6	-2.728799000	-0.246259000	-1.553400000
6	-3.893498000	0.480104000	-1.375372000
6	-2.779608000	-1.634406000	-1.591019000
6	-5.102518000	-0.182863000	-1.206769000
1	-3.854221000	1.561014000	-1.359822000
6	-3.986031000	-2.285562000	-1.420855000
1	-1.872975000	-2.202403000	-1.754752000
6	-5.168277000	-1.570804000	-1.217594000
1	-6.008854000	0.393927000	-1.062289000
1	-4.016251000	-3.369215000	-1.446698000
6	-6.469707000	-2.295049000	-1.027538000
1	-7.291326000	-1.598432000	-0.860763000
1	-6.709307000	-2.900259000	-1.904999000
1	-6.416531000	-2.972199000	-0.171931000
6	5.707494000	-2.620289000	-0.804085000
1	6.686949000	-2.373460000	-1.218985000
1	5.850085000	-2.962454000	0.224486000
1	5.292379000	-3.448630000	-1.382113000
6	5.392492000	-0.223104000	-0.084101000
1	5.626470000	-0.486461000	0.950085000
1	6.325329000	0.083604000	-0.560606000
1	4.715027000	0.632905000	-0.080684000
1	3.719849000	-1.301792000	1.722874000
1	1.499114000	-2.091524000	2.492215000
1	2.648155000	-2.226293000	-2.342255000
1	0.391623000	-2.861436000	-1.593891000

Complex (S)-1a₈

7	-1.082847000	2.024089000	-0.702723000
1	-1.350575000	0.583565000	-2.709249000
6	0.862046000	0.860203000	0.303745000
1	0.739341000	1.331743000	1.285686000
6	0.354644000	1.852613000	-0.765880000
1	0.609907000	1.405133000	-1.733243000
6	-3.037132000	1.139910000	1.622377000
6	-3.727562000	1.566301000	0.452159000
6	-2.857699000	-0.249767000	1.779840000
6	-4.037112000	-0.757654000	-0.296947000

6	-3.394542000	-1.193682000	0.865595000	6	-2.396542000	1.275834000	-1.381684000
6	-2.488215000	2.124582000	2.606733000	6	-0.587999000	2.896522000	-0.948206000
1	-3.242885000	2.375969000	3.356325000	6	-1.193243000	1.939326000	-1.764735000
1	-1.620599000	1.713238000	3.123250000	6	-3.046157000	0.288622000	-2.296758000
1	-2.193205000	3.050401000	2.110075000	1	-3.540552000	0.817626000	-3.116195000
6	-4.549757000	-1.710247000	-1.351921000	1	-2.301804000	-0.380905000	-2.726246000
1	-4.437915000	-1.199213000	-2.313447000	1	-3.793352000	-0.301565000	-1.768636000
7	-0.021545000	-0.319607000	0.212244000	7	0.002685000	-0.875672000	-0.396298000
16	0.289200000	-1.487058000	1.256389000	16	0.810528000	-1.164448000	-1.723678000
8	0.643527000	-0.985824000	2.569101000	8	0.962900000	-2.586937000	-1.945892000
8	-0.775263000	-2.462161000	1.207724000	8	0.264350000	-0.402111000	-2.821738000
6	2.339861000	0.610076000	0.090900000	6	1.025847000	-2.159292000	1.556762000
6	3.262537000	1.033592000	1.038672000	6	2.151101000	-2.843044000	1.098235000
6	2.813518000	0.022488000	-1.079632000	6	1.019893000	-1.746878000	2.888174000
6	4.625646000	0.866901000	0.833489000	6	3.251131000	-3.058553000	1.914735000
1	2.907536000	1.493597000	1.953875000	1	2.157334000	-3.219404000	0.084114000
6	4.170893000	-0.152007000	-1.288459000	6	2.114511000	-1.965955000	3.713258000
1	2.109323000	-0.324848000	-1.826165000	1	0.149521000	-1.235988000	3.278499000
6	5.084562000	0.270345000	-0.330559000	6	3.241767000	-2.612221000	3.228035000
1	5.328557000	1.200760000	1.587333000	1	4.113594000	-3.585789000	1.524346000
1	4.519558000	-0.624296000	-2.199219000	1	2.082370000	-1.630574000	4.743312000
1	6.146727000	0.131614000	-0.491788000	1	4.097351000	-2.780136000	3.870923000
6	1.086190000	3.174298000	-0.677794000	6	-2.703131000	-2.085603000	0.478448000
6	1.897985000	3.614125000	-1.716887000	6	-3.965579000	-1.813331000	1.008178000
6	0.968185000	3.978004000	0.455093000	6	-2.649132000	-2.743017000	-0.746963000
6	2.576866000	4.822621000	-1.632333000	6	-5.126423000	-2.170121000	0.341294000
1	2.005483000	2.997977000	-2.602549000	1	-4.047411000	-1.319280000	1.970537000
6	1.643021000	5.185293000	0.545509000	6	-3.809096000	-3.111229000	-1.417894000
1	0.347282000	3.653009000	1.283036000	1	-1.698272000	-2.966357000	-1.211231000
6	2.451777000	5.612677000	-0.499714000	6	-5.053336000	-2.824865000	-0.881607000
1	3.206198000	5.145267000	-2.453145000	1	-6.090738000	-1.945780000	0.781910000
1	1.541681000	5.793468000	1.436502000	1	-3.732334000	-3.615866000	-2.373699000
1	2.981719000	6.554733000	-0.429255000	1	-5.957087000	-3.108781000	-1.406870000
6	-4.208104000	0.648678000	-0.495715000	6	-1.130526000	3.189155000	0.335327000
44	-2.091598000	0.322343000	-0.160786000	6	-0.496278000	4.197893000	1.274173000
7	-1.529422000	-0.261785000	-2.176852000	1	-0.426272000	3.717878000	2.254973000
1	-0.660616000	-0.782329000	-2.106281000	44	-0.883030000	1.002948000	0.215522000
1	-1.281111000	2.744234000	-0.017631000	7	0.873310000	1.107304000	1.473390000
1	-2.199157000	-0.821695000	-2.692220000	1	1.618876000	0.509710000	1.132937000
6	1.715633000	-2.370259000	0.656199000	1	-2.385795000	-0.044103000	2.042169000
6	2.892202000	-2.402567000	1.382278000	1	1.266434000	2.023664000	1.648634000
6	1.622300000	-3.056027000	-0.547368000	6	2.463517000	-0.514964000	-1.522173000
6	3.984242000	-3.102320000	0.890429000	6	3.565609000	-1.351780000	-1.529539000
1	2.957633000	-1.870324000	2.321203000	6	2.644264000	0.854969000	-1.354254000
6	2.715349000	-3.751945000	-1.028949000	6	4.838095000	-0.825915000	-1.344569000
1	0.697201000	-3.038739000	-1.110534000	1	3.433773000	-2.414247000	-1.680762000
6	3.918226000	-3.778475000	-0.322846000	6	3.912861000	1.368380000	-1.164493000
1	4.906822000	-3.114603000	1.459450000	1	1.788468000	1.516614000	-1.367942000
1	2.638122000	-4.282942000	-1.971060000	6	5.033537000	0.535657000	-1.152124000
6	5.119987000	-4.486581000	-0.878425000	1	5.692640000	-1.492806000	-1.350214000
1	4.830519000	-5.346813000	-1.483604000	1	4.041189000	2.436876000	-1.029618000
1	5.696118000	-3.812281000	-1.518705000	6	6.406396000	1.110448000	-0.952933000
1	5.782342000	-4.829369000	-0.082646000	1	6.677729000	1.763048000	-1.786450000
6	-6.044133000	-1.955122000	-1.129513000	1	6.449878000	1.712359000	-0.042617000
1	-6.605769000	-1.018820000	-1.124990000	1	7.158897000	0.325140000	-0.879845000
1	-6.446934000	-2.589702000	-1.921531000	6	-1.418703000	5.413064000	1.410984000
1	-6.211393000	-2.456990000	-0.173138000	1	-2.402998000	5.131588000	1.787549000
6	-3.782288000	-3.025240000	-1.421934000	1	-0.985881000	6.139241000	2.101854000
1	-3.960545000	-3.641544000	-0.538266000	1	-1.551995000	5.903632000	0.443310000
1	-4.108592000	-3.597604000	-2.292157000	6	0.898175000	4.653925000	0.855625000
1	-2.706183000	-2.860262000	-1.503548000	1	1.585712000	3.825242000	0.676005000
1	-3.185427000	-2.238879000	1.020296000	1	0.857816000	5.251290000	-0.058415000
1	-2.257885000	-0.609285000	2.605113000	1	1.328435000	5.279661000	1.638988000
1	-4.667709000	1.009833000	-1.406079000	1	-3.813255000	1.051762000	0.216609000
1	-3.796626000	2.625934000	0.238528000	1	-0.713798000	1.651665000	-2.688011000
Complex (S)-1a_s				1	0.330647000	3.361588000	-1.273437000
7	-1.455283000	-0.289487000	1.725901000	1	-2.723178000	2.717992000	1.715179000
1	0.543236000	0.716825000	2.350804000	Complex (S)-1b_s			
6	-0.151260000	-1.964745000	0.595543000	7	-0.975344000	2.163853000	-0.524846000
1	-0.225866000	-2.911011000	0.062431000	1	-1.333642000	2.590672000	-1.372788000
6	-1.473267000	-1.686524000	1.302418000	6	0.893649000	0.883859000	0.374501000
1	-1.506133000	-2.331819000	2.192983000	1	0.814843000	1.375399000	1.352016000
6	-2.941127000	1.591509000	-0.128815000	6	0.458819000	1.892980000	-0.695575000
6	-2.317452000	2.537705000	0.728573000	1	0.554239000	1.413599000	-1.668163000

6	-3.189146000	1.174742000	1.640038000
6	-3.760696000	1.618067000	0.413528000
6	-2.983850000	-0.204281000	1.767164000
6	-4.021533000	-0.682874000	-0.409991000
6	-3.412503000	-1.128711000	0.768373000
6	-2.740554000	2.147672000	2.686217000
1	-3.573927000	2.418360000	3.339449000
1	-1.951564000	1.717056000	3.303318000
1	-2.365654000	3.068070000	2.233787000
6	-4.477489000	-1.622909000	-1.500241000
1	-4.327785000	-1.097749000	-2.448401000
7	-0.040058000	-0.257677000	0.315655000
16	0.266103000	-1.425506000	1.355803000
8	0.728105000	-0.923660000	2.634629000
8	-0.849770000	-2.340433000	1.390208000
6	2.358527000	0.558698000	0.145795000
6	3.307143000	0.904097000	1.097570000
6	2.782988000	-0.040564000	-1.036406000
6	4.655476000	0.650619000	0.882359000
1	2.986622000	1.370060000	2.022154000
6	4.124840000	-0.300490000	-1.254640000
1	2.052621000	-0.325447000	-1.784480000
6	5.067626000	0.044797000	-0.293885000
1	5.382257000	0.923519000	1.637900000
1	4.437901000	-0.779462000	-2.174549000
1	6.117542000	-0.161197000	-0.462983000
6	1.287478000	3.156879000	-0.683310000
6	2.079434000	3.485825000	-1.776617000
6	1.285485000	4.003554000	0.422630000
6	2.857265000	4.635269000	-1.768238000
1	2.092452000	2.830807000	-2.640160000
6	2.058624000	5.153722000	0.434127000
1	0.683457000	3.758928000	1.291520000
6	2.848622000	5.472253000	-0.662573000
1	3.471745000	4.875640000	-2.627227000
1	2.049267000	5.800528000	1.302957000
1	3.455821000	6.369044000	-0.653289000
6	-4.189290000	0.722287000	-0.587197000
44	-2.101212000	0.389169000	-0.151624000
7	-1.508217000	-0.019567000	-2.100630000
1	-0.679452000	-0.603381000	-2.024457000
1	-1.120865000	2.828137000	0.229529000
1	-2.193432000	-0.604989000	-2.568362000
6	1.600715000	-2.399547000	0.687934000
6	2.790889000	-2.545420000	1.374437000
6	1.414820000	-3.042749000	-0.529771000
6	3.806307000	-3.322596000	0.832706000
1	2.929850000	-2.041017000	2.320920000
6	2.429499000	-3.816128000	-1.058740000
1	0.481427000	-2.925061000	-1.066724000
6	3.645915000	-3.964103000	-0.389032000
1	4.741615000	-3.423948000	1.371099000
1	2.281608000	-4.312818000	-2.011233000
6	4.755018000	-4.774970000	-0.994875000
1	4.387896000	-5.737281000	-1.356802000
1	5.191009000	-4.250919000	-1.849755000
1	5.551617000	-4.959390000	-0.273806000
6	-5.978365000	-1.879838000	-1.343286000
1	-6.546919000	-0.947672000	-1.353172000
1	-6.341592000	-2.508302000	-2.158911000
1	-6.183501000	-2.393859000	-0.400731000
6	-3.697579000	-2.930735000	-1.554587000
1	-2.621784000	-2.751079000	-1.592299000
1	-3.907733000	-3.560332000	-0.687104000
1	-3.983573000	-3.493107000	-2.445296000
1	-2.444464000	-0.583646000	2.624012000
1	-3.184251000	-2.172349000	0.904648000
1	-4.594477000	1.105374000	-1.513953000
1	-3.823639000	2.682548000	0.219513000

Complex (S)-1b₈

7	-0.982261000	0.484135000	-1.705468000
1	-0.311660000	-0.063149000	-2.243094000
6	0.782577000	1.496982000	-0.371480000
1	0.947564000	2.397320000	0.222132000

6	-0.403550000	1.784604000	-1.301957000
1	-0.020207000	2.291192000	-2.192030000
6	-3.250443000	0.215174000	0.808048000
6	-3.508646000	-0.589286000	-0.326261000
6	-2.523581000	-0.316585000	1.878535000
6	-2.467710000	-2.490114000	0.730507000
6	-2.124851000	-1.687095000	1.827588000
6	-2.205214000	0.521350000	3.075394000
1	-2.976082000	0.359701000	3.834192000
1	-1.242974000	0.244670000	3.499011000
1	-2.196070000	1.580804000	2.824823000
7	0.410589000	0.384046000	0.515712000
16	1.290416000	0.230822000	1.825216000
8	1.582926000	1.519486000	2.419800000
8	0.695975000	-0.767517000	2.680103000
6	2.059410000	1.329777000	-1.192182000
6	2.920285000	2.418633000	-1.294154000
6	2.395394000	0.156827000	-1.859323000
6	4.093774000	2.338952000	-2.029496000
1	2.678965000	3.337763000	-0.770970000
6	3.569665000	0.070799000	-2.591913000
1	1.747940000	-0.707305000	-1.790981000
6	4.426050000	1.159466000	-2.678801000
1	4.754597000	3.195820000	-2.083869000
1	3.819976000	-0.857536000	-3.091646000
1	5.347201000	1.086987000	-3.244129000
6	-1.487015000	2.672784000	-0.718226000
6	-2.539477000	3.056213000	-1.547045000
6	-1.479858000	3.126161000	0.594663000
6	-3.570714000	3.851241000	-1.073416000
1	-2.552817000	2.734184000	-2.583143000
6	-2.503874000	3.934560000	1.069520000
1	-0.689566000	2.831786000	1.272157000
6	-3.556042000	4.294369000	0.242229000
1	-4.380594000	4.134050000	-1.734768000
1	-2.481128000	4.273686000	2.098013000
1	-4.356658000	4.920360000	0.616419000
6	-3.176342000	-1.963757000	-0.383349000
6	-3.656347000	-2.800581000	-1.548039000
1	-3.801280000	-2.112767000	-2.386056000
44	-1.391277000	-0.758825000	-0.022744000
7	-0.039785000	-1.988827000	-1.013974000
1	0.837648000	-1.896610000	-0.513313000
1	-1.789554000	0.629640000	-2.301451000
1	-0.297729000	-2.960925000	-0.879226000
6	2.874633000	-0.443542000	1.358158000
6	3.983378000	0.376129000	1.220008000
6	2.980521000	-1.799450000	1.082067000
6	5.182176000	-0.155144000	0.772721000
1	3.904851000	1.429578000	1.450375000
6	4.183671000	-2.322291000	0.639733000
1	2.123227000	-2.447376000	1.215507000
6	5.300123000	-1.507350000	0.464673000
1	6.041081000	0.496089000	0.656596000
1	4.257039000	-3.382456000	0.425544000
6	6.587651000	-2.062725000	-0.071656000
1	7.450693000	-1.577036000	0.386153000
1	6.661190000	-3.136787000	0.102396000
1	6.652161000	-1.895795000	-1.150749000
6	-2.688093000	-3.886513000	-2.000751000
1	-1.740531000	-3.461532000	-2.331315000
1	-2.486444000	-4.608750000	-1.206039000
1	-3.122174000	-4.437596000	-2.837514000
6	-5.019201000	-3.400207000	-1.190137000
1	-4.924300000	-4.096798000	-0.352575000
1	-5.732800000	-2.624400000	-0.904831000
1	-5.431582000	-3.947848000	-2.040219000
1	-1.520488000	-2.092056000	2.625173000
1	-2.110498000	-3.510924000	0.703523000
1	-3.534301000	1.257884000	0.809024000
1	-3.976255000	-0.136243000	-1.192932000

Complex 2

7	0.084630000	1.018370000	-1.669247000
1	-0.164768000	1.635932000	-2.430793000

6	1.736218000	-0.383293000	-0.644259000
1	2.752461000	-0.346137000	-0.251121000
6	1.515931000	0.848512000	-1.544304000
1	1.951606000	0.629073000	-2.523720000
6	-2.623801000	1.914699000	-0.034182000
6	-2.960279000	1.222171000	-1.230382000
6	-2.516343000	1.201266000	1.205020000
6	-2.873497000	-0.918662000	0.021099000
6	-2.707963000	-0.202913000	1.230070000
6	-3.185108000	1.976956000	-2.513998000
1	-3.480811000	3.004296000	-2.316821000
1	-2.294532000	1.999602000	-3.146121000
1	-3.985645000	1.512469000	-3.088245000
6	-2.410649000	3.402274000	-0.064152000
1	-3.368403000	3.920523000	0.038822000
1	-1.766598000	3.729888000	0.747153000
1	-1.951939000	3.719655000	-0.998051000
6	-2.262677000	1.976781000	2.469033000
1	-3.053861000	2.717516000	2.609179000
1	-2.238196000	1.337871000	3.344480000
1	-1.311378000	2.505009000	2.429724000
6	-2.676054000	-0.926573000	2.548913000
1	-3.503913000	-0.574643000	3.169038000
1	-2.786767000	-1.999422000	2.433966000
1	-1.749490000	-0.735642000	3.085021000
6	-2.991137000	-2.419670000	0.048052000
1	-3.933321000	-2.705901000	0.522399000
1	-2.984359000	-2.851096000	-0.947334000
1	-2.183513000	-2.880284000	0.614412000
7	0.763377000	-0.259481000	0.447467000
16	1.281874000	-0.337852000	1.914055000
8	2.676898000	-0.022667000	2.059842000
8	0.347131000	0.244193000	2.832068000
6	1.595441000	-1.676417000	-1.431981000
6	2.557458000	-1.978103000	-2.393816000
6	0.556416000	-2.575181000	-1.232916000
6	2.473555000	-3.137534000	-3.147829000
1	3.387521000	-1.297579000	-2.550778000
6	0.466609000	-3.738318000	-1.986680000
1	-0.187022000	-2.369277000	-0.475798000
6	1.421735000	-4.023018000	-2.949640000
1	3.234216000	-3.353744000	-3.888306000
1	-0.353207000	-4.425605000	-1.814150000
1	1.354746000	-4.931036000	-3.536285000
6	2.238958000	2.071122000	-0.997641000
6	3.585824000	2.253188000	-1.301055000
6	1.613749000	2.994282000	-0.168812000
6	4.294127000	3.326496000	-0.784154000
1	4.086206000	1.541858000	-1.950039000
6	2.319328000	4.070190000	0.353352000
1	0.565665000	2.866563000	0.070095000
6	3.661365000	4.240146000	0.048769000
1	5.341320000	3.451739000	-1.032198000
1	1.816876000	4.777204000	1.002835000
1	4.211799000	5.079923000	0.455073000
6	-2.976012000	-0.201282000	-1.219122000
6	-3.099237000	-0.953215000	-2.516425000
1	-2.865945000	-0.321573000	-3.368590000
1	-2.413168000	-1.797357000	-2.548177000
1	-4.115682000	-1.336292000	-2.640473000
44	-1.141785000	0.420792000	-0.338663000
6	1.248943000	-2.133465000	2.386036000
9	1.584514000	-2.288929000	3.667801000
9	0.035809000	-2.662131000	2.215290000
9	2.110004000	-2.835585000	1.648494000

Complex (R)-2a₁

7	-0.009764000	-1.875224000	-0.718006000
1	-0.187063000	-2.805031000	-0.350502000
1	-0.764008000	-0.779077000	-2.689846000
6	1.443994000	0.036158000	-0.590488000
1	1.703420000	-0.049744000	-1.648807000
6	1.190159000	-1.386081000	-0.069296000
1	1.072053000	-1.297130000	1.024050000
6	-3.622912000	-1.343727000	-0.072132000

6	-2.766123000	-2.169092000	0.693265000
6	-3.659961000	0.074823000	0.157413000
6	-1.938702000	-0.185783000	1.896936000
6	-2.849605000	0.643239000	1.150734000
6	-2.695308000	-3.648937000	0.425648000
1	-3.526388000	-4.167171000	0.911567000
1	-2.739871000	-3.862293000	-0.640389000
1	-1.771775000	-4.082080000	0.800261000
6	-4.552976000	-1.929308000	-1.100612000
1	-5.575862000	-1.621076000	-0.874673000
1	-4.334840000	-1.581717000	-2.111188000
1	-4.531483000	-3.014243000	-1.108750000
6	-4.556236000	0.947176000	-0.675273000
1	-5.539221000	1.046305000	-0.204866000
1	-4.136597000	1.943032000	-0.793549000
1	-4.707711000	0.533985000	-1.670088000
6	-2.962571000	2.118317000	1.432779000
1	-4.014428000	2.392640000	1.528737000
1	-2.468518000	2.394018000	2.359624000
1	-2.535656000	2.712671000	0.626057000
6	-0.997979000	0.460473000	2.874601000
1	-1.493933000	0.631140000	3.834186000
1	-0.120593000	-0.154290000	3.052596000
1	-0.647805000	1.418205000	2.499980000
7	0.154914000	0.756834000	-0.459726000
16	0.020446000	2.100586000	-1.243183000
8	0.929505000	2.242325000	-2.351221000
8	-1.362747000	2.435714000	-1.463769000
6	2.608825000	0.677153000	0.128501000
6	3.801453000	0.905629000	-0.546498000
6	2.536024000	0.994809000	1.481039000
6	4.899410000	1.442569000	0.111231000
1	3.869529000	0.662772000	-1.600715000
6	3.628386000	1.532113000	2.142877000
1	1.610207000	0.832700000	2.016943000
6	4.815898000	1.758057000	1.459091000
1	5.820369000	1.617017000	-0.431960000
1	3.553056000	1.778385000	3.195348000
1	5.669993000	2.180508000	1.974321000
6	2.392231000	-2.277585000	-0.306213000
6	3.194971000	-2.679295000	0.755550000
6	2.728176000	-2.698978000	-1.590518000
6	4.311196000	-3.478239000	0.544873000
1	2.945570000	-2.355909000	1.760431000
6	3.841509000	-3.495935000	-1.807062000
1	2.105720000	-2.397935000	-2.424600000
6	4.638654000	-3.888398000	-0.738659000
1	4.925344000	-3.779158000	1.385247000
1	4.090842000	-3.811741000	-2.813226000
1	5.508918000	-4.510938000	-0.907662000
6	-1.936956000	-1.587554000	1.714685000
6	-1.080235000	-2.497917000	2.554038000
1	-0.251538000	-2.920101000	1.981833000
1	-0.668234000	-1.993137000	3.422086000
1	-1.682510000	-3.330622000	2.919954000
44	-1.569234000	-0.612956000	-0.216854000
7	-1.673398000	-0.463025000	-2.364390000
1	-1.837356000	0.486847000	-2.681823000
1	-2.371243000	-1.061208000	-2.791970000
6	0.550122000	3.511383000	-0.132655000
9	0.084624000	3.363323000	1.108508000
9	0.060700000	4.656846000	-0.615517000
9	1.870874000	3.639859000	-0.066819000

Complex (R)-2a₂

7	0.759893000	0.987735000	1.527150000
1	0.452829000	0.521194000	2.372283000
1	1.134635000	1.741506000	-1.472981000
6	-1.418510000	1.219958000	0.385204000
1	-1.990302000	1.945369000	-0.190249000
6	-0.279939000	1.932067000	1.156362000
1	-0.732635000	2.326532000	2.074278000
6	3.230924000	-1.228098000	0.103127000
6	2.746973000	-1.300204000	1.431486000
6	2.554608000	-1.923850000	-0.955889000

6	0.816733000	-2.615533000	0.650687000
6	1.336300000	-2.566480000	-0.689444000
6	3.489131000	-0.646334000	2.564719000
1	4.521566000	-0.431654000	2.303570000
1	3.007277000	0.289711000	2.859431000
1	3.504894000	-1.304851000	3.433171000
6	4.458314000	-0.408630000	-0.195943000
1	5.363659000	-0.995608000	-0.019998000
1	4.479599000	-0.071543000	-1.229323000
1	4.502308000	0.477376000	0.433863000
6	3.123846000	-1.951435000	-2.350407000
1	2.987138000	-2.936956000	-2.794248000
1	2.635285000	-1.230055000	-3.010077000
1	4.190860000	-1.744929000	-2.352126000
6	0.622103000	-3.291771000	-1.793806000
1	1.021834000	-4.307431000	-1.879729000
1	-0.443952000	-3.369197000	-1.609243000
1	0.747807000	-2.789558000	-2.747408000
6	-0.396797000	-3.467660000	0.907195000
1	-0.169961000	-4.493892000	0.607974000
1	-0.679534000	-3.489317000	1.954675000
1	-1.260437000	-3.147339000	0.329367000
7	-0.789446000	0.244803000	-0.526960000
16	-1.342769000	0.161941000	-1.976547000
8	-1.916096000	1.387699000	-2.475406000
8	-0.445551000	-0.554336000	-2.838359000
6	-2.392329000	0.602418000	1.366639000
6	-3.434016000	1.380081000	1.866948000
6	-2.264147000	-0.701512000	1.818115000
6	-4.322945000	0.863459000	2.796691000
1	-3.553181000	2.400187000	1.517295000
6	-3.150300000	-1.226209000	2.748648000
1	-1.466650000	-1.308018000	1.422057000
6	-4.184068000	-0.445048000	3.242747000
1	-5.132114000	1.480585000	3.168605000
1	-3.033706000	-2.250181000	3.084549000
1	-4.881485000	-0.852177000	3.964660000
6	0.303983000	3.160352000	0.455939000
6	-0.240177000	3.759976000	-0.675404000
6	1.447986000	3.737943000	1.010116000
6	0.351756000	4.881626000	-1.248241000
1	-1.118708000	3.347765000	-1.152181000
6	2.035126000	4.859591000	0.450054000
1	1.885479000	3.277330000	1.886895000
6	1.491401000	5.436388000	-0.691896000
1	-0.086450000	5.317037000	-2.138480000
1	2.922170000	5.285973000	0.903854000
1	1.951834000	6.309149000	-1.138666000
6	1.510841000	-1.981769000	1.702538000
6	0.984995000	-1.995715000	3.110875000
1	1.291229000	-1.106740000	3.658215000
1	-0.099904000	-2.034277000	3.142974000
1	1.372474000	-2.864199000	3.650635000
44	1.209284000	-0.473744000	0.137127000
7	1.890570000	1.158139000	-1.132542000
1	2.378941000	0.800885000	-1.946336000
1	2.527483000	1.770450000	-0.633954000
6	-2.849124000	-0.929341000	-1.951453000
9	-2.595300000	-2.121782000	-1.409308000
9	-3.291676000	-1.136133000	-3.193971000
9	-3.837958000	-0.368387000	-1.254417000

Complex (R)-2b_a

7	-0.013273000	-1.927938000	-0.633066000
1	-0.175314000	-2.871165000	-0.296168000
1	0.020217000	-1.974476000	-1.650470000
6	1.435159000	0.023219000	-0.589065000
1	1.704007000	-0.058840000	-1.646385000
6	1.229373000	-1.402918000	-0.058266000
1	1.065079000	-1.341961000	1.019304000
6	-3.695712000	-1.249803000	-0.110072000
6	-2.881683000	-2.098435000	0.674025000
6	-3.648430000	0.170471000	0.095624000
6	-2.006285000	-0.162639000	1.918957000
6	-2.836033000	0.699290000	1.122109000

6	-2.865901000	-3.575745000	0.388921000
1	-3.677989000	-4.076607000	0.923483000
1	-2.990604000	-3.771312000	-0.674192000
1	-1.933114000	-4.040510000	0.700842000
6	-4.586286000	-1.840648000	-1.169237000
1	-5.399691000	-1.165551000	-1.423253000
1	-4.029235000	-2.058432000	-2.083835000
1	-5.030321000	-2.772118000	-0.819852000
6	-4.452375000	1.085125000	-0.783503000
1	-5.485673000	1.151682000	-0.430247000
1	-4.031593000	2.085818000	-0.802651000
1	-4.474082000	0.725127000	-1.811094000
6	-2.886642000	2.179041000	1.399844000
1	-3.928192000	2.493609000	1.485259000
1	-2.392159000	2.435191000	2.331680000
1	-2.429315000	2.753752000	0.597081000
6	-1.067030000	0.438165000	2.928238000
1	-1.580643000	0.640020000	3.872402000
1	-0.228112000	-0.220725000	3.136125000
1	-0.653017000	1.375042000	2.564208000
7	0.151414000	0.746093000	-0.458919000
16	0.035690000	2.091975000	-1.249736000
8	0.914490000	2.190189000	-2.387322000
8	-1.334822000	2.483839000	-1.416124000
6	2.601816000	0.649535000	0.145030000
6	3.802720000	0.875458000	-0.513518000
6	2.508069000	0.953624000	1.498841000
6	4.892766000	1.402236000	0.165100000
1	3.883725000	0.641514000	-1.568700000
6	3.592500000	1.481170000	2.180279000
1	1.572843000	0.789584000	2.019095000
6	4.790176000	1.707102000	1.513997000
1	5.822305000	1.577329000	-0.362768000
1	3.503752000	1.719630000	3.233347000
1	5.638497000	2.121941000	2.044572000
6	2.430281000	-2.285474000	-0.310368000
6	3.220079000	-2.702356000	0.754405000
6	2.777636000	-2.677235000	-1.600275000
6	4.340505000	-3.492137000	0.538717000
1	2.960101000	-2.396705000	1.761652000
6	3.893754000	-3.469510000	-1.818916000
1	2.178199000	-2.357991000	-2.445686000
6	4.679724000	-3.877820000	-0.749395000
1	4.948822000	-3.804863000	1.378527000
1	4.153444000	-3.765650000	-2.827873000
1	5.553642000	-4.493961000	-0.921380000
6	-2.057575000	-1.557735000	1.723049000
6	-1.261111000	-2.507710000	2.581044000
1	-0.365933000	-2.875764000	2.074397000
1	-0.950359000	-2.046759000	3.514231000
1	-1.869316000	-3.375163000	2.837287000
44	-1.621854000	-0.596104000	-0.224676000
7	-1.694759000	-0.662850000	-2.303018000
1	-1.044907000	0.011360000	-2.697819000
1	-2.600666000	-0.338255000	-2.626982000
6	0.659257000	3.482583000	-0.157619000
9	0.249369000	3.337020000	1.103955000
9	0.173156000	4.641864000	-0.609928000
9	1.984430000	3.585748000	-0.153772000

Complex (R)-2b_a

7	-0.091154000	-1.407811000	-1.583957000
1	0.362051000	-1.372276000	-2.489444000
1	-0.167334000	-2.387706000	-1.326844000
6	-1.454368000	0.512342000	-0.811332000
1	-2.498915000	0.711490000	-0.566371000
6	-1.431596000	-0.774005000	-1.671551000
1	-1.586919000	-0.471533000	-2.705563000
6	3.199568000	-1.660840000	0.265820000
6	3.064322000	-1.106073000	-1.026695000
6	2.913984000	-0.843519000	1.409160000
6	2.507085000	1.090669000	-0.084643000
6	2.556422000	0.510847000	1.233117000
6	3.243951000	-1.988397000	-2.232123000
1	4.299062000	-2.044140000	-2.514518000

1	2.894066000	-2.999459000	-2.033891000
1	2.693552000	-1.612147000	-3.091606000
6	3.612118000	-3.098797000	0.430761000
1	4.121276000	-3.250864000	1.379979000
1	2.754190000	-3.775025000	0.396699000
1	4.301925000	-3.395098000	-0.357646000
6	2.962067000	-1.423765000	2.793723000
1	3.946987000	-1.255883000	3.239365000
1	2.216608000	-0.965051000	3.438388000
1	2.777675000	-2.495401000	2.794205000
6	2.300862000	1.349248000	2.458471000
1	3.149609000	1.266608000	3.140456000
1	2.173283000	2.399627000	2.220103000
1	1.411842000	1.012505000	2.989565000
6	2.128010000	2.538371000	-0.220396000
1	2.951704000	3.179950000	0.104089000
1	1.869913000	2.802870000	-1.239849000
1	1.260931000	2.768124000	0.394155000
7	-0.692084000	0.279350000	0.430614000
16	-1.475170000	0.231017000	1.780581000
8	-2.841886000	-0.207207000	1.676158000
8	-0.658980000	-0.316554000	2.827685000
6	-0.956203000	1.739459000	-1.574033000
6	-1.270136000	3.008114000	-1.090293000
6	-0.245261000	1.665291000	-2.765173000
6	-0.873631000	4.155897000	-1.754685000
1	-1.848895000	3.105329000	-0.184507000
6	0.151385000	2.810971000	-3.442969000
1	0.017140000	0.710041000	-3.196399000
6	-0.155585000	4.062953000	-2.939366000
1	-1.136283000	5.126133000	-1.350929000
1	0.709074000	2.716788000	-4.366791000
1	0.152542000	4.957444000	-3.466465000
6	-2.596945000	-1.691160000	-1.352790000
6	-3.847384000	-1.316040000	-1.845381000
6	-2.504335000	-2.853555000	-0.600584000
6	-4.975156000	-2.075475000	-1.587355000
1	-3.936263000	-0.412519000	-2.439330000
6	-3.634597000	-3.621480000	-0.345376000
1	-1.552853000	-3.165472000	-0.186447000
6	-4.872105000	-3.237867000	-0.833606000
1	-5.935404000	-1.763295000	-1.979720000
1	-3.540814000	-4.522693000	0.248574000
1	-5.751167000	-3.837018000	-0.630233000
6	2.810471000	0.299326000	-1.204963000
6	2.945184000	0.861225000	-2.593953000
1	2.205592000	0.458013000	-3.283955000
1	2.867609000	1.942584000	-2.617686000
1	3.929113000	0.590678000	-2.984371000
44	1.224935000	-0.765517000	0.038160000
7	0.399406000	-2.497181000	0.836102000
1	-0.402509000	-2.257957000	1.410371000
1	1.050280000	-2.892537000	1.506616000
6	-1.722419000	1.975382000	2.405285000
9	-0.629401000	2.724899000	2.264320000
9	-2.031683000	1.945675000	3.702104000
9	-2.727095000	2.590453000	1.773268000

Complex (S)-2a₆

7	-0.247416000	1.725785000	-0.883802000
1	-1.250755000	0.560480000	-2.902373000
6	1.260349000	0.144292000	0.283144000
1	0.967458000	0.563709000	1.252285000
6	1.130130000	1.256142000	-0.781973000
1	1.399483000	0.783862000	-1.733289000
6	-2.246058000	0.266411000	1.820509000
6	-2.308454000	1.599746000	1.359517000
6	-3.009331000	-0.759553000	1.160940000
6	-3.736585000	0.874080000	-0.519138000
6	-3.758569000	-0.462780000	0.012976000
6	-1.535929000	2.689456000	2.050777000
1	-2.092311000	3.058433000	2.916603000
1	-0.569290000	2.333740000	2.398634000
1	-1.348328000	3.535591000	1.394632000

6	-1.445012000	-0.110275000	3.038078000
1	-2.105127000	-0.547647000	3.790370000
1	-0.683838000	-0.853897000	2.798859000
1	-0.952964000	0.742660000	3.493759000
6	-3.048399000	-2.142019000	1.747408000
1	-3.864250000	-2.192542000	2.476226000
1	-3.214083000	-2.900744000	0.990506000
1	-2.127188000	-2.398100000	2.262162000
6	-4.564671000	-1.548202000	-0.653049000
1	-5.114759000	-2.120929000	0.093879000
1	-5.295673000	-1.141572000	-1.346521000
1	-3.928614000	-2.248281000	-1.198373000
6	-4.409598000	1.174037000	-1.831973000
1	-5.450006000	1.473283000	-1.678202000
1	-3.898853000	1.975441000	-2.360699000
1	-4.408622000	0.305586000	-2.486913000
7	0.209657000	-0.814629000	-0.119434000
16	0.191866000	-2.333673000	0.199330000
8	0.601079000	-2.720880000	1.526047000
8	-1.015090000	-2.911914000	-0.328769000
6	2.676235000	-0.370332000	0.437650000
6	3.150342000	-0.673298000	1.710064000
6	3.551799000	-0.489985000	-0.638653000
6	4.455152000	-1.099172000	1.906157000
1	2.483220000	-0.577575000	2.558689000
6	4.859785000	-0.906954000	-0.448233000
1	3.216689000	-0.260590000	-1.641247000
6	5.315999000	-1.216781000	0.824755000
1	4.800766000	-1.334736000	2.905473000
1	5.525269000	-0.990702000	-1.298940000
1	6.337873000	-1.543970000	0.973606000
6	2.075032000	2.414914000	-0.562289000
6	2.859524000	2.890696000	-1.607511000
6	2.153363000	3.061448000	0.669800000
6	3.703047000	3.979002000	-1.432238000
1	2.810641000	2.397528000	-2.572063000
6	2.996385000	4.147021000	0.852125000
1	1.551838000	2.712459000	1.500845000
6	3.775409000	4.610758000	-0.199574000
1	4.306606000	4.331813000	-2.259971000
1	3.048048000	4.631497000	1.819893000
1	4.435576000	5.457660000	-0.057552000
6	-3.090566000	1.913890000	0.193723000
6	-3.172321000	3.340374000	-0.282354000
1	-2.272777000	3.640182000	-0.825939000
1	-4.027280000	3.496186000	-0.934748000
1	-3.288373000	4.013028000	0.566907000
44	-1.663268000	0.342204000	-0.292321000
7	-1.479433000	-0.263955000	-2.356709000
1	-0.700705000	-0.909903000	-2.429769000
1	-0.328908000	2.525255000	-0.267039000
1	-2.293735000	-0.708412000	-2.765027000
6	1.464654000	-3.208076000	-0.874130000
9	1.043769000	-4.453858000	-1.110544000
9	1.604832000	-2.601692000	-2.056737000
9	2.659074000	-3.304905000	-0.303773000

Complex (S)-2a₆

7	0.585343000	1.103646000	1.546380000
1	-0.700606000	-0.785725000	2.746425000
6	-1.226794000	1.634079000	0.004777000
1	-1.444394000	2.307915000	-0.823446000
6	-0.016695000	2.181734000	0.761098000
1	-0.404836000	2.946474000	1.448166000
6	2.926026000	-0.405347000	0.170585000
6	2.749946000	-1.047247000	1.442789000
6	2.356459000	-0.990148000	-0.985879000
6	1.459085000	-2.853346000	0.355519000
6	1.673865000	-2.257706000	-0.893933000
6	3.373506000	-0.470198000	2.687696000
1	3.657464000	-1.262685000	3.377915000
1	4.274854000	0.090175000	2.451958000
1	2.691556000	0.200048000	3.217367000
6	3.744821000	0.853385000	0.114938000
1	4.807910000	0.597611000	0.082676000

1	3.517599000	1.466076000	-0.749437000
1	3.581165000	1.473699000	0.992842000
6	2.554415000	-0.380482000	-2.346323000
1	3.268718000	-0.981691000	-2.915695000
1	1.617488000	-0.352225000	-2.897405000
1	2.941274000	0.630313000	-2.296682000
6	1.262150000	-2.998030000	-2.139371000
1	1.442789000	-2.424464000	-3.039714000
1	1.845142000	-3.920910000	-2.204695000
1	0.208304000	-3.262487000	-2.133011000
6	0.741143000	-4.169064000	0.485385000
1	1.399839000	-4.905177000	0.952657000
1	-0.147372000	-4.091090000	1.112965000
1	0.426246000	-4.564499000	-0.474475000
7	-0.811790000	0.317351000	-0.563861000
16	-1.511245000	-0.172974000	-1.863535000
8	-2.398553000	0.799089000	-2.447303000
8	-0.627595000	-0.874072000	-2.750524000
6	-2.492041000	1.612295000	0.859673000
6	-3.728609000	1.818658000	0.250899000
6	-2.464471000	1.457988000	2.244812000
6	-4.901535000	1.828018000	0.991234000
1	-3.771289000	1.965264000	-0.820256000
6	-3.635048000	1.464771000	2.989612000
1	-1.508695000	1.336129000	2.738712000
6	-4.861175000	1.642008000	2.365112000
1	-5.849596000	1.986537000	0.491249000
1	-3.586460000	1.339871000	4.065007000
1	-5.775649000	1.648803000	2.945873000
6	0.982598000	2.918166000	-0.121555000
6	1.828053000	3.841502000	0.493960000
6	1.127244000	2.713400000	-1.489503000
6	2.797342000	4.523933000	-0.222769000
1	1.721440000	4.025808000	1.558321000
6	2.090655000	3.401297000	-2.216342000
1	0.495252000	2.002272000	-2.003194000
6	2.934009000	4.304024000	-1.587539000
1	3.441069000	5.235424000	0.280830000
1	2.183802000	3.222284000	-3.281022000
1	3.686265000	4.837994000	-2.155268000
6	1.961831000	-2.214583000	1.539728000
6	1.701272000	-2.817996000	2.892809000
1	1.558406000	-2.048120000	3.649206000
1	0.819301000	-3.453194000	2.894415000
1	2.550351000	-3.435435000	3.198903000
44	0.788818000	-0.694478000	0.550951000
7	-0.870279000	-1.237546000	1.854385000
1	-1.757155000	-0.886918000	1.510703000
1	1.500477000	1.430646000	1.835105000
1	-0.977981000	-2.232828000	2.014382000
6	-2.664902000	-1.553008000	-1.379759000
9	-3.287007000	-2.032810000	-2.458418000
9	-2.002271000	-2.564640000	-0.809609000
9	-3.598876000	-1.149679000	-0.518447000

Complex (S)-2b₁

7	-0.127168000	1.510055000	-1.102473000
1	-0.351406000	1.478741000	-2.093861000
6	1.193782000	0.101391000	0.379624000
1	0.829107000	0.728336000	1.199900000
6	1.246791000	0.994167000	-0.874203000
1	1.483114000	0.356813000	-1.724280000
6	-2.135790000	0.554594000	1.920663000
6	-2.168247000	1.813311000	1.292153000
6	-2.915661000	-0.529910000	1.386995000
6	-3.754342000	0.942945000	-0.396393000
6	-3.739811000	-0.339757000	0.258014000
6	-1.316925000	2.948966000	1.791354000
1	-1.842055000	3.508972000	2.570021000
1	-0.380157000	2.590527000	2.211323000
1	-1.069822000	3.649250000	0.996580000
6	-1.292516000	0.301921000	3.141730000
1	-1.893544000	-0.169301000	3.920795000
1	-0.462418000	-0.371645000	2.917988000
1	-0.884931000	1.217809000	3.558385000

6	-2.861164000	-1.860127000	2.084293000
1	-3.602088000	-1.874730000	2.889851000
1	-3.059549000	-2.684382000	1.409921000
1	-1.885129000	-2.041468000	2.525544000
6	-4.602132000	-1.449705000	-0.282339000
1	-4.760032000	-2.234133000	0.451871000
1	-5.583393000	-1.063275000	-0.558025000
1	-4.160899000	-1.905941000	-1.171382000
6	-4.543870000	1.130942000	-1.662531000
1	-5.503955000	1.610068000	-1.452066000
1	-4.001424000	1.749444000	-2.375036000
1	-4.746636000	0.182242000	-2.151935000
7	0.111980000	-0.867963000	0.118715000
16	0.233109000	-2.414277000	0.143549000
8	1.036061000	-2.955120000	1.206398000
8	-1.053934000	-3.003600000	-0.092143000
6	2.551735000	-0.404728000	0.816082000
6	2.834657000	-0.464469000	2.176700000
6	3.547796000	-0.756085000	-0.086197000
6	4.074838000	-0.882209000	2.630039000
1	2.066915000	-0.183117000	2.888964000
6	4.792320000	-1.174951000	0.360744000
1	3.360815000	-0.707304000	-1.150971000
6	5.059379000	-1.241415000	1.719567000
1	4.274889000	-0.925368000	3.693725000
1	5.556354000	-1.446758000	-0.357274000
1	6.031877000	-1.566704000	2.068376000
6	2.252729000	2.117208000	-0.814308000
6	3.178670000	2.278594000	-1.838493000
6	2.263919000	3.018128000	0.247489000
6	4.099992000	3.315463000	-1.804918000
1	3.181189000	1.580864000	-2.668287000
6	3.183163000	4.054931000	0.284997000
1	1.552497000	2.909840000	1.057375000
6	4.105238000	4.206120000	-0.741702000
1	4.816295000	3.425373000	-2.609909000
1	3.182672000	4.744173000	1.120567000
1	4.825340000	5.014493000	-0.711536000
6	-3.004665000	2.015624000	0.137350000
6	-3.061119000	3.384029000	-0.492627000
1	-2.156112000	3.620269000	-1.056491000
1	-3.906291000	3.482589000	-1.167503000
1	-3.171333000	4.143392000	0.282254000
44	-1.691504000	0.313839000	-0.249742000
7	-1.703014000	-0.372914000	-2.210333000
1	-1.087949000	-1.176472000	-2.285165000
1	-0.185605000	2.476462000	-0.800942000
1	-2.619644000	-0.741087000	-2.445870000
6	1.176993000	-2.999389000	-1.389395000
9	0.169069000	-4.108353000	-1.876760000
9	1.155023000	-2.080258000	-2.362732000
9	2.450979000	-3.280997000	-1.128790000

Complex (S)-2b₂

7	0.474213000	1.150079000	1.574430000
1	-0.082565000	0.771912000	2.339617000
6	-1.405174000	1.425606000	0.001624000
1	-1.616663000	2.060489000	-0.857402000
6	-0.295439000	2.136815000	0.787029000
1	-0.777512000	2.831719000	1.478866000
6	3.034081000	-0.072106000	-0.195073000
6	3.016005000	-0.538586000	1.161786000
6	2.400575000	-0.840027000	-1.186335000
6	1.948943000	-2.630292000	0.453028000
6	1.887809000	-2.149360000	-0.867810000
6	3.563142000	0.342628000	2.252471000
1	4.605992000	0.087399000	2.458735000
1	3.533631000	1.394155000	1.975125000
1	3.000384000	0.225895000	3.177108000
6	3.770170000	1.204232000	-0.504295000
1	4.759091000	1.165440000	-0.043238000
1	3.915358000	1.345475000	-1.570395000
1	3.261676000	2.085452000	-0.115250000
6	2.311076000	-0.336423000	-2.599707000
1	3.125783000	-0.749429000	-3.201671000

1	1.366710000	-0.625962000	-3.050443000
1	2.372491000	0.746580000	-2.644311000
6	1.409492000	-3.085870000	-1.946134000
1	1.520541000	-2.660181000	-2.937069000
1	2.004258000	-4.001839000	-1.905620000
1	0.363750000	-3.356095000	-1.824220000
6	1.404480000	-3.990963000	0.780012000
1	2.188295000	-4.744582000	0.658344000
1	1.048375000	-4.051132000	1.806205000
1	0.578437000	-4.258690000	0.126377000
7	-0.868558000	0.132260000	-0.494779000
16	-1.618671000	-0.489381000	-1.711849000
8	-2.570210000	0.407225000	-2.314646000
8	-0.752000000	-1.226752000	-2.585563000
6	-2.718163000	1.377270000	0.775196000
6	-3.830116000	1.992290000	0.206179000
6	-2.862497000	0.794530000	2.031904000
6	-5.053388000	2.017928000	0.860597000
1	-3.739020000	2.447415000	-0.772551000
6	-4.082566000	0.818394000	2.690544000
1	-2.030508000	0.286909000	2.501602000
6	-5.184811000	1.428112000	2.108026000
1	-5.903983000	2.497134000	0.391080000
1	-4.171875000	0.352793000	3.664827000
1	-6.137820000	1.441954000	2.622747000
6	0.652586000	2.959247000	-0.064667000
6	1.391414000	3.960969000	0.561770000
6	0.817263000	2.768162000	-1.431025000
6	2.275107000	4.751955000	-0.155717000
1	1.262998000	4.131243000	1.625714000
6	1.694465000	3.563832000	-2.154343000
1	0.270422000	1.987874000	-1.942674000
6	2.427312000	4.555769000	-1.521264000
1	2.836371000	5.528289000	0.349644000
1	1.808833000	3.399704000	-3.218905000
1	3.111164000	5.175172000	-2.088324000
6	2.529035000	-1.827038000	1.487579000
6	2.628071000	-2.359045000	2.892300000
1	1.697002000	-2.219338000	3.447225000
1	2.851541000	-3.424957000	2.879507000
1	3.425204000	-1.870068000	3.447117000
44	0.958435000	-0.663774000	0.545598000
7	-0.406130000	-1.350032000	1.955857000
1	-1.318294000	-1.432315000	1.519765000
1	1.275143000	1.613316000	1.989627000
1	-0.176701000	-2.301745000	2.222370000
6	-2.701296000	-1.867496000	-1.082161000
9	-3.377718000	-2.407741000	-2.099579000
9	-1.976323000	-2.837097000	-0.518872000
9	-3.588775000	-1.445938000	-0.184017000

Complex 3

7	0.188623000	1.043432000	-1.620560000
1	-0.050591000	1.640641000	-2.398047000
6	1.614537000	0.905900000	-1.424741000
6	1.808571000	-0.325602000	-0.517468000
1	2.101549000	0.694028000	-2.380649000
6	2.294151000	2.135844000	-0.839702000
1	2.786022000	-0.256482000	-0.041636000
7	0.750986000	-0.236765000	0.497369000
6	1.774560000	-1.615055000	-1.322956000
6	3.638683000	2.361554000	-1.122941000
6	1.637033000	3.016835000	0.009997000
6	2.851542000	-1.894380000	-2.161703000
6	0.724968000	-2.522327000	-1.270673000
6	4.314151000	3.436370000	-0.566333000
1	4.163549000	1.683338000	-1.787835000
6	2.309744000	4.093035000	0.572792000
1	0.590372000	2.856609000	0.234830000
6	2.871830000	-3.040700000	-2.939504000
1	3.688498000	-1.205360000	-2.202348000
6	0.739249000	-3.671740000	-2.050022000
1	-0.110138000	-2.336976000	-0.609988000
6	3.649955000	4.306872000	0.287657000
1	5.360031000	3.595931000	-0.799759000
1	1.783205000	4.765929000	1.239080000

6	1.809565000	-3.934330000	-2.890195000
1	3.720755000	-3.240282000	-3.582188000
1	-0.091625000	-4.365062000	-1.994363000
1	4.174338000	5.147189000	0.725972000
1	1.822236000	-4.831769000	-3.496485000
16	1.145382000	-0.371894000	2.005868000
8	2.515369000	-0.033382000	2.269635000
8	0.124739000	0.153551000	2.862721000
77	-1.109794000	0.400451000	-0.345444000
6	-2.920645000	-0.774920000	-0.416998000
6	-3.011857000	0.374702000	-1.302001000
6	-2.814364000	-0.300839000	0.921465000
6	-3.037694000	-2.197174000	-0.845001000
6	-2.897205000	1.546450000	-0.502230000
6	-3.232401000	0.317218000	-2.775309000
6	-2.738257000	1.120620000	0.878180000
6	-2.833382000	-1.128260000	2.161522000
1	-4.091108000	-2.488688000	-0.878240000
1	-2.617068000	-2.345876000	-1.839047000
1	-2.524009000	-2.864244000	-0.153593000
6	-2.997076000	2.959398000	-0.965867000
1	-2.728644000	-0.543360000	-3.215206000
1	-4.300496000	0.231266000	-2.990882000
1	-2.859136000	1.214921000	-3.266859000
6	-2.653189000	2.024079000	2.059038000
1	-3.821088000	-1.059111000	2.625245000
1	-2.639674000	-2.176699000	1.944872000
1	-2.093256000	-0.783218000	2.880398000
1	-4.025720000	3.313120000	-0.857292000
1	-2.353923000	3.613725000	-0.377827000
1	-2.715970000	3.056079000	-2.013838000
1	-3.659429000	2.275869000	2.406149000
1	-2.115710000	1.546040000	2.875843000
1	-2.141681000	2.954136000	1.811438000
6	1.117110000	-2.188345000	2.388646000
9	-0.056225000	-2.735596000	2.072700000
9	1.328273000	-2.391438000	3.689178000
9	2.068074000	-2.830226000	1.711134000

Complex (R)-3a.

7	0.068923000	-1.874214000	-0.667367000
1	-0.125545000	-2.794386000	-0.286006000
1	-2.441943000	-1.094382000	-2.684401000
6	1.266310000	-1.382357000	-0.015273000
6	1.522629000	0.040406000	-0.542943000
1	1.142039000	-1.298452000	1.076841000
6	2.473144000	-2.266407000	-0.253748000
1	1.864303000	-0.053034000	-1.576156000
7	0.215422000	0.740601000	-0.526699000
6	2.607687000	0.719249000	0.259197000
6	3.298613000	-2.635613000	0.802046000
6	2.792584000	-2.707947000	-1.535422000
6	3.846239000	0.973608000	-0.314855000
6	2.406625000	1.052264000	1.595090000
6	4.421588000	-3.424012000	0.587477000
1	3.062086000	-2.295431000	1.804367000
6	3.911665000	-3.495728000	-1.755228000
1	2.152380000	-2.430358000	-2.364152000
6	4.866930000	1.551623000	0.427560000
1	4.011742000	0.719055000	-1.355456000
6	3.420676000	1.631711000	2.340026000
1	1.440731000	0.869631000	2.049042000
6	4.731712000	-3.856413000	-0.693040000
1	5.054210000	-3.699836000	1.422669000
1	4.147445000	-3.829000000	-2.758990000
6	4.656590000	1.882974000	1.757587000
1	5.826467000	1.746034000	-0.036205000
1	3.247091000	1.890950000	3.377609000
1	5.606720000	-4.471522000	-0.864653000
1	5.450003000	2.338074000	2.337880000
16	0.116437000	2.078621000	-1.331951000
8	1.117870000	2.223566000	-2.354816000
8	-1.248635000	2.381371000	-1.671162000
77	-1.490487000	-0.594041000	-0.199193000
6	-2.016575000	-0.207670000	1.865756000

6	-2.167386000	-1.595516000	1.579696000
6	-2.951641000	0.530776000	1.033099000
6	-1.166640000	0.385647000	2.937470000
6	-3.138781000	-1.732997000	0.521928000
6	-1.454191000	-2.714378000	2.259585000
6	-3.633521000	-0.403122000	0.221167000
6	-3.207274000	1.997663000	1.110001000
1	-1.751294000	0.516451000	3.852221000
1	-0.316918000	-0.255562000	3.171032000
1	-0.785785000	1.362341000	2.642189000
6	-3.688118000	-3.014269000	-0.012614000
1	-0.459487000	-2.411113000	2.586036000
1	-2.016245000	-3.034075000	3.140781000
1	-1.346564000	-3.576007000	1.601075000
6	-4.695741000	-0.095876000	-0.779461000
1	-3.968642000	2.205045000	1.867596000
1	-2.306324000	2.541754000	1.384821000
1	-3.557470000	2.392244000	0.157816000
1	-4.539665000	-3.348482000	0.586675000
1	-4.030083000	-2.899234000	-1.041434000
1	-2.936344000	-3.803600000	0.003170000
1	-5.682204000	-0.197347000	-0.319425000
1	-4.601797000	0.920611000	-1.160026000
1	-4.654645000	-0.783301000	-1.624920000
6	0.526626000	3.498614000	-0.183267000
9	0.022302000	4.629421000	-0.682145000
9	0.000409000	3.317667000	1.028706000
9	1.836126000	3.673056000	-0.043643000
7	-1.645966000	-0.569304000	-2.339766000
1	-1.711323000	0.375532000	-2.705752000
1	-0.799003000	-1.013161000	-2.687776000

Complex (R)-3a.

7	0.103648000	-1.929602000	-0.562701000
1	-0.058633000	-2.869491000	-0.216324000
1	0.127246000	-1.963985000	-1.584448000
6	1.342142000	-1.387304000	0.008640000
6	1.532051000	0.040316000	-0.528983000
1	1.181474000	-1.333499000	1.086192000
6	2.554733000	-2.250361000	-0.251551000
1	1.892558000	-0.043184000	-1.556897000
7	0.217054000	0.718245000	-0.527920000
6	2.597511000	0.728573000	0.296066000
6	3.364523000	-2.643528000	0.806936000
6	2.896192000	-2.640415000	-1.543707000
6	3.839204000	1.011269000	-0.255148000
6	2.361684000	1.044955000	1.629907000
6	4.499353000	-3.410220000	0.582663000
1	3.108872000	-2.337967000	1.815223000
6	4.025868000	-3.410670000	-1.770182000
1	2.281593000	-2.336487000	-2.383905000
6	4.832371000	1.605475000	0.511536000
1	4.028247000	0.769510000	-1.294563000
6	3.348612000	1.639814000	2.397914000
1	1.390309000	0.837526000	2.063030000
6	4.831909000	-3.796154000	-0.707006000
1	5.123950000	-3.704575000	1.417104000
1	4.281030000	-3.706383000	-2.780386000
6	4.589102000	1.921816000	1.839454000
1	5.795995000	1.824721000	0.068096000
1	3.150447000	1.887757000	3.433721000
1	5.717076000	-4.394124000	-0.885533000
1	5.361305000	2.389556000	2.437926000
16	0.125745000	2.046482000	-1.357041000
8	1.137339000	2.169726000	-2.372693000
8	-1.232211000	2.358454000	-1.697889000
77	-1.512118000	-0.610782000	-0.203004000
6	-2.115025000	-0.122409000	1.862223000
6	-2.251151000	-1.513131000	1.631799000
6	-2.972626000	0.569691000	0.914721000
6	-1.315428000	0.536489000	2.935286000
6	-3.175111000	-1.710838000	0.530909000
6	-1.578080000	-2.611125000	2.384741000
6	-3.643399000	-0.406621000	0.129584000
6	-3.225640000	2.038348000	0.894006000

1	-1.949931000	0.767052000	3.795540000
1	-0.504639000	-0.104987000	3.280174000
1	-0.881248000	1.471180000	2.583120000
6	-3.698097000	-3.023428000	0.049098000
1	-0.661540000	-2.266895000	2.862762000
1	-2.242757000	-2.991876000	3.164459000
1	-1.329602000	-3.446713000	1.728967000
6	-4.670089000	-0.136374000	-0.916471000
1	-4.025558000	2.282211000	1.599315000
1	-2.339529000	2.597969000	1.184901000
1	-3.525305000	2.377153000	-0.095465000
1	-4.585247000	-3.317893000	0.616675000
1	-3.974482000	-2.975191000	-1.004305000
1	-2.951906000	-3.810029000	0.163455000
1	-5.662013000	-0.088552000	-0.459276000
1	-4.481561000	0.810756000	-1.420742000
1	-4.686732000	-0.924511000	-1.668906000
6	0.543108000	3.477839000	-0.221505000
9	0.048606000	4.604638000	-0.739406000
9	0.007699000	3.318794000	0.990322000
9	1.852504000	3.650198000	-0.073402000
7	-1.555548000	-0.765109000	-2.289999000
1	-2.454496000	-1.151141000	-2.563908000
1	-1.562446000	0.173688000	-2.676284000

Complex (R)-3a.

7	0.713242000	0.964472000	1.565550000
1	0.379903000	0.475977000	2.387812000
1	2.530383000	1.752750000	-0.470940000
6	-0.299102000	1.945406000	1.204857000
6	-1.446803000	1.271359000	0.416423000
1	-0.741444000	2.334996000	2.128294000
6	0.319975000	3.160849000	0.517912000
1	-2.032048000	2.022827000	-0.110904000
7	-0.813433000	0.362824000	-0.554595000
6	-2.392797000	0.594380000	1.388717000
6	-0.171539000	3.743297000	-0.645670000
6	1.446998000	3.734725000	1.108492000
6	-3.292143000	1.381863000	2.105139000
6	-2.376058000	-0.770404000	1.624074000
6	0.455765000	4.847578000	-1.214286000
1	-1.035062000	3.330654000	-1.149166000
6	2.069477000	4.838849000	0.551616000
1	1.844587000	3.286301000	2.010450000
6	-4.144797000	0.815747000	3.039018000
1	-3.325469000	2.451425000	1.926017000
6	-3.226075000	-1.344784000	2.559780000
1	-1.700204000	-1.386462000	1.054020000
6	1.578669000	5.399425000	-0.622011000
1	0.059283000	5.271045000	-2.129437000
1	2.942798000	5.263901000	1.032250000
6	-4.112499000	-0.553688000	3.273763000
1	-4.840635000	1.443468000	3.582774000
1	-3.195979000	-2.415439000	2.725669000
1	2.067223000	6.258229000	-1.065896000
1	-4.779633000	-0.998058000	4.002257000
16	-1.400371000	0.282208000	-1.993800000
8	-2.082618000	1.478142000	-2.418600000
8	-0.473702000	-0.328771000	-2.903272000
77	1.126620000	-0.475137000	0.124962000
6	0.869663000	-2.602003000	0.646431000
6	1.776106000	-1.967013000	1.542961000
6	1.432147000	-2.530263000	-0.689175000
6	-0.303278000	-3.440790000	1.025713000
6	2.885202000	-1.457675000	0.777199000
6	1.625794000	-1.867458000	3.022302000
6	2.671369000	-1.859682000	-0.600215000
6	0.866544000	-3.193106000	-1.898681000
1	0.010420000	-4.487724000	1.069852000
1	-0.697140000	-3.170513000	2.003954000
1	-1.107277000	-3.370307000	0.294992000
6	4.114175000	-0.813188000	1.327078000
1	0.577053000	-1.892807000	3.318107000
1	2.134957000	-2.705551000	3.504874000
1	2.065297000	-0.945294000	3.402350000

6	3.617624000	-1.613237000	-1.725818000
1	1.215063000	-4.228806000	-1.952244000
1	-0.220750000	-3.206057000	-1.871193000
1	1.169805000	-2.683127000	-2.811129000
1	4.852753000	-1.568096000	1.610293000
1	4.575706000	-0.153129000	0.592250000
1	3.881695000	-0.218277000	2.210320000
1	4.311373000	-2.453053000	-1.815645000
1	3.091299000	-1.510364000	-2.674998000
1	4.213777000	-0.715145000	-1.560533000
6	-2.806168000	-0.934552000	-1.976303000
9	-3.251912000	-1.140078000	-3.217406000
9	-2.434120000	-2.115263000	-1.478439000
9	-3.825973000	-0.484478000	-1.246216000
7	1.931354000	1.165524000	-1.041979000
1	2.483476000	0.816905000	-1.817872000
1	1.215957000	1.769791000	-1.433040000

Complex (R)-3a_i

7	-0.249598000	1.267029000	1.524157000
1	-0.073788000	0.802524000	2.409225000
1	-0.008788000	2.244458000	1.649926000
6	-1.695706000	1.146970000	1.196041000
6	-1.888688000	-0.185572000	0.452056000
1	-2.238380000	1.071984000	2.140024000
6	-2.217749000	2.400415000	0.517282000
1	-2.867465000	-0.159660000	-0.027061000
7	-0.834360000	-0.316709000	-0.560994000
6	-1.931657000	-1.318451000	1.469414000
6	-2.823333000	2.405716000	-0.732153000
6	-2.123484000	3.604748000	1.213971000
6	-3.039895000	-1.423174000	2.307970000
6	-0.907943000	-2.240624000	1.605404000
6	-3.297282000	3.589869000	-1.283066000
1	-2.920542000	1.493331000	-1.303455000
6	-2.592393000	4.786529000	0.666596000
1	-1.680829000	3.622191000	2.204514000
6	-3.112840000	-2.421479000	3.265474000
1	-3.858570000	-0.718804000	2.204573000
6	-0.973568000	-3.242390000	2.564834000
1	-0.060437000	-2.179211000	0.942595000
6	-3.179308000	4.783925000	-0.591817000
1	-3.757131000	3.571762000	-2.263626000
1	-2.504690000	5.710309000	1.225216000
6	-2.074281000	-3.334866000	3.401441000
1	-3.984949000	-2.491270000	3.904260000
1	-0.161548000	-3.954790000	2.651187000
1	-3.546326000	5.705991000	-1.025367000
1	-2.130634000	-4.117183000	4.148356000
16	-1.232384000	-0.813988000	-1.983628000
8	-2.596673000	-0.518347000	-2.342673000
8	-0.199762000	-0.556874000	-2.942127000
77	1.153925000	0.510586000	0.054103000
6	2.537584000	-1.207988000	0.506363000
6	2.661711000	-0.198720000	1.483391000
6	2.826407000	-0.616021000	-0.787776000
6	2.364902000	-2.669048000	0.749018000
6	3.051233000	1.036783000	0.822109000
6	2.465635000	-0.358306000	2.953212000
6	3.204852000	0.740664000	-0.576615000
6	2.916118000	-1.370561000	-2.070268000
1	3.342704000	-3.156398000	0.694883000
1	1.949088000	-2.871086000	1.734801000
1	1.727392000	-3.135508000	0.000315000
6	3.402657000	2.321978000	1.494225000
1	1.776487000	-1.172740000	3.177047000
1	3.419698000	-0.575699000	3.440434000
1	2.071630000	0.554951000	3.402007000
6	3.688874000	1.690585000	-1.617037000
1	3.898757000	-1.844191000	-2.154572000
1	2.158950000	-2.150487000	-2.121999000
1	2.777741000	-0.715279000	-2.928214000
1	4.469333000	2.354535000	1.732112000
1	3.171123000	3.174133000	0.855042000
1	2.849350000	2.442509000	2.426081000

1	4.777729000	1.628431000	-1.689399000
1	3.272496000	1.455307000	-2.596244000
1	3.428580000	2.719544000	-1.369895000
6	-1.284046000	-2.672510000	-1.954902000
9	-1.533814000	-3.141498000	-3.178693000
9	-0.124945000	-3.195463000	-1.550469000
9	-2.242206000	-3.120291000	-1.143302000
7	0.568191000	2.221617000	-0.959193000
1	1.157899000	2.315764000	-1.779794000
1	-0.365259000	2.105924000	-1.339114000

Complex (S)-3a_i

7	-0.182743000	1.776126000	-0.753027000
1	-0.786097000	0.524648000	-2.873658000
6	1.399164000	0.141169000	0.276715000
1	1.248995000	0.497777000	1.301102000
6	1.198524000	1.334977000	-0.690375000
1	1.485336000	0.964825000	-1.680216000
7	0.316690000	-0.811478000	-0.056367000
16	0.277325000	-2.219550000	0.634052000
8	0.830402000	-2.264361000	1.961759000
8	-0.987611000	-2.855757000	0.393814000
6	2.817878000	-0.369684000	0.163578000
6	3.632467000	-0.397838000	1.289471000
6	3.367543000	-0.735124000	-1.063119000
6	4.961609000	-0.785088000	1.199393000
1	3.218035000	-0.113542000	2.249572000
6	4.694865000	-1.119668000	-1.159526000
1	2.752025000	-0.733203000	-1.953985000
6	5.498040000	-1.146056000	-0.027556000
1	5.578705000	-0.802804000	2.089587000
1	5.104065000	-1.403104000	-2.121783000
1	6.535816000	-1.447385000	-0.101899000
6	2.128307000	2.475689000	-0.341878000
6	3.114025000	2.895154000	-1.227214000
6	2.012005000	3.133051000	0.881932000
6	3.965622000	3.943045000	-0.902928000
1	3.220007000	2.390589000	-2.180845000
6	2.858669000	4.179804000	1.210796000
1	1.252422000	2.819550000	1.589997000
6	3.840730000	4.588784000	0.317793000
1	4.728938000	4.253892000	-1.606087000
1	2.754818000	4.676199000	2.168236000
1	4.504435000	5.405525000	0.574043000
7	-1.177573000	-0.271680000	-2.379373000
1	-0.487232000	-1.015889000	-2.387508000
1	-0.309015000	2.512520000	-0.069323000
1	-1.993120000	-0.590279000	-2.890831000
6	1.393370000	-3.397075000	-0.314005000
9	0.950401000	-4.642542000	-0.123178000
9	1.355159000	-3.153168000	-1.626371000
9	2.657512000	-3.370124000	0.086998000
77	-1.582259000	0.325196000	-0.331097000
6	-3.504873000	-0.614041000	0.294093000
6	-3.716290000	0.562744000	-0.506687000
6	-2.765482000	-0.206243000	1.445432000
6	-4.070422000	-1.968415000	0.024781000
6	-3.142064000	1.690273000	0.164060000
6	-4.477700000	0.607418000	-1.788325000
6	-2.522290000	1.207839000	1.377460000
6	-2.395122000	-1.060563000	2.608774000
1	-5.093379000	-2.040310000	0.405768000
1	-4.099278000	-2.179222000	-1.044950000
1	-3.470098000	-2.742427000	0.497615000
6	-3.221397000	3.115669000	-0.265334000
1	-4.381880000	-0.328816000	-2.338513000
1	-5.539853000	0.764861000	-1.583916000
1	-4.133385000	1.419440000	-2.428191000
6	-1.891147000	2.051790000	2.433306000
1	-3.119804000	-0.894672000	3.410913000
1	-2.397810000	-2.115885000	2.351144000
1	-1.407922000	-0.807105000	2.993569000
1	-4.099259000	3.592302000	0.178767000
1	-2.341580000	3.674800000	0.054301000
1	-3.299472000	3.202058000	-1.348669000

1	-2.646344000	2.431672000	3.126965000
1	-1.161077000	1.482553000	3.008632000
1	-1.381034000	2.911097000	1.995687000

Complex (S)-3a₁

7	-0.086240000	1.874490000	-0.477680000
1	-0.282751000	2.409068000	-1.318133000
6	1.429981000	0.121814000	0.345241000
1	1.357093000	0.446109000	1.388668000
6	1.288839000	1.358422000	-0.556801000
1	1.420038000	1.034505000	-1.587486000
7	0.297884000	-0.776805000	0.036355000
16	0.251956000	-2.183642000	0.726387000
8	0.888874000	-2.237588000	2.016154000
8	-1.046282000	-2.773162000	0.573965000
6	2.819049000	-0.445499000	0.128637000
6	3.699292000	-0.551679000	1.196817000
6	3.262460000	-0.794118000	-1.143847000
6	4.998149000	-0.999912000	1.003477000
1	3.363175000	-0.281743000	2.190832000
6	4.558493000	-1.239660000	-1.342409000
1	2.587546000	-0.729408000	-1.988818000
6	5.431877000	-1.343179000	-0.268086000
1	5.671859000	-1.079023000	1.847951000
1	4.887756000	-1.509434000	-2.338486000
1	6.445876000	-1.691419000	-0.422327000
6	2.307765000	2.426283000	-0.233848000
6	3.249373000	2.811126000	-1.179682000
6	2.321774000	3.037369000	1.017912000
6	4.190859000	3.786974000	-0.883430000
1	3.249387000	2.337141000	-2.154274000
6	3.258763000	4.013658000	1.316303000
1	1.599307000	2.744673000	1.773339000
6	4.197729000	4.390277000	0.365153000
1	4.920752000	4.074590000	-1.630077000
1	3.259985000	4.478003000	2.294812000
1	4.932612000	5.150821000	0.598317000
7	-1.062463000	0.062076000	-2.322846000
1	-0.396983000	-0.705106000	-2.353004000
1	-0.179584000	2.509614000	0.308482000
1	-1.866178000	-0.272406000	-2.845270000
6	1.260918000	-3.405443000	-0.285134000
9	0.782875000	-4.633013000	-0.064752000
9	1.153451000	-3.158183000	-1.591062000
9	2.548214000	-3.428436000	0.039097000
77	-1.596437000	0.360253000	-0.330244000
6	-3.480076000	-0.610352000	0.157742000
6	-3.708087000	0.550464000	-0.657973000
6	-2.888451000	-0.148708000	1.398266000
6	-3.999660000	-1.980330000	-0.123956000
6	-3.211305000	1.694827000	0.041824000
6	-4.383828000	0.561577000	-1.986424000
6	-2.724631000	1.254732000	1.335911000
6	-2.605560000	-0.984308000	2.600891000
1	-5.055630000	-2.048931000	0.154113000
1	-3.915248000	-2.223085000	-1.183488000
1	-3.445145000	-2.731182000	0.432531000
6	-3.282436000	3.112736000	-0.417581000
1	-4.246339000	-0.385186000	-2.508125000
1	-5.457523000	0.717685000	-1.853158000
1	-4.002875000	1.360635000	-2.621952000
6	-2.209837000	2.139543000	2.422387000
1	-3.424022000	-0.866674000	3.316682000
1	-2.517379000	-2.035845000	2.345150000
1	-1.683931000	-0.678113000	3.095775000
1	-4.210043000	3.574783000	-0.069757000
1	-2.452814000	3.700083000	-0.022267000
1	-3.257608000	3.179325000	-1.504943000
1	-3.035774000	2.525584000	3.026164000
1	-1.534284000	1.598378000	3.084845000
1	-1.671515000	3.000041000	2.020899000

Complex (S)-3a₁

7	-0.466668000	1.171910000	-1.526478000
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1	0.651282000	-0.719127000	-2.765945000
6	1.309265000	1.586939000	0.088296000
1	1.512397000	2.209754000	0.958529000
6	0.134735000	2.201424000	-0.678215000
1	0.563031000	2.981537000	-1.321180000
7	0.856084000	0.248176000	0.569532000
16	1.505457000	-0.337819000	1.860032000
8	2.398881000	0.580172000	2.513510000
8	0.578898000	-1.062089000	2.682317000
6	2.598831000	1.564726000	-0.724863000
6	3.814854000	1.765517000	-0.075357000
6	2.615292000	1.394256000	-2.107988000
6	5.012575000	1.754636000	-0.775189000
1	3.822251000	1.921297000	0.995495000
6	3.810741000	1.380187000	-2.811722000
1	1.674851000	1.283297000	-2.632445000
6	5.016679000	1.551633000	-2.147132000
1	5.944901000	1.908309000	-0.245117000
1	3.798202000	1.243132000	-3.886633000
1	5.950433000	1.540623000	-2.696224000
6	-0.884687000	2.914361000	0.199248000
6	-1.696484000	3.872823000	-0.407486000
6	-1.090945000	2.641933000	1.547199000
6	-2.690699000	4.528897000	0.299606000
1	-1.542602000	4.106160000	-1.456235000
6	-2.081479000	3.301606000	2.263847000
1	-0.487230000	1.899790000	2.051777000
6	-2.888673000	4.243051000	1.644356000
1	-3.306698000	5.269975000	-0.195817000
1	-2.223616000	3.071310000	3.313075000
1	-3.661240000	4.755435000	2.204553000
7	0.790409000	-1.240200000	-1.906300000
1	1.714083000	-1.000477000	-1.561527000
1	-1.359236000	1.531571000	-1.845390000
1	0.790990000	-2.231288000	-2.121628000
6	2.632609000	-1.717829000	1.319320000
9	3.230229000	-2.261067000	2.380762000
9	1.953228000	-2.683929000	0.694896000
9	3.583598000	-1.292016000	0.489151000
77	-0.794733000	-0.629963000	-0.549168000
6	-1.961330000	-2.452880000	-0.856789000
6	-2.632037000	-1.294268000	-1.393901000
6	-1.811035000	-2.291915000	0.544611000
6	-1.534711000	-3.640998000	-1.650015000
6	-2.933931000	-0.424437000	-0.282338000
6	-3.083122000	-1.104566000	-2.804117000
6	-2.400354000	-1.018116000	0.897533000
6	-1.328247000	-3.322552000	1.508756000
1	-2.351015000	-4.366677000	-1.691768000
1	-1.284134000	-3.368773000	-2.675554000
1	-0.671845000	-4.133277000	-1.201588000
6	-3.737994000	0.827820000	-0.363289000
1	-2.410414000	-1.600063000	-3.504512000
1	-4.084856000	-1.518148000	-2.949358000
1	-3.116946000	-0.046599000	-3.066080000
6	-2.584870000	-0.521125000	2.290030000
1	-2.174301000	-3.911796000	1.875370000
1	-0.622393000	-4.008703000	1.041764000
1	-0.836257000	-2.860868000	2.361139000
1	-4.801778000	0.584827000	-0.292517000
1	-3.490230000	1.517645000	0.441552000
1	-3.579650000	1.342369000	-1.310977000
1	-3.407845000	-1.066926000	2.760670000
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1	-2.830854000	0.538617000	2.305276000

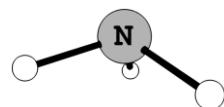
Complex (S)-3a₁

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1	1.702875000	1.971205000	0.971858000
6	0.426060000	2.157503000	-0.702041000
1	0.944462000	2.859641000	-1.358413000
7	0.910936000	0.083540000	0.500813000
16	1.555218000	-0.591243000	1.752729000

8	2.564678000	0.227328000	2.369289000
8	0.597567000	-1.231094000	2.608403000
6	2.818197000	1.313752000	-0.666930000
6	3.904723000	1.999197000	-0.132038000
6	2.990124000	0.637214000	-1.871222000
6	5.133529000	2.011612000	-0.776741000
1	3.789914000	2.522159000	0.810265000
6	4.216338000	0.647605000	-2.518843000
1	2.171335000	0.072996000	-2.300419000
6	5.293613000	1.333956000	-1.975525000
1	5.966600000	2.546131000	-0.336414000
1	4.331325000	0.110308000	-3.452767000
1	6.251590000	1.336180000	-2.481165000
6	-0.530942000	2.969645000	0.148489000
6	-1.223308000	4.010974000	-0.465568000
6	-0.758958000	2.722135000	1.496117000
6	-2.126863000	4.784329000	0.245009000
1	-1.046139000	4.221881000	-1.515151000
6	-1.653870000	3.502792000	2.214677000
1	-0.251222000	1.908811000	1.996476000
6	-2.343046000	4.532469000	1.592839000
1	-2.653827000	5.590399000	-0.250594000
1	-1.817511000	3.296086000	3.265180000
1	-3.042472000	5.138452000	2.155416000
7	0.383538000	-1.323550000	-2.007980000
1	1.228810000	-1.666670000	-1.563645000
1	-1.142955000	1.700066000	-1.945232000
1	-0.028824000	-2.150686000	-2.427041000
6	2.522239000	-2.058510000	1.146146000
9	3.142392000	-2.643148000	2.173489000
9	1.729214000	-2.968703000	0.578806000
9	3.447147000	-1.706562000	0.256532000
77	-0.925686000	-0.591387000	-0.551642000
6	-2.344151000	-2.214293000	-0.761042000
6	-2.885030000	-0.986304000	-1.269387000
6	-2.065543000	-2.043241000	0.624310000
6	-2.136252000	-3.467158000	-1.540150000
6	-3.024868000	-0.076906000	-0.144916000
6	-3.390138000	-0.747121000	-2.653611000
6	-2.512515000	-0.714301000	1.007034000
6	-1.655445000	-3.126991000	1.562696000
1	-3.008524000	-4.116020000	-1.425581000
1	-2.012006000	-3.263173000	-2.603557000
1	-1.261164000	-4.013292000	-1.188921000
6	-3.661445000	1.268528000	-0.226905000
1	-2.816402000	-1.315192000	-3.385880000
1	-4.438259000	-1.046783000	-2.738207000
1	-3.323198000	0.307738000	-2.921401000
6	-2.539883000	-0.201985000	2.406757000
1	-2.545729000	-3.651833000	1.922511000
1	-1.012849000	-3.856936000	1.071614000
1	-1.120256000	-2.725647000	2.418361000
1	-4.749585000	1.161870000	-0.212829000
1	-3.369254000	1.905657000	0.605355000
1	-3.395289000	1.778419000	-1.153301000
1	-3.340432000	-0.698103000	2.963071000
1	-1.598945000	-0.407835000	2.914347000
1	-2.723215000	0.870318000	2.436767000

Cartesian Coordinates for all optimized geometries under B3LYP/SDD(Ru)/6-31G*(C,H,N,O,S,F)/C-PCM(CH₂Cl₂).

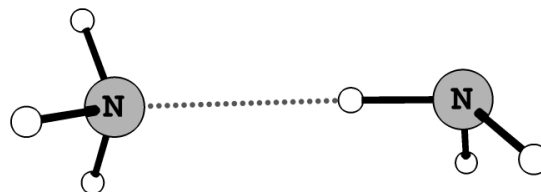
NH₃



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1	0.000000000	0.934306000	-0.286916000
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NH₃...NH₃



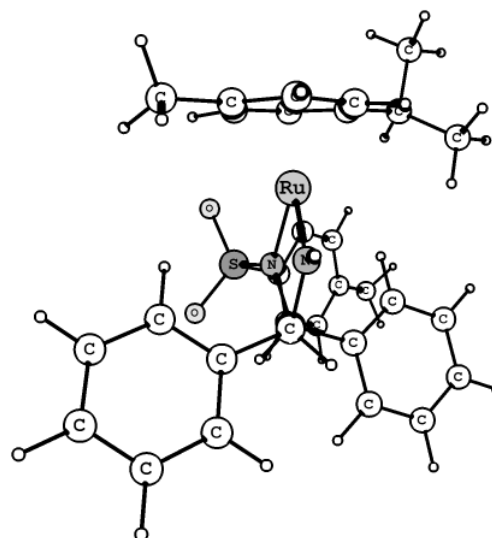
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1	-0.652625000	-0.001105000	0.100159000
7	1.514610000	-0.000343000	-0.006460000
1	1.903172000	0.915934000	-0.229323000
1	1.887249000	-0.634350000	-0.713111000
1	1.955909000	-0.278187000	0.870039000

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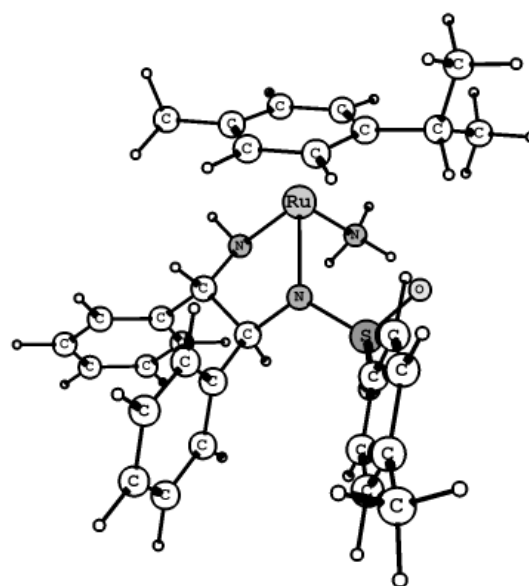
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1	2.740274000	0.269832000	-1.951544000
6	0.391969000	-1.588931000	-0.454204000
1	0.475563000	-2.508176000	0.133441000
6	1.747306000	-1.383090000	-1.198515000
1	1.642415000	-1.837112000	-2.193398000
6	2.476337000	2.790112000	0.745762000
6	2.354502000	3.117737000	-0.639684000
6	1.281212000	2.743748000	1.529629000
6	-0.125224000	3.266469000	-0.433703000
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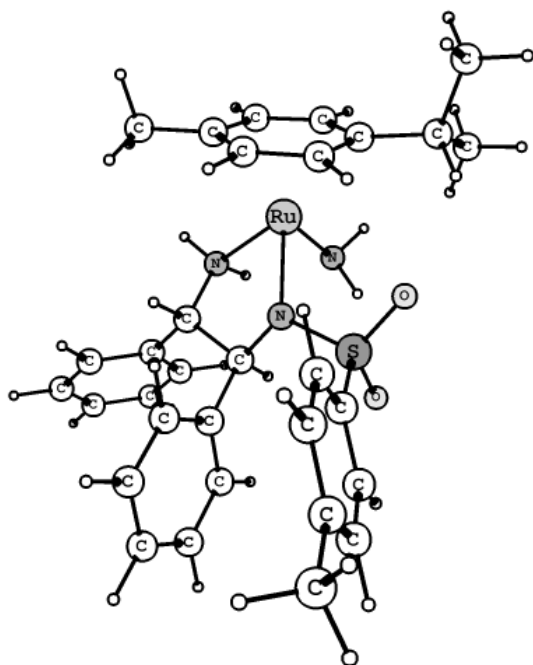
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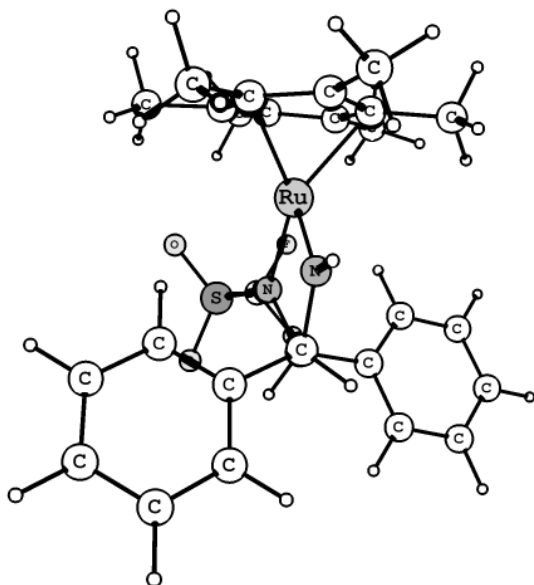


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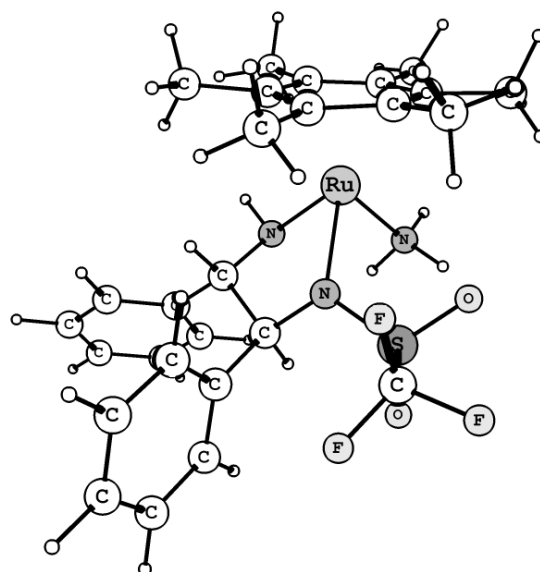
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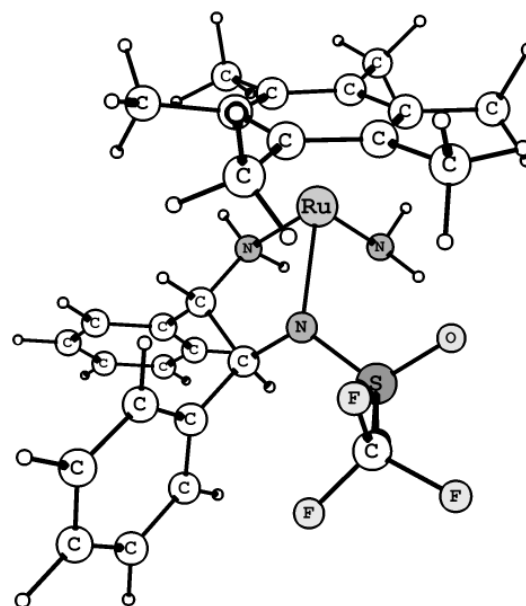
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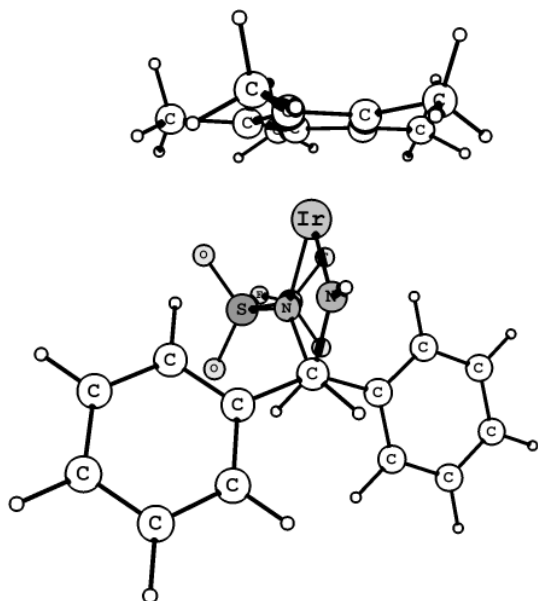
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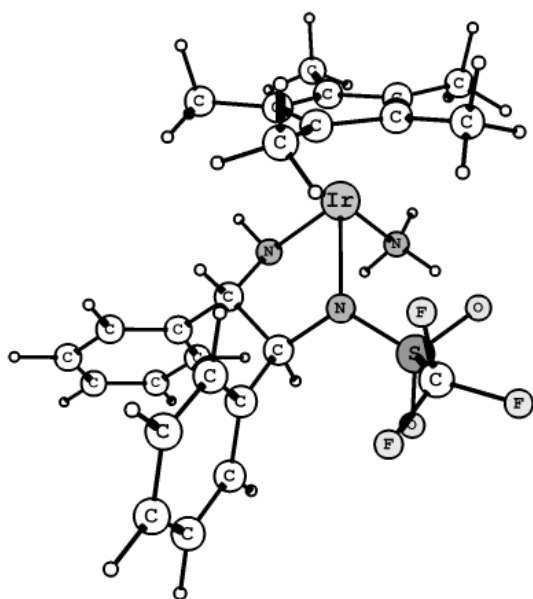
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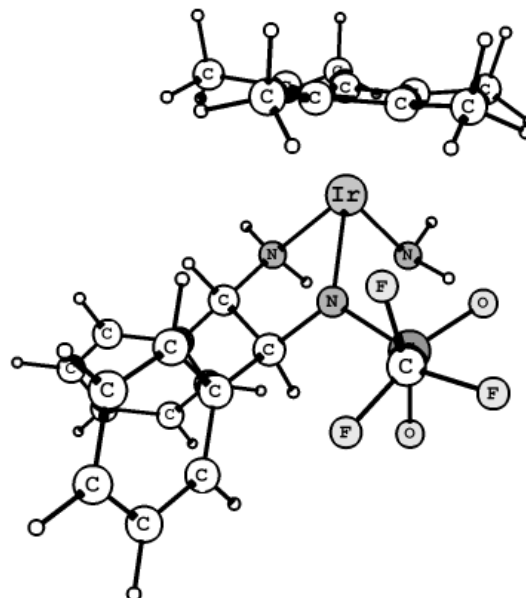
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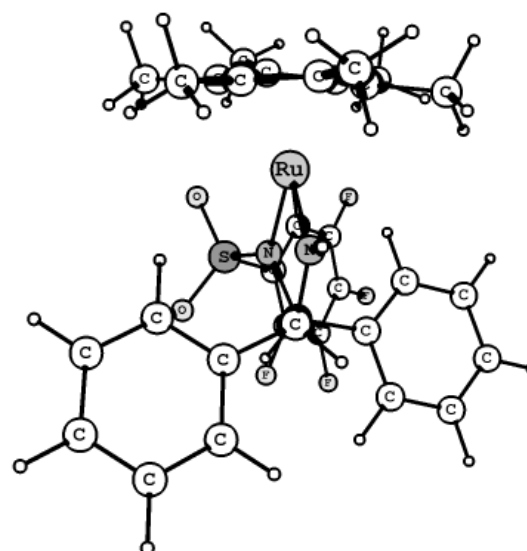
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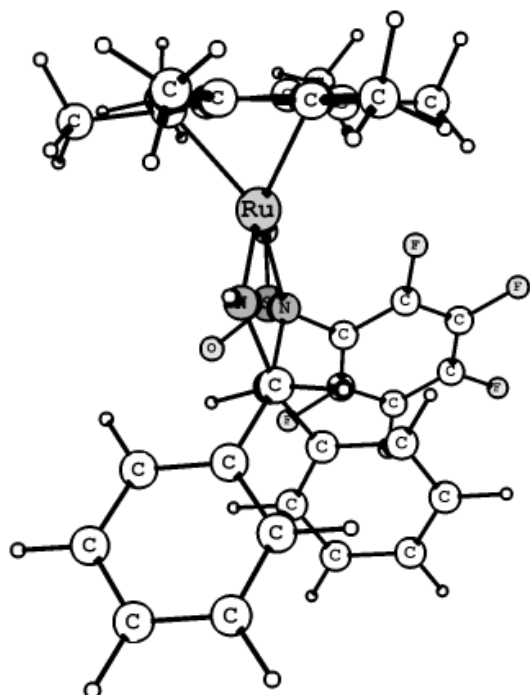
4-ee (δ -isomer)



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8	-0.273947000	-0.730590000	-2.554123000
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1	3.506868000	5.874258000	-2.180337000
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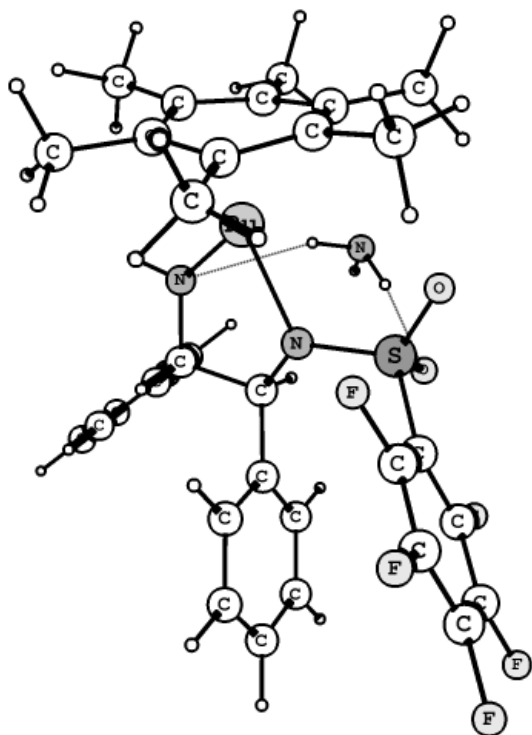
4-aa (λ -isomer)



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1	5.854225000	-0.110688000	1.670669000
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1	1.672432000	-2.947098000	-2.778795000
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1	0.674545000	6.618898000	1.885358000
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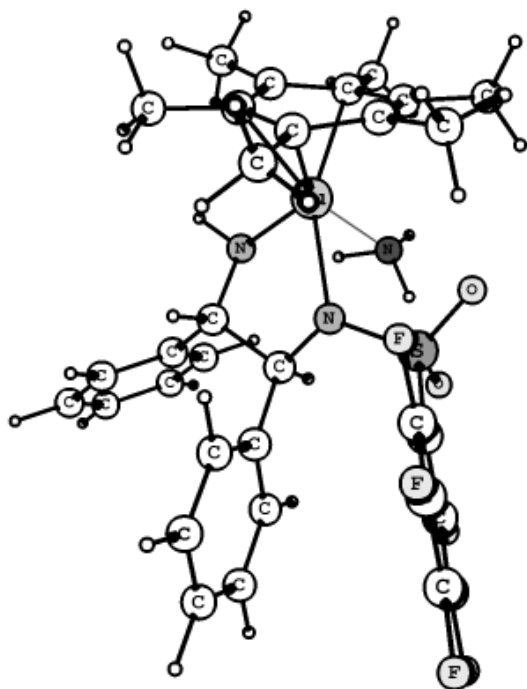
4R·NH₃



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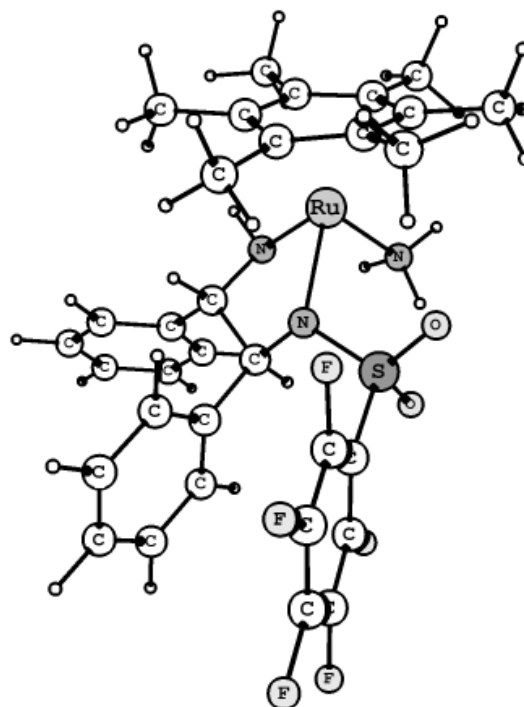
TS1^R, ν 155 cm⁻¹



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6	2.476561000	2.594815000	0.464521000
6	1.987001000	1.362505000	-1.548181000
6	3.704407000	2.991281000	-0.073128000

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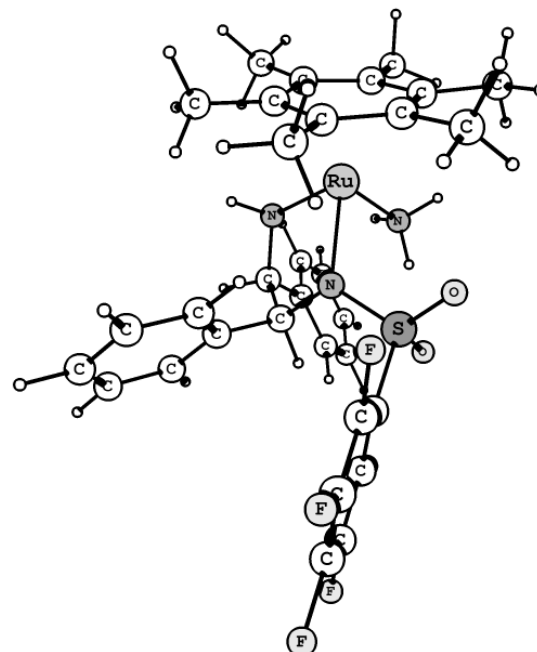
4a_R (λ-isomer)



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6	0.317623000	1.254107000	0.420237000
1	0.389016000	1.533471000	1.479474000
6	-0.863473000	2.052036000	-0.182594000
1	-0.863988000	1.825730000	-1.264767000
6	-4.286647000	-1.377399000	0.315113000
6	-4.266161000	-0.334563000	-0.660164000
6	-3.411184000	-2.530223000	0.176686000
6	-2.326954000	-1.420835000	-1.752415000
6	-2.470284000	-2.563489000	-0.869420000
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6	-5.322147000	-1.360514000	1.420741000
1	-6.105809000	-2.101493000	1.215717000
1	-4.895870000	-1.612577000	2.395961000
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1	-4.061726000	-4.532160000	0.661817000
1	-2.534099000	-4.068895000	1.424305000
1	-4.058517000	-3.443293000	2.044340000
6	-1.609484000	-3.785234000	-1.111292000
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1	-1.568577000	-4.006791000	-2.182784000
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1	-0.346371000	-1.977806000	-2.408452000
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6	2.577420000	2.404187000	0.406729000
6	1.903393000	1.219593000	-1.579857000
6	3.761772000	2.795515000	-0.223943000
1	2.384082000	2.716252000	1.429895000
6	3.084516000	1.607983000	-2.213854000
1	1.189053000	0.591418000	-2.103764000
6	4.018779000	2.399569000	-1.538089000
1	4.482321000	3.407157000	0.312839000
1	3.277228000	1.292206000	-3.236107000
1	4.939102000	2.701205000	-2.031084000
6	-0.694317000	3.561637000	-0.044262000
6	-0.582224000	4.370395000	-1.182707000
6	-0.675187000	4.180445000	1.216020000
6	-0.448495000	5.757758000	-1.072725000
1	-0.597187000	3.907720000	-2.167253000
6	-0.537876000	5.564324000	1.331949000
1	-0.773219000	3.571384000	2.110057000
6	-0.424614000	6.359628000	0.186739000
1	-0.364495000	6.365360000	-1.970226000
1	-0.520959000	6.024246000	2.316946000
1	-0.321108000	7.437748000	0.277233000
6	-3.274675000	-0.356911000	-1.715690000
6	-3.286345000	0.732410000	-2.768327000
1	-3.123791000	1.727314000	-2.340368000
1	-2.528992000	0.574682000	-3.534578000
1	-4.258876000	0.748511000	-3.274090000
44	-2.261313000	-0.469833000	0.274873000
6	2.454429000	-1.325687000	0.692157000
6	3.553839000	-0.761333000	1.346411000

6	2.711348000	-2.078069000	-0.459695000
6	4.853965000	-0.957722000	0.882098000
6	4.001575000	-2.281922000	-0.934169000
6	5.080202000	-1.721640000	-0.256045000
9	1.713502000	-2.623546000	-1.171102000
9	4.210757000	-3.007958000	-2.039192000
9	6.323573000	-1.910087000	-0.702744000
9	5.886947000	-0.404893000	1.529546000
9	3.422414000	0.006897000	2.431268000
7	-2.176753000	-0.247277000	2.441946000
1	-1.281659000	-0.506148000	2.865112000
1	-2.924073000	-0.684422000	2.978875000

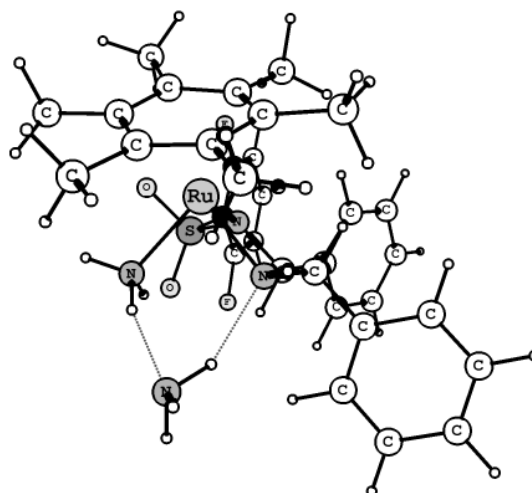
4a_R (δ-isomer)



7	1.892105000	1.067529000	1.348365000
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1	2.829063000	1.026093000	-2.293627000
6	-0.551529000	1.066200000	0.811585000
1	-1.266004000	1.739009000	0.328900000
6	0.687066000	1.901923000	1.280819000
1	0.462642000	2.227407000	2.307867000
6	4.152698000	-1.089875000	-0.432320000
6	3.863210000	-1.220788000	0.955020000
6	3.374824000	-1.824056000	-1.412078000
6	1.900149000	-2.634903000	0.401414000
6	2.263140000	-2.593442000	-1.001648000
6	4.742785000	-0.559114000	1.994272000
1	4.931696000	-1.244677000	2.825503000
1	5.712108000	-0.274246000	1.585318000
1	4.269248000	0.343793000	2.399516000
6	5.329889000	-0.249371000	-0.888650000
1	6.266111000	-0.818017000	-0.809003000
1	5.230750000	0.060783000	-1.929772000
1	5.438881000	0.656662000	-0.289352000
6	3.803793000	-1.778223000	-2.864850000
1	4.857524000	-2.065596000	-2.955732000
1	3.222616000	-2.456619000	-3.486962000
1	3.710656000	-0.777111000	-3.302718000
6	1.496007000	-3.421696000	-2.011670000
1	2.085414000	-4.305167000	-2.292875000
1	0.542997000	-3.769346000	-1.619378000
1	1.272029000	-2.853599000	-2.914040000

6	0.749184000	-3.525605000	0.819689000
1	0.999547000	-4.570027000	0.593246000
1	0.542523000	-3.468245000	1.886701000
1	-0.172672000	-3.288857000	0.284482000
7	-0.096412000	0.024598000	-0.150758000
16	-0.835766000	0.061525000	-1.576872000
8	-0.767344000	1.374007000	-2.273460000
8	-0.434148000	-1.095674000	-2.396940000
6	-1.293198000	0.465565000	2.010567000
6	-1.899994000	1.326941000	2.940713000
6	-1.412857000	-0.912495000	2.211200000
6	-2.587958000	0.823890000	4.045191000
1	-1.841932000	2.403893000	2.795375000
6	-2.098584000	-1.422539000	3.319489000
1	-0.976482000	-1.578514000	1.478492000
6	-2.685854000	-0.557397000	4.243352000
1	-3.052067000	1.510101000	4.749018000
1	-2.177065000	-2.498706000	3.454157000
1	-3.221051000	-0.951131000	5.103283000
6	0.934492000	3.221661000	0.521481000
6	2.182711000	3.849907000	0.688216000
6	-0.034185000	3.899553000	-0.233754000
6	2.461272000	5.089306000	0.110202000
1	2.935922000	3.341338000	1.281253000
6	0.241906000	5.141365000	-0.817476000
1	-1.013582000	3.467435000	-0.402497000
6	1.489373000	5.743118000	-0.652466000
1	3.436850000	5.545940000	0.259468000
1	-0.527379000	5.635268000	-1.405909000
1	1.700674000	6.707402000	-1.107028000
6	2.697724000	-1.968931000	1.379206000
6	2.362942000	-2.058287000	2.854620000
1	1.287507000	-1.995862000	3.031345000
1	2.720576000	-3.004734000	3.281330000
1	2.826256000	-1.251304000	3.424034000
44	2.053926000	-0.424683000	-0.088691000
6	-2.614521000	-0.187960000	-1.207849000
6	-3.545406000	0.855865000	-1.181281000
6	-3.087692000	-1.474419000	-0.922693000
6	-4.893466000	0.624268000	-0.912935000
6	-4.429774000	-1.721667000	-0.655043000
6	-5.337974000	-0.667114000	-0.654665000
9	-2.259473000	-2.527385000	-0.880739000
9	-4.849848000	-2.964469000	-0.391832000
9	-6.627003000	-0.893545000	-0.396127000
9	-5.760782000	1.643070000	-0.896686000
9	-3.191294000	2.131440000	-1.386693000
7	2.251795000	1.254653000	-1.485495000
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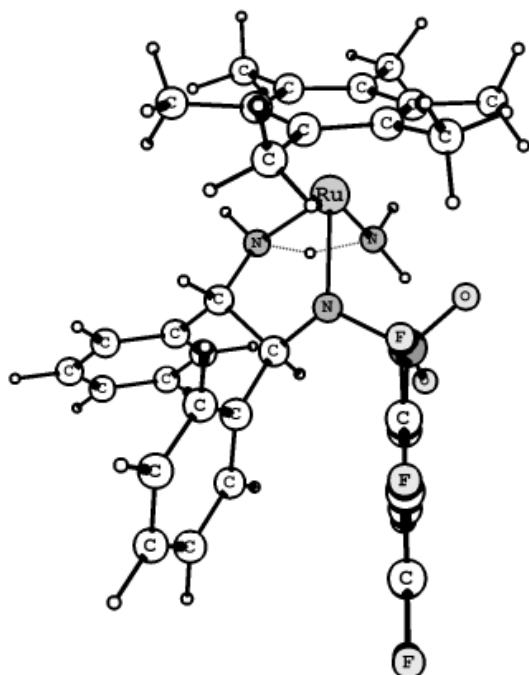
4a_R...NH₃



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1	-0.366068000	1.573555000	-1.358048000
6	0.882527000	1.925379000	0.347344000
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6	4.137560000	-1.648856000	-0.051927000
6	4.072015000	-0.636544000	0.950345000
6	3.180780000	-2.742243000	-0.046626000
6	2.018187000	-1.677984000	1.857808000
6	2.163588000	-2.780973000	0.926899000
6	5.120729000	0.458481000	0.996759000
1	6.066031000	0.065322000	1.392738000
1	5.324132000	0.873371000	0.006433000
1	4.821140000	1.286621000	1.638956000
6	5.266840000	-1.675431000	-1.064136000
1	5.829101000	-2.612163000	-0.970977000
1	4.904752000	-1.617896000	-2.095849000
1	5.971154000	-0.857550000	-0.920906000
6	3.292536000	-3.842855000	-1.080556000
1	3.866442000	-4.691744000	-0.684299000
1	2.310308000	-4.213715000	-1.378400000
1	3.804997000	-3.506082000	-1.983225000
6	1.222180000	-3.962631000	1.033603000
1	1.643309000	-4.851327000	0.560766000
1	1.045001000	-4.208526000	2.085228000
1	0.258760000	-3.750819000	0.563274000
6	0.841222000	-1.692654000	2.808556000
1	1.067599000	-2.288559000	3.703306000
1	0.572982000	-0.687704000	3.135733000
1	-0.040404000	-2.121281000	2.332046000
7	-0.039702000	-0.233146000	-0.261102000
16	-0.857209000	-1.100714000	-1.354867000
8	-0.909117000	-0.464043000	-2.697389000
8	-0.407766000	-2.506771000	-1.337413000
6	-1.636297000	1.632556000	0.363163000
6	-2.504747000	2.538253000	-0.260620000
6	-1.970488000	1.159071000	1.640728000
6	-3.675438000	2.964298000	0.372931000
1	-2.262877000	2.911968000	-1.252272000
6	-3.138725000	1.580956000	2.277288000
1	-1.316979000	0.441421000	2.127124000
6	-3.996000000	2.487856000	1.645837000
1	-4.336610000	3.665349000	-0.129932000
1	-3.381630000	1.201117000	3.266551000
1	-4.906433000	2.815836000	2.140407000
6	0.808503000	3.447449000	0.283119000

6	0.716959000	4.205122000	1.457950000
6	0.862652000	4.127369000	-0.944258000
6	0.674736000	5.602026000	1.415131000
1	0.675974000	3.694534000	2.417887000
6	0.816413000	5.521241000	-0.993402000
1	0.946779000	3.557518000	-1.865015000
6	0.722943000	6.265204000	0.187558000
1	0.605119000	6.169203000	2.339922000
1	0.855245000	6.029116000	-1.953963000
1	0.690310000	7.350881000	0.149245000
6	3.010167000	-0.658639000	1.935869000
6	3.011221000	0.374079000	3.045207000
1	2.856766000	1.392209000	2.671935000
1	2.244406000	0.176783000	3.792969000
1	3.977342000	0.360294000	3.562594000
44	2.140879000	-0.657204000	-0.137819000
6	-2.602433000	-1.196991000	-0.801264000
6	-3.643729000	-0.494129000	-1.415709000
6	-2.939713000	-2.029942000	0.271641000
6	-4.964170000	-0.631146000	-0.989065000
6	-4.251428000	-2.177800000	0.706773000
6	-5.270957000	-1.476911000	0.069447000
9	-2.002119000	-2.713502000	0.945327000
9	-4.537043000	-2.984681000	1.736175000
9	-6.533925000	-1.610046000	0.480002000
9	-5.939048000	0.056216000	-1.596704000
9	-3.434257000	0.355891000	-2.424939000
7	2.185034000	-0.552073000	-2.310100000
1	1.272154000	-0.278930000	-2.681199000
1	3.112730000	2.089505000	-2.070481000
7	3.713289000	1.957624000	-2.896592000
1	3.329164000	2.540965000	-3.639969000
1	2.863469000	0.164450000	-2.613842000
1	2.425638000	-1.437772000	-2.754636000
1	4.625734000	2.352592000	-2.669423000

TS₃^R, *i*1402 cm⁻¹

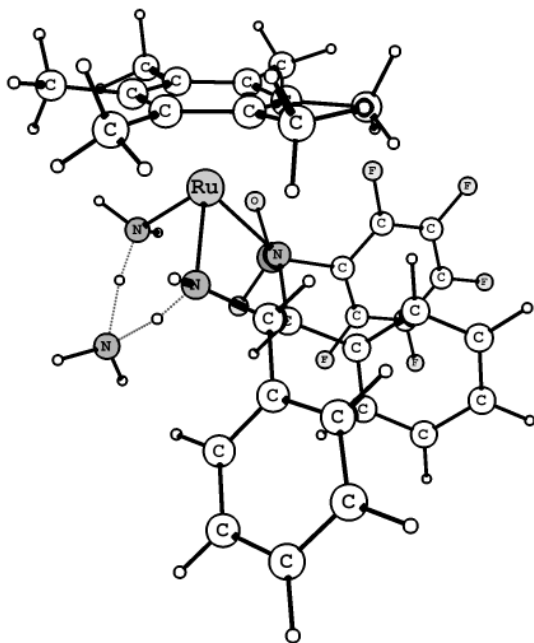


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6	0.335133000	1.293230000	0.346248000
1	0.452378000	1.619639000	1.387267000

6	-0.827243000	2.121451000	-0.259582000
1	-0.843180000	1.923108000	-1.340719000
6	-4.296846000	-1.357579000	0.346898000
6	-4.258200000	-0.417051000	-0.725925000
6	-3.375011000	-2.477621000	0.362323000
6	-2.340973000	-1.621897000	-1.726035000
6	-2.440087000	-2.626821000	-0.685347000
6	-5.243100000	0.735480000	-0.769672000
1	-5.397423000	1.180160000	0.216155000
1	-4.909289000	1.532497000	-1.434565000
1	-6.219746000	0.393119000	-1.135978000
6	-5.356475000	-1.272286000	1.427025000
1	-5.962141000	-2.186332000	1.423047000
1	-4.924309000	-1.180854000	2.428824000
1	-6.034148000	-0.432520000	1.282297000
6	-3.438180000	-3.496246000	1.481184000
1	-4.029125000	-4.371881000	1.179343000
1	-2.440132000	-3.840855000	1.756908000
1	-3.901146000	-3.085297000	2.378836000
6	-1.564156000	-3.858174000	-0.782681000
1	-1.928671000	-4.661285000	-0.141536000
1	-1.571217000	-4.233167000	-1.811720000
1	-0.531894000	-3.645312000	-0.500256000
6	-1.262995000	-1.770677000	-2.778522000
1	-1.615609000	-2.384619000	-3.618516000
1	-0.953682000	-0.804301000	-3.179043000
1	-0.372869000	-2.246930000	-2.368027000
7	-0.069635000	-0.146869000	0.305560000
16	0.725405000	-1.060741000	1.387469000
8	0.881672000	-0.415035000	2.713233000
8	0.178870000	-2.430369000	1.397875000
6	1.634708000	1.592505000	-0.394132000
6	2.613045000	2.402440000	0.196357000
6	1.854192000	1.114200000	-1.694380000
6	3.784684000	2.728961000	-0.492576000
1	2.458252000	2.778112000	1.204519000
6	3.022920000	1.436875000	-2.385199000
1	1.111283000	0.470984000	-2.157307000
6	3.992805000	2.247633000	-1.786627000
1	4.533580000	3.356197000	-0.016219000
1	3.178197000	1.055193000	-3.391104000
1	4.903519000	2.498106000	-2.324024000
6	-0.646230000	3.621711000	-0.064827000
6	-0.427598000	4.457989000	-1.166937000
6	-0.710613000	4.199020000	1.213066000
6	-0.268662000	5.836558000	-1.001369000
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6	-0.551559000	5.575064000	1.382759000
1	-0.889355000	3.568347000	2.080122000
6	-0.329034000	6.399161000	0.275090000
1	-0.099621000	6.468465000	-1.869294000
1	-0.602544000	6.004787000	2.379763000
1	-0.206915000	7.470831000	0.407166000
6	-3.284084000	-0.563199000	-1.789615000
6	-3.322028000	0.399861000	-2.960700000
1	-4.334101000	0.435392000	-3.378782000
1	-3.052562000	1.421802000	-2.672711000
1	-2.652748000	0.095186000	-3.764199000
44	-2.267539000	-0.454515000	0.232135000
6	2.435495000	-1.285320000	0.759822000
6	3.556906000	-0.694494000	1.350685000
6	2.661263000	-2.124957000	-0.336548000
6	4.845080000	-0.947709000	0.879846000
6	3.938468000	-2.387901000	-0.816742000
6	5.038632000	-1.798616000	-0.200977000
9	1.641851000	-2.702904000	-0.990295000

9	4.114289000	-3.197920000	-1.868020000
9	6.270412000	-2.041930000	-0.653547000
9	5.898548000	-0.366040000	1.466407000
9	3.461051000	0.154684000	2.377671000
1	-2.122625000	1.313228000	1.564491000
7	-2.242252000	0.193207000	2.270043000
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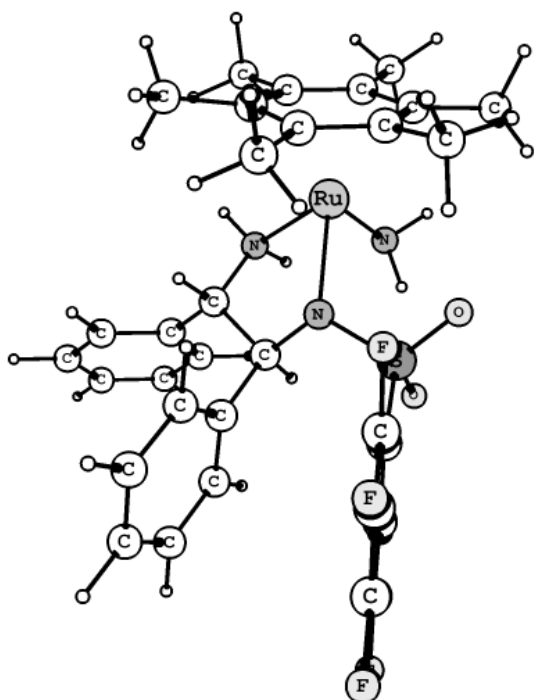
TS₃^R...NH₃, *i*458 cm⁻¹



7	2.115581000	1.498742000	-0.431367000
1	2.927018000	1.946006000	-0.002125000
6	-0.298776000	1.269696000	-0.425074000
1	-0.342887000	1.613301000	-1.466162000
6	0.893508000	1.995084000	0.242959000
1	0.920773000	1.665491000	1.288029000
6	4.228750000	-1.568135000	0.002890000
6	4.102122000	-0.518306000	0.957492000
6	3.253402000	-2.638880000	-0.009771000
6	2.053339000	-1.559638000	1.870500000
6	2.199815000	-2.656783000	0.932544000
6	5.114126000	0.610112000	0.979774000
1	6.019047000	0.302203000	1.519794000
1	5.412525000	0.907206000	-0.027723000
1	4.728548000	1.498446000	1.482111000
6	5.413949000	-1.638386000	-0.940570000
1	5.862635000	-2.636385000	-0.897794000
1	5.142377000	-1.453341000	-1.986136000
1	6.191129000	-0.922338000	-0.675686000
6	3.377022000	-3.757906000	-1.020024000
1	3.951610000	-4.593892000	-0.598283000
1	2.397288000	-4.139081000	-1.312176000
1	3.892198000	-3.436420000	-1.926831000
6	1.264714000	-3.847903000	0.987891000
1	1.823194000	-4.774520000	0.825889000
1	0.782806000	-3.927815000	1.963416000
1	0.484704000	-3.775750000	0.226116000
6	0.867547000	-1.555379000	2.809206000
1	1.063078000	-2.184590000	3.687974000
1	0.635866000	-0.550798000	3.163499000
1	-0.025019000	-1.935692000	2.313451000
7	0.019763000	-0.191353000	-0.376268000

16	-0.840397000	-1.068367000	-1.436221000
8	-1.028781000	-0.407586000	-2.747120000
8	-0.320075000	-2.450020000	-1.480387000
6	-1.610615000	1.644992000	0.256047000
6	-2.507642000	2.511909000	-0.380467000
6	-1.923423000	1.181612000	1.542393000
6	-3.689245000	2.910470000	0.250584000
1	-2.280173000	2.876559000	-1.378835000
6	-3.102098000	1.576775000	2.176282000
1	-1.246873000	0.492326000	2.038437000
6	-3.989720000	2.444919000	1.532219000
1	-4.374347000	3.581183000	-0.261215000
1	-3.329710000	1.206192000	3.172498000
1	-4.908606000	2.751714000	2.024578000
6	0.774650000	3.514299000	0.242446000
6	0.462300000	4.182038000	1.435377000
6	0.969811000	4.273621000	-0.922534000
6	0.334255000	5.572478000	1.468309000
1	0.310526000	3.607253000	2.346064000
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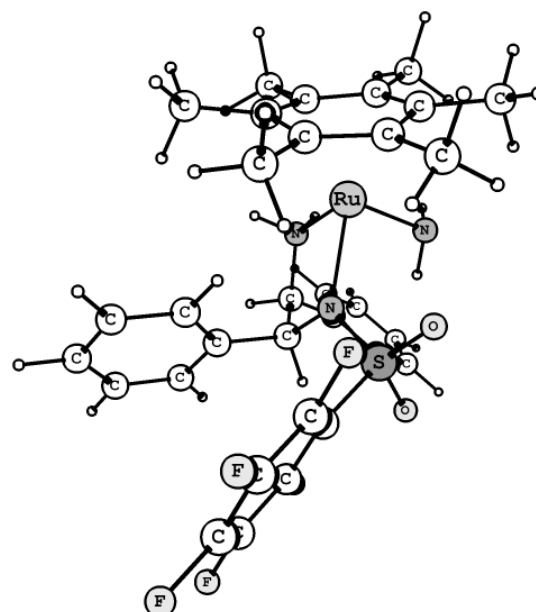
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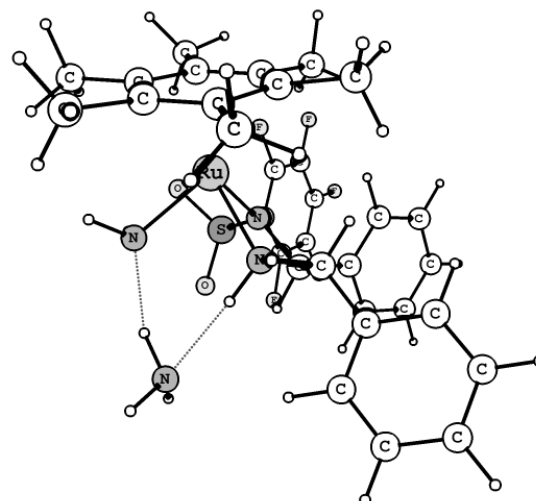


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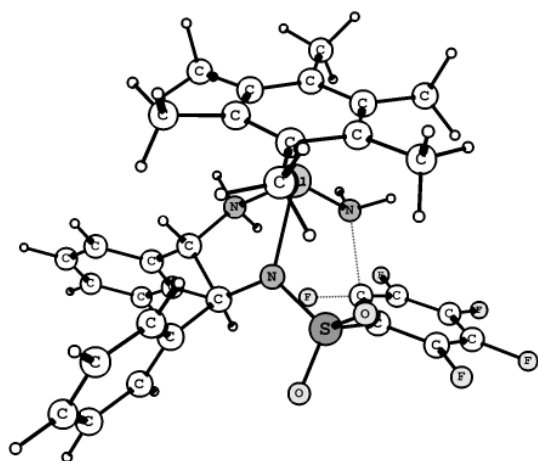
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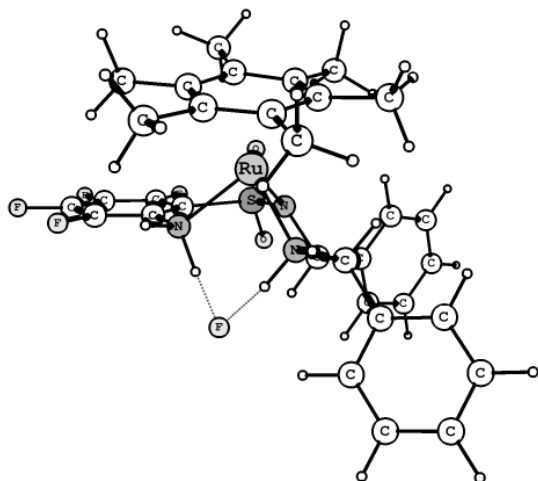


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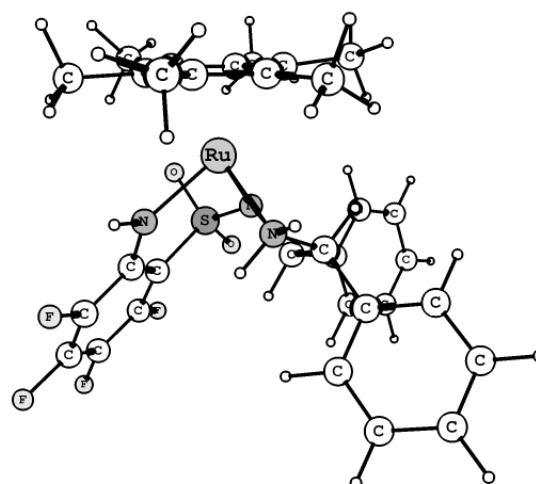
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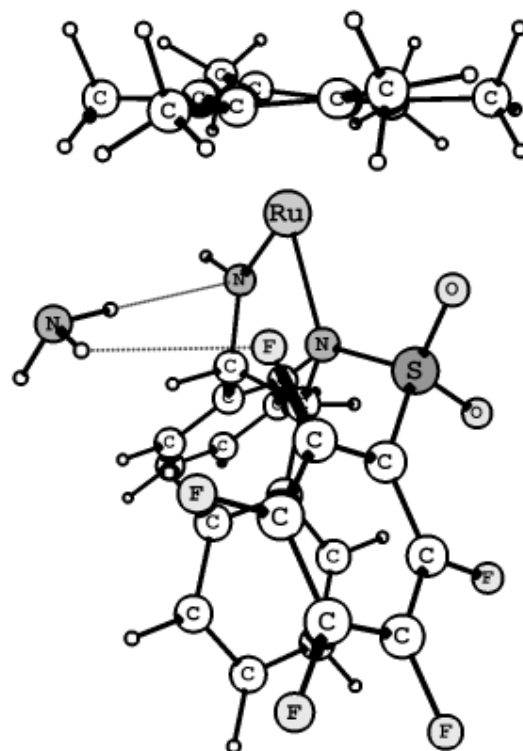


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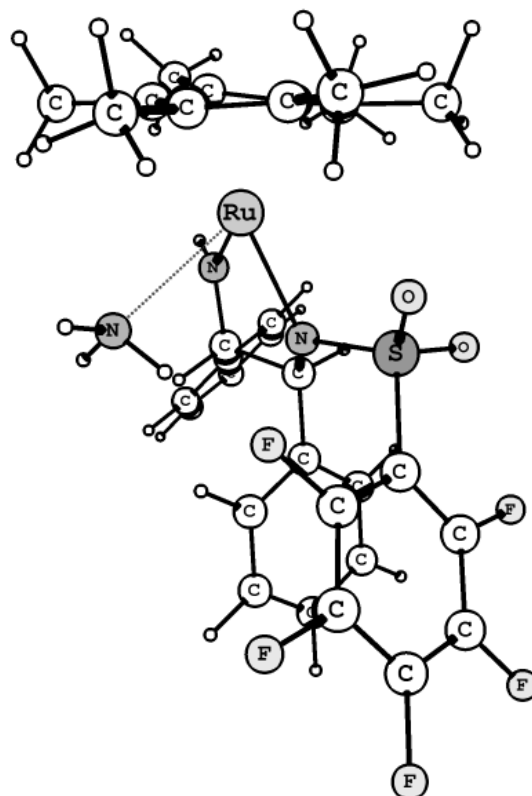
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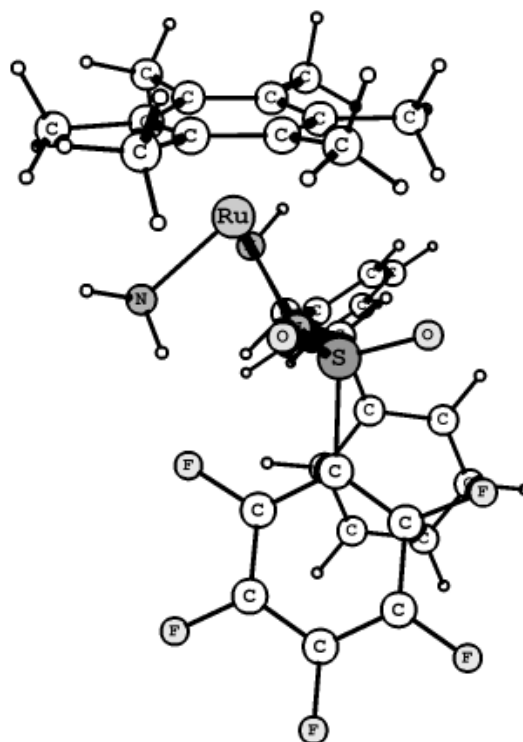
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1	5.372871000	-1.657691000	2.728300000
44	2.205954000	-0.478261000	0.163304000
6	-2.511597000	-1.229214000	-0.583744000
6	-3.663943000	-0.800406000	-1.247494000
6	-2.686055000	-1.919914000	0.619543000
6	-4.934255000	-1.047486000	-0.725716000
6	-3.943095000	-2.173883000	1.152799000
6	-5.076193000	-1.737505000	0.471350000
9	-1.626161000	-2.352657000	1.325150000
9	-4.071051000	-2.833570000	2.311118000
9	-6.291633000	-1.976587000	0.970027000
9	-6.021703000	-0.622841000	-1.381537000
9	-3.619175000	-0.129091000	-2.401356000
7	0.871014000	-0.794353000	2.707239000
1	0.008947000	-0.917757000	2.179952000
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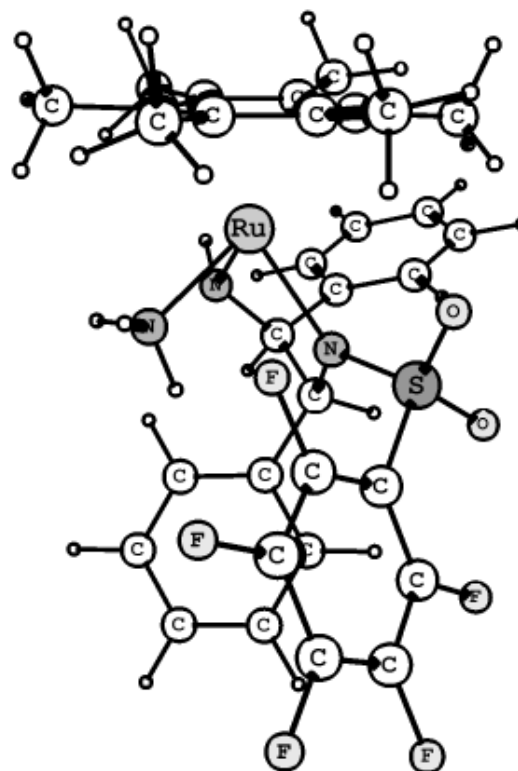
4as (λ -isomer)



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1	0.178326000	1.463023000	-1.341386000
6	0.576411000	1.978001000	0.737789000
1	0.065204000	1.756359000	1.684204000
6	3.176496000	-0.716983000	-1.684714000
6	4.022623000	0.019172000	-0.803427000
6	2.805681000	-2.072761000	-1.335508000
6	3.900263000	-1.820001000	0.852936000
6	3.177566000	-2.637978000	-0.092895000
6	4.537010000	1.391880000	-1.182210000
1	5.470737000	1.293457000	-1.751426000
1	3.833592000	1.946024000	-1.804753000
1	4.752761000	2.004943000	-0.305972000
6	2.771848000	-0.191887000	-3.047412000
1	3.262196000	-0.771973000	-3.840060000
1	1.691959000	-0.275935000	-3.198383000
1	3.047686000	0.851375000	-3.193760000
6	2.117184000	-2.917946000	-2.382625000
1	2.868226000	-3.235104000	-3.120775000
1	1.653627000	-3.806265000	-1.961622000
1	1.341986000	-2.366347000	-2.913963000
6	2.820244000	-4.080446000	0.208435000
1	3.234593000	-4.741179000	-0.562070000
1	3.221255000	-4.417808000	1.163606000
1	1.736026000	-4.227029000	0.220624000
6	4.212629000	-2.361445000	2.233810000
1	5.153596000	-2.926993000	2.227513000
1	4.311994000	-1.560723000	2.968656000
1	3.432228000	-3.035953000	2.591506000
7	0.025996000	-0.214447000	-0.044571000
16	-0.748103000	-1.331656000	-0.918138000
8	-0.836435000	-1.026414000	-2.364353000
8	-0.248484000	-2.669615000	-0.541176000
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6	-2.284333000	2.155244000	-1.515866000
6	-2.474885000	1.630885000	0.826354000

6	-3.602735000	2.618602000	-1.523640000
1	-1.699998000	2.179821000	-2.432207000
6	-3.791125000	2.092439000	0.824306000
1	-2.051737000	1.237092000	1.746189000
6	-4.361459000	2.589484000	-0.352390000
1	-4.034759000	3.000440000	-2.444976000
1	-4.372931000	2.064940000	1.742040000
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6	0.184373000	4.321907000	1.626476000
6	0.978290000	4.094389000	-0.634630000
6	0.212760000	5.713192000	1.501176000
1	-0.138701000	3.872595000	2.562907000
6	1.006574000	5.484262000	-0.766148000
1	1.278531000	3.477221000	-1.477808000
6	0.623832000	6.299967000	0.302313000
1	-0.086869000	6.336930000	2.339481000
1	1.325753000	5.930121000	-1.704754000
1	0.645569000	7.381664000	0.200377000
6	4.418074000	-0.539153000	0.465627000
6	5.362872000	0.239843000	1.360275000
1	4.869226000	1.098664000	1.831541000
1	5.782198000	-0.381715000	2.151591000
1	6.206104000	0.623432000	0.776979000
44	2.185242000	-0.521988000	0.340492000
6	-2.474109000	-1.387590000	-0.299816000
6	-3.600160000	-1.172992000	-1.098698000
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6	-3.972055000	-1.867124000	1.566379000
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9	-4.145366000	-2.199679000	2.851779000
9	-6.311550000	-1.761957000	1.248366000
9	-5.950871000	-1.077850000	-1.367807000
9	-3.510641000	-0.830867000	-2.386656000
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1	0.336951000	-0.861448000	2.212449000
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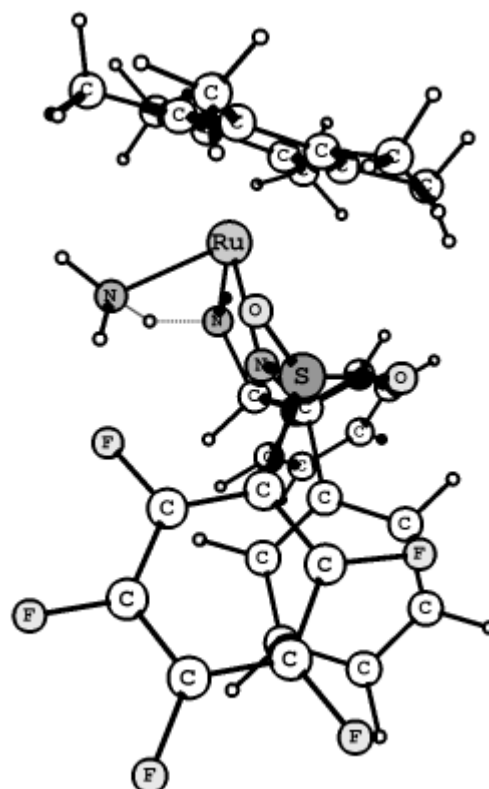
4as (δ -isomer)



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6	1.393022000	2.084060000	1.002769000
1	1.273246000	2.822845000	1.813325000
6	3.547350000	-1.056931000	-0.487739000
6	3.516843000	-1.626182000	0.840245000
6	2.587384000	-1.490165000	-1.448945000
6	1.709545000	-3.176631000	0.127971000
6	1.733324000	-2.628182000	-1.170195000
6	4.492474000	-1.135737000	1.892156000
1	5.275537000	-1.884402000	2.067096000
1	4.986039000	-0.211378000	1.593116000
1	3.997416000	-0.946218000	2.848386000
6	4.656030000	-0.087328000	-0.845278000
1	4.665429000	0.150071000	-1.907413000
1	4.588175000	0.856524000	-0.298006000
1	5.624519000	-0.542990000	-0.606038000
6	2.556238000	-0.861548000	-2.826053000
1	3.232989000	-1.393431000	-3.509208000
1	1.549381000	-0.887886000	-3.239162000
1	2.863359000	0.184419000	-2.795348000
6	0.907391000	-3.287141000	-2.256131000
1	1.175909000	-2.923065000	-3.247058000
1	1.080213000	-4.369382000	-2.243937000
1	-0.161154000	-3.106857000	-2.119876000
6	0.786656000	-4.336099000	0.433915000
1	1.264113000	-5.285581000	0.154349000
1	0.542271000	-4.403931000	1.495492000
1	-0.150008000	-4.264194000	-0.122339000
7	-0.017048000	0.574954000	-0.309324000
16	-0.990061000	0.435939000	-1.577417000
8	-1.176320000	1.722431000	-2.283460000
8	-0.614603000	-0.731733000	-2.395363000
6	-1.141682000	2.163318000	1.355446000
6	-2.314643000	2.788320000	0.903469000

6	-1.052212000	1.840917000	2.720342000
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1	-2.393578000	3.080327000	-0.139243000
6	-2.114996000	2.096803000	3.591038000
1	-0.131472000	1.404321000	3.096391000
6	-3.287520000	2.691886000	3.118746000
1	-4.277608000	3.526518000	1.392213000
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6	2.444925000	2.696874000	0.070031000
6	3.551492000	3.330821000	0.661470000
6	2.373462000	2.676316000	-1.330930000
6	4.561573000	3.906077000	-0.111727000
1	3.614649000	3.384067000	1.747292000
6	3.378555000	3.258407000	-2.110275000
1	1.525990000	2.210914000	-1.822353000
6	4.478947000	3.870643000	-1.506783000
1	5.403028000	4.394143000	0.373800000
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1	5.257075000	4.324750000	-2.114545000
6	2.588082000	-2.660230000	1.158401000
6	2.582406000	-3.316688000	2.525120000
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1	2.844639000	-4.377612000	2.431214000
1	3.300301000	-2.862579000	3.206354000
44	1.469536000	-0.879175000	0.445064000
6	-2.696965000	-0.035022000	-1.027221000
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9	-6.171200000	1.097722000	-1.074580000
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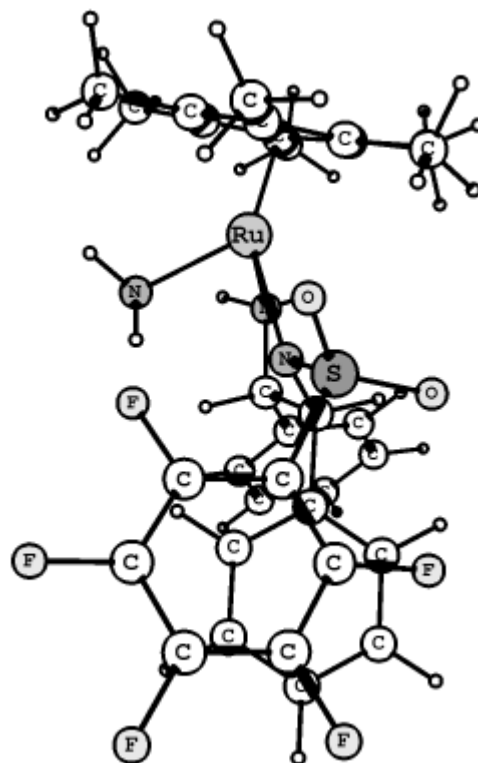
TS₃^S, $i1420\text{ cm}^{-1}$



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1	-0.086700000	1.891422000	1.845915000
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6	2.872117000	-2.710760000	-0.593204000
6	4.695629000	1.270611000	-0.350184000
1	5.669526000	1.275191000	-0.857187000
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6	1.934515000	-2.167905000	-2.891403000
1	2.663415000	-2.479886000	-3.652997000
1	1.254410000	-2.996087000	-2.707314000
1	1.347398000	-1.348422000	-3.304767000
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1	2.647899000	-4.773326000	0.058348000
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1	3.985297000	-2.752661000	2.655920000
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1	0.538376000	6.448202000	2.145066000
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6	4.298047000	-1.052614000	0.603574000
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1	4.760386000	-0.250797000	2.592169000
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6	-2.617699000	-1.222894000	-0.313458000
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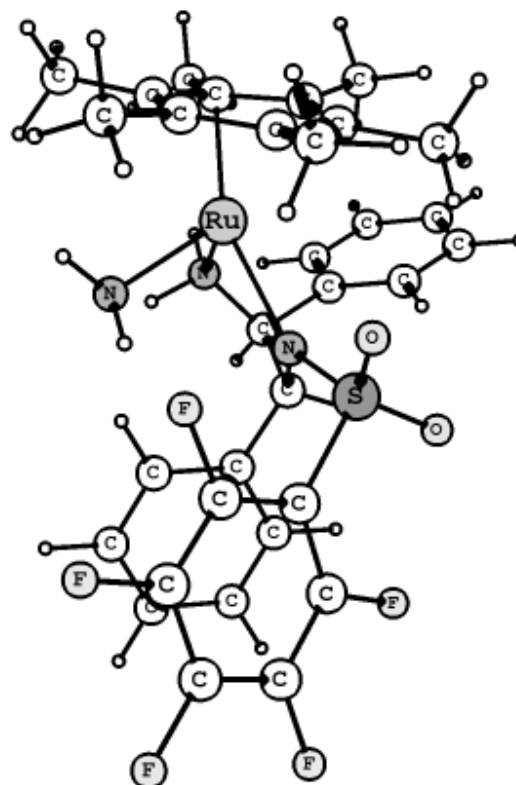
4bs (λ -isomer)



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1	-0.018130000	1.622462000	-1.450627000
6	0.526133000	2.095873000	0.589603000
1	0.217071000	1.772941000	1.584266000
6	3.804181000	-0.467352000	-1.442264000
6	4.334778000	-0.095511000	-0.152183000
6	3.028126000	-1.648800000	-1.545075000
6	3.522288000	-2.217634000	0.819790000
6	2.922224000	-2.559432000	-0.419023000
6	5.072051000	1.222351000	-0.015519000
1	6.147435000	1.074935000	-0.180055000
1	4.733126000	1.959662000	-0.745935000
1	4.950504000	1.661939000	0.976320000
6	4.092879000	0.400689000	-2.654622000
1	4.007238000	-0.169462000	-3.580622000
1	3.418422000	1.262084000	-2.737292000
1	5.114394000	0.789227000	-2.612530000
6	2.400287000	-2.016284000	-2.872590000
1	3.099488000	-2.618194000	-3.469676000
1	1.484545000	-2.586438000	-2.732012000
1	2.141699000	-1.129741000	-3.453555000
6	2.310340000	-3.938569000	-0.566924000
1	2.021515000	-4.150690000	-1.594282000
1	3.042366000	-4.697230000	-0.264132000
1	1.418818000	-4.059888000	0.051377000
6	3.425031000	-3.175927000	1.985524000
1	4.240651000	-3.910349000	1.937571000
1	3.505589000	-2.665281000	2.946645000
1	2.484141000	-3.729208000	1.977293000
7	0.039371000	-0.133334000	-0.244549000
16	-0.767570000	-1.159905000	-1.191516000
8	-1.008179000	-0.643788000	-2.556589000
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6	-0.101520000	5.741146000	1.548835000
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6	0.206704000	6.413073000	0.364141000
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1	5.507871000	-1.542344000	2.627344000
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44	2.210709000	-0.453757000	0.285188000
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6	-3.631863000	-1.163302000	-1.118042000
6	-2.512113000	-1.947484000	0.838750000
6	-4.862427000	-1.432527000	-0.517659000
6	-3.729141000	-2.219808000	1.450555000
6	-4.913289000	-1.963880000	0.764562000
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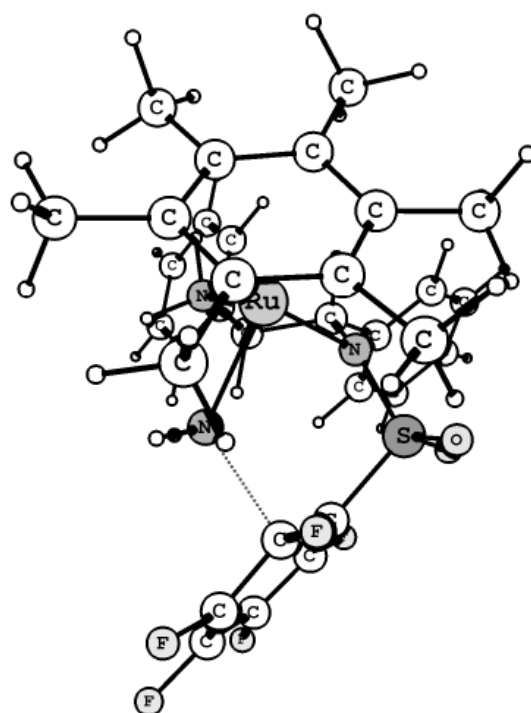
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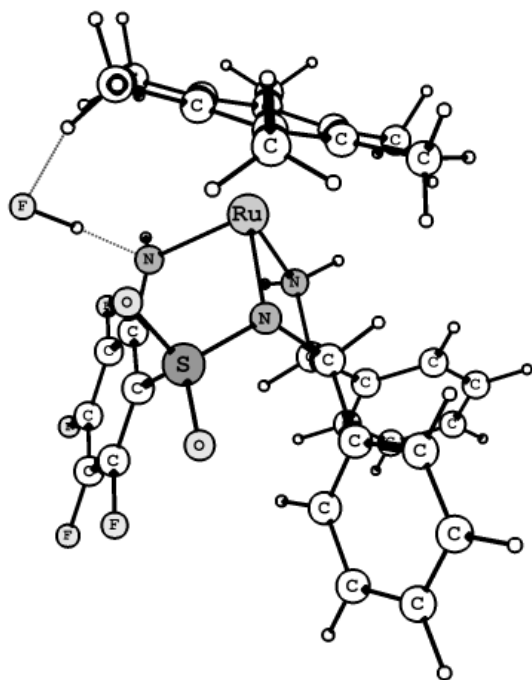
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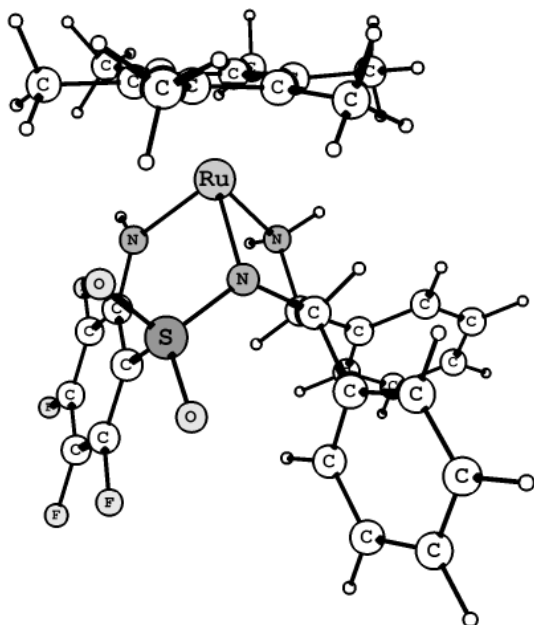


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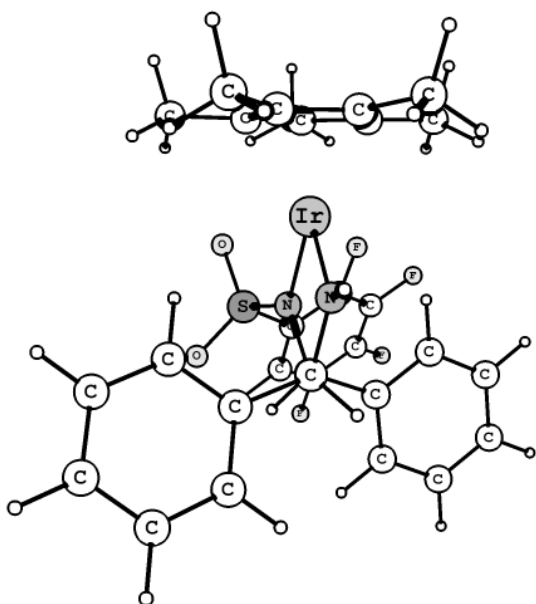
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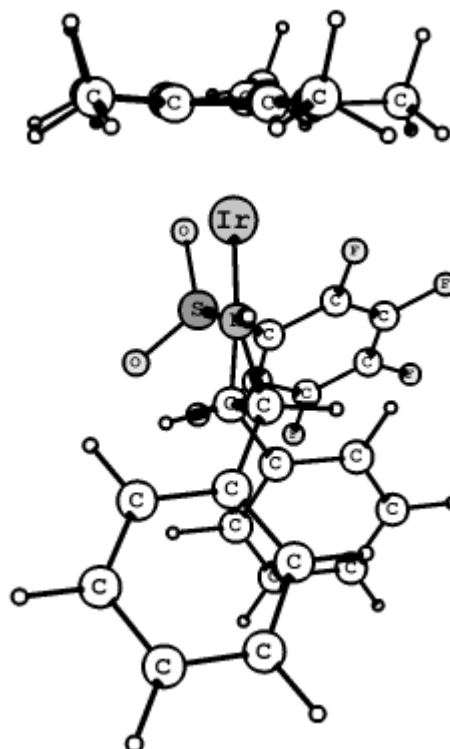
5-ee (δ -isomer)



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6	-0.23912400	1.62206600	0.61690500
1	0.93455200	2.45953800	2.21543500
6	1.79734900	3.18479700	0.41536300
1	-0.61658300	2.45453600	0.01753700
7	0.02800300	0.46064100	-0.27223900
6	-1.26766700	1.34544300	1.71310800
6	1.59909800	4.51341600	0.81865000
6	2.57634300	2.94086900	-0.72431500
6	-2.17427900	2.35980200	2.05406700
6	-1.31505300	0.14059000	2.42951100
6	2.15423600	5.57371800	0.09916700
1	1.00445600	4.71880500	1.70663500
6	3.13184500	3.99933900	-1.44780800
1	2.74848700	1.91661000	-1.04003000
6	-3.10065300	2.18289400	3.08477500
1	-2.15653500	3.29898200	1.50506600
6	-2.24090900	-0.04007900	3.45984700
1	-0.62844600	-0.65848100	2.17422400
6	2.92270300	5.31923900	-1.03974800
1	1.99172000	6.59589700	0.43109100
1	3.73156900	3.79171300	-2.33051600
6	-3.13657900	0.97976200	3.79291100
1	-3.79669700	2.98152000	3.32772100
1	-2.26343200	-0.98172900	4.00278100
1	3.35943100	6.14132300	-1.60044800
1	-3.85801400	0.83571200	4.59271400
16	-0.83223800	0.42454500	-1.64462800
8	-0.95272300	1.76460500	-2.24724700
8	-0.35104600	-0.66688900	-2.50501900
77	1.71828500	-0.71165800	0.20769700
6	1.88776100	-2.90230000	0.56894600
6	3.12149300	-2.21057600	0.93643300
6	1.69300800	-2.77191600	-0.84428700
6	1.04740000	-3.72532500	1.49795700
6	3.64305000	-1.60255200	-0.25365500
6	3.76645100	-2.23384000	2.29127700
6	2.72817000	-1.91959500	-1.35410700
6	0.66046000	-3.49313300	-1.65769500
1	1.40352600	-4.76457600	1.50479500
1	1.09771500	-3.35133800	2.52404800

1	-0.00036400	-3.73249400	1.18799300
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1	4.41115500	-1.36429800	2.44596800
6	2.93442400	-1.55487900	-2.79321300
1	1.06309400	-4.46582300	-1.97215900
1	-0.25065800	-3.67805000	-1.08595400
1	0.38713400	-2.92718200	-2.54781300
1	5.73561900	-1.56833800	-0.69979200
1	4.88515000	-0.08089900	-1.14240100
1	5.25468100	-0.41677600	0.55545300
1	3.48876200	-2.35036600	-3.30994900
1	1.97703700	-1.41614600	-3.29987700
1	3.51081900	-0.63086600	-2.89287000
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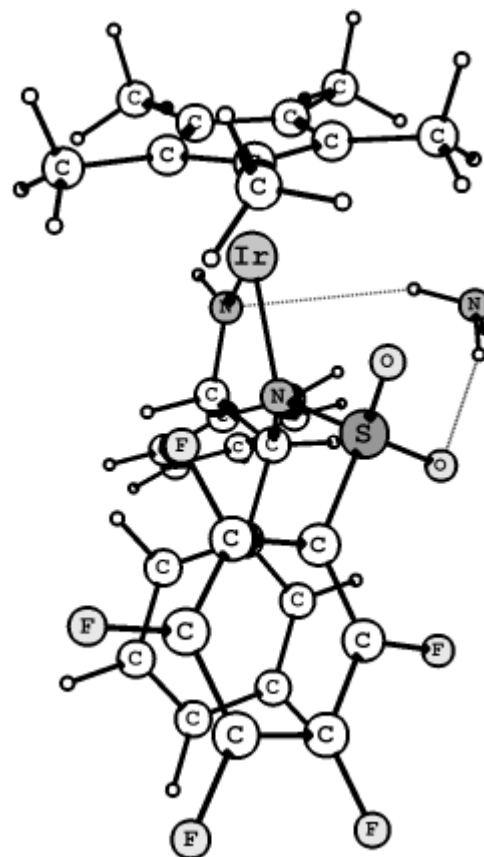
5-aa (λ -isomer)



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1	0.02708300	1.98736600	1.33673600
7	-0.02410000	0.08783900	0.39289400
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6	2.392338000	2.786677000	0.727637000
6	2.115833000	1.604005000	-1.354298000
6	-0.916525000	5.936800000	-1.142359000
1	-0.228751000	4.226739000	-2.259836000
6	-1.936573000	5.455923000	0.993885000
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1	2.010346000	3.080353000	1.701765000
6	3.383884000	2.019924000	-1.761014000
1	1.524095000	0.970435000	-2.009814000
6	-1.532024000	6.383536000	0.028592000
1	-0.601681000	6.649557000	-1.899973000
1	-2.418318000	5.795594000	1.907074000
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1	3.765414000	1.716116000	-2.732286000
1	-1.698394000	7.445502000	0.188149000
1	5.148781000	3.151113000	-1.240572000
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77	-1.999852000	-0.547846000	-0.049269000
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6	-2.079134000	-2.671104000	-2.586495000
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6	-2.995051000	-2.257374000	1.044163000
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1	-2.195583000	-1.866590000	-3.317637000
1	-1.018652000	-2.928931000	-2.527445000
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1	-3.987209000	-0.462475000	-2.936420000
1	-5.378729000	-1.420290000	-2.410099000
1	-5.076174000	0.166913000	-1.692093000
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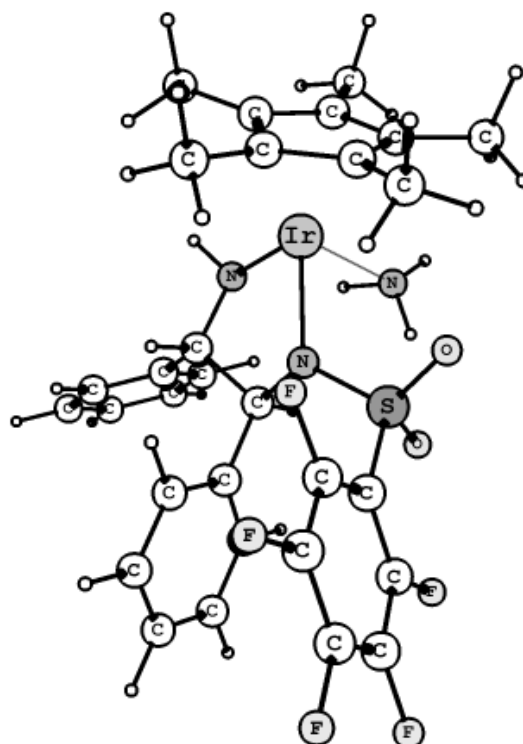
5R·NH₃



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1	1.623760000	0.845374000	-2.155969000
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1	-1.963344000	5.870781000	1.741376000
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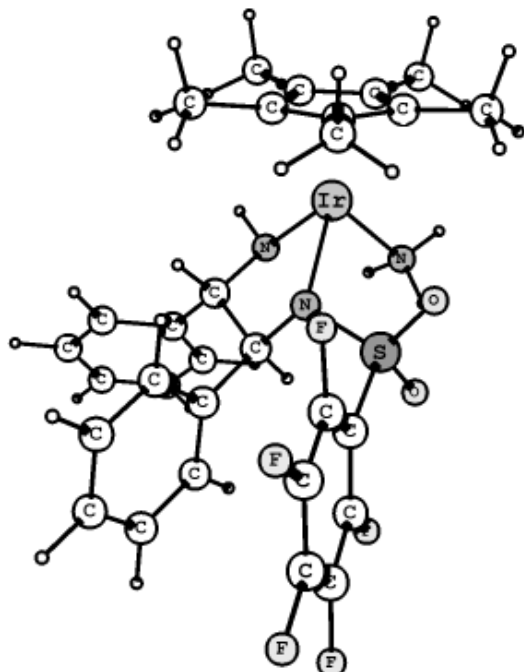
TS₂^R, *i*168 cm⁻¹



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6	1.279184000	5.625311000	-0.959721000
1	1.476291000	3.613712000	-1.697228000
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5a_R (λ-isomer)

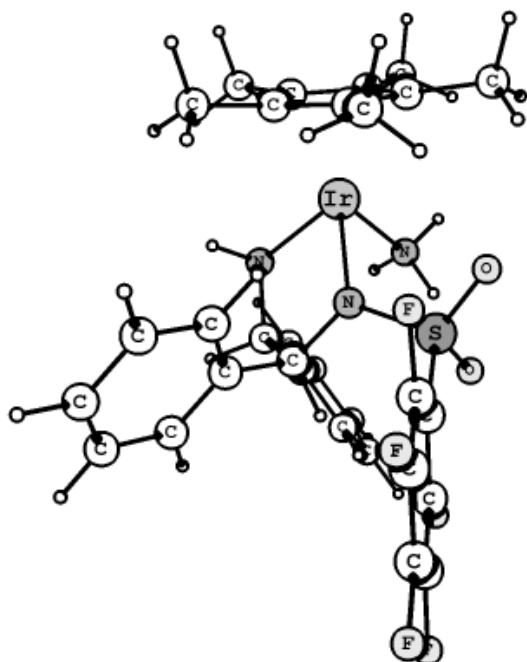


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1	-0.519069000	1.513246000	-1.393420000
7	0.011770000	-0.189110000	-0.208625000
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6	-2.723586000	2.295705000	-0.274151000
6	-1.953876000	1.146226000	1.699446000
6	0.164028000	5.781654000	1.084179000
1	0.390322000	3.955856000	2.206113000
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1	0.599875000	3.566392000	-2.065342000
6	-3.908688000	2.637848000	0.383147000
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8	-0.218846000	-2.587137000	-1.032266000
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6	4.179270000	-1.381887000	-0.089642000
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6	1.352347000	-2.942284000	1.878212000
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1	5.759830000	0.441483000	1.893974000
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1	0.623714000	-2.330250000	2.414539000
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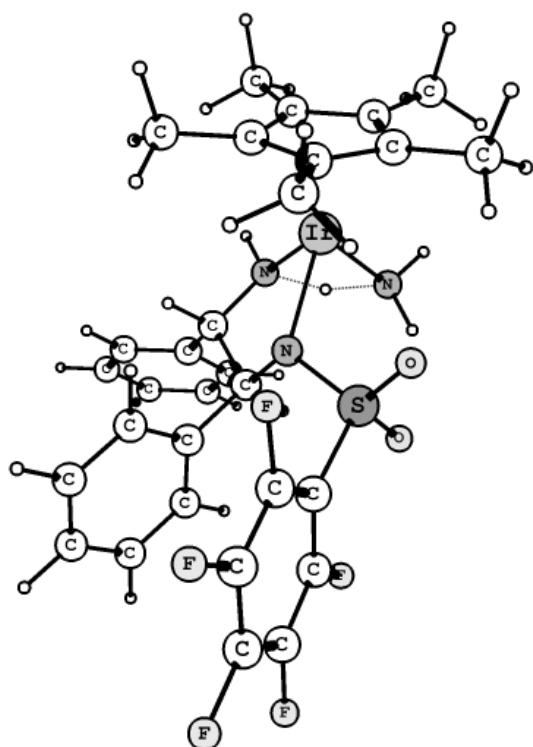
5a_R (δ -isomer)



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8	-0.489319000	-1.153344000	-2.367603000
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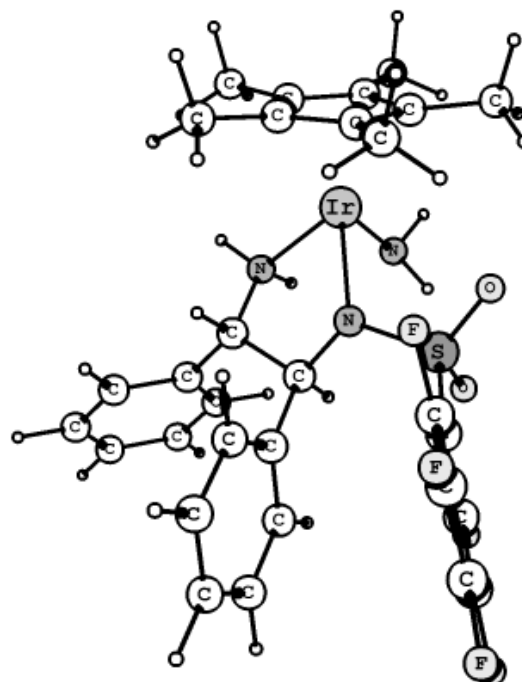
TS₄^R, ν 1442 cm⁻¹



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1	0.646774000	3.588991000	-2.023429000
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16	-0.745309000	-1.111831000	-1.309512000
8	-0.866856000	-0.505907000	-2.657256000
8	-0.176077000	-2.469776000	-1.256833000
77	2.207165000	-0.391152000	-0.196727000
6	2.946272000	-1.057243000	1.808231000
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6	2.418354000	-2.215486000	1.131198000
6	2.575334000	-0.580480000	3.183466000

6	4.165615000	-1.388622000	-0.168424000
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9	-4.189025000	-3.190610000	1.917134000
9	-6.326214000	-2.138576000	0.581599000
7	2.152868000	0.317690000	-2.220700000
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5b_R (λ-isomer)

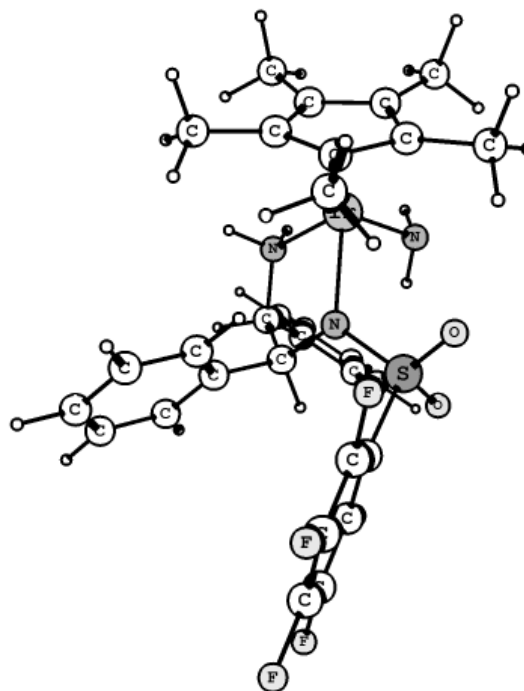


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1	-5.179172000	2.448825000	1.975764000
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8	-0.195905000	-2.497509000	-1.175841000
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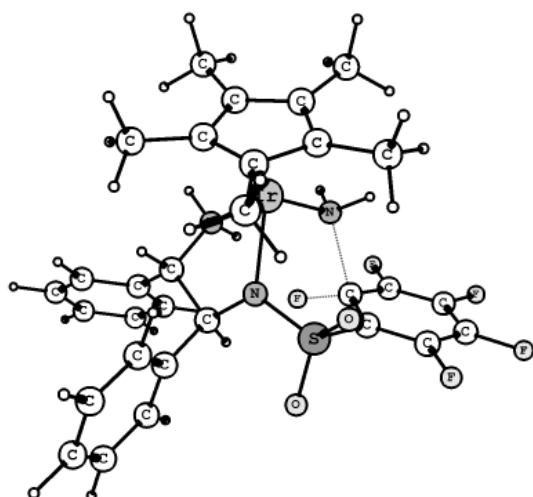
5b_R (δ -isomer)



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8	-0.991698000	1.249136000	-2.485948000
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6	1.679365000	4.355975000	1.074188000
6	0.356352000	3.724946000	-0.840948000
6	1.970664000	5.584437000	0.481543000
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1	2.590107000	6.304443000	1.009237000
1	0.230785000	5.188954000	-2.411213000
1	1.670553000	6.848808000	-1.243341000
6	-2.660964000	-0.272155000	-1.166396000

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6	-4.467961000	-1.809024000	-0.592405000
6	-5.361489000	-0.748517000	-0.488901000
9	-2.332934000	-2.633100000	-0.974646000
9	-4.888307000	-3.059794000	-0.369887000
9	-6.636945000	-0.973907000	-0.169983000
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9	-3.219414000	2.057464000	-1.199628000
7	2.435363000	0.928301000	-1.630387000
1	1.732326000	1.668612000	-1.615501000
1	3.306100000	1.402154000	-1.372761000
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TS₆^R, i235 cm⁻¹

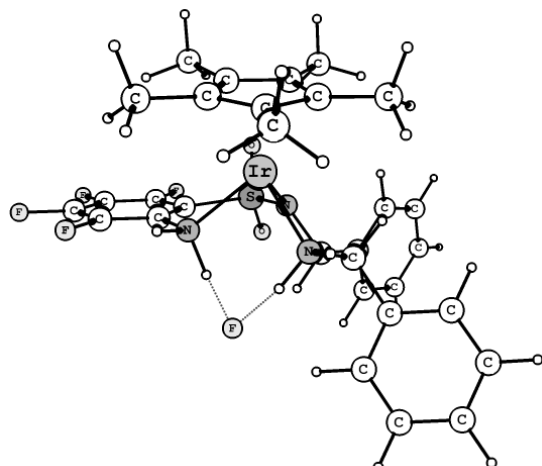


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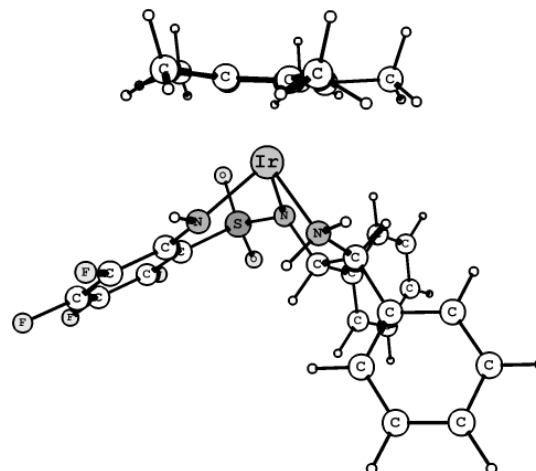
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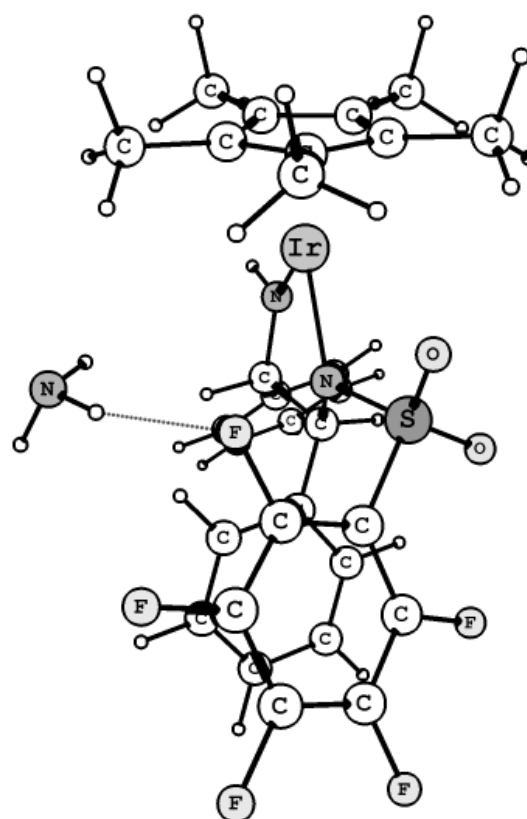
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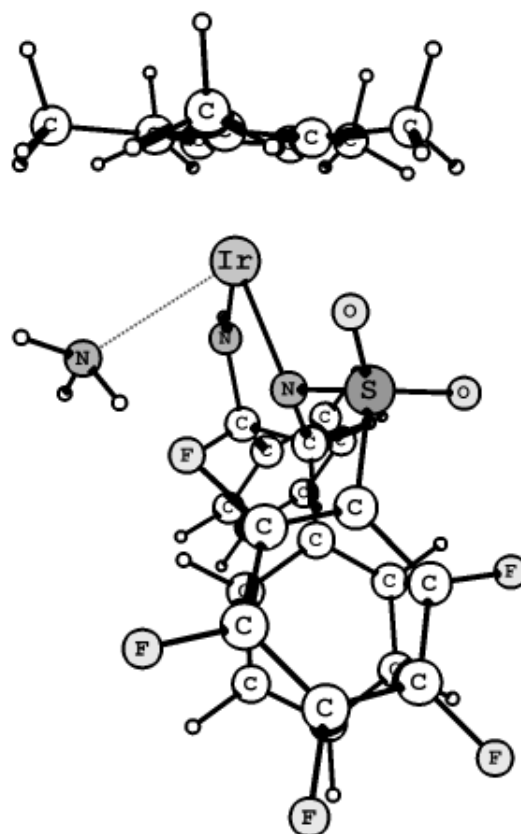
5s⁺NH₃



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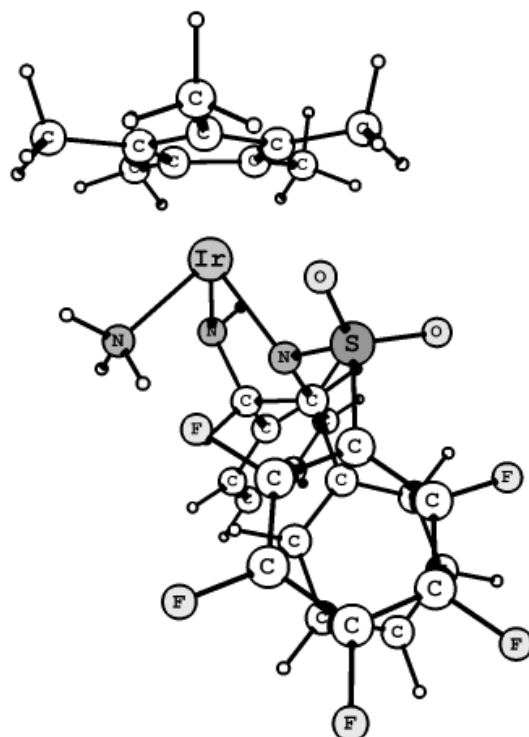
TS₂^S, *i*167 cm⁻¹



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6	4.454833000	2.556923000	-0.545826000
1	4.421319000	3.357744000	1.457065000
1	4.175967000	1.657422000	-2.488891000
1	-0.805084000	7.420689000	0.187690000
1	5.473982000	2.875627000	-0.747291000
16	0.824407000	-1.064070000	1.202786000
8	0.956201000	-0.453737000	2.541557000
8	0.286716000	-2.434278000	1.132250000
77	-2.124863000	-0.442904000	-0.164307000
6	-3.677844000	-1.879441000	-0.849145000

6	-4.269375000	-0.700824000	-0.252762000
6	-2.908756000	-2.578562000	0.151027000
6	-3.921070000	-2.349483000	-2.250688000
6	-3.817799000	-0.646768000	1.124678000
6	-5.255530000	0.223824000	-0.904720000
6	-2.980336000	-1.820762000	1.364340000
6	-2.250217000	-3.914265000	-0.031508000
1	-4.842979000	-2.945856000	-2.283786000
1	-4.040027000	-1.511165000	-2.941579000
1	-3.103605000	-2.976061000	-2.613366000
6	-4.290755000	0.313809000	2.175595000
1	-5.074656000	0.309624000	-1.979985000
1	-6.279721000	-0.146524000	-0.765948000
1	-5.208452000	1.229047000	-0.475707000
6	-2.453394000	-2.227200000	2.707135000
1	-2.966799000	-4.721016000	0.175195000
1	-1.891450000	-4.048067000	-1.056482000
1	-1.398064000	-4.026629000	0.638872000
1	-5.171240000	-0.096631000	2.688461000
1	-3.520124000	0.495881000	2.929672000
1	-4.576884000	1.276420000	1.743481000
1	-3.226502000	-2.790934000	3.247612000
1	-1.565642000	-2.852239000	2.613925000
1	-2.192768000	-1.356802000	3.315875000
6	2.530445000	-1.279243000	0.569826000
6	2.716891000	-1.951827000	-0.642392000
6	3.676080000	-0.879293000	1.263275000
6	3.980168000	-2.212576000	-1.157216000
6	4.951976000	-1.133438000	0.759081000
6	5.106265000	-1.803449000	-0.447829000
9	6.326789000	-2.049592000	-0.929111000
9	4.120194000	-2.853932000	-2.323887000
9	6.032431000	-0.735721000	1.441897000
9	3.618745000	-0.231071000	2.429062000
9	1.665574000	-2.361164000	-1.373089000
7	-0.893158000	-0.882312000	-2.660816000
1	-1.050142000	-1.622756000	-3.343530000
1	-0.872176000	-0.000317000	-3.169374000

5a_S (λ -isomer)



7	-1.909577000	1.525706000	-0.739111000
1	-0.190145000	-0.871559000	-2.149599000
1	-2.443062000	2.018607000	-0.022369000
6	-0.536306000	2.038116000	-0.685625000
6	0.328387000	1.307687000	0.384896000
1	-0.060960000	1.815306000	-1.649861000
6	-0.528309000	3.551270000	-0.520343000
1	-0.028388000	1.595938000	1.383055000
7	0.051264000	-0.142777000	0.160669000
6	1.790715000	1.718315000	0.269783000
6	-0.113097000	4.378554000	-1.572673000
6	-0.971637000	4.158151000	0.666113000
6	2.439866000	2.309515000	1.361757000
6	2.505591000	1.580174000	-0.932193000
6	-0.136176000	5.770093000	-1.448946000
1	0.233632000	3.926485000	-2.499115000
6	-0.996084000	5.548183000	0.795118000
1	-1.300169000	3.543420000	1.500830000
6	3.762519000	2.749645000	1.263757000
1	1.903212000	2.421075000	2.300304000
6	3.826222000	2.017161000	-1.035050000
1	2.031950000	1.116587000	-1.793103000
6	-0.577844000	6.360281000	-0.262836000
1	0.190795000	6.391156000	-2.278919000
1	-1.339965000	5.996984000	1.723445000
6	4.461172000	2.605050000	0.063917000
1	4.245178000	3.202742000	2.125711000
1	4.361058000	1.899440000	-1.973988000
1	-0.596258000	7.442172000	-0.162624000
1	5.489932000	2.945763000	-0.016368000
16	0.829550000	-1.175291000	1.142719000
8	1.006560000	-0.671616000	2.519564000
8	0.268831000	-2.530939000	0.983789000
77	-2.087810000	-0.508022000	-0.290283000
6	-3.829102000	-1.849654000	-0.630501000
6	-4.260422000	-0.559376000	-0.146112000
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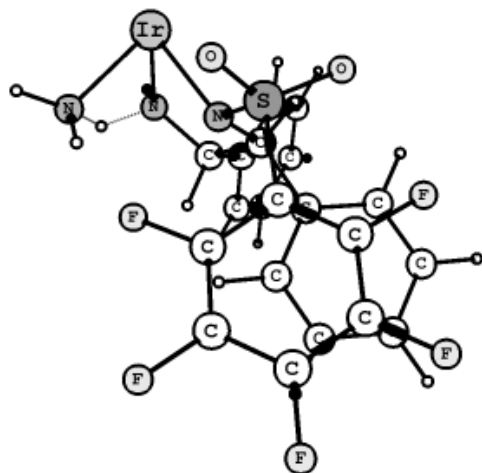
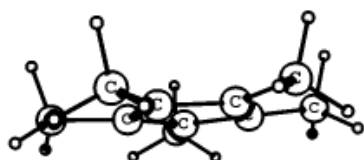
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6	-2.534152000	-3.909252000	0.355501000
1	-5.136036000	-3.055763000	-1.820477000
1	-4.420245000	-1.702713000	-2.704432000
1	-3.446306000	-3.135296000	-2.324299000
6	-4.018032000	0.733312000	2.134737000
1	-5.212144000	0.246681000	-1.907065000
1	-6.244300000	0.195381000	-0.469907000
1	-4.976013000	1.422023000	-0.610241000
6	-2.338313000	-1.888549000	2.833124000
1	-3.276628000	-4.592051000	0.792113000
1	-2.344409000	-4.245234000	-0.668821000
1	-1.603729000	-4.006472000	0.916345000
1	-4.943661000	0.525031000	2.688242000
1	-3.218506000	0.878657000	2.866475000
1	-4.165168000	1.678918000	1.603383000
1	-3.087927000	-2.375124000	3.472312000
1	-1.482707000	-2.556646000	2.733501000
1	-2.005787000	-0.981529000	3.343884000
6	2.512160000	-1.369582000	0.442565000
6	2.643601000	-1.880015000	-0.852999000
6	3.688751000	-1.103871000	1.147754000
6	3.882002000	-2.104633000	-1.439268000
6	4.941330000	-1.325820000	0.573868000
6	5.040217000	-1.828566000	-0.717204000
9	6.238036000	-2.043646000	-1.265913000
9	3.968603000	-2.586098000	-2.685364000
9	6.053154000	-1.058988000	1.269976000
9	3.684476000	-0.618159000	2.391574000
9	1.558662000	-2.159301000	-1.599673000
7	-1.193132000	-0.721672000	-2.266611000
1	-1.568930000	-1.487038000	-2.825103000
1	-1.336831000	0.147128000	-2.783077000

5as (δ -isomer)

7	1.685476000	0.857955000	1.645097000
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6	-0.202360000	1.805628000	0.386373000
1	-0.362610000	2.526723000	-0.418952000
6	1.176409000	2.096883000	1.017890000
1	0.999313000	2.824690000	1.826114000
7	-0.143199000	0.431189000	-0.221160000
16	-1.043454000	0.208123000	-1.536116000
8	-1.167948000	1.436750000	-2.348553000
8	-0.641662000	-1.026115000	-2.233937000
6	-1.365357000	2.008480000	1.363523000
6	-2.557529000	2.577522000	0.889568000
6	-1.281478000	1.703220000	2.731265000
6	-3.644763000	2.796840000	1.739790000
1	-2.635799000	2.855596000	-0.158000000
6	-2.364313000	1.921806000	3.585874000
1	-0.346861000	1.321053000	3.130110000
6	-3.554809000	2.462344000	3.092240000
1	-4.556806000	3.237240000	1.345144000
1	-2.272740000	1.680034000	4.641873000
1	-4.396707000	2.634212000	3.757553000
6	2.166471000	2.787176000	0.072732000
6	3.210765000	3.529956000	0.648999000
6	2.095224000	2.731088000	-1.327169000
6	4.163709000	4.178480000	-0.138169000
1	3.270232000	3.609500000	1.733385000
6	3.043231000	3.385756000	-2.120832000
1	1.292033000	2.182615000	-1.807482000
6	4.083940000	4.107401000	-1.531846000

1	4.958217000	4.749975000	0.335143000
1	2.962304000	3.334157000	-3.203966000
1	4.817085000	4.618092000	-2.150516000
6	-2.777372000	-0.183976000	-1.031872000
6	-3.893537000	0.567894000	-1.412029000
6	-3.024923000	-1.342799000	-0.292466000
6	-5.187025000	0.182750000	-1.057499000
6	-4.303055000	-1.743825000	0.073272000
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9	-4.488168000	-2.859405000	0.788828000
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9	-6.232930000	0.929832000	-1.430829000
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1	2.676524000	1.010790000	1.837748000
77	1.538489000	-0.843946000	0.427989000
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6	2.510551000	-2.861986000	0.339130000
6	4.285912000	-1.834800000	1.993606000
6	2.717738000	-1.360563000	-1.419780000
6	4.627256000	0.169655000	-0.471829000
6	2.056605000	-2.583103000	-0.986893000
6	2.127609000	-4.057773000	1.161395000
1	5.225588000	-2.380401000	1.832436000
1	4.545819000	-0.817791000	2.302538000
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6	2.619519000	-0.774639000	-2.797038000
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1	4.340298000	0.935196000	-1.194667000
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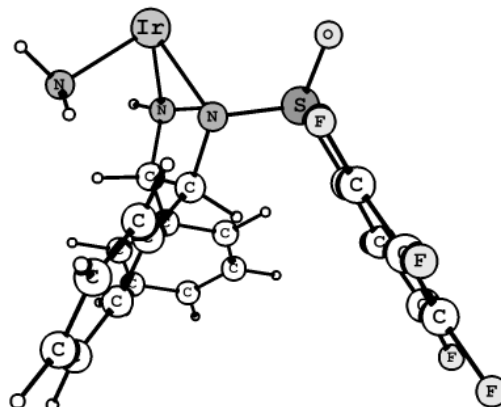
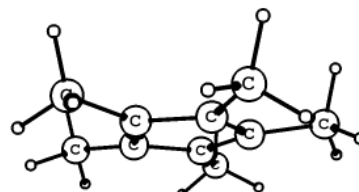
TS₄^S, $i1453\text{ cm}^{-1}$



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6	-0.880384000	3.390813000	-0.671423000
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6	-0.759857000	5.758953000	-1.226221000
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6	-2.045727000	5.041464000	0.687269000
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1	1.486735000	2.431687000	2.293095000
6	3.821768000	2.321698000	-0.793180000
1	2.217124000	1.304130000	-1.790343000
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1	-0.388991000	6.549713000	-1.872869000
1	-2.679470000	5.272802000	1.539361000
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1	4.473135000	2.285514000	-1.662348000
1	-1.843614000	7.101159000	0.071053000
1	5.262737000	3.346003000	0.448052000
16	0.929393000	-1.193478000	0.958240000
8	0.974612000	-0.708708000	2.353793000
8	0.492672000	-2.585329000	0.737607000
77	-2.013871000	-0.690319000	-0.337264000
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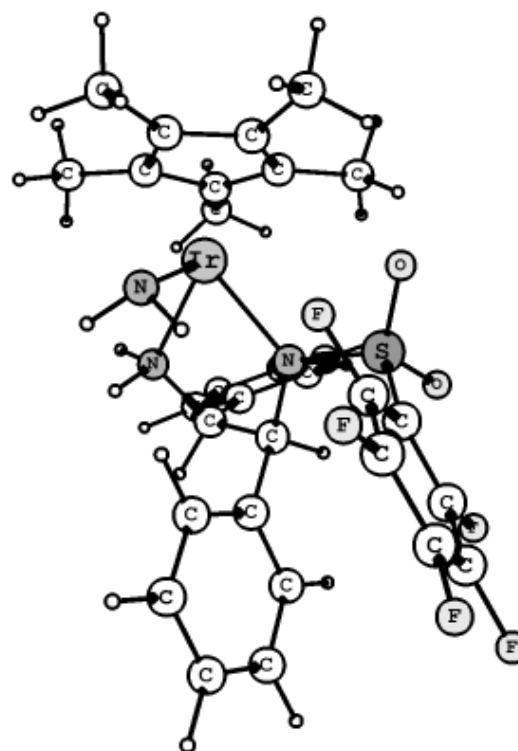
5bs (λ -isomer)



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6	-0.761663000	0.934088000	0.486870000
1	0.616906000	2.357233000	1.371013000
6	-0.400439000	3.434307000	-0.186676000
1	-1.567706000	1.125981000	-0.230133000
7	-0.073543000	-0.337044000	0.129634000

6	-1.435882000	0.852634000	1.864203000
6	-0.225555000	4.648206000	0.494406000
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6	-1.532151000	-0.357858000	2.563114000
6	-0.738570000	5.840665000	-0.021561000
1	0.313234000	4.657525000	1.439119000
6	-1.606937000	4.634118000	-1.924896000
1	-1.246152000	2.515892000	-1.956401000
6	-2.672039000	1.931191000	3.666074000
1	-1.985974000	2.944535000	1.906050000
6	-2.178955000	-0.422778000	3.801485000
1	-1.103222000	-1.251565000	2.125401000
6	-1.431048000	5.836594000	-1.234101000
1	-0.596436000	6.769578000	0.523978000
1	-2.145187000	4.622572000	-2.868816000
6	-2.749290000	0.721101000	4.360913000
1	-3.118009000	2.829921000	4.084193000
1	-2.237543000	-1.373683000	4.325009000
1	-1.832051000	6.762149000	-1.637830000
1	-3.252513000	0.671385000	5.322705000
16	-0.650741000	-0.965460000	-1.251037000
8	-0.571122000	-0.042149000	-2.410208000
8	-0.119101000	-2.322483000	-1.458679000
77	2.186950000	-0.195632000	0.185363000
6	3.873654000	-1.482204000	0.770941000
6	4.349338000	-0.255356000	0.153642000
6	3.101734000	-2.196679000	-0.204346000
6	4.219158000	-1.960904000	2.150086000
6	3.925846000	-0.286209000	-1.241367000
6	5.293211000	0.738815000	0.766417000
6	3.173477000	-1.473278000	-1.471676000
6	2.498052000	-3.557560000	-0.021432000
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1	4.388368000	-1.131184000	2.842695000
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6	2.720552000	-1.988778000	-2.806005000
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1	1.570164000	-3.647776000	-0.587229000
1	5.242506000	0.472908000	-2.747897000
1	3.533993000	0.806717000	-3.062493000
1	4.412384000	1.734043000	-1.833881000
1	3.490896000	-2.647447000	-3.231394000
1	1.792361000	-2.553857000	-2.719590000
1	2.556435000	-1.174661000	-3.518343000
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9	-4.539814000	-3.570642000	0.911923000
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9	-3.170134000	0.600567000	-2.318740000
9	-1.946937000	-3.034865000	0.525995000
7	1.868409000	0.548640000	2.127358000
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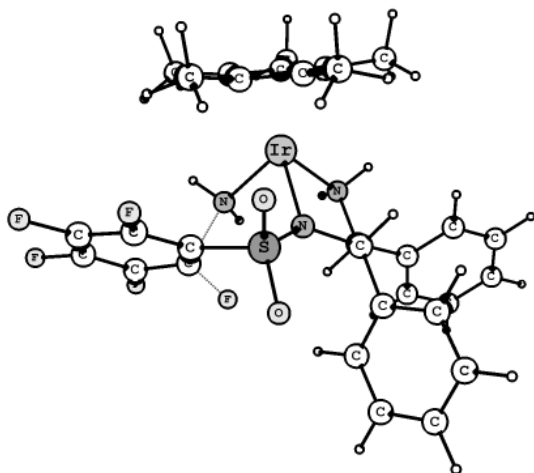
5bs (δ -isomer)



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6	2.490280000	2.902430000	-0.967789000
6	2.012986000	0.887579000	-2.196276000
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6	3.126676000	1.119744000	-3.006538000
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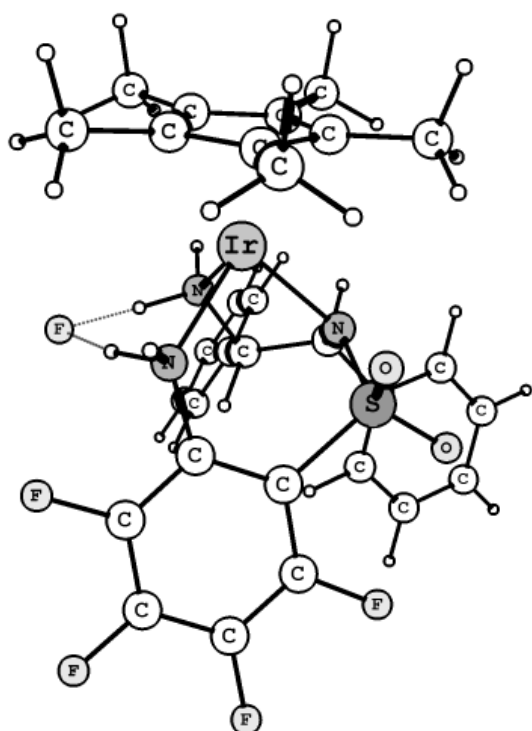
TS₆^S, i251 cm⁻¹



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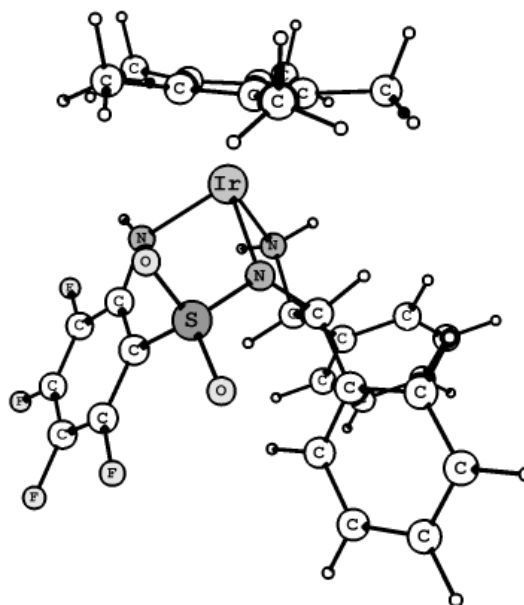
[7s-H]⁺F⁻



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6	4.664820000	-2.223718000	-2.590954000
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1	3.321497000	-5.346786000	3.537745000
1	5.615879000	-2.437243000	-3.071084000
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8	-0.587719000	1.814358000	-2.377437000
77	-1.753729000	-0.068893000	-0.013761000
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6	-3.263381000	-1.515187000	-0.658175000

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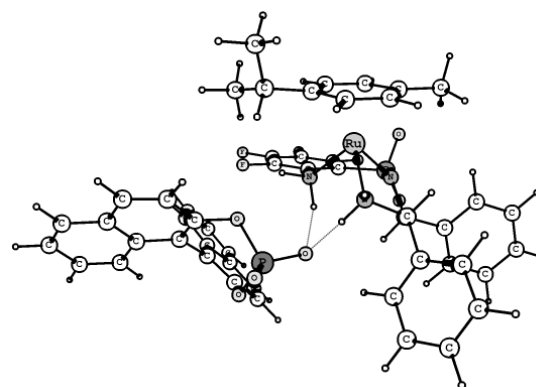
7_R



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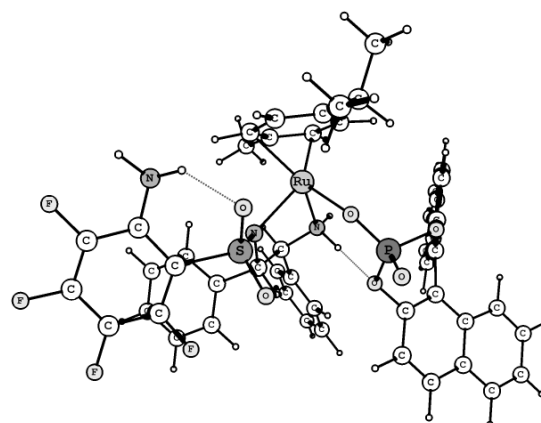
17_A (chloroform)



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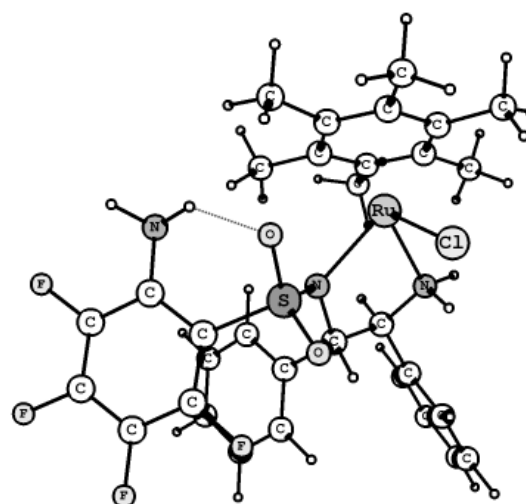
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Complex 12



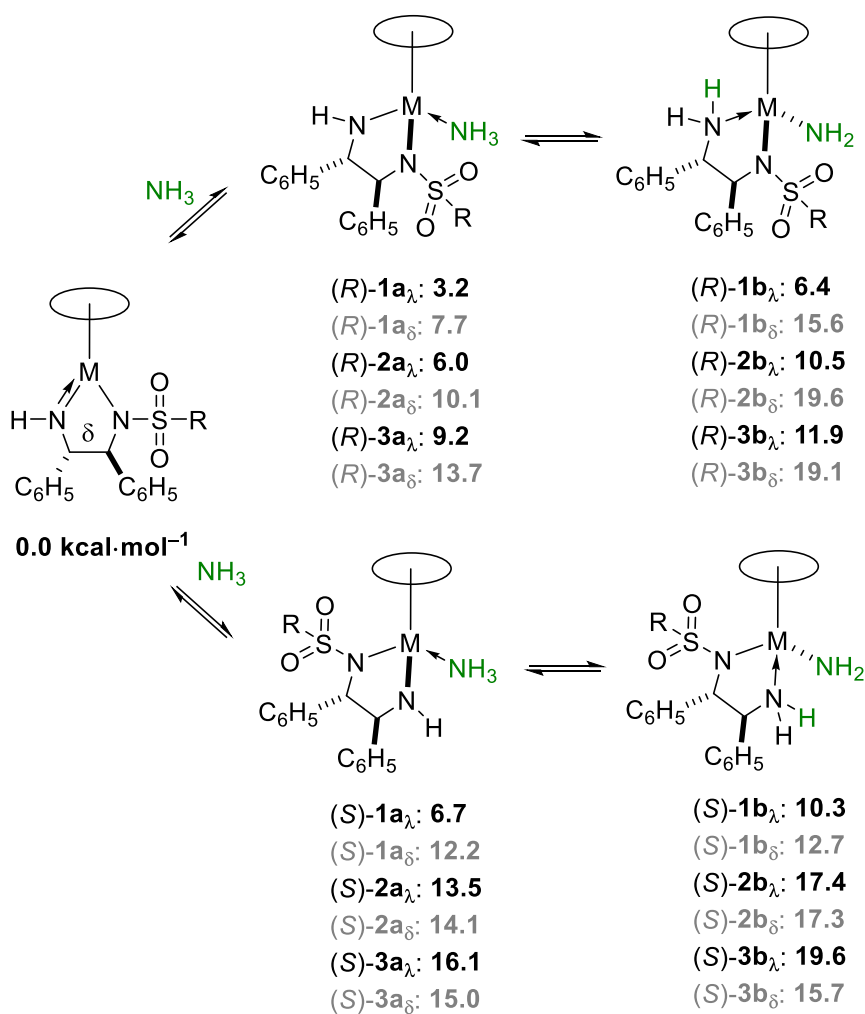
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1	-1.027743000	-3.375833000	0.112764000

7. Energy Data

7.1. Table of Energy Data (unit is Hartree or kcal/mol for ΔE or ΔG°_{298K} , 1 M) under DFT/ ω B97X-D/def2-TZVP/SMD(dichloromethane) level of theory.

	E	ΔE	G°_{298K} , 1 atm	G°_{298K} , 1M	ΔG°_{298K} , 1M
NH ₃	-56.56977949		-56.553471	-56.550461	
1	-1955.034584		-1954.512405	-1954.509395	
(R)-1a _λ	-2011.61696	-7.90	-2011.057834	-2011.054824	3.16
(R)-1a _δ	-2011.609801		-2011.05056	-2011.04755	7.72
(R)-1b _λ	-2011.612099		-2011.052732	-2011.049722	6.36
(R)-1b _δ	-2011.599051		-2011.03801	-2011.035	15.60
(S)-1a _λ	-2011.611795		-2011.052265	-2011.049255	6.65
(S)-1a _δ	-2011.604713		-2011.043403	-2011.040393	12.21
(S)-1b _λ	-2011.606926		-2011.046533	-2011.043523	10.25
(S)-1b _δ	-2011.604811		-2011.042703	-2011.039693	12.65
2	-2100.386077		-2099.915464	-2099.912454	
(R)-2a _λ	-2156.967442	-7.27	-2156.456347	-2156.453337	6.01
(R)-2a _δ	-2156.961662	-3.64	-2156.44987	-2156.44686	10.07
(R)-2b _λ	-2156.961554	-3.58	-2156.449195	-2156.446185	10.50
(R)-2b _δ	-2156.949336	4.09	-2156.434673	-2156.431663	19.61
(S)-2a _λ	-2156.954937	0.58	-2156.444451	-2156.441441	13.48
(S)-2a _δ	-2156.959197	-2.10	-2156.443396	-2156.440386	14.14
(S)-2b _λ	-2156.949757	3.83	-2156.438256	-2156.435246	17.36
(S)-2b _δ	-2156.95522	0.40	-2156.438367	-2156.435357	17.29
3	-2031.847103		-2031.421554	-2031.418544	
(R)-3a _λ	-2088.421353	-2.81	-2087.957421	-2087.954411	9.16
(R)-3a _δ	-2088.417887	-0.63	-2087.953062	-2087.950052	11.89
(R)-3b _λ	-2088.415207	1.05	-2087.950197	-2087.947187	13.69
(R)-3b _δ	-2088.413942		-2087.941589	-2087.938579	19.09
(S)-3a _λ	-2088.410864		-2087.946304	-2087.943294	16.13
(S)-3a _δ	-2088.417928		-2087.94805	-2087.94504	15.04
(S)-3b _λ	-2088.405661		-2087.940729	-2087.937719	19.63
(S)-3b _δ	-2088.413942		-2087.946589	-2087.943579	15.96



1_δ : Ru-(η^6 -*p*-cymene), R = *p*-CH₃C₆H₄

2_δ : Ru-(η^6 -hmb), R = CF₃

3_δ : Ir-(η^5 -Cp*), R = CF₃

$\Delta G^\circ_{298\text{K}}, 1 \text{ M}$

7.2. Table of Energy Data (unit is Hartree or kcal/mol for ΔE or $\Delta G^\circ_{298\text{K}}, 1 \text{ atm}$) under B3LYP31/SDD(Ru,Ir)/6-31G*(C,H,N,O,S,F,P)/C-PCM32(dichloromethane) level of theory.

	E	ΔE	E_{ZPVE}	$G^\circ_{298\text{K}} (1 \text{ atm})$	ν, cm^{-1}
NH₃	-56.55341224		-56.51888	-56.536923	
NH₃... NH₃	-113.1120148		-113.040684	-113.069489	
HF	-100.4251041		-100.416117	-100.432552	
1	-1954.810071		-1954.225273	-1954.296724	
1a	-2011.375031		-2010.750955	-2010.824676	
1b	-2011.36909		-2010.74502	-2010.817561	
2	-2100.093468		-2099.557156	-2099.626404	
2a	-2156.657326		-2156.082208	-2156.155117	
2b	-2156.650687		-2156.074864	-2156.145895	

3	-2031.543447		-2031.053709	-2031.121435	
3a	-2088.104496		-2087.575355	-2087.644816	
3b	-2088.098092		-2087.568486	-2087.637655	
4-ee (δ -isomer)	-2490.237427	0.00	-2489.66591	-2489.743035	
4-aa (λ -isomer)	-2490.237436	-0.01	-2489.6659	-2489.741185	
4_R·NH₃	-2546.795806	-3.12	-2546.187584	-2546.267867	
TS₁^R	-2546.786315	2.84	-2546.178306	-2546.256079	i155
4a_R (λ -isomer)	-2546.804364	-8.49	-2546.193475	-2546.270661	
4a_R (δ -isomer)	-2546.791633	-0.50	-2546.179985	-2546.256793	
4a_R···NH₃	-2603.365997	-10.39	-2602.717531	-2602.798742	
TS₃^R	-2546.788767	1.30	-2546.178545	-2546.255716	i1402
TS₃^R···NH₃	-2603.336188	8.32	-2602.70808	-2602.771238	i458
4b_R (λ -isomer)	-2546.796733	-3.70	-2546.185393	-2546.26145	
4b_R (δ -isomer)	-2546.780212	6.67	-2546.168469	-2546.245018	
4b_R···NH₃	-2603.356323	-4.32	-2602.70808	-2602.788856	
TS₅^R	-2546.778834	7.53	-2546.16727	-2546.241893	i231
[6^{hmb}_R·H]⁺F⁻	-2546.858052	-42.18	-2546.244115	-2546.317675	
6^{hmb}_R	-2446.394314		-2445.795523	-2445.869676	
4_S·NH₃	-2546.79461	-2.37	-2546.186635	-2546.267973	
TS₁^S	-2546.781383	5.93	-2546.173841	-2546.252777	i147
4a_S (λ -isomer)	-2546.796823	-3.76	-2546.186263	-2546.264118	
4a_S (δ -isomer)	-2546.790077	0.48	-2546.177955	-2546.252541	
TS₃^S	-2546.773911	10.62	-2546.167887	-2546.245462	i1420
4b_S (λ -isomer)	-2546.788865	1.24	-2546.177287	-2546.253582	
4b_S (δ -isomer)	-2546.787766	1.93	-2546.175192	-2546.249906	
TS₅^S	-2546.764005	16.84	-2546.152423	-2546.226332	i263
6^{hmb}_S·HF	-2546.836892	-28.90	-2546.224638	-2546.299768	
6^{hmb}_S	-2446.383828		-2445.785118	-2445.860007	
5-ee (δ -isomer)	-2421.687883	0.00	-2421.162966	-2421.237952	
5-aa (λ -isomer)	-2421.687809	0.05	-2421.163493	-2421.23866	
5_R·NH₃	-2478.246299	-3.14	-2477.684707	-2477.763184	
TS₂^R	-2478.235056	3.92	-2477.673194	-2477.750287	i168
5a_R (λ -isomer)	-2478.250543	-5.80	-2477.686382	-2477.762043	
5a_R (δ -isomer)	-2478.239155	1.34	-2477.674984	-2477.752556	
TS₄^R	-2478.229626	7.32	-2477.67006	-2477.745567	i1442
5b_R (λ -isomer)	-2478.243317	-1.27	-2477.679006	-2477.754692	
5b_R (δ -isomer)	-2478.22737	8.74	-2477.662227	-2477.737206	
TS₆^R	-2478.225953	9.63	-2477.660699	-2477.733447	i235
[7_R·H]⁺F⁻	-2478.301596	-37.84	-2477.735375	-2477.808269	
7_R	-2377.839512	-14.63	-2377.2872	-2377.359462	

5_S·NH₃	-2478.244519	-2.02	-2477.683401	-2477.763281	
TS₂^S	-2478.229423	7.45	-2477.668774	-2477.746421	i167
5a_S (λ-isomer)	-2478.244919	-2.27	-2477.680982	-2477.75731	
5a_S (δ-isomer)	-2478.239137	1.35	-2477.674165	-2477.748528	
TS₄^S	-2478.221676	12.31	-2477.662116	-2477.736891	i1453
5b_S (λ-isomer)	-2478.230867	6.54	-2477.666067	-2477.741826	
5b_S (δ-isomer)	-2478.228834	7.82	-2477.663391	-2477.738027	
TS₆^S	-2478.211723	18.56	-2477.647337	-2477.721207	i251
[7_S·H]⁺F⁻	-2478.285914	-28.00	-2477.719948	-2477.79384	
7_R	-2377.82776	-7.26	-2377.276257	-2377.349464	
17_A (chloroform)	-3780.102797		-3779.212415	-3779.365797	
17_B (chloroform)	-3780.091096	7.34	-3779.201517	-3779.355975	

References

1. Dub, P. A.; Wang, H.; Matsunami, A.; Gridnev, I. D.; Kuwata, S.; Ikariya, T., C-F bond breaking through aromatic nucleophilic substitution with a hydroxo ligand mediated via water bifunctional activation. *Bull. Chem. Soc. Jpn.* **2013**, *86*, 557-568.
2. (a) Bennett, M. A.; Smith, A. K., ARENE RUTHENIUM(II) COMPLEXES FORMED BY DEHYDROGENATION OF CYCLOHEXADIENES WITH RUTHENIUM(III) TRICHLORIDE. *Journal of the Chemical Society-Dalton Transactions* **1974**, 233-241; (b) Komiya, S., *Synthesis of Organometallic Compounds: A Practical Guide*. Wiley: 2002.
3. Kang, J. W.; Moseley, K.; Maitlis, P. M., PENTAMETHYLCYCLOPENTADIENYL RHODIUM AND -IRIDIUM HALIDES. I. SYNTHESIS AND PROPERTIES. *J. Am. Chem. Soc.* **1969**, *91*, 5970-&.
4. Haack, K.-J.; Hashiguchi, S.; Fujii, A.; Ikariya, T.; Noyori, R., The catalyst precursor, catalyst and intermediate in the RuII-promoted asymmetric hydrogen transfer between alcohols and ketones. *Angew. Chem., Int. Ed. Engl.* **1997**, *36*, 285-288.
5. Ikariya, T.; Wang, H.; Watanabe, M.; Murata, K., Asymmetric Michael reactions of alpha-substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes. *J. Organomet. Chem.* **2004**, *689*, 1377-1381.
6. Matsunami, A.; Kayaki, Y.; Kuwata, S.; Ikariya, T., Nucleophilic Aromatic Substitution in Hydrodefluorination Exemplified by Hydrido-iridium(III) Complexes with Fluorinated Phenylsulfonyl-1,2-diphenylethylenediamine Ligands. *Organometallics* **2018**, *37*, 1958-1969.
7. Dub, P. A.; Wang, H.; Matsunami, A.; Gridnev, I. D.; Kuwata, S.; Ikariya, T., C-F Bond Breaking through Aromatic Nucleophilic Substitution with a Hydroxo Ligand Mediated via Water Bifunctional Activation. *Bull. Chem. Soc. Jap.* **2013**, *86*, 557-568.
8. We noted if the reagents were mixed directly under ammonia atmosphere and mixed for further 48 h, < 2% of the *S*-diastereomer were detected during the course of the reaction.
9. (a) Kohn, W.; Sham, L. J., Self-Consistent Equations Including Exchange and Correlation Effects. *Phys. Rev.* **1965**, *140*, A1133-A1138; (b) Hohenberg, P.; Kohn, W., Inhomogeneous Electron Gas. *Phys. Rev.* **1964**, *136*, B864-B871.
10. Chai, J.-D.; Head-Gordon, M., Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620.
11. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
12. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
13. Becke, A. D., DENSITY-FUNCTIONAL THERMOCHEMISTRY .3. THE ROLE OF EXACT EXCHANGE. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

14. Cossi, M.; Rega, N.; Scalmani, G.; Barone, V., Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. *J. Comp. Chem.* **2003**, *24*, 669-681.
15. Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
16. <http://www.gsic.titech.ac.jp/en>. Accessed on April 1st 2013.
17. Fukui, K., The path of chemical reactions - the IRC approach. *Acc. Chem. Res.* **1981**, *14*, 363-368.
18. Wolinski, K.; Hinton, J. F.; Pulay, P., Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. *J. Am. Chem. Soc.* **1990**, *112*, 8251-8260.
19. Pettersen, E. F.; Goddard, T. D.; Huang, C. C.; Couch, G. S.; Greenblatt, D. M.; Meng, E. C.; Ferrin, T. E., UCSF Chimera—A visualization system for exploratory research and analysis. *J. Comp. Chem.* **2004**, *25*, 1605-1612.
20. <http://www.chemcraftprog.com/index.html>. Accessed on January 11th 2019.
21. This crystal contains two crystallographically independent molecules.