Electronic Supplementary Information

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Abbreviations

COD = 1,5-cyclooctadiene

Cor = corrole trianion

KC_8 = potassium graphite

Mes = 2,4,6-trimethylphenyl or mesityl

Dipp = 2,6-diisopropylphenyl

Tipp = 2,4,6-triisopropylphenyl

DCP = 2,6-dichlorophenyl

BTF = 3,5-*bis*(trifluoromethyl)phenyl

TBP = 4-*tert*-butyl-phenyl

EA = ethyl acetate

KIE = kinetic isotope effect

General

ATR-FTIR spectra were recorded using a "Spectrum Two™" spectrometer (manufacturer: PerkinElmer; detector: $LiTaO_3$). Resonance Raman experiments were carried out according to the procedure reported elsewhere.[1,2] X-band EPR spectroscopy was performed using a Bruker EMXplus-10/12 instrument (microwave frequency: 9.27-9.60 GHz; power: 2-20 mW; power attenuation: 10-20 dB; ModAmp: 2-4 G; ModFreq: 100.00 kHz). NMR experiments were conducted using DPX-600, DPX-500, or DPX-400 spectrometer. UV-vis and GC-MS spectra were acquired by a Cary 8454 spectrometer and Agilent 7890B GC system (5977A MS detector; GC-MS temperature profile: 0-10 min: 60 ^{o}C, 10-20 min: 20 ^{o}C/min, 20-21 min: 260 ^{o}C), respectively, manufactured by Agilent Technologies. A maXis II UHR-TOF mass spectrometer (Bruker) was used to record HR-ESI-MS spectra.

The X-ray diffraction data were collected on a Bruker PLATINUM135 CCD detector with monochromated Cu-Kα radiation at 100 K or a Bruker SMART 1000 CCD detector with graphite monochromated Mo-Kα radiation. Cell refinement and data reduction were processed with the Protenum2 program package.[3] By using SHELXTL, the structure was solved with the ShelXS6 structure solution program using direct methods and refined with the XL refinement package using least squares minimization.[4] All non-hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms were included in idealized positions and refined with fixed geometry with respect to their carrier atoms.

All chemicals were used as received unless otherwise specified. ^{15}N-Sodium azide ($Na^{+}[^{15}N{\equiv}NN]^{-}$ & $Na^{+}[NN{\equiv}^{15}N]^{-}$; 98 atom%), D_2O, d_8-THF, C_6D_6 and $CDCl_3$ were purchased from Cambridge Isotope Laboratories. d_8-THF and C_6D_6 were dried over 3 and 4 Å molecular sieves, respectively (activated in a 350 ^{o}C furnace for 3 h and spontaneous cooling in a small antechamber of glovebox under dynamic vacuum for 2 h), followed by five freeze-thaw cycles. Benzene (pre-treated with conc. H_2SO_4 to remove any reductant(s)) was dried and distilled over Na cubes/benzophenone (deep blue in colour), followed by three freeze-thaw cycles and stored over 4 Å molecular sieves. Anhydrous THF (J & K Scientific) was deaerated by five freeze-thaw cycles and stirred with shiny Li granules (Merck, 99% trace metals basis without paraffin oil; 20% w/v) under argon for 48 h and stored over 3 Å molecular sieves. Pentane was stirred with shiny Li granules (10% w/v) under argon for 24 h and stored over 4 Å molecular sieves. All the anhydrous solvents were tested with a purple sodium ketyl indicator dissolved in THF (qualified solvents should result in no colour change upon mixing), similar to the literature procedure.[5] Potassium graphite (KC_8) was purchased from Strem Chemical, INC. and stored at -35 ^{o}C freezer inside the glovebox. $InCl_3$, benzaldehyde, 3,4,5,6-tetrachloro-1,2-benzoquinone (TCQ), 2,4,6-trimethylphenylboronic acid, 2,4,6-triisopropylphenylboronic acid, styrene, 1,1-diphenylethylene, *α*-methylstyrene, *cis*-stilbene, cyclohexene, cyclohexa-1,4-diene, triphenylphosphine, indane, tetralin, isochroman, indene, ferrocene, 4-*tert*-butyl-benzaldehyde, phthalane, 10% Pd on activated charcoal were used as received from commercial vendors without further purification. Pyrrole was freshly distilled prior to use for the synthesis of 5-phenyldipyrromethane. d_4-Tetralin (*ca*. 90% *d*-content at the benzylic positions) was prepared according to the literature method.[6] Except for the synthesis of 5-phenyldipyrromethane, corrole ligand and

$[Ru^{III}(^{t}Bu\text{-}Cor)]_2$, all the reactions were conducted using sealed Schlenk tubes, which were dried in a 120 ^{o}C oven overnight and subsequently placed into high-vacuum antechamber for further drying (16 h). The reactions involving the highly reducing species **2** were all performed using Pyrex® spinbars (dried in a similar way as glassware). 2-mL polypropylene centrifuge tubes (Thomas Scientific) were used for the preparation of **2** to remove (potassium) graphite whereas polytetrafluoroethylene (PTFE, 0.22 or 0.45 μm) filters were used for the purification of Ru(V)-arylimido species. Glass Pasteur pipettes and gas tight EPR tubes were dried in antechamber for 24 h and placed in a well-circulated glovebox for one week prior to use.

General procedure for EPR spectroscopy

A typical EPR sample was prepared by dissolving *ca*. 1.0 μmol of Ru(V)-imido corrole with dry and deaerated benzene and transferring the solution (total volume: 200-400 μL) to a gas-tight EPR tube inside a glovebox. For cryogenic samples, the tube was then taken out of the glovebox, followed by immersing into a liquid nitrogen bath until frozen. The frozen sample was placed in a sample holder of EPR instrument after removal of ice on the surface of EPR tube. Spectral simulation was carried out using the EasySpin toolbox.[7]

Synthesis of aryl azides

General method A (not applicable for terminal ^{15}N-labelling as C_{Ar}–N is not cleaved[8]): Aniline ($DippNH_2$, $BTFNH_2$, $DCPNH_2$, $TBPNH_2$ or $MesNH_2$) was diazotized using HCl(aq) + $NaNO_2$(aq) according to the reported procedure for preparation of aryl azides.[9] The aryl azide was obtained by extracting the reaction mixture with Et_2O four times (15 mL each). If applicable, the azide was further purified by column chromatography with silica as a stationary phase and *n*-hexane or EA/*n*-hexane as an eluent.

General method B (suitable for ^{15}N-labelling): According to another reported method for preparing aryl azides,[10] arylboronic acid ($MesB(OH)_2$ or $TippB(OH)_2$; 3 mmol) was dissolved in methanol (10 mL) containing $Cu(OAc)_2$ (0.3 mmol) and non-labelled NaN_3 (4.5 mmol; or ^{15}N-labelled NaN_3). The reaction mixture was stirred under aerobic conditions until a nearly colourless mixture was obtained. The mixture was concentrated to dryness under high vacuum prior to flash column chromatography with *n*-hexane as an eluent and silica as a stationary phase.

For characterization data of $DippN_3$,[11] $BTFN_3$,[9,12] $DCPN_3$,[13] $TBPN_3$,[14] $MesN_3$,[9,15] and $TippN_3$,[16] see the corresponding literature reports.

Synthesis of 5-phenyldipyrromethane

To an oven-dried two-neck round bottom flask, benzaldehyde (1.3 mL, 13 mmol) and pyrrole (40 mL, 580 mmol) were added and mixed thoroughly, followed by purging the solution with a positive argon flow for 10 min. After that, anhydrous $InCl_3$ (1.3 mmol) was added. The reaction mixture was stirred for 1.5 h prior to quenching by $NaOH_{(s)}$ (2.5 g, 63 mmol). The reaction was stirred for additional 45 min before quick

filtration and subsequent vacuum distillation at temperature not greater than 50 ^{o}C. The viscous mixture was first dissolved with minimal amount of MeOH, followed by precipitation with brine and then washed with deionized water 3 times. The beige solid obtained was then dried under high vacuum (84% yield).

5-Phenyldipyrromethane: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ 5.48 (s, 1H), 5.98 (s, 2H), 6.24 (d, 2H), 6.69 (s, 2H), 7.27 (d, 2H), 7.32−7.42 (m, 3H), 7.84 (s, 2H); FAB-MS ($C_{15}H_{14}N_2$, $[M]^+$): *m*/*z* 222.1. For other characterizations, please refer to the literature data.[17]

Synthesis of H_3(*t*Bu-Cor)

In a typical experiment, 5-phenyldipyrromethane (2 mmol, 444 mg) and 4-*tert*-butylbenzaldehyde (1 mmol) were dissolved in CH_2Cl_2 (250 mL). Under stirring, trifluoroacetic acid (0.015 mmol, 1.15 μL) was added with a syringe. The reaction was stirred at RT in the absence of light. After 5 h, the reaction mixture was treated with TCQ (3 mmol, 738 mg) dissolved in toluene, followed by stirring in the dark for 45 min. After removal of the volatile(s), the crude product was purified by silica gel column chromatography using CH_2Cl_2/*n*-hexane (v/v = 1:3; the first greenish band) as an eluent.

H_3(*t*Bu-Cor): Yield: 10%; ^{1}H NMR (400 MHz, $CDCl_3$, 298 K; aromatic protons resolved at <0.5 mM): δ 1.36 (s, 9H), 7.54-7.56 (d, 2H), 7.72-7.74 (t, 4H), 7.80-7.82 (t, 2H), 8.17-8.19 (d, 2H), 8.36-8.38 (d, 4H), 8.55-8.57 (d, 2H), 8.61-8.62 (d, 2H), 8.88-8.89 (d, 2H), 8.99-9.00 (d, 2H); FAB-MS ($C_{41}H_{34}N_4$, $[M]^+$): *m*/*z* 582.2; UV-vis (CH_2Cl_2): λ_{max} 421, 644 nm.

Synthesis of $[Ru^{III}$(*t*Bu-Cor)$]_2$ (1)

H_3(*t*Bu-Cor) (0.13 mmol) and $[Ru(COD)Cl_2]_n$ (0.26 mmol) were added to an oven-dried two-neck flask. The flask was evacuated and filled with argon for three times. Under argon atmosphere, 2-methoxyethanol (40 mL) was added and purged with a positive argon flow for deaeration. The reaction flask was immersed onto a pre-heated oil bath (135 ^{o}C), followed by addition of triethylamine (1 mL) when the solution started to boil. The reaction was terminated after 30 min. After that, the volatiles were removed under high vacuum. The crude product was purified by silica gel column chromatography using CH_2Cl_2/*n*-hexane (v/v = 1:3) as the eluent, giving the title compound as a black solid.

$[Ru^{III}$(*t*Bu-Cor)$]_2$ (**1**): Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K; integral per Ru corrole): δ 1.66 (s, 9H), 7.18 (d, 1H), 7.31 (br, 2H), 7.49−7.54 (m, 3H), 7.74 (t, 2H), 7.89−7.94 (m, 3H), 8.33 (d, 2H), 8.39 (d, 2H), 8.58 (d, 2H), 8.75 (d, 2H), 8.92 (d, 1H), 9.06 (s, 2H); UV-vis (THF): λ_{max} (ε x 10^{-4}): 329, 399, 538 nm; HR-ESI-MS ($C_{82}H_{62}N_8Ru_2$): *m*/*z* calcd for 1362.3157, found: 1362.3215; elemental analysis for $C_{82}H_{62}N_8Ru_2$•$2H_2O$•$2CH_2Cl_2$, calcd (found): C, 64.37 (64.48); H, 4.50 (4.37); N, 7.15 (7.20).

Synthesis of 2

To an oven-dried Schlenk tube (containing a Pyrex® spinbar) was added $[Ru^{III}(^{t}Bu\text{-}Cor)]_2$ (10 mg, 7.34 µmol) together with excess KC_8 (8 mg; 4 equiv). The flask was then charged with THF (anhydrous and rigorously deaerated, 4 mL). A glassy stopper equipped with a Glindemann PTFE sealing ring was used to seal the tube tightly (or a sealed tube could be used instead; the solution should not be in contact with parts made of PTFE). The red solution was stirred gently at RT overnight, followed by centrifugation using a mini centrifuge placed inside the glovebox to remove precipitate. The resulting brown solution was transferred to another Schlenk tube and evaporated to dryness under high vacuum inside the glovebox. If necessary, the solid was further washed with benzene (1 mL) until the benzene solution became colourless.

2 (assigned as $K_2[Ru(^{t}Bu\text{-}Cor)]_2$)**:** Yield: *7*6%. UV-vis (THF): λ_{max} 411, 445, 600 nm; effective magnetic moment (by Evans method): 2.81 μ_B (*S* = 1); elemental analysis for $K_2C_{82}H_{62}N_8Ru_2 \bullet 2C_4H_8O$, calcd (found): C, 68.24 (68.37); H, 4.96 (5.07); N, 7.07 (6.95). Titration of **2** with $[Cp_2Fe]PF_6$ generated 2 equiv. of Cp_2Fe and 1 equiv. of **1**.

Synthesis of Ru(V)-arylimido corroles (3)

Complex **2** (8 mg, 5.56 µmol) suspended in benzene (1 mL) was treated with ArN_3 (2.5 equiv; standard solution was prepared by dissolving 138 µmol ArN_3 in 1000 µL benzene). The reaction was stirred for several minutes using Pyrex® spinbar (0.5 h is needed for ArN_3 with Ar = Dipp, Tipp). After that, the solution was filtered using a syringe equipped with PTFE filter (pore size: 0.22 µm). The solvent was removed under high vacuum inside a glovebox. For preparing **3d**, it was first washed with chilled 1:1 benzene/pentane solution (pre-equilibrated at -35 ^{o}C freezer overnight), followed by pentane. For other hydrophobic complexes, they were all washed by chilled pentane twice to minimize sample loss (-35 ^{o}C). The undissolved solid was subjected to high vacuum for further drying. All the Ru(V)-imido species were freshly prepared as they underwent gradual decomposition upon standing overnight, particularly in solution state. The effective magnetic moments of **3a-3d** were consistently determined to be *ca*. 1.73 μ_B (*S* = 1/2; by Evans method) by dissolving the freshly prepared samples in C_6D_6.

[Ru^{V}(*t*Bu-Cor)(NMes)] (**3a**)**:** Yield: 36%. UV-vis (benzene): λ_{max} 411, 587 nm; HR ESI-MS: *m*/*z* Calcd for $C_{50}H_{42}N_5Ru$ (M^+): 814.2492, found: 814.2479; Elemental analysis for $C_{50}H_{42}N_5Ru$, calcd. (found): C, 74.36 (74.01); H, 5.20 (5.34); N, 8.60 (8.72).

[Ru^{V}(*t*Bu-Cor)(NDipp)] (**3b**)**:** Yield: 32**%**. UV-vis (benzene): λ_{max} 411, 580 (sh) nm; HR ESI-MS: *m*/*z* Calcd for $C_{53}H_{48}N_5Ru$ (M^+): 856.2953, found: 856.2975; Elemental analysis for $C_{53}H_{48}N_5Ru$, calcd. (found): C, 74.36 (74.39); H, 5.55 (5.62); N, 8.18 (8.24).

[Ru^{V}(*t*Bu-Cor)(NTipp)] (**3c**)**:** Yield: 25**%.** UV-vis (benzene): λ_{max} 407, 580 (sh) nm; HR ESI-MS m/z Calcd

for $C_{56}H_{54}N_5Ru$ (M^+): 898.3423, found: 898.3423; Elemental analysis for $C_{56}H_{54}N_5Ru$, calcd. (found): C, 74.89 (74.94); H, 6.06 (6.20); N, 7.80 (7.94).

[Ru^V(^{t}Bu-Cor)(NBTF)] (**3d**)**:** Yield: 32%. UV-vis (benzene): λ_{max} 406, 580 nm; MADLI-TOF MS: *m*/*z* Calcd for $C_{49}H_{34}F_6N_5Ru$ (M^+): 908.176, found: 907.961; Elemental analysis for $C_{49}H_{34}F_6N_5Ru$, calcd. (found): C, 64.82 (64.78); H, 3.77 (3.83); N, 7.71 (7.80).

General procedure of stoichiometric aziridination/C–H amination

In an argon-filled glovebox, an oven-dried seal tube was charged with Ru(V)-imido corrole complex **3** (5.50 μmol), substrate (1.65 mmol) and benzene (1 mL) sequentially. The tube was then sealed tightly, and heating was performed using a pre-equilibrated hot plate (85 ^oC) placed in a fumehood. After 24 h, the reaction mixture was cooled to RT, followed by quantitative analysis. The quantification methods, according to different volatility/thermostability of products, are depicted as follows:

Entry[a]	Qualitative and quantitative analyses
1	^{1}H NMR
2	GC-MS, ^{1}H NMR and ^{19}F NMR
3, 4	^{1}H, ^{19}F NMR
6	GC-MS (compare with authentic standard)
5, 7, 8, 9, 10, 11	GC-MS, ^{19}F NMR

[a] Corresponding to the same entries in the Table 1 of the main text.

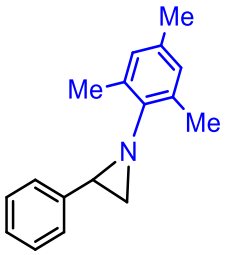
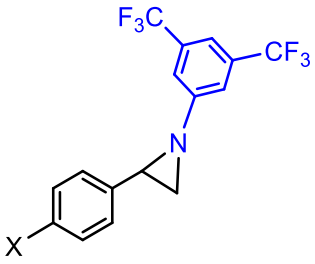
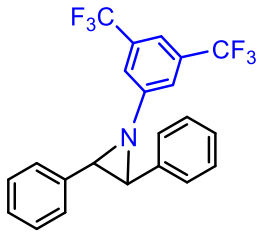
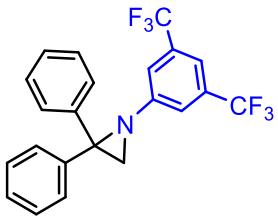
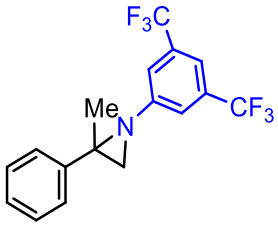
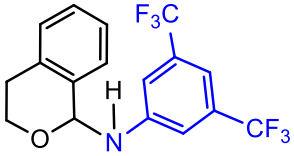
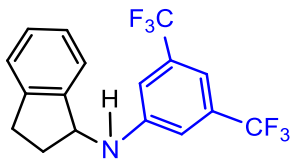
Aziridine characterization

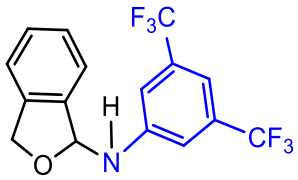
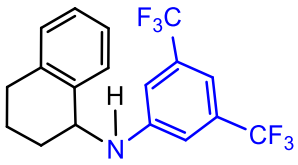
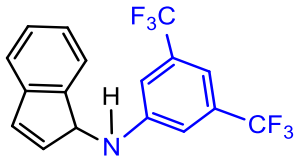
1-(3,5-Bis(trifluoromethyl)phenyl)-2-(4-chlorophenyl)aziridine: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K): δ 2.48-2.50 (d, 1H), 2.56-2.58 (d, 1H), 3.19-3.22 (dd, 1H), 7.30-7.32 (d, 2H), 7.34-7.36 (d, 2H), 7.41 (s, 2H), 7.49 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K): δ 38.15, 41.36, 116.16 (q, $J_{H\text{-}F}$ = 3 Hz), 120.59, 122.23 (q, $J_{H\text{-}F}$ = 271 Hz), 127.43, 128.86, 132.17 (q, $J_{H\text{-}F}$ = 33 Hz), 133.71, 136.46, 155.44; ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ -63.4; HR EI-MS: *m*/*z* Calcd for $C_{16}H_9ClF_6N$ ([M – H]$^+$): 364.0328, found: 364.0328; GC-MS (EI; [M – H]$^+$): 364 (t_R = 18.967 min).

1-(3,5-Bis(trifluoromethyl)phenyl)-2-(4-(trifluoromethyl)phenyl)aziridine: ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 2.52-2.53 (d, 1H), 2.61-2.63 (d, 1H), 3.27-3.29 (dd, 1H), 7.42 (s, 2H), 7.50-7.52 (m, 3H), 7.64-7.66 (d, 2H); ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ -62.05, -63.03; ^{13}C NMR (125 MHz, 298 K): δ 38.30, 41.36, 116.31 (q, $J_{H\text{-}F}$ = 3 Hz), 120.55, 122.00 (q, $J_{H\text{-}F}$ = 271 Hz), 122.96 (q, $J_{H\text{-}F}$ = 271 Hz), 125.56 (q, $J_{H\text{-}F}$ = 3 Hz), 126.45, 130.01 (q, $J_{C\text{-}F}$ = 33 Hz), 132.42 (q, $J_{C\text{-}F}$ = 33 Hz), 142.03, 155.20. HR EI-MS: *m*/*z* Calcd for $C_{17}H_9F_9N$ ([M – H]$^+$): 398.0591, found: 398.0592; GC-MS (EI; [M]$^+$): 398 (t_R = 17.928 min).

1-(3,5-Bis(trifluoromethyl)phenyl)-2-(4-fluorophenyl)aziridine: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K): δ 2.48-2.49 (d, 1H), 2.55-2.56 (d, 1H), 3.21-3.22 (dd, 1H), 7.06-7.08 (d, 2H), 7.33-7.34 (d, 2H), 7.42 (s, 2H), 7.49 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K): δ 38.06, 41.38, 115.51, 115.66, 116.19 (q, J_{H-F} = 3 Hz), 120.61, 124.07 (q, J_{H-F} = 271 Hz), 127.67, 132.37 (q, J_{H-F} = 33 Hz), 133.61,155.57; ^{19}F NMR (376 MHz, $CDCl_3$, 298 K): δ -62.99, -114.37; HR EI-MS: *m*/*z* Calcd for $C_{16}H_9F_7N$ ($[M - H]^+$): 349.0701, found: 349.0710.

References for the reported compounds

Compound	Reference
	9
	X = H, Br 19,19 X = Me 18
	20
	19
	19,21
	22a
	22b

	20
	20,22b
	23

Hammett analysis

In an argon-filled glovebox, an oven-dried seal tube was charged with Ru(V)-imido corrole complex **3e** (5.50 μmol), styrene + *para*-substituted styrene *p*-X-$C_6H_4CH=CH_2$ (0.0825 mmol each) and benzene (1 mL) sequentially. The tube was then sealed tightly, and heating was performed using a pre-equilibrated hot plate (85 ^oC). After 24 h, the reaction mixture was cooled to RT and concentrated by *ca*. 10 times. The product ratio was determined by GC-MS.

The values for the dual-parameter Hammett plot are shown as follows:

Substituent X in *p*-X-$C_6H_4CH=CH_2$	$\sigma_{JJ}^{\bullet}$	σ_{mb} [a]	k_{rel}	log (k_{rel})
H	0	0	1	0.00
Me	0.15	-0.29	1.99	0.21
Cl	0.22	0.11	1.09	0.04
Br	0.23	0.13	1.04	0.02
CF_3	-0.01	0.49	0.52	-0.28

[a] Values from literature report.[24]

KIE experiment

The procedure is similar to that for the Hammett analysis, except that equimolar amounts of tetralin and d_4-tetralin, instead of styrenes, were used. The product ratio was determined by GC-MS.

Computational details

DFT (density functional theory) and CASSCF (complete active space self-consistent field) calculations were performed using Gaussian 09 Revision D.01 (Gaussian Inc., Wallingford CT, **2013**). Geometries were optimized using the B3LYP functional[25,26] with a mixed basis set (BSI) combining the SDD pseudopotential and corresponding basis set[27,28] for Ru and the all-electron 6-31G* basis set for other atoms. Frequency calculations were carried out at the same B3LYP/BSI level. Raman spectra (scaled by 0.9520), spin density plots and bond order were generated by using Multiwfn.[29] Solvent effect was included by means of the polarizable continuum model (PCM).[30] In the reaction mechanism calculations, single-point energy correction with a larger basis set 6-311G** for C, H, N and F was used. The EPR *g*-tensors calculations were performed by ADF2014 [31] based on Gaussian 09 optimized structures.

For the CASSCF calculations, an active space consisting of 11 orbitals and 9 electrons was employed, which would yield a total of 10584 electronic configurations to describe the Ru(V)-arylimido species. Specifically, the active space used to give a balanced description of metal-ligand interactions involves the non-bonding d_{xy} orbital of Ru, σ and σ* orbitals between Ru-d_{z^2} and N-p_z, two sets of π and π* orbitals between Ru-$d_{xz/yz}$ and N-$p_{x/y}$, and a pair of π and π* orbitals of the corrole ligand. The ground state configuration reveals a major electronic occupation of $(d_{xy})^2(d_{\pi(xz)})^2(d_{\pi(yz)})^2(d_{\sigma})^2(d_{\pi(xz)^*})^1(d_{\pi(yz)^*})^0(d_{\sigma^*})^0$ (CI vector, -0.927), and a minor electronic occupation of $(d_{xy})^2(d_{\pi(xz)})^2(d_{\pi(yz)})^2(d_{\sigma})^2(d_{\pi(yz)^*})^1(d_{\pi(xz)^*})^0(d_{\sigma^*})^0$ (CI vector, 0.188). The major one with singly occupied molecular orbital (SOMO) located on $d_{\pi(xz)^*}$ shows a greater metal-based character (Ru 48.1% *vs* N_{imido} 36.2%), while the minor one with SOMO located on $d_{\pi(yz)^*}$ is more characteristic of N_{imido}-based radical (Ru 44.9% *vs* N_{imido} 47.3%). Therefore, it can be concluded that the ground state of **3b** exhibits a major Ru^{V}=NAr configuration with a minor Ru^{IV}–•NAr contribution.

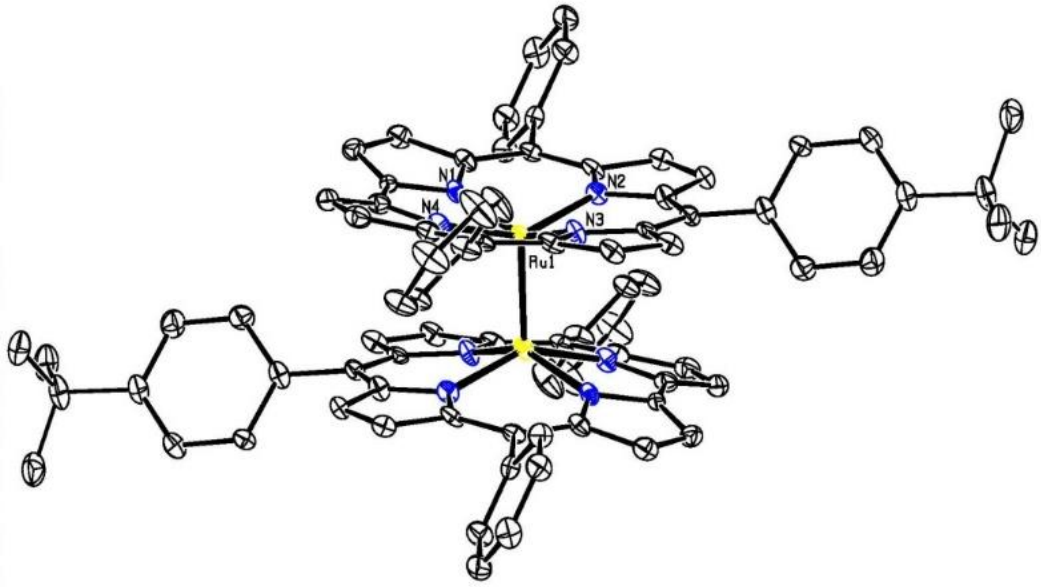


Fig. S1 ORTEP drawing of **1** at ellipsoid probability level of 30% (hydrogen atoms and solvent molecules were omitted).

Table S1 X-ray crystallographic data of **1**.

Empirical formula	$C_{82}H_{62}N_8Ru_2 \cdot 2CH_2Cl_2$
Formula weight	1531.38
T [K]	100
Wavelength [Å]	1.54178
Crystal system	monoclinic
Space group	$P2_1/c$
a [Å]	10.4207(6)
b [Å]	12.7439(7)
c [Å]	26.3116(13)
α [°]	90
β [°]	93.427(2)
γ [°]	90
V [Å^3]	3487.9(2)
Z	2
ρ [g cm^{-3}]	1.458
μ [mm^{-1}]	5.329
F(000)	1564.0
2θ range [°]	6.73 to 135.376
Index ranges	$-12 \le h \le 12$, $0 \le k \le 14$, $0 \le l \le 31$
Reflections collected	5478
Independent reflections	5478
Completeness	0.867
restraints	81
Goodness-of-fit on F^2	1.090
R_1 (all data)	0.0842
wR_2 (all data)	0.1879

Table S2 Selected bond distances (Å) and angles (°) of **1**.

Ru_1-Ru_1^1	2.1842(15)	Ru_1-N_4	1.969(8)
Ru_1-N_1	1.982(7)	Ru_1-N_3	1.992(7)
Ru_1-N_2	1.996(7)		
N_1-Ru_1-Ru_1^1	105.5(2)	N_1-Ru_1-N_2	88.0(3)
N_1-Ru_1-N_3	150.2(3)	N_2-Ru_1-Ru_1^1	103.5(2)
N_3-Ru_1-Ru_1^1	103.5(3)	N_3-Ru_1-N_2	91.9(3)
N_4-Ru_1-Ru_1^1	105.8(2)	N_4-Ru_1-N_1	78.4(3)
N_4-Ru_1-N_2	150.1(3)	N_4-Ru_1-N_3	87.3(3)
C_1-N_1-Ru_1	116.9(6)	C_4-N_1-Ru_1	131.5(6)
C_{12}-N_2-Ru_1	126.3(5)	C_{15}-N_2-Ru_1	124.7(6)
C_{27}-N_3-Ru_1	123.4(6)	C_{30}-N_3-Ru_1	126.4(6)
C_{38}-N_4-Ru_1	132.7(7)	C_{41}-N_4-Ru_1	117.2(6)

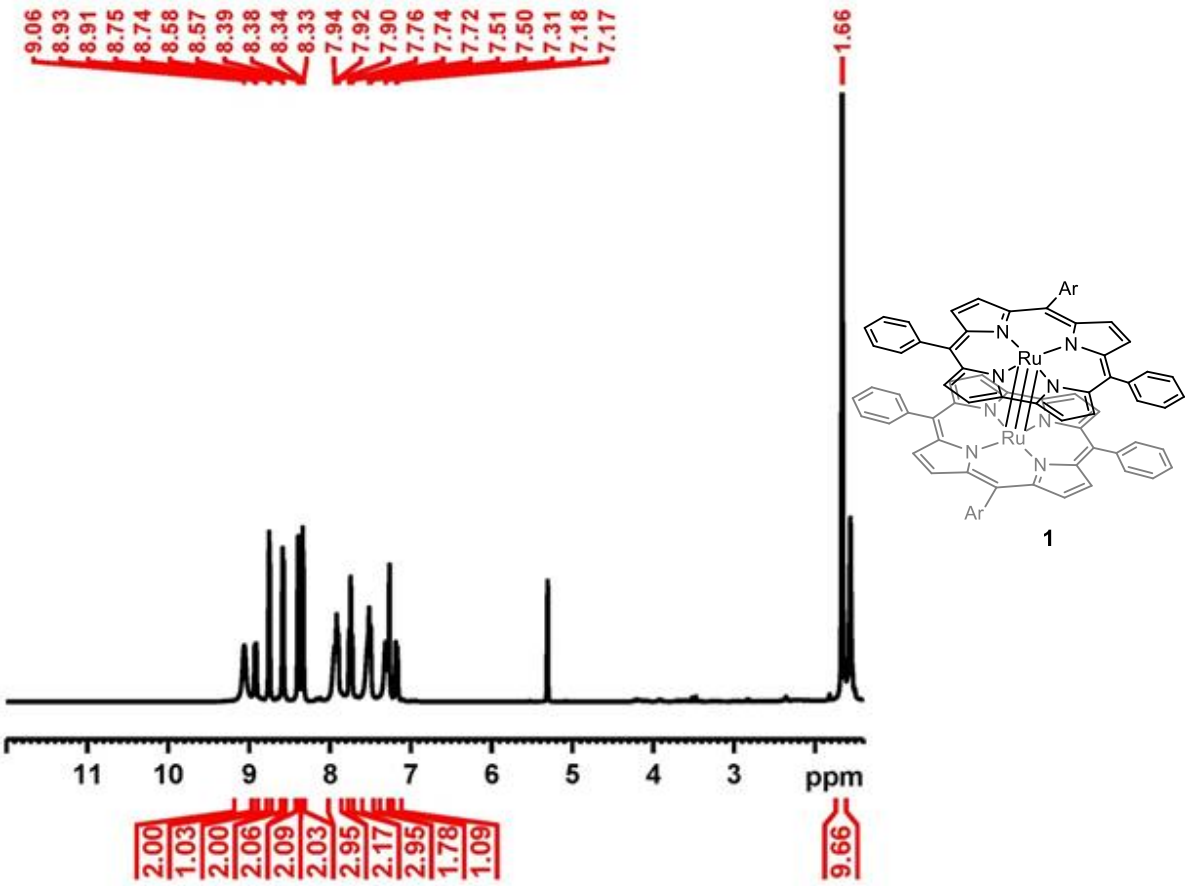


Fig. S2 ^{1}H NMR spectrum of **1** in $CDCl_3$ at 298 K.

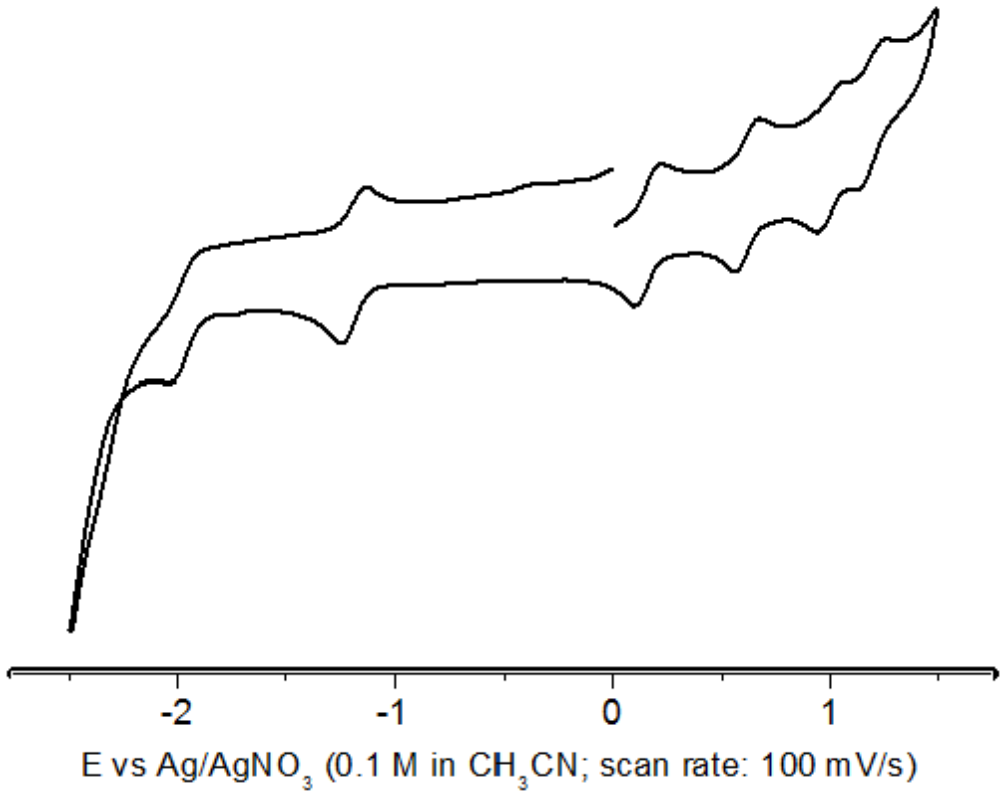


Fig. S3 Cyclic voltammogram of **1** in CH_2Cl_2 at 298 K with 0.1 M [^{n}Bu$_4$N]PF_6 as electrolyte.

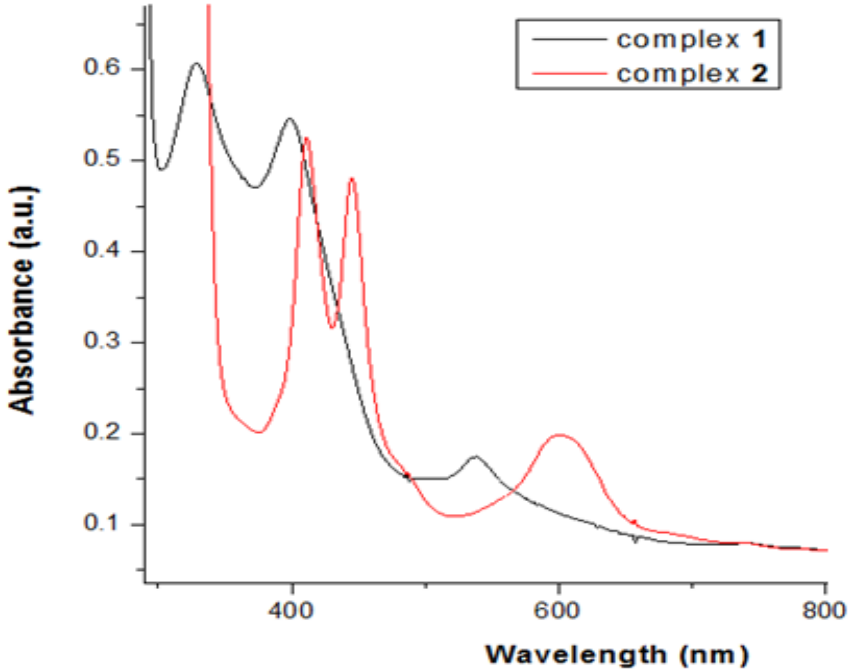


Fig. S4 UV-vis spectra of complexes **1** and **2** (concentration = 5.45 μM, solvent = THF, under Ar).

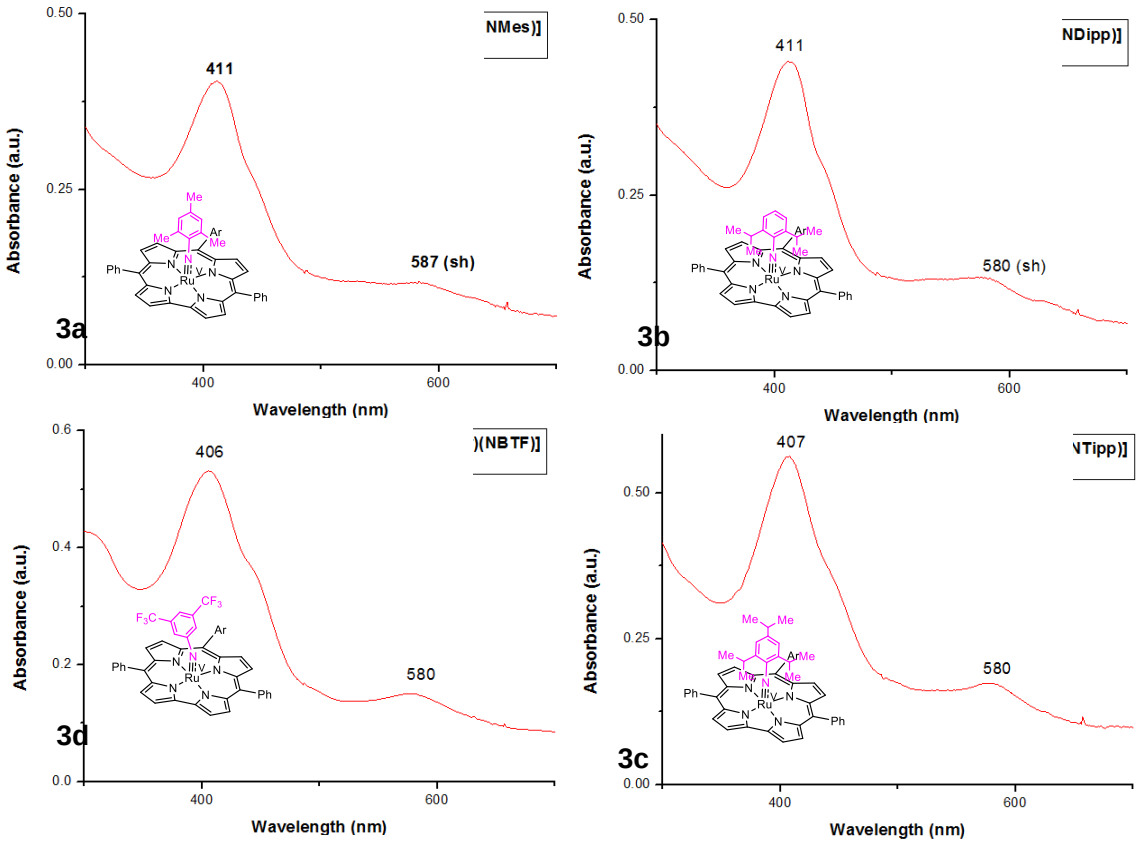


Fig. S5 UV–vis spectra of Ru(V)-arylimido corroles in benzene under argon.

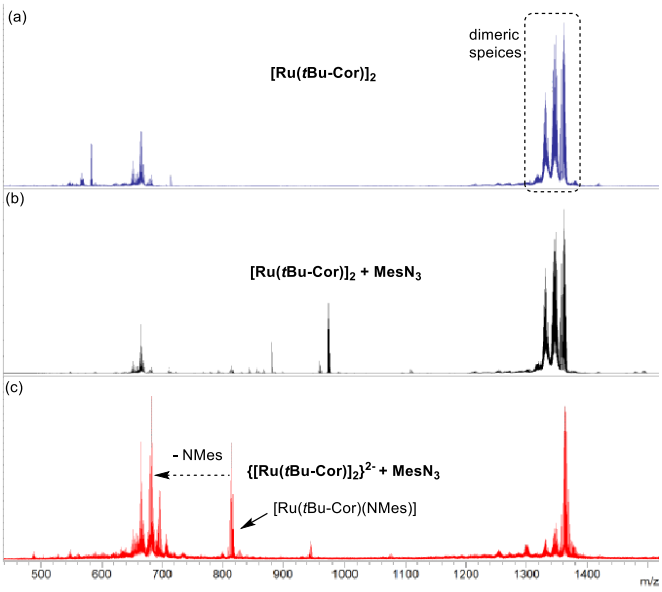


Fig. S6 MALDI-TOF MS spectra of a) **1**, b) a crude mixture of **1** and $MesN_3$, c) a crude mixture of **2** and $MesN_3$.

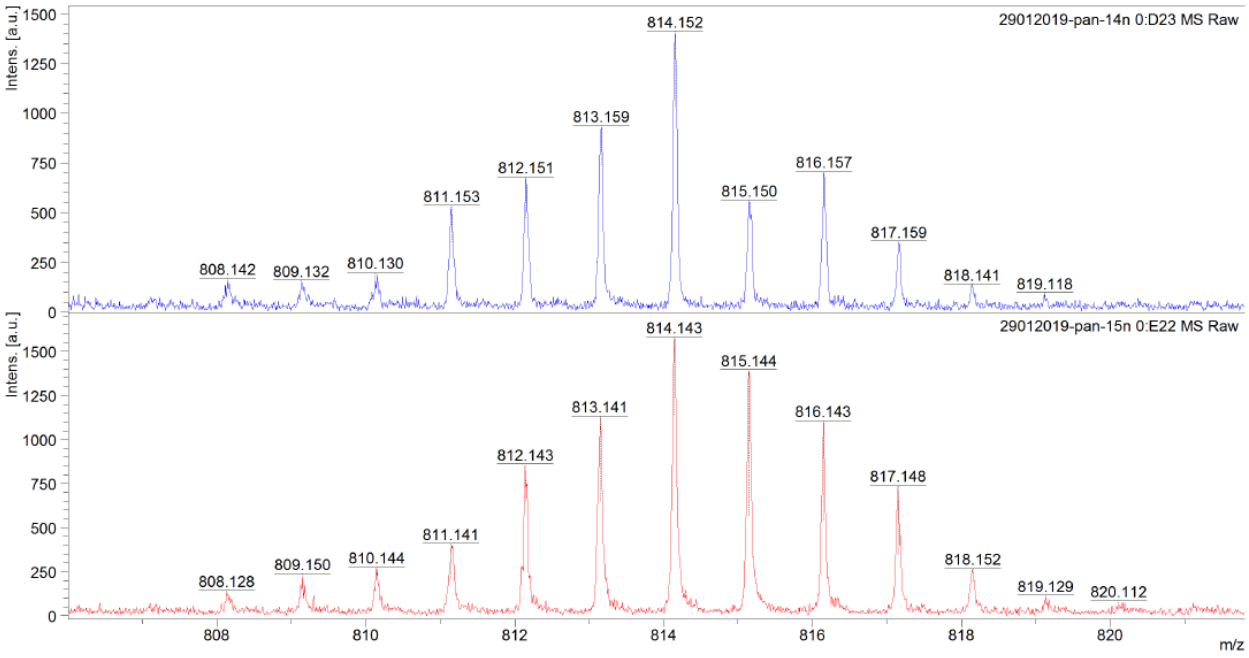


Fig. S7 MADLI-TOF MS spectra showing the experimental isotope patterns of **3a** (top) and ^{14,15}N-**3a** (bottom).

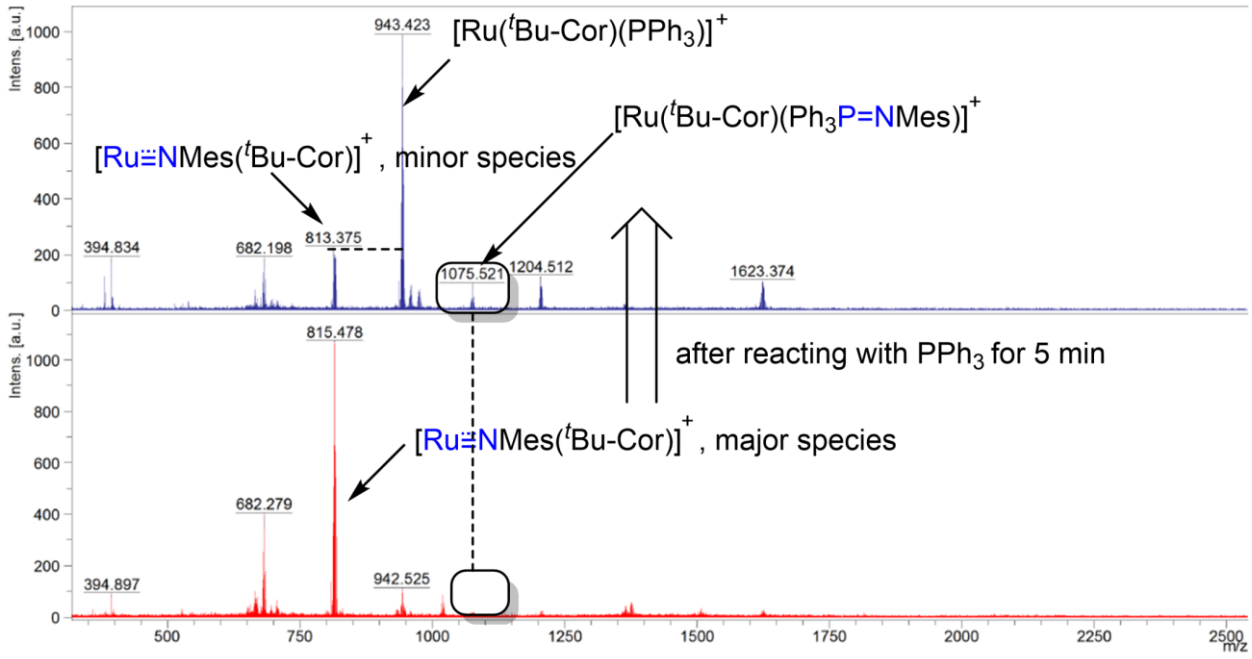


Fig. S8 MADLI-TOF MS spectra before (bottom) and after (top) addition of PPh_3 to **3a**.

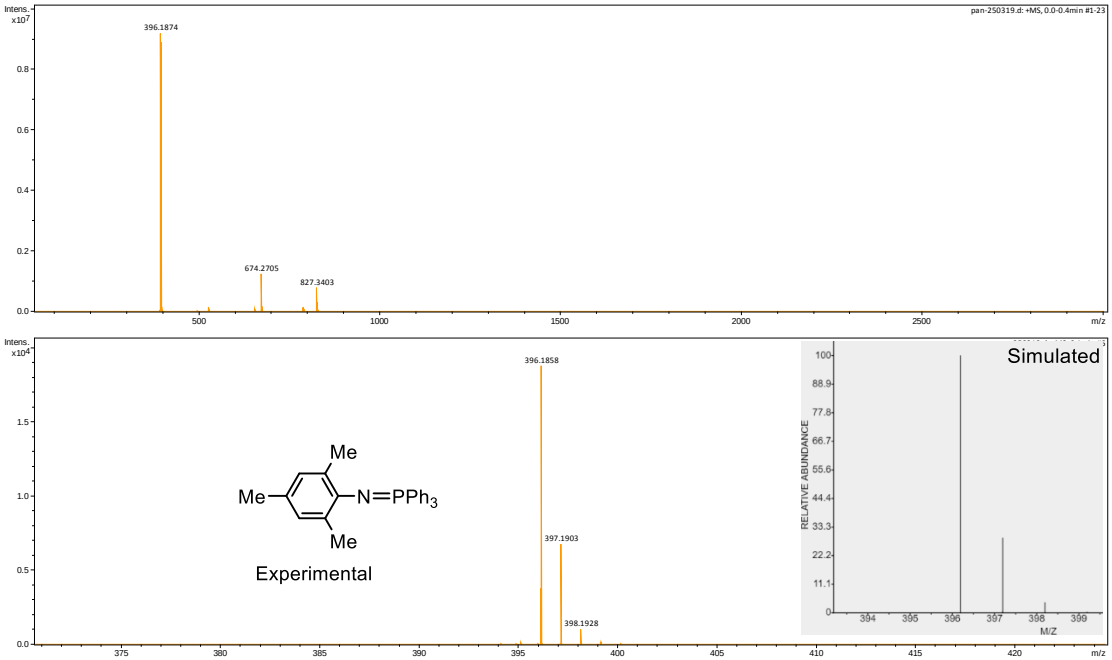


Fig. S9 a) HR-ESI-MS spectrum of PPh_3=NMes generated from the reaction between **3a** and PPh_3. b) HR-ESI-MS spectra showing the experimental and simulated isotope patterns of PPh_3=NMes.

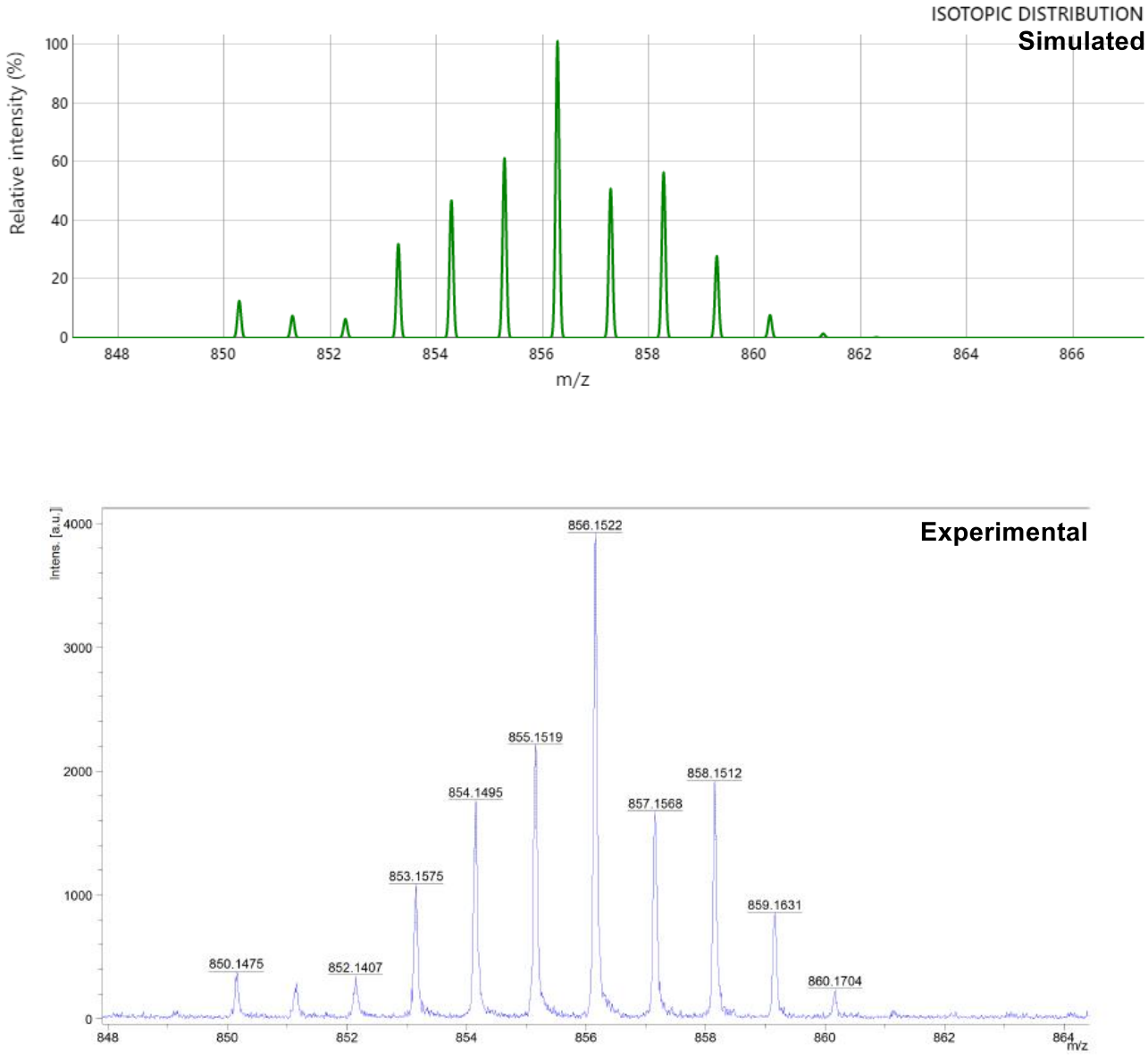


Fig. S10 MADLI-TOF MS spectra showing the experimental and simulated isotope patterns of **3b**.

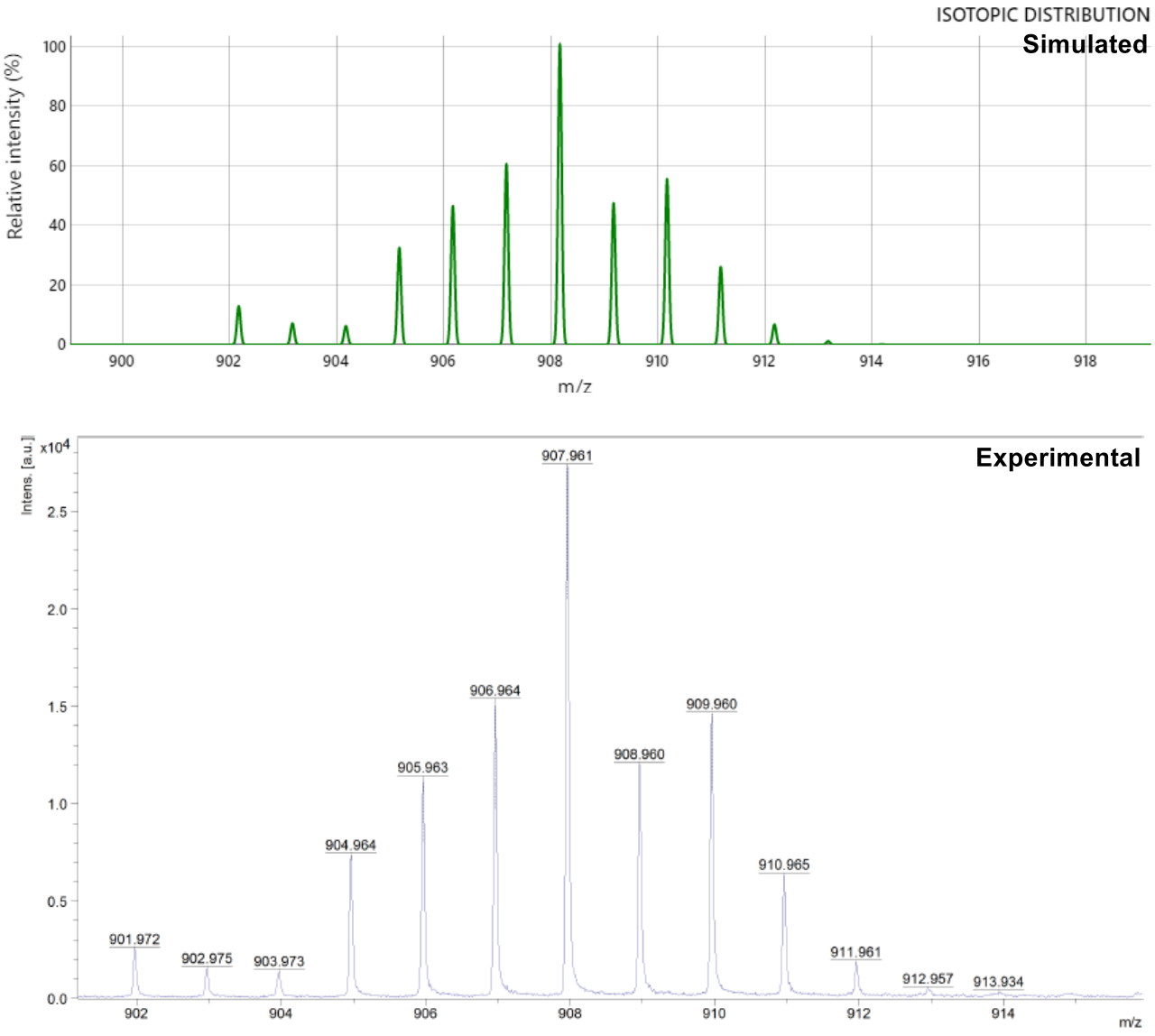


Fig. S11 MADLI-TOF MS spectra showing the experimental and simulated isotope patterns of **3d**.

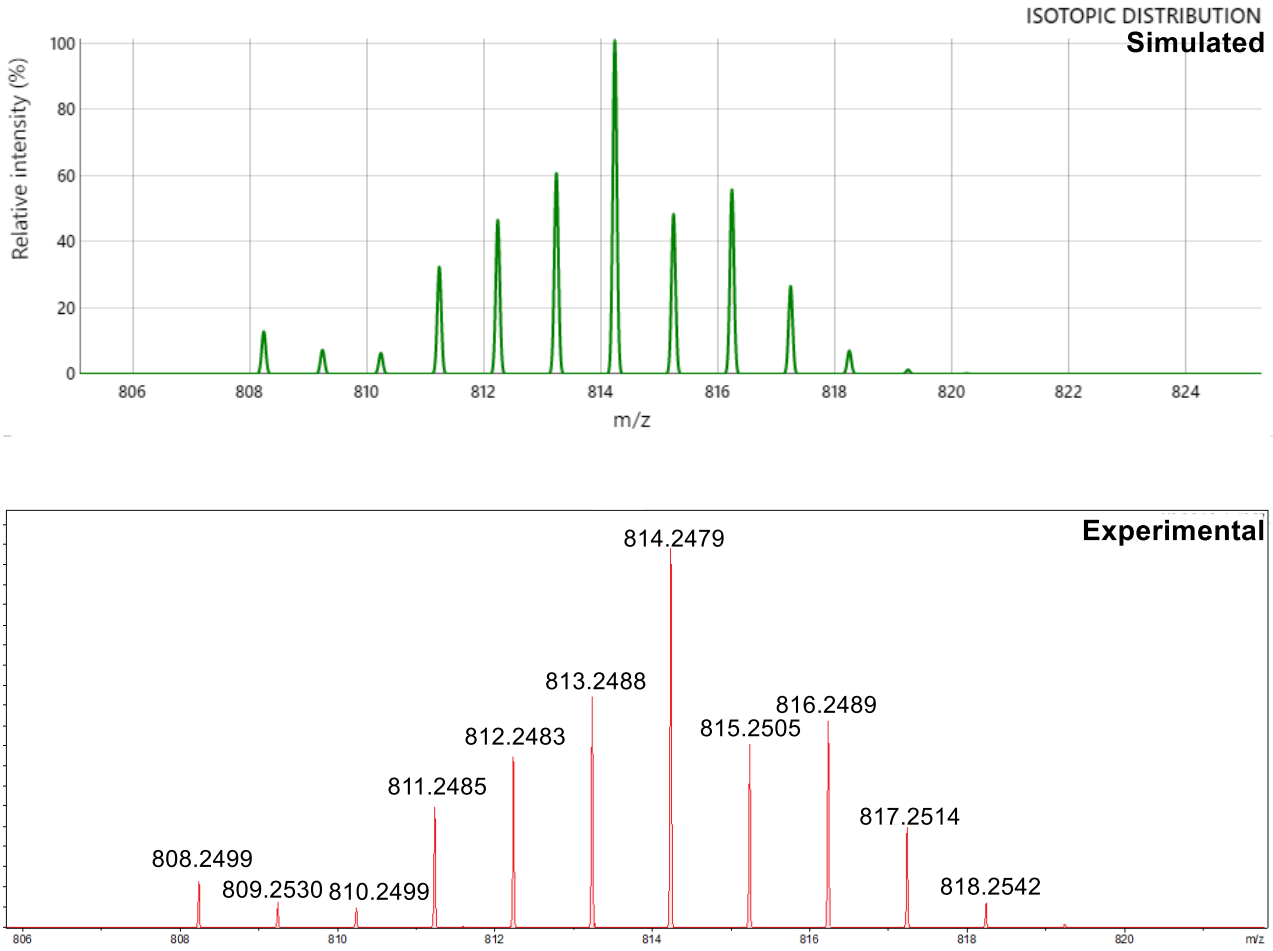


Fig. S12 HR-ESI-MS spectra showing the experimental and simulated isotope patterns of **3a**.

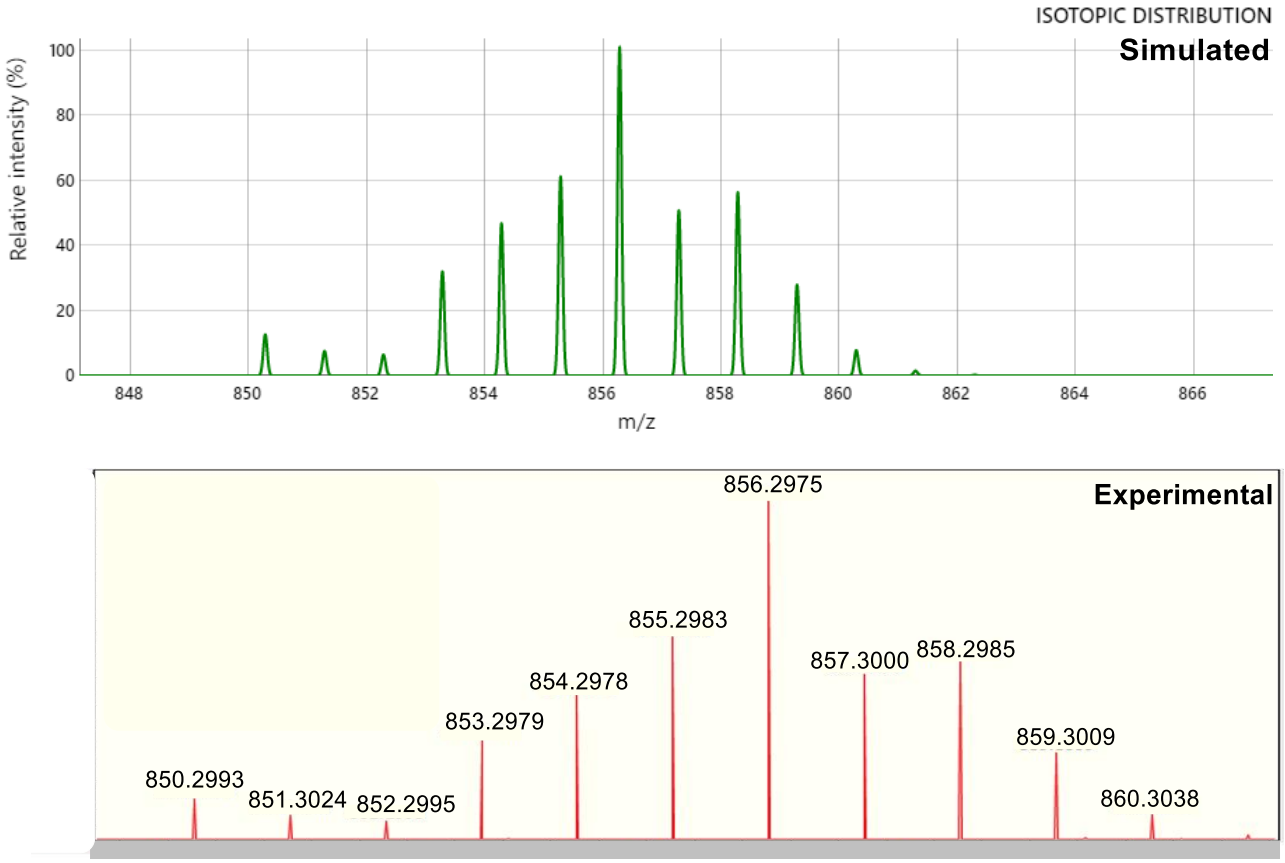


Fig. S13 HR-ESI-MS spectra showing the experimental and simulated isotope patterns of **3b**.

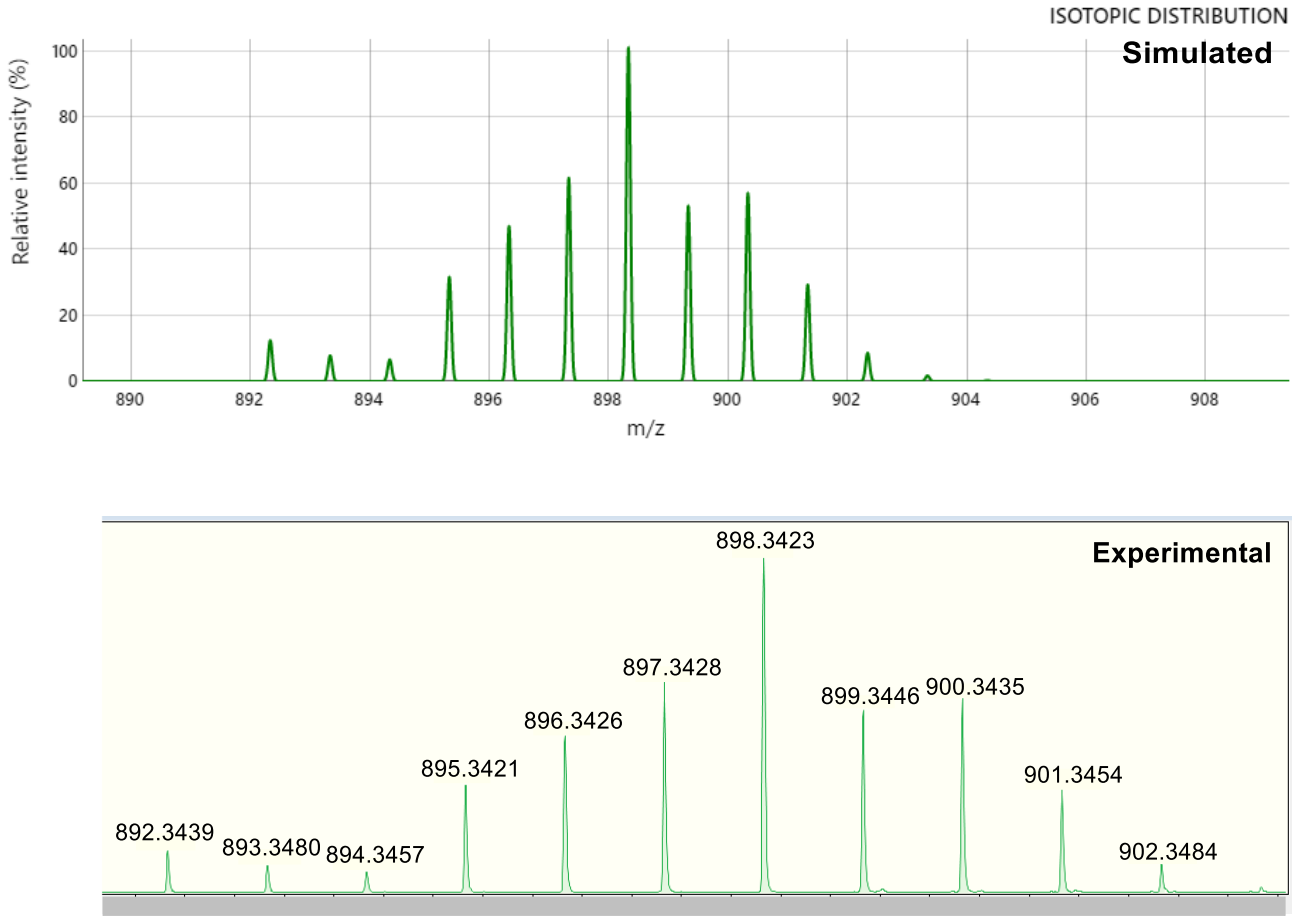


Fig. S14 HR-ESI-MS spectra showing the experimental and simulated isotope patterns of **3c**.

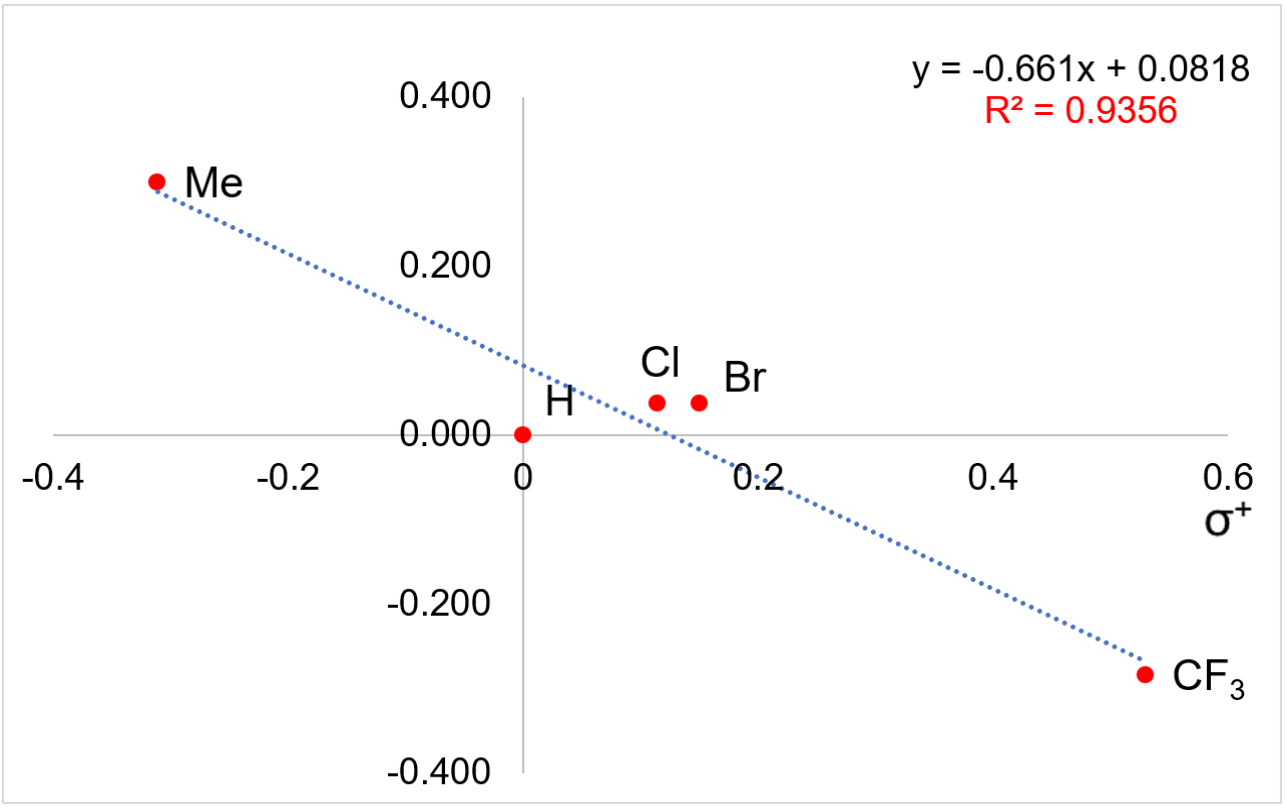


Fig. S15 Hammett correlation for the aziridination of *para*-substituted styrenes mediated by **3d** using a single-parameter method (σ^+).

Table S3 Comparison between the DFT-calculated *g* values and the ones based on experimental EPR spectra.

Complex	g_x	g_y	g_z	g_{iso}[a]	Δ[b]
3a (Simulated)	2.010	2.000	1.890	1.967	0.017
3a (Experimental)	2.010	2.005	1.880	1.965	
3b (Simulated)	2.010	1.970	1.870	1.950	0.000
3b (Experimental)	2.000	1.980	1.870	1.950	

[a] $g_{iso} = (g_x + g_y + g_z)/3$. [b] Δ = absolute difference between the g_{iso} values obtained experimentally and theoretically.

Table S4. Selected examples of the structural and electronic information of Ru-imido (Ru(NR)) species.

Ru terminal imido species	CN[a]	M–N_{NR} distance (Å)	M-N-R angle (^{o})	%$SD_{Ru/NR}$	Ref.
$[Ru(PNP)(NPh)]^+$	4	1.716	177.5	N/A	32
$[Ru^{II}(p\text{-cymene})(NAr)]$[b]	2	1.751	178.5	N/A	33
$[Ru^{V}(^t\text{Bu-Cor})(NMes)]$ (**3a**)	5	1.756[c]	146.0	44:40[c]	This work
$[Ru^{V}(^t\text{Bu-Cor})(NBTF)]$ (**3d**)	5	1.763[c]	138.0	53:26[c]	This work
$[Ru^{V}(^t\text{Bu-Cor})(NDipp)]$ (**3b**)	5	1.779[c]	160.0	35:54[c] 48:52[d]	This work
$[Ru^{IV}(NDipp)_2(PMe_3)_2]$	4	1.785	178.7	N/A	18
$[Ru^{VI}(TMP)(NSO_2Ar)_2]$[e]	6	1.793	162.5	N/A	34
$[Ru^{VI}(TPP)(NBTF)_2]$[f]	6	1.806, 1.808	143.7, 139.8	N/A	23
[Ru(PNP)(NPh)]	4	1.806	162.0	30:68[c]	32
$[Ru^{II}(NDipp)(PMe_3)_3]$	4	1.811	174.9	N/A	35
$[(SiP^{iPr}{}_3)Ru(NAr)]$[g]	5	1.869	172.0	40:54[c]	36
$[Ru^{IV}(NTs)(SeMes)_2\text{-}(PPh_3)]$[h]	5	1.895	96.7	N/A	37

[a] Coordination number. [b] Ar = 2,4,6-$(^t\text{Bu})_3$-C_6H_2. [c] Obtained by DFT calculations. [d] Obtained by CASSCF calculations. [e] Ar = *p*-OMe-C_6H_4. [f] Ar = 3,5-$(CF_3)_2$-C_6H_3 (Ru=N_1, Ru=N_2 not identical). [g] Ar = *p*-CF_3-C_6H_4. [h] κ^2-NTs (as a bidentate N^O ligand).

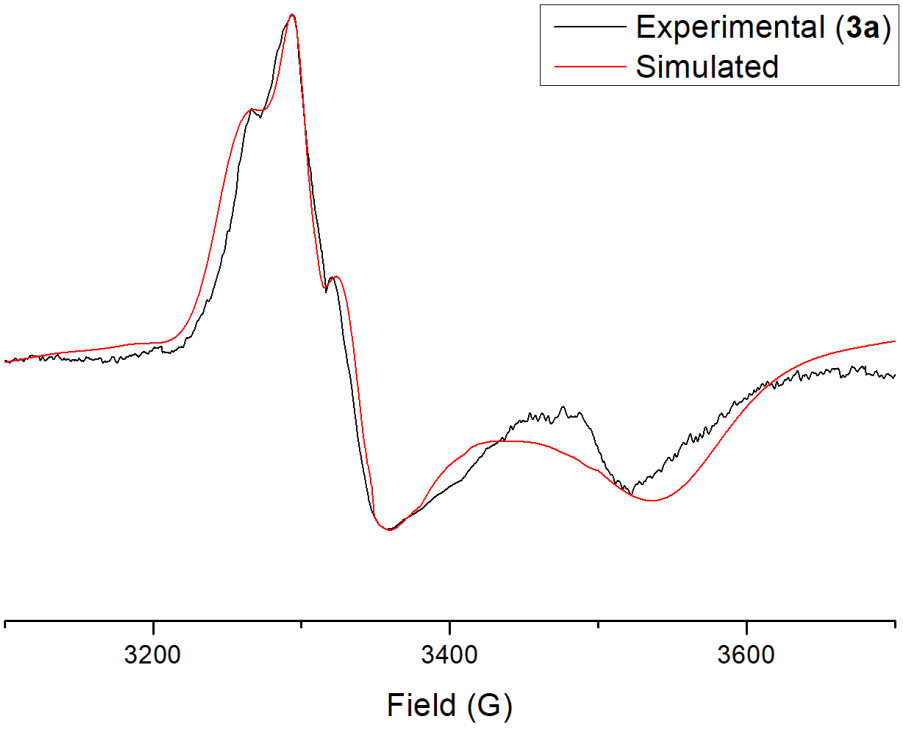


Fig. S16 X-band EPR spectra of **3a** (experimental and simulated) recorded at 100 K.

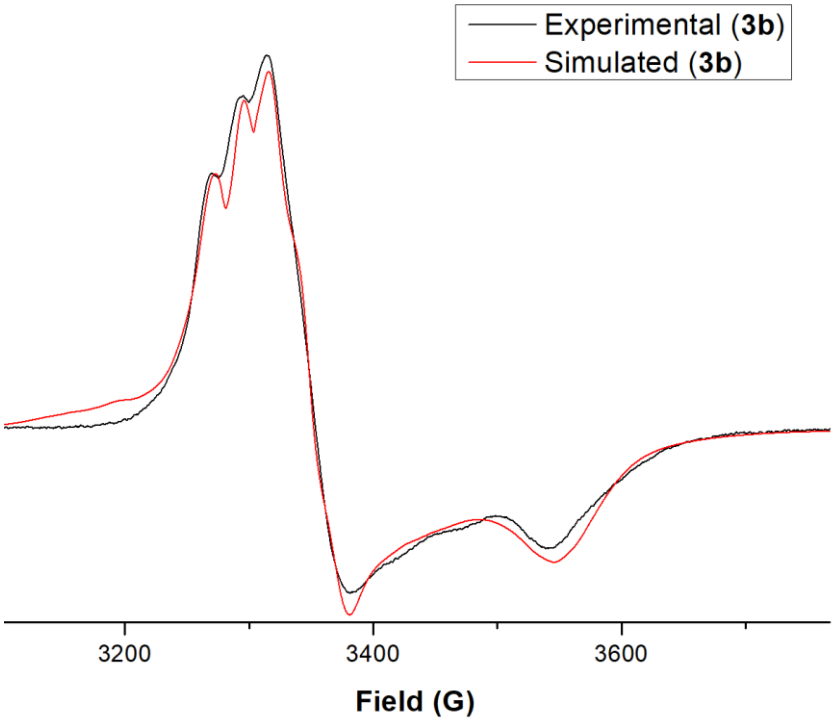


Fig. S17 X-band EPR spectra of **3b** (experimental and simulated) recorded at 100 K.

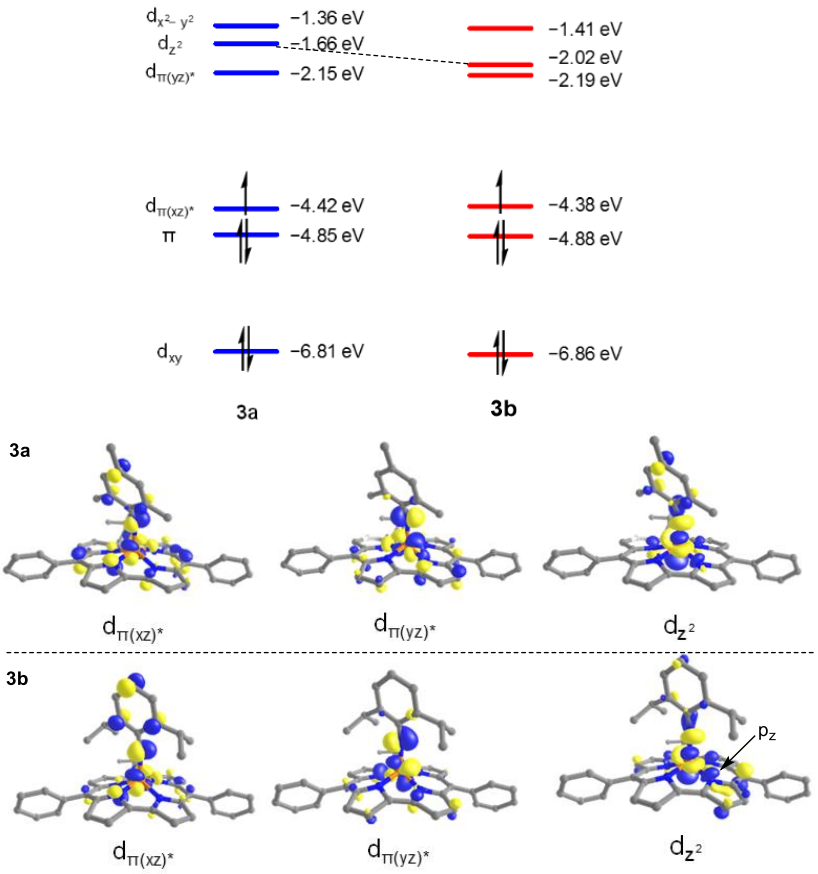


Fig. S18 DFT-calculated molecular orbital energy diagrams of **3a** (left) and **3b** (right).

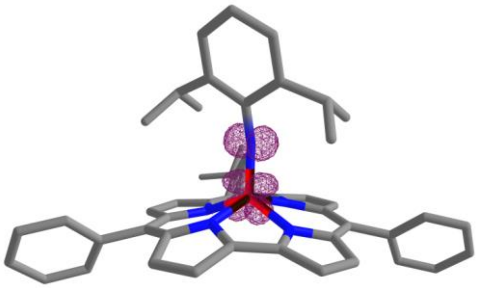


Fig. S19 Spin density plot (contour value: 0.01) for **3b** obtained from the CASSCF calculation.

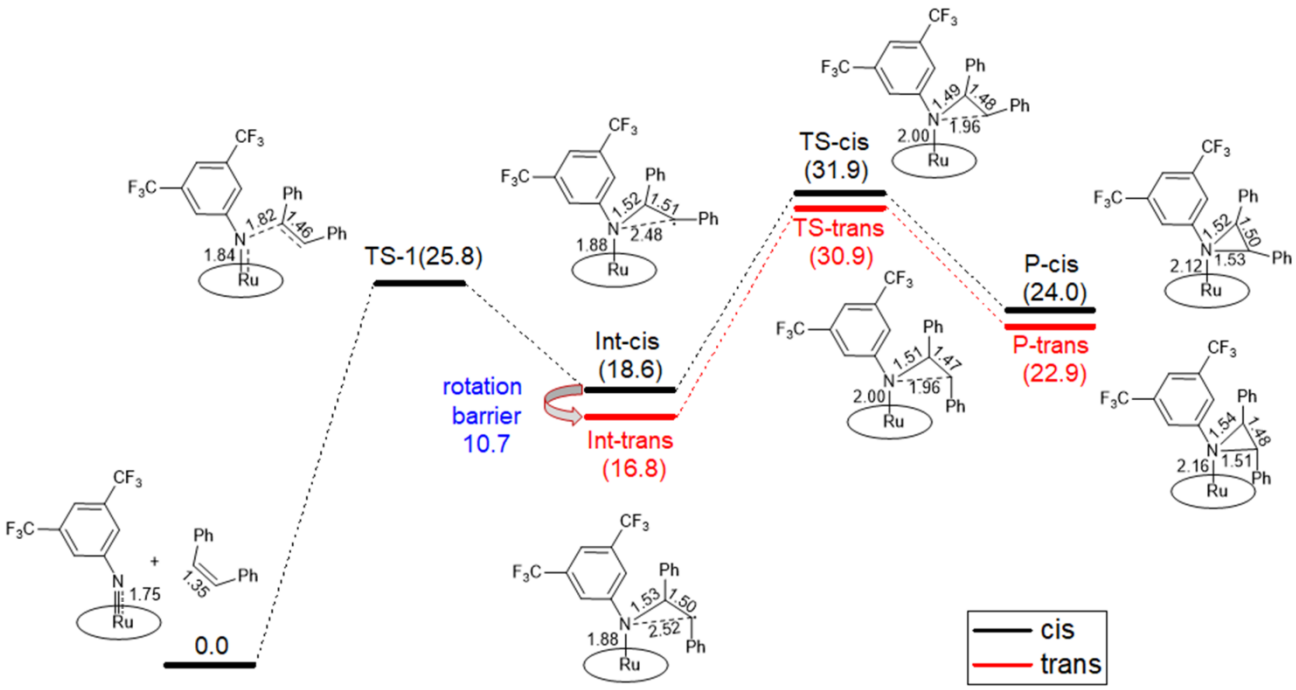
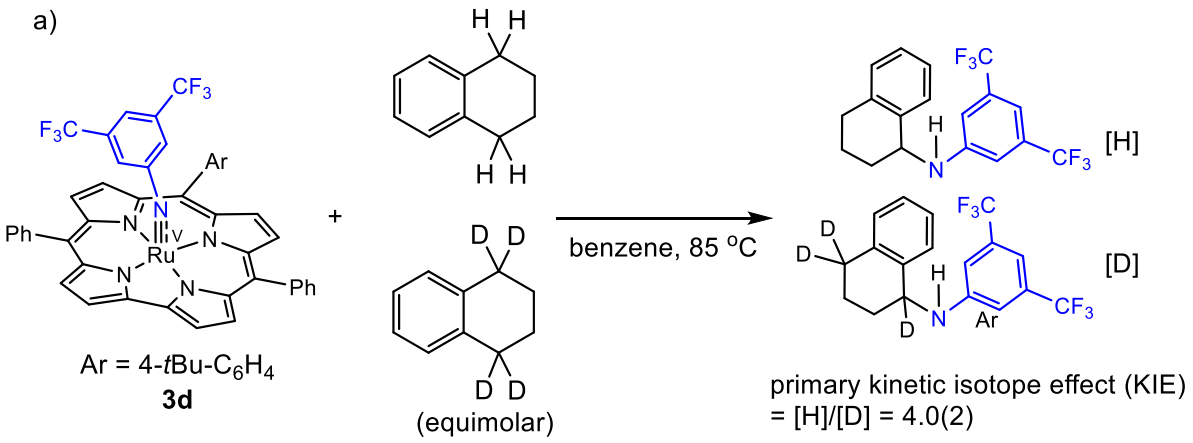


Fig. S20 DFT-calculated reaction profile of **3d**-mediated aziridination of *cis*-stilbene.



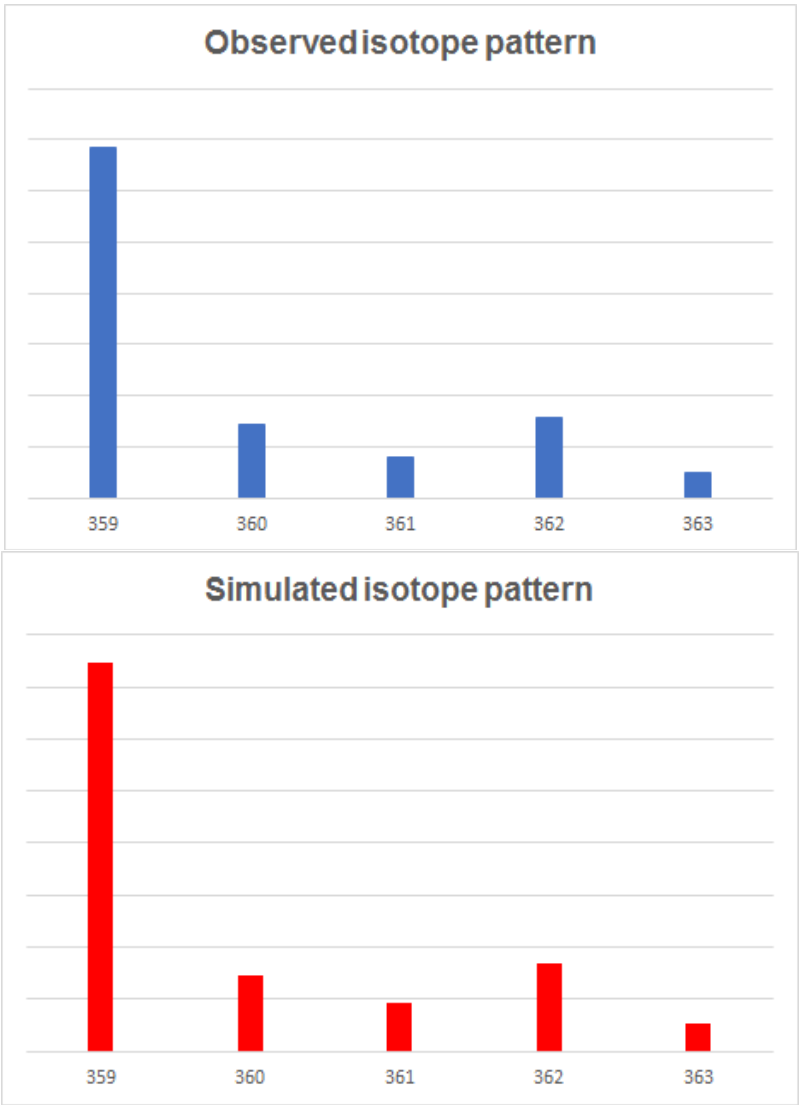
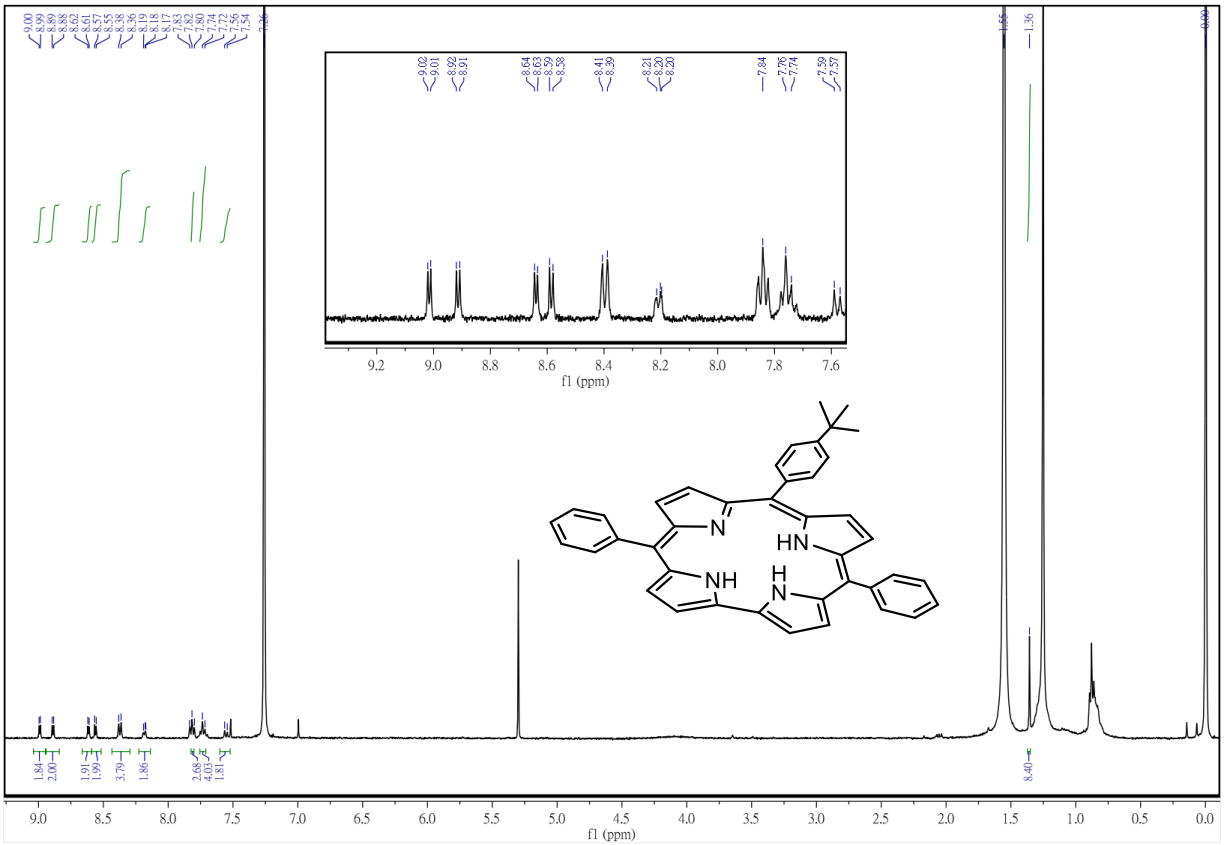
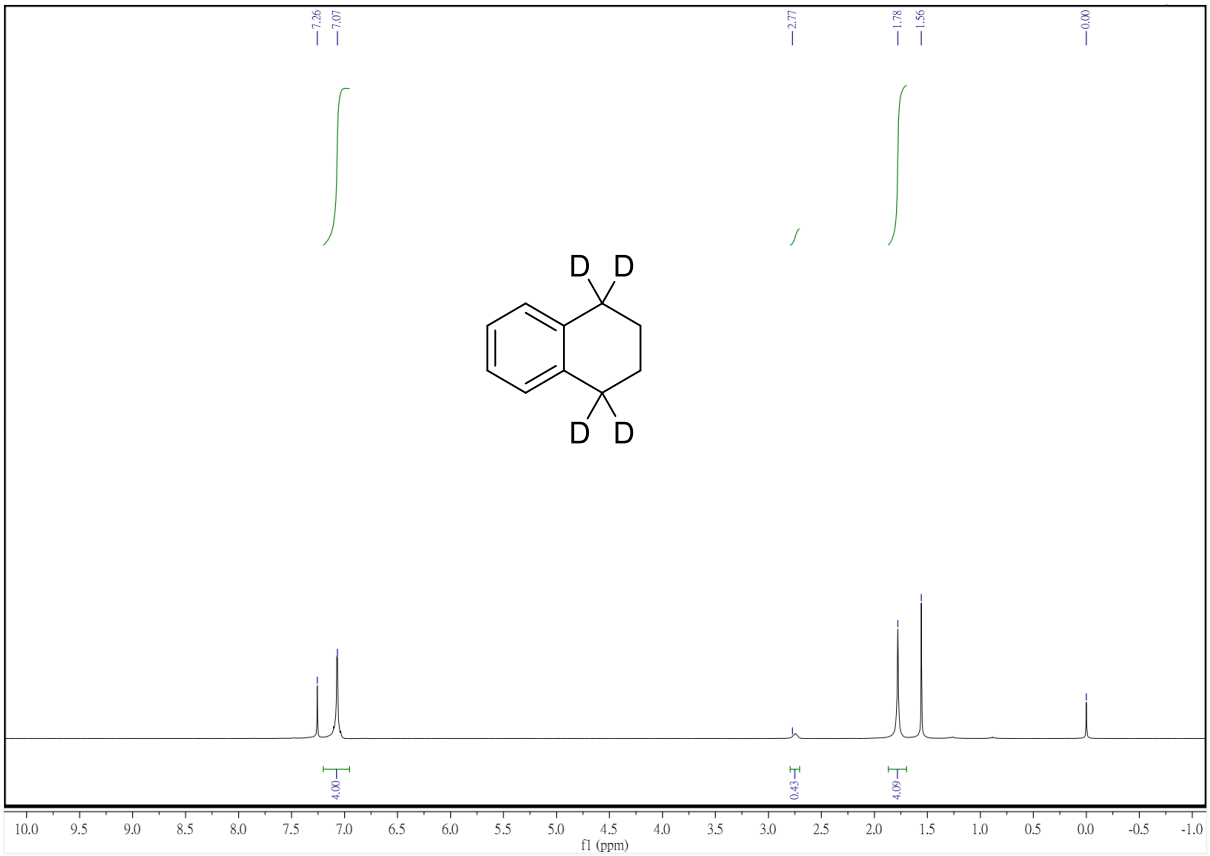
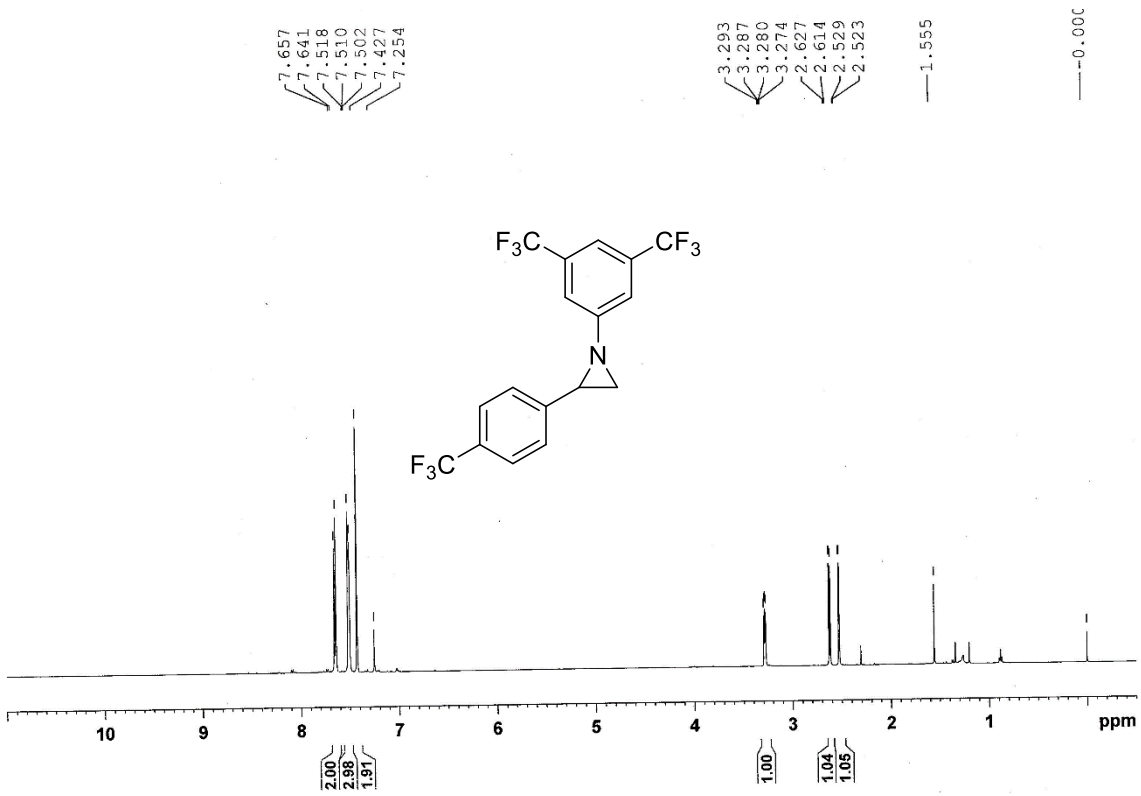


Fig. S21 a) KIE experiment for the reaction of **3d** with tetralin. b) Isotope pattern of the aminated products by GC-MS.

NMR spectra of the organic starting materials and products



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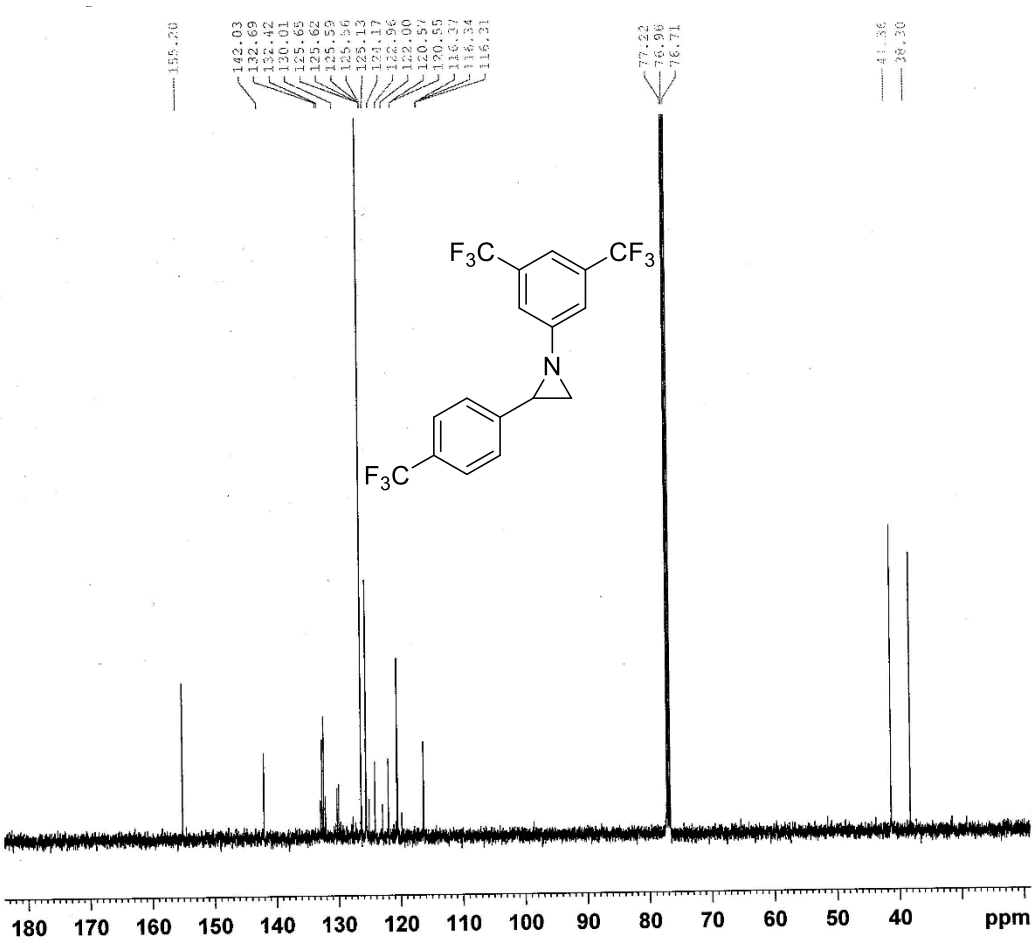
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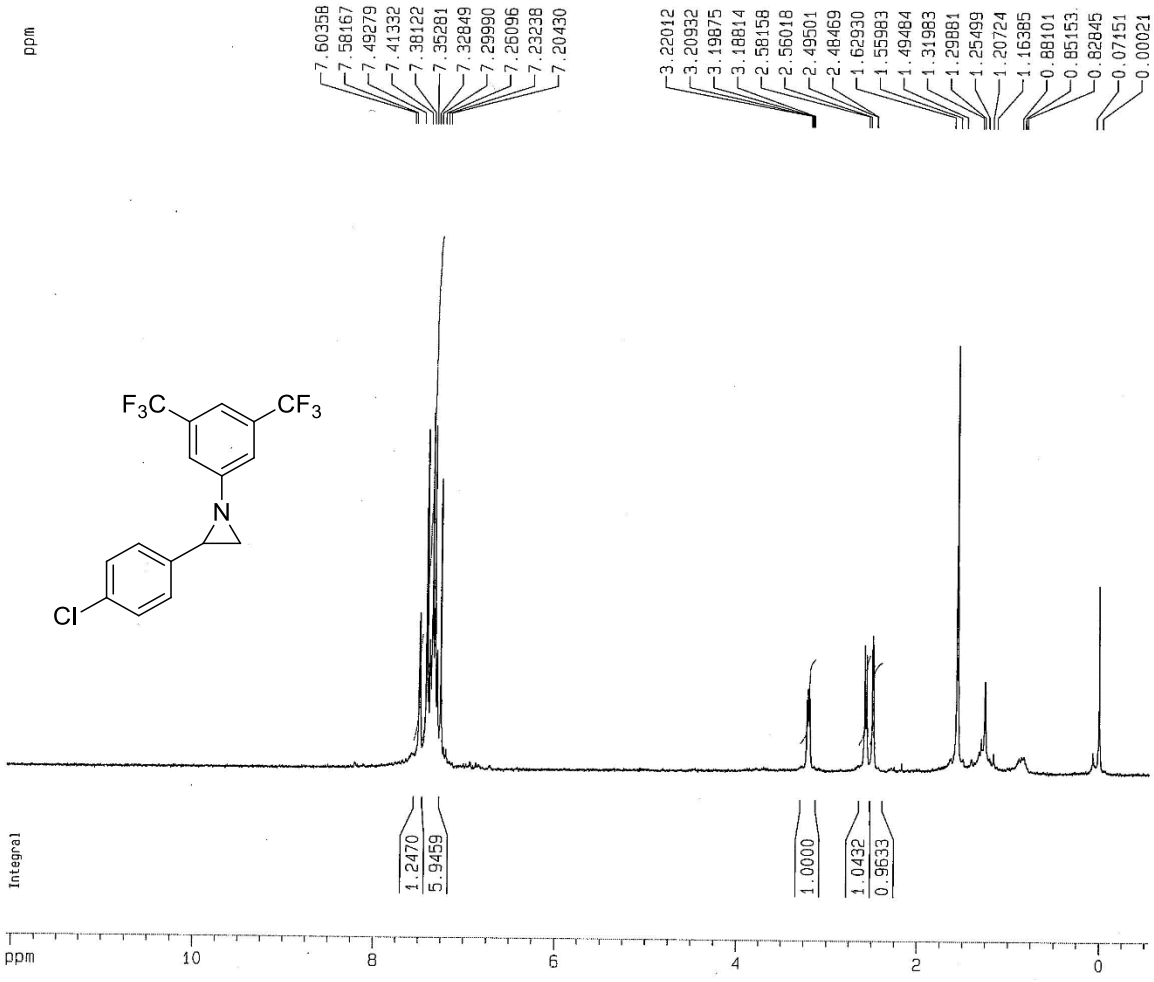
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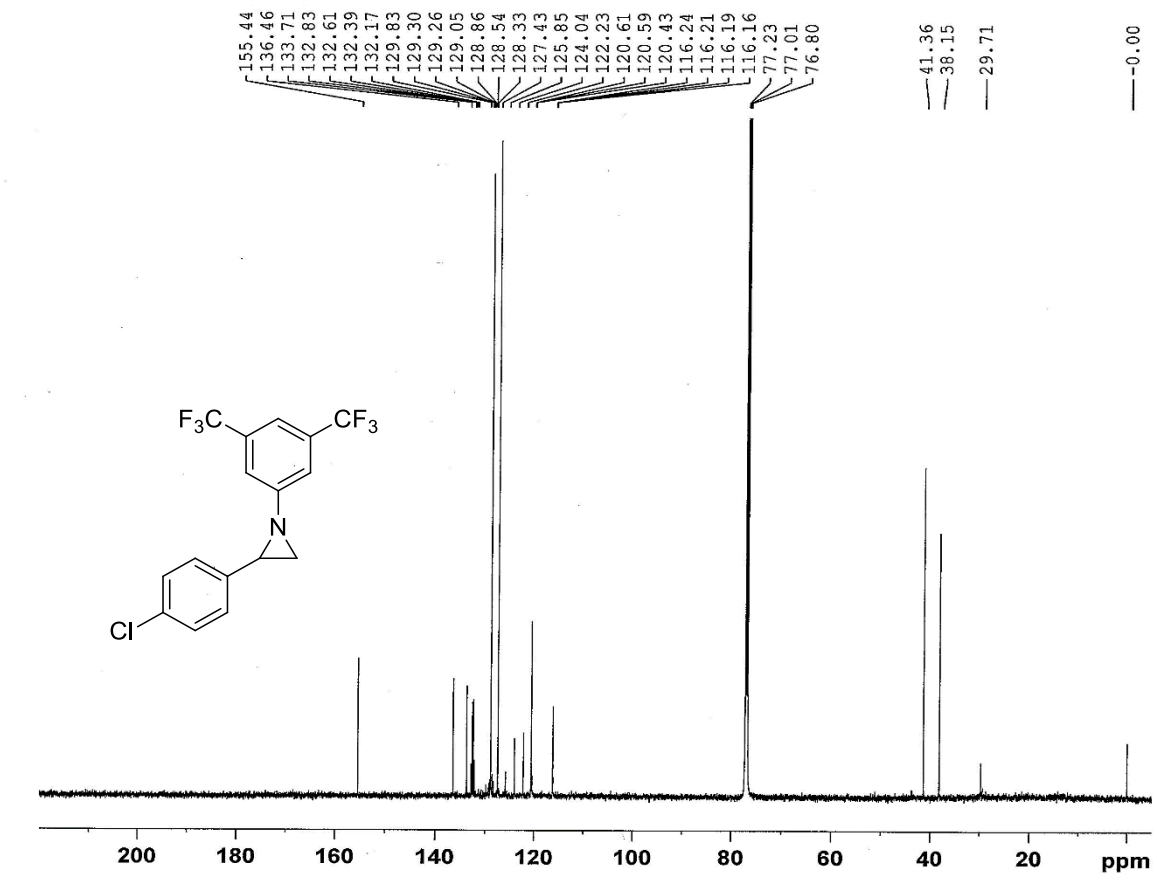
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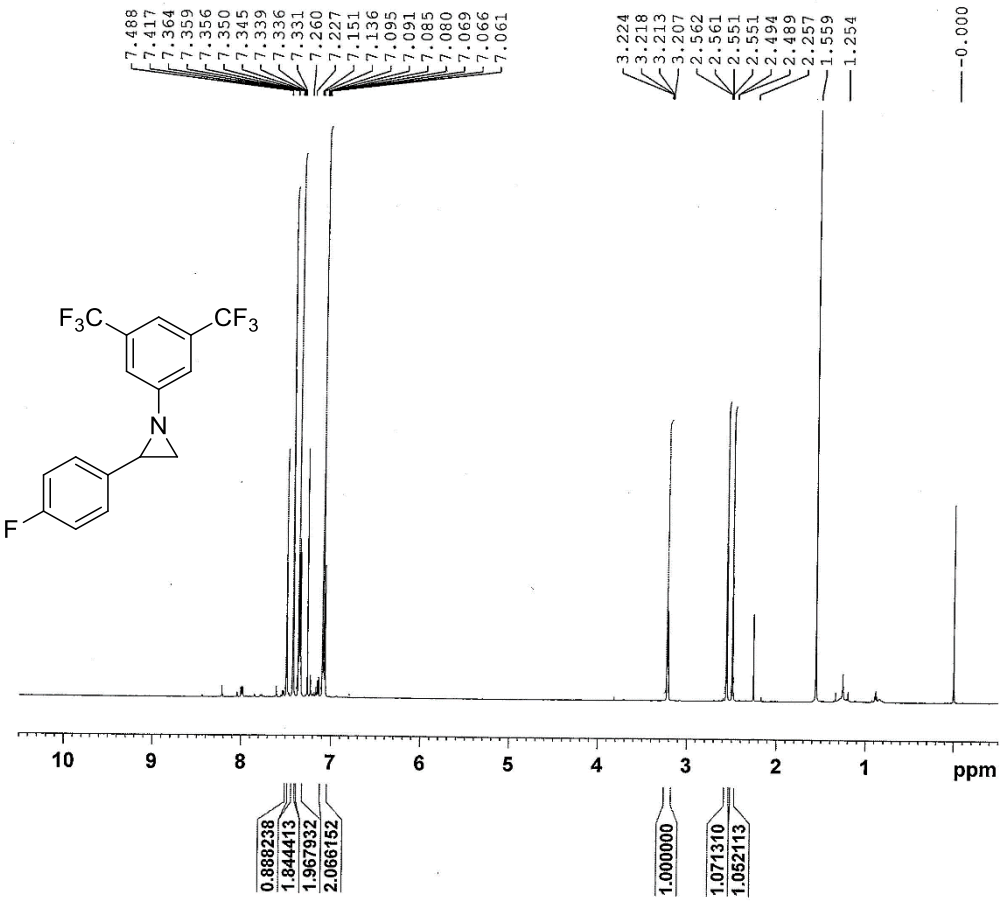
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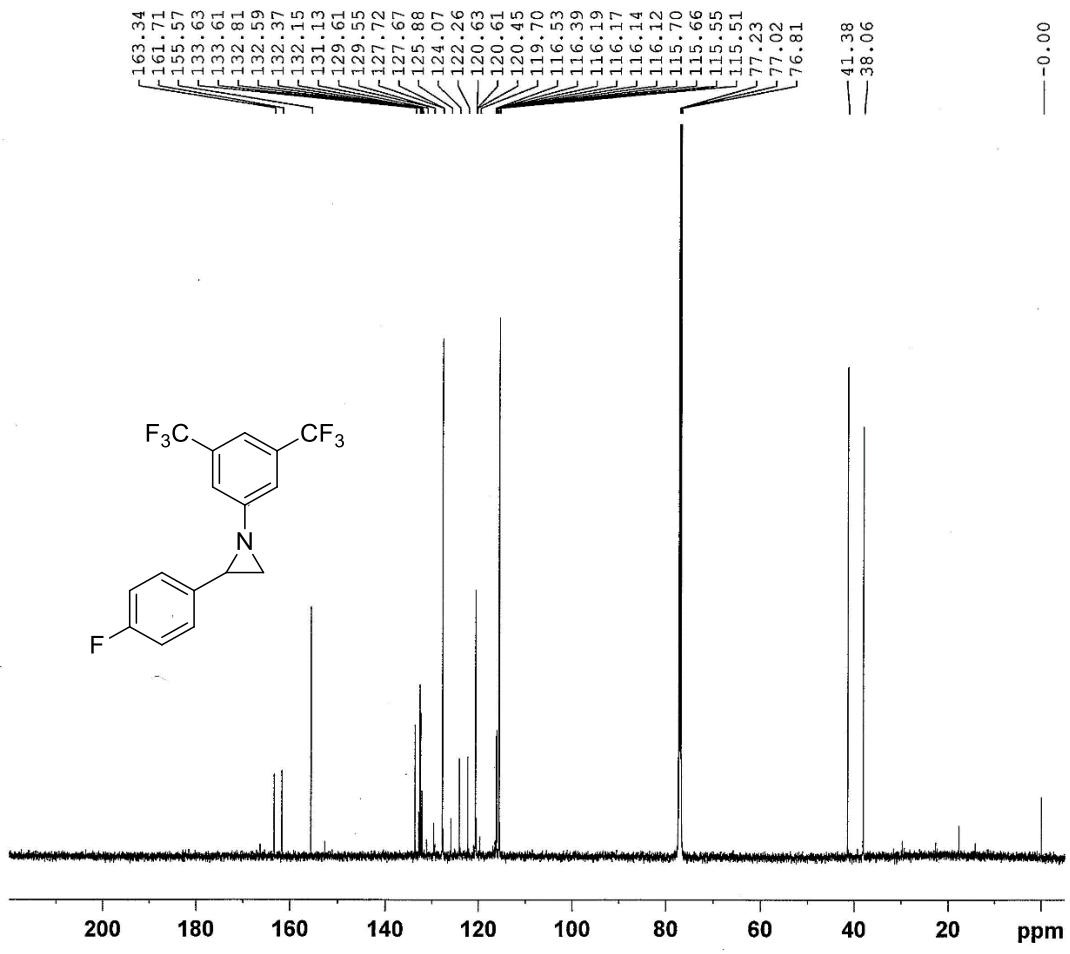
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116.19
116.17
116.14
116.12
115.70
115.66
115.55
115.51
77.23
77.02
76.81
41.38
38.06
0.00
F3C
CF3
N
F
200
180
160
140
120
100
80
60
40
20
ppm

Cartesian coordinates for DFT calculations

3a

Ru	8.427333000	12.043157000	0.050626000	H	14.137744000	18.465356000	2.193358000
N	9.208513000	13.664192000	-0.846081000	C	13.942363000	16.341254000	1.861833000
N	8.098549000	11.665691000	-1.846807000	H	14.983522000	16.127016000	2.088693000
C	8.285059000	12.699003000	-2.751016000	C	13.085730000	15.299863000	1.505507000
N	9.969450000	12.139563000	1.325334000	H	13.463250000	14.283288000	1.446284000
C	10.119586000	11.246628000	2.390321000	N	6.981967000	12.735640000	0.768182000
C	7.665764000	9.114266000	-0.482454000	C	6.176576000	13.845306000	0.869563000
C	8.733590000	9.371742000	1.479687000	C	5.120085000	14.043073000	-0.063081000
C	8.965346000	13.809018000	-2.190930000	C	6.330980000	14.719254000	1.983165000
C	10.148777000	14.577992000	-0.445534000	C	4.276159000	15.137800000	0.118522000
N	8.301846000	10.026530000	0.347547000	C	5.455459000	15.794933000	2.105761000
C	7.487709000	10.592035000	-2.471423000	C	4.427340000	16.033606000	1.183535000
C	10.418045000	15.428622000	-1.575044000	H	3.467562000	15.291958000	-0.593466000
H	11.118157000	16.252406000	-1.581634000	H	5.574425000	16.465966000	2.954504000
C	10.935071000	11.884499000	3.379495000	C	7.406602000	14.472090000	3.008961000
H	11.208099000	11.448127000	4.329321000	H	7.324425000	15.185960000	3.834393000
C	10.812155000	14.453101000	0.793850000	H	7.337926000	13.458177000	3.421334000
C	12.134032000	17.918699000	1.605808000	H	8.408650000	14.565825000	2.576455000
H	11.755756000	18.936847000	1.646275000	C	4.903274000	13.081615000	-1.202637000
C	11.276102000	13.129057000	2.914807000	H	5.704059000	13.145963000	-1.948045000
H	11.876237000	13.868110000	3.425972000	H	4.885320000	12.044108000	-0.849119000
C	11.736415000	15.549518000	1.198440000	H	3.955318000	13.291644000	-1.708065000
C	9.548983000	9.957397000	2.473931000	C	3.516817000	17.228864000	1.330730000
C	7.241088000	9.372736000	-1.807179000	H	2.551829000	17.060916000	0.840912000
C	8.292975000	8.004386000	1.399192000	H	3.326828000	17.462336000	2.384318000
H	8.489826000	7.242434000	2.139593000	H	3.960637000	18.125619000	0.876505000
C	7.286996000	10.978201000	-3.834778000	C	9.867807000	9.124922000	3.672885000
H	6.840531000	10.353349000	-4.595802000	C	8.852505000	8.671274000	4.525295000
C	7.629549000	7.852584000	0.209686000	C	11.186798000	8.750152000	3.978547000
H	7.187686000	6.945658000	-0.177516000	C	9.141884000	7.879091000	5.638617000
C	7.242865000	7.089683000	-2.889760000	C	11.468822000	7.959826000	5.089342000
H	8.266129000	6.953526000	-2.551612000	C	10.455371000	7.502091000	5.949918000
C	11.276948000	16.877437000	1.248653000	H	7.822007000	8.946968000	4.317877000
H	10.236780000	17.085355000	1.014471000	H	11.995488000	9.073842000	3.328966000
C	9.690523000	14.949254000	-2.649681000	H	8.318296000	7.560084000	6.267932000
H	9.711088000	15.322436000	-3.665430000	H	12.503617000	7.688770000	5.281202000
C	7.777345000	12.266845000	-4.003907000	C	10.812287000	6.626059000	7.163868000
H	7.789867000	12.837515000	-4.923510000	C	11.772756000	7.403393000	8.095393000
C	10.686549000	13.309469000	1.621473000	H	12.045379000	6.788627000	8.962124000
C	4.631701000	7.454772000	-3.796645000	H	12.698477000	7.685166000	7.582687000
H	3.612555000	7.602295000	-4.144429000	H	11.302221000	8.321985000	8.464312000
C	6.573378000	8.286769000	-2.585844000	C	11.506874000	5.331431000	6.677160000
C	5.306086000	6.266983000	-4.086290000	H	11.773975000	4.696875000	7.531193000
H	4.816919000	5.487190000	-4.663855000	H	10.845432000	4.755553000	6.019737000
C	6.614333000	6.088798000	-3.631594000	H	12.425987000	5.544825000	6.121268000
H	7.151145000	5.171896000	-3.860667000	C	9.570270000	6.224652000	7.982629000
C	5.260391000	8.456092000	-3.055236000	H	8.857095000	5.645367000	7.385120000
H	4.731086000	9.376850000	-2.826277000	H	9.873100000	5.600703000	8.831065000
C	13.469668000	17.654543000	1.915494000	H	9.047538000	7.099239000	8.386732000

3b

Ru	8.475538000	12.166972000	-0.011883000	C	8.512093000	12.751416000	-2.843379000
N	9.361605000	13.756257000	-0.926884000	N	10.052544000	12.187766000	1.231254000
N	8.246864000	11.750436000	-1.921308000	C	10.191672000	11.285024000	2.297157000

C	7.714622000	9.217439000	-0.558558000	C	6.075601000	14.546120000	2.217151000
C	8.687077000	9.487538000	1.442503000	C	3.816831000	14.726836000	0.562834000
C	9.174610000	13.866037000	-2.281829000	C	5.058425000	15.470424000	2.462587000
C	10.378082000	14.599497000	-0.551841000	C	3.948706000	15.601023000	1.635667000
N	8.306516000	10.142247000	0.291159000	H	2.919404000	14.767964000	-0.049650000
C	7.702471000	10.652546000	-2.576634000	H	5.143032000	16.100333000	3.344785000
C	10.722089000	15.400929000	-1.699349000	C	7.183389000	14.499309000	3.264789000
H	11.484328000	16.167299000	-1.716099000	H	6.787046000	15.066191000	4.117660000
C	11.107875000	11.852398000	3.237039000	C	4.411548000	12.820303000	-0.889695000
H	11.390040000	11.396566000	4.174679000	H	3.337346000	12.985736000	-1.046104000
C	11.081782000	14.414272000	0.652112000	C	9.815012000	9.214289000	3.633224000
C	12.746787000	17.737945000	1.423521000	C	8.782122000	8.870015000	4.514732000
H	12.460521000	18.783288000	1.504821000	C	11.103110000	8.734716000	3.922210000
C	11.534300000	13.057129000	2.742394000	C	9.027093000	8.086578000	5.644748000
H	12.227182000	13.741291000	3.210638000	C	11.340544000	7.953543000	5.049904000
C	12.121695000	15.420098000	1.010457000	C	10.310527000	7.609280000	5.943228000
C	9.536780000	10.043354000	2.421332000	H	7.774524000	9.226186000	4.317868000
C	7.406816000	9.444956000	-1.919162000	H	11.922400000	8.969495000	3.248167000
C	8.222146000	8.128690000	1.368165000	H	8.192802000	7.855467000	6.297774000
H	8.377054000	7.376219000	2.127940000	H	12.352571000	7.600884000	5.229692000
C	7.629975000	10.996375000	-3.963005000	C	10.617609000	6.744894000	7.179231000
H	7.261695000	10.343516000	-4.741941000	C	11.654843000	7.471096000	8.069219000
C	7.620728000	7.967407000	0.148662000	H	11.892412000	6.864574000	8.951935000
H	7.191059000	7.060313000	-0.251341000	H	12.591017000	7.659441000	7.533142000
C	7.545963000	7.136598000	-2.932388000	H	11.267403000	8.436559000	8.414365000
H	8.526364000	7.022039000	-2.479097000	C	11.196723000	5.383390000	6.725412000
C	11.781365000	16.780192000	1.111059000	H	11.428059000	4.757882000	7.596319000
H	10.749322000	17.079721000	0.952969000	H	10.478818000	4.841658000	6.098954000
C	9.981688000	14.940089000	-2.768199000	H	12.119080000	5.504680000	6.147834000
H	10.045833000	15.269405000	-3.797134000	C	9.362138000	6.472289000	8.029520000
C	8.126822000	12.280900000	-4.124062000	H	8.595034000	5.932590000	7.462393000
H	8.224900000	12.826021000	-5.053834000	H	9.628894000	5.854370000	8.894376000
C	10.892396000	13.284599000	1.483785000	H	8.917725000	7.398912000	8.410381000
C	5.048285000	7.444664000	-4.131949000	C	5.090268000	13.194871000	-2.217643000
H	4.072692000	7.570315000	-4.594311000	H	6.175763000	13.151447000	-2.144429000
C	6.834961000	8.332479000	-2.736232000	H	4.776790000	12.513658000	-3.017831000
C	5.762342000	6.258892000	-4.313624000	H	4.814458000	14.214110000	-2.512568000
H	5.348224000	5.458432000	-4.920812000	C	4.543063000	11.331848000	-0.525283000
C	7.014185000	6.109553000	-3.712829000	H	3.991644000	11.112205000	0.396652000
H	7.582781000	5.194575000	-3.857067000	H	4.114433000	10.715804000	-1.324979000
C	5.581006000	8.472954000	-3.353168000	H	5.577431000	11.023029000	-0.377507000
H	5.021015000	9.392564000	-3.211641000	C	7.479684000	13.093970000	3.813055000
C	14.072906000	17.355813000	1.635057000	H	6.562432000	12.633062000	4.198814000
H	14.825314000	18.101573000	1.877240000	H	7.898946000	12.429187000	3.058805000
C	14.426985000	16.008704000	1.529413000	H	8.198403000	13.162214000	4.638145000
H	15.459069000	15.702878000	1.679806000	C	8.435462000	15.258528000	2.796557000
C	13.461886000	15.050539000	1.219748000	H	9.222356000	15.221694000	3.558988000
H	13.746011000	14.006795000	1.121601000	H	8.836068000	14.836412000	1.875621000
N	6.997530000	12.835395000	0.719721000	H	8.191398000	16.310297000	2.605221000
C	5.997375000	13.724768000	1.030585000	H	3.178915000	16.336679000	1.850679000
C	4.782491000	13.768853000	0.247806000				

3d

Ru	8.367972000	11.997041000	0.135543000	C	7.600977000	9.074729000	-0.401907000
N	9.108590000	13.611969000	-0.776962000	C	8.758422000	9.316320000	1.514058000
N	7.918681000	11.651099000	-1.740665000	C	8.792444000	13.784576000	-2.106977000
C	8.078141000	12.688066000	-2.646424000	C	10.043932000	14.542171000	-0.396147000
N	9.959787000	12.092828000	1.353547000	N	8.279804000	9.980678000	0.403568000
C	10.146538000	11.196015000	2.408008000	C	7.295612000	10.576686000	-2.353806000

C	10.241456000	15.418555000	-1.518708000	N	6.955993000	12.692255000	0.929602000
H	10.918181000	16.261417000	-1.538001000	C	6.219705000	13.858891000	0.885652000
C	10.962244000	11.844126000	3.390002000	C	5.710621000	14.376247000	-0.323719000
H	11.257827000	11.407148000	4.332713000	C	5.917099000	14.514300000	2.097319000
C	10.736701000	14.427149000	0.826584000	C	4.927610000	15.527587000	-0.308429000
C	11.980306000	17.918410000	1.646720000	C	5.147851000	15.673641000	2.086824000
H	11.575686000	18.925264000	1.706787000	C	4.643498000	16.187986000	0.888959000
C	11.263824000	13.101671000	2.932095000	C	9.954267000	9.061429000	3.675589000
H	11.851466000	13.852315000	3.440788000	C	8.964353000	8.590359000	4.548269000
C	11.639020000	15.544217000	1.222390000	C	11.285762000	8.709577000	3.952610000
C	9.597902000	9.897716000	2.490572000	C	9.290881000	7.804827000	5.655878000
C	7.101664000	9.345490000	-1.698466000	C	11.604229000	7.925205000	5.057612000
C	8.315654000	7.951449000	1.439526000	C	10.617219000	7.452214000	5.940443000
H	8.540905000	7.184349000	2.166289000	H	7.925383000	8.850191000	4.364069000
C	7.036276000	10.977166000	-3.703964000	H	12.075157000	9.047289000	3.286631000
H	6.562034000	10.357507000	-4.452133000	H	8.486559000	7.473121000	6.303149000
C	7.597904000	7.809464000	0.279512000	H	12.647267000	7.672953000	5.228573000
H	7.135708000	6.906738000	-0.093208000	C	11.015856000	6.590387000	7.151553000
C	7.066236000	7.075825000	-2.807246000	C	11.976955000	7.394318000	8.059653000
H	8.106684000	6.943631000	-2.524364000	H	12.278048000	6.791402000	8.925171000
C	11.144406000	16.858286000	1.295455000	H	12.887111000	7.691340000	7.528028000
H	10.093931000	17.040282000	1.087184000	H	11.494280000	8.305499000	8.431166000
C	9.472746000	14.948350000	-2.569896000	C	11.728590000	5.307996000	6.658923000
H	9.434363000	15.348504000	-3.574616000	H	12.023777000	4.684398000	7.511677000
C	7.516753000	12.267109000	-3.880846000	H	11.067790000	4.714383000	6.016809000
H	7.492015000	12.845990000	-4.794830000	H	12.633375000	5.536728000	6.085820000
C	10.650631000	13.276978000	1.649719000	C	9.798589000	6.167620000	7.996453000
C	4.408131000	7.431633000	-3.572548000	H	9.086668000	5.569226000	7.416546000
H	3.371244000	7.574850000	-3.864852000	H	10.131545000	5.555701000	8.842278000
C	6.403630000	8.263258000	-2.454444000	H	9.265154000	7.033074000	8.406095000
C	5.076052000	6.253573000	-3.912576000	H	5.939937000	13.874723000	-1.255931000
H	4.563554000	5.477358000	-4.474404000	H	6.306317000	14.111268000	3.025624000
C	6.407549000	6.079813000	-3.529053000	H	4.050262000	17.094227000	0.888258000
H	6.938397000	5.170419000	-3.798129000	C	4.337652000	16.037372000	-1.598548000
C	5.066780000	8.428889000	-2.852077000	F	4.142862000	17.373472000	-1.567749000
H	4.543081000	9.341928000	-2.582799000	F	5.130690000	15.764270000	-2.656791000
C	13.328549000	17.686756000	1.926592000	F	3.136302000	15.468705000	-1.848808000
H	13.979984000	18.512413000	2.199954000	C	4.803796000	16.345881000	3.391550000
C	13.835351000	16.387397000	1.850419000	F	4.587912000	17.669387000	3.230800000
H	14.886026000	16.199262000	2.055074000	F	3.680281000	15.825383000	3.934842000
C	12.999883000	15.326704000	1.500852000	F	5.787547000	16.199541000	4.304596000
H	13.402720000	14.321001000	1.424611000				
C	4.126479000	18.381586000	1.945556000	H	5.109374000	18.740210000	1.619074000
H	4.236251000	17.974404000	2.956133000	H	3.451791000	19.244235000	2.005046000

3d + *cis*-stilbene (in Figure S20)

Ru	8.090943000	11.661182000	0.393876000	H	10.237739000	16.187282000	-1.160780000
N	8.666557000	13.374697000	-0.459553000	C	10.900756000	11.500284000	3.467588000
N	7.624377000	11.366058000	-1.498898000	H	11.298560000	11.028972000	4.354434000
C	7.588102000	12.483487000	-2.316171000	C	10.344029000	14.200332000	1.083545000
N	9.715351000	11.803095000	1.538066000	C	11.518099000	17.677430000	2.061792000
C	10.044445000	10.858381000	2.515794000	H	11.079539000	18.652316000	2.257254000
C	7.491105000	8.724329000	-0.270511000	C	11.097998000	12.794829000	3.061699000
C	8.744537000	8.935322000	1.585744000	H	11.689417000	13.548369000	3.561708000
C	8.250043000	13.602310000	-1.751427000	C	11.231232000	15.333695000	1.474018000
C	9.561776000	14.344644000	-0.081226000	C	9.602062000	9.520059000	2.545241000
N	8.119448000	9.631304000	0.572677000	C	6.897602000	9.030878000	-1.521431000
C	6.979689000	10.305794000	-2.115725000	C	8.456192000	7.538697000	1.411317000
C	9.620923000	15.299500000	-1.152460000	H	8.827094000	6.744472000	2.043113000

C	6.514046000	10.796468000	-3.378246000	H	13.466762000	7.231584000	7.113858000
H	5.959066000	10.216442000	-4.102319000	H	12.125152000	7.681157000	8.177670000
C	7.691167000	7.411640000	0.280132000	C	12.393690000	4.832289000	6.179346000
H	7.339509000	6.493823000	-0.169226000	H	12.807474000	4.178571000	6.956870000
C	6.673576000	7.570247000	-3.562088000	H	11.717118000	4.234608000	5.557719000
H	7.528195000	8.084566000	-3.991979000	H	13.223407000	5.163721000	5.546267000
C	10.690675000	16.607909000	1.717171000	C	10.540045000	5.463979000	7.735125000
H	9.617502000	16.755959000	1.655212000	H	9.822320000	4.850334000	7.178849000
C	8.813801000	14.838709000	-2.180199000	H	10.988320000	4.828862000	8.507552000
H	8.678552000	15.295199000	-3.152059000	H	9.987258000	6.262036000	8.243874000
C	6.898091000	12.124873000	-3.502993000	H	4.192184000	12.780219000	0.703818000
H	6.707222000	12.775772000	-4.346320000	H	7.749964000	14.323709000	2.570301000
C	10.373940000	13.006534000	1.843469000	H	4.161905000	16.704098000	2.486451000
C	4.506991000	6.219900000	-2.441340000	C	2.574086000	14.899926000	1.209688000
H	3.658675000	5.702477000	-2.001319000	F	2.195407000	16.192838000	1.118417000
C	6.227750000	7.934489000	-2.279803000	F	2.269387000	14.300014000	0.041822000
C	4.959083000	5.868722000	-3.714884000	F	1.790121000	14.328469000	2.159753000
H	4.469363000	5.072250000	-4.268613000	C	6.759982000	16.751408000	3.273300000
C	6.045256000	6.546797000	-4.272164000	F	7.358706000	17.561107000	2.359720000
H	6.410222000	6.274679000	-5.259060000	F	5.933189000	17.531869000	3.999329000
C	5.136041000	7.241652000	-1.729083000	F	7.732950000	16.305315000	4.093178000
H	4.769291000	7.519971000	-0.745470000	C	3.373459000	9.467399000	3.451192000
C	12.898664000	17.495991000	2.162638000	C	3.168798000	9.843447000	4.732561000
H	13.541925000	18.330141000	2.429732000	H	4.068438000	8.638323000	3.315722000
C	13.448610000	16.235731000	1.916937000	H	3.661103000	9.221561000	5.480818000
H	14.523202000	16.086935000	1.983127000	C	2.411583000	10.965170000	5.318007000
C	12.623051000	15.164449000	1.576414000	C	2.235662000	12.204681000	4.675068000
H	13.055613000	14.189283000	1.371547000	C	1.896830000	10.820226000	6.620005000
N	6.688912000	12.230171000	1.291406000	C	1.547617000	13.242820000	5.298880000
C	6.055224000	13.423964000	1.580729000	C	1.202624000	11.856369000	7.243030000
C	4.700231000	13.582958000	1.226554000	C	1.022370000	13.073459000	6.583045000
C	6.713397000	14.454208000	2.282475000	H	2.644577000	12.360713000	3.683901000
C	4.035875000	14.763916000	1.549173000	H	2.041139000	9.877732000	7.143754000
C	6.025828000	15.622539000	2.599257000	H	1.427375000	14.186737000	4.774993000
C	4.687559000	15.791042000	2.235680000	H	0.808099000	11.714684000	8.245955000
C	10.116716000	8.635992000	3.633744000	H	0.486092000	13.885236000	7.067287000
C	9.240920000	8.030641000	4.544421000	C	2.809634000	9.969086000	2.183713000
C	11.488701000	8.369934000	3.775575000	C	3.592673000	9.885068000	1.016445000
C	9.716750000	7.200476000	5.561871000	C	1.497608000	10.463575000	2.063402000
C	11.956030000	7.538870000	4.789595000	C	3.100940000	10.317043000	-0.216563000
C	11.084441000	6.933571000	5.712379000	C	1.005611000	10.894322000	0.832805000
H	8.174100000	8.220807000	4.462862000	C	1.805126000	10.830391000	-0.312059000
H	12.191958000	8.811812000	3.074968000	H	4.605792000	9.495462000	1.083496000
H	8.996948000	6.764930000	6.246088000	H	0.860949000	10.505527000	2.940774000
H	13.025092000	7.355880000	4.855151000	H	3.730315000	10.247704000	-1.099907000
C	11.645875000	6.025574000	6.821357000	H	-0.009798000	11.275933000	0.766109000
C	12.630703000	6.834577000	7.699094000	H	1.418566000	11.168332000	-1.269579000
H	13.048804000	6.197809000	8.488371000				

TS-1 (in Figure S20)

Ru	8.265586000	11.838092000	0.057904000	C	9.758086000	14.568460000	-0.175921000
N	8.879842000	13.641927000	-0.660452000	N	8.187583000	9.797930000	0.247724000
N	8.061084000	11.597343000	-1.859054000	C	7.507397000	10.540703000	-2.579918000
C	8.107100000	12.740445000	-2.655547000	C	10.010964000	15.518018000	-1.235716000
N	9.723242000	11.957147000	1.375166000	H	10.666442000	16.374736000	-1.163498000
C	9.907337000	10.994287000	2.385233000	C	10.606274000	11.629808000	3.458649000
C	7.727145000	8.909640000	-0.709934000	H	10.864011000	11.153494000	4.393476000
C	8.724636000	9.076086000	1.288988000	C	10.401940000	14.376092000	1.064557000
C	8.669319000	13.863033000	-1.992204000	C	11.590042000	17.804075000	2.190577000

H	11.174897000	18.800204000	2.319186000	H	12.623841000	7.532701000	5.046409000
C	10.856931000	12.931456000	3.101417000	C	11.042918000	6.045765000	6.728229000
H	11.359783000	13.679258000	3.698052000	C	11.867029000	6.836338000	7.772412000
C	11.276235000	15.469418000	1.576412000	H	12.197403000	6.171302000	8.579783000
C	9.465255000	9.653731000	2.347423000	H	12.759760000	7.290663000	7.329906000
C	7.331785000	9.254656000	-2.027259000	H	11.268681000	7.639773000	8.217236000
C	8.519026000	7.673679000	1.024896000	C	11.916939000	4.913091000	6.137761000
H	8.855403000	6.865007000	1.657821000	H	12.246003000	4.231348000	6.931746000
C	7.201054000	11.058929000	-3.875357000	H	11.355565000	4.329341000	5.399283000
H	6.737137000	10.496323000	-4.673590000	H	12.811449000	5.305269000	5.642650000
C	7.909189000	7.573871000	-0.196414000	C	9.845430000	5.400683000	7.451570000
H	7.662560000	6.667246000	-0.730799000	H	9.235017000	4.795195000	6.771761000
C	7.375915000	7.847616000	-4.121213000	H	10.207606000	4.738727000	8.246338000
H	8.279523000	8.368027000	-4.425073000	H	9.197206000	6.151936000	7.917015000
C	10.769241000	16.770336000	1.737834000	H	4.853352000	13.402543000	-0.840838000
H	9.723491000	16.966002000	1.526312000	H	7.429675000	14.316825000	2.470151000
C	9.339405000	15.077066000	-2.357381000	H	4.835896000	17.352429000	0.858011000
H	9.360621000	15.519592000	-3.344938000	C	3.657505000	15.810779000	-1.057718000
C	7.579534000	12.396760000	-3.922192000	F	3.591080000	17.147881000	-1.231959000
H	7.479488000	13.064555000	-4.768126000	F	3.849107000	15.248826000	-2.270834000
C	10.323100000	13.162348000	1.794753000	F	2.438897000	15.406052000	-0.627318000
C	5.080689000	6.480657000	-3.322287000	C	6.722479000	16.948221000	2.736074000
H	4.183004000	5.954853000	-3.007486000	F	7.506009000	17.861998000	2.104282000
C	6.769598000	8.182601000	-2.898247000	F	5.727344000	17.646127000	3.326668000
C	5.691915000	6.159053000	-4.536039000	F	7.468414000	16.392165000	3.709483000
H	5.276385000	5.378614000	-5.167881000	C	5.665384000	11.210138000	1.793161000
C	6.842038000	6.845371000	-4.931661000	C	5.722301000	11.680412000	3.173306000
H	7.330574000	6.595282000	-5.869813000	H	6.344076000	10.371773000	1.661881000
C	5.614716000	7.481557000	-2.509984000	H	6.579276000	11.301550000	3.726785000
H	5.129481000	7.739233000	-1.572965000	C	4.930820000	12.636901000	3.879967000
C	12.932846000	17.560243000	2.484699000	C	3.851002000	13.383065000	3.326238000
H	13.571320000	18.366413000	2.836199000	C	5.250335000	12.879224000	5.247846000
C	13.451087000	16.273143000	2.322733000	C	3.145335000	14.296849000	4.096855000
H	14.497897000	16.075329000	2.538421000	C	4.536782000	13.791538000	6.010588000
C	12.631520000	15.238467000	1.872903000	C	3.475911000	14.507847000	5.441809000
H	13.042700000	14.243164000	1.731230000	H	3.582381000	13.247729000	2.286045000
N	6.669889000	12.365479000	0.816426000	H	6.075321000	12.329418000	5.694422000
C	6.185349000	13.699707000	0.824646000	H	2.330734000	14.856603000	3.645240000
C	5.218740000	14.105947000	-0.103484000	H	4.806529000	13.952274000	7.050873000
C	6.671460000	14.626611000	1.761645000	H	2.918534000	15.225949000	6.036381000
C	4.739340000	15.418523000	-0.086412000	C	4.363589000	10.926373000	1.081570000
C	6.185014000	15.930719000	1.766336000	C	4.325797000	10.787772000	-0.315814000
C	5.211903000	16.335931000	0.848081000	C	3.201071000	10.625056000	1.808798000
C	9.862498000	8.753022000	3.470435000	C	3.154935000	10.399306000	-0.966861000
C	8.896832000	8.069748000	4.222047000	C	2.030532000	10.230162000	1.157732000
C	11.211188000	8.535314000	3.799913000	C	1.999322000	10.122815000	-0.232571000
C	9.260109000	7.211652000	5.262217000	H	5.220584000	10.982955000	-0.895936000
C	11.567506000	7.676576000	4.835654000	H	3.212484000	10.689383000	2.891378000
C	10.603273000	6.991554000	5.596396000	H	3.151442000	10.306551000	-2.049502000
H	7.844438000	8.213599000	3.991751000	H	1.143428000	10.004872000	1.743709000
H	11.985763000	9.035885000	3.225658000	H	1.086960000	9.820196000	-0.739223000
H	8.470936000	6.713993000	5.815076000				

Int-*cis* (in Figure S20)

Ru	8.271449000	11.876142000	0.087250000	C	9.946466000	10.992918000	2.367297000
N	8.886717000	13.688792000	-0.624958000	C	7.704248000	8.954623000	-0.704936000
N	8.023795000	11.658633000	-1.819905000	C	8.725640000	9.095650000	1.280098000
C	8.070500000	12.808932000	-2.611205000	C	8.654759000	13.920306000	-1.950403000
N	9.759675000	11.966415000	1.364101000	C	9.794230000	14.594658000	-0.157116000

N	8.182425000	9.831286000	0.253681000	C	10.638702000	6.963130000	5.546446000
C	7.467748000	10.607239000	-2.549938000	H	7.873001000	8.230296000	3.989068000
C	10.042778000	15.546009000	-1.217603000	H	12.013241000	9.006448000	3.170261000
H	10.715433000	16.390010000	-1.154550000	H	8.506358000	6.710383000	5.793364000
C	10.665139000	11.613930000	3.434708000	H	12.658011000	7.483461000	4.972341000
H	10.925442000	11.129604000	4.364684000	C	11.082103000	6.003969000	6.665482000
C	10.464938000	14.381259000	1.064738000	C	11.928466000	6.777575000	7.704610000
C	11.752982000	17.777470000	2.177631000	H	12.262049000	6.102853000	8.502542000
H	11.364514000	18.783303000	2.313749000	H	12.820247000	7.225455000	7.253681000
C	10.927810000	12.914856000	3.082250000	H	11.344942000	7.584081000	8.163352000
H	11.445445000	13.653048000	3.678207000	C	11.935659000	4.866112000	6.055370000
C	11.372276000	15.452357000	1.564827000	H	12.266625000	4.174410000	6.839843000
C	9.487453000	9.658753000	2.330846000	H	11.358483000	4.294621000	5.319493000
C	7.296685000	9.314804000	-2.012512000	H	12.828448000	5.252025000	5.552317000
C	8.509199000	7.695946000	1.006537000	C	9.886761000	5.366870000	7.399302000
H	8.849755000	6.880155000	1.627942000	H	9.260761000	4.773799000	6.722704000
C	7.151971000	11.138777000	-3.836420000	H	10.251520000	4.694526000	8.184082000
H	6.679220000	10.584130000	-4.635030000	H	9.253162000	6.121609000	7.879000000
C	7.885475000	7.611687000	-0.207699000	H	5.004673000	13.486876000	-0.902510000
H	7.627036000	6.712415000	-0.748772000	H	7.407089000	14.404553000	2.532539000
C	7.328401000	7.930470000	-4.121624000	H	5.098399000	17.499838000	0.630947000
H	8.231451000	8.452573000	-4.424402000	C	3.970360000	15.942781000	-1.301584000
C	10.900142000	16.765226000	1.735629000	F	3.995792000	17.272298000	-1.533408000
H	9.856814000	16.987602000	1.539205000	F	4.214761000	15.318272000	-2.474544000
C	9.338946000	15.124438000	-2.325629000	F	2.702657000	15.625664000	-0.947268000
H	9.346727000	15.570660000	-3.311681000	C	6.827368000	17.076414000	2.650199000
C	7.531448000	12.477012000	-3.874663000	F	7.663312000	17.949498000	2.027603000
H	7.425176000	13.152484000	-4.713648000	F	5.830277000	17.819050000	3.178469000
C	10.380901000	13.161958000	1.785299000	F	7.515169000	16.526937000	3.669401000
C	5.034613000	6.559338000	-3.325955000	C	5.838351000	11.474045000	1.768901000
H	4.137487000	6.031763000	-3.012530000	C	5.747736000	12.009165000	3.177612000
C	6.728019000	8.253644000	-2.892660000	H	6.472061000	10.587788000	1.837055000
C	5.639910000	6.248861000	-4.545552000	H	6.589847000	11.718089000	3.802580000
H	5.220254000	5.475441000	-5.183280000	C	4.813623000	12.892654000	3.781417000
C	6.789353000	6.937191000	-4.939660000	C	3.693385000	13.478382000	3.120141000
H	7.273209000	6.695759000	-5.882489000	C	5.003092000	13.232306000	5.155568000
C	5.573687000	7.551112000	-2.505723000	C	2.834439000	14.335132000	3.793695000
H	5.093040000	7.800874000	-1.564322000	C	4.136703000	14.086921000	5.818701000
C	13.093593000	17.500084000	2.451401000	C	3.042531000	14.645972000	5.144243000
H	13.756851000	18.289557000	2.794758000	H	3.512835000	13.257915000	2.075406000
C	13.577480000	16.200995000	2.279318000	H	5.851572000	12.804613000	5.684417000
H	14.622256000	15.977045000	2.478627000	H	1.992233000	14.769972000	3.262004000
C	12.726060000	15.187803000	1.840236000	H	4.310582000	14.325331000	6.864634000
H	13.110855000	14.183181000	1.690571000	H	2.364566000	15.318105000	5.662374000
N	6.668445000	12.414781000	0.911752000	C	4.539058000	10.995537000	1.105066000
C	6.235367000	13.781803000	0.837849000	C	4.416615000	10.916420000	-0.288386000
C	5.360734000	14.197947000	-0.168840000	C	3.500553000	10.473752000	1.891823000
C	6.712749000	14.720947000	1.764411000	C	3.275636000	10.368595000	-0.880067000
C	4.956332000	15.535039000	-0.239056000	C	2.363121000	9.920007000	1.302702000
C	6.300997000	16.047954000	1.686177000	C	2.240940000	9.871706000	-0.087030000
C	5.415443000	16.464893000	0.687873000	H	5.223840000	11.265821000	-0.921421000
C	9.890223000	8.747660000	3.443243000	H	3.579309000	10.502980000	2.973762000
C	8.926515000	8.071471000	4.203575000	H	3.205465000	10.325028000	-1.963610000
C	11.240640000	8.511630000	3.752118000	H	1.570544000	9.528284000	1.934910000
C	9.293766000	7.202031000	5.232739000	H	1.352364000	9.446671000	-0.545878000
C	11.600733000	7.641558000	4.777076000				

Int-*trans* (in Figure S20)

Ru	8.184073000	11.854683000	0.205991000	N	8.808285000	13.656546000	-0.515733000

N	7.839700000	11.665261000	-1.684703000	C	9.939720000	8.651796000	3.437269000
C	7.926120000	12.805731000	-2.485595000	C	9.011565000	8.013821000	4.271558000
N	9.733451000	11.907370000	1.422593000	C	11.299152000	8.358777000	3.638528000
C	9.981976000	10.909059000	2.383917000	C	9.422655000	7.125180000	5.267808000
C	7.563181000	8.945253000	-0.600132000	C	11.702524000	7.471003000	4.631874000
C	8.652072000	9.052929000	1.353097000	C	10.776918000	6.829401000	5.474122000
C	8.545328000	13.901200000	-1.833724000	H	7.952065000	8.219305000	4.145022000
C	9.723024000	14.557251000	-0.057695000	H	12.043549000	8.823866000	2.998206000
N	8.098456000	9.807260000	0.344240000	H	8.661901000	6.664478000	5.888261000
C	7.273676000	10.621126000	-2.411681000	H	12.764478000	7.269584000	4.743420000
C	9.947012000	15.521624000	-1.113395000	C	11.266805000	5.851693000	6.557089000
H	10.617236000	16.367924000	-1.053587000	C	12.204049000	6.596723000	7.537744000
C	10.780117000	11.496209000	3.413514000	H	12.572817000	5.909866000	8.309487000
H	11.105561000	10.984655000	4.307694000	H	13.074653000	7.021176000	7.026714000
C	10.427684000	14.326601000	1.141234000	H	11.676565000	7.417170000	8.037933000
C	11.639439000	17.714601000	2.350602000	C	12.043369000	4.691557000	5.889037000
H	11.218352000	18.694731000	2.558429000	H	12.402190000	3.985869000	6.648249000
C	11.017905000	12.807487000	3.083458000	H	11.402030000	4.142288000	5.190307000
H	11.577432000	13.527789000	3.663066000	H	12.913938000	5.051854000	5.331117000
C	11.323292000	15.407551000	1.642564000	C	10.105538000	5.246739000	7.368890000
C	9.490627000	9.585029000	2.359857000	H	9.416939000	4.676886000	6.734446000
C	7.116411000	9.324810000	-1.886153000	H	10.502500000	4.559611000	8.124639000
C	8.355958000	7.663650000	1.100592000	H	9.529180000	6.017199000	7.893754000
H	8.672135000	6.836432000	1.719866000	H	5.348081000	13.419814000	-1.096016000
C	6.998239000	11.142020000	-3.712685000	H	6.947792000	14.509540000	2.734476000
H	6.547686000	10.579331000	-4.518591000	H	5.048260000	17.488184000	0.274051000
C	7.683199000	7.600997000	-0.090054000	C	4.399849000	15.837112000	-1.809558000
H	7.345266000	6.711419000	-0.602594000	F	4.234058000	17.167541000	-1.961709000
C	7.320116000	7.247056000	-3.308481000	F	5.064448000	15.381583000	-2.894362000
H	8.373586000	7.199252000	-3.047198000	F	3.169026000	15.273204000	-1.843893000
C	10.805974000	16.687720000	1.905169000	C	6.357490000	17.163450000	2.620842000
H	9.743209000	16.869610000	1.779434000	F	7.487190000	17.834373000	2.275401000
C	9.222378000	15.109790000	-2.211070000	F	5.378056000	18.089328000	2.716906000
H	9.208688000	15.566289000	-3.192279000	F	6.563020000	16.654482000	3.851916000
C	7.396951000	12.473234000	-3.755206000	C	5.726464000	11.568502000	1.918955000
H	7.324771000	13.141178000	-4.603601000	C	5.259592000	12.277009000	3.157906000
C	10.383396000	13.090244000	1.834755000	H	6.379057000	10.740222000	2.192211000
C	4.624315000	7.389829000	-4.006745000	H	4.350335000	12.865063000	3.068499000
H	3.572539000	7.450048000	-4.274447000	C	5.861402000	12.224918000	4.440431000
C	6.530481000	8.285215000	-2.788532000	C	7.067566000	11.520403000	4.720629000
C	5.418088000	6.359141000	-4.513754000	C	5.238081000	12.907575000	5.527684000
H	4.988795000	5.615409000	-5.179827000	C	7.599884000	11.496859000	6.002301000
C	6.767906000	6.291185000	-4.162530000	C	5.779012000	12.877873000	6.803069000
H	7.395307000	5.497123000	-4.559000000	C	6.963763000	12.170189000	7.053350000
C	5.175628000	8.346221000	-3.152088000	H	7.588927000	11.002566000	3.923512000
H	4.554280000	9.141427000	-2.750571000	H	4.318235000	13.456339000	5.340460000
C	13.004094000	17.484151000	2.535002000	H	8.520201000	10.948646000	6.184065000
H	13.652406000	18.285063000	2.880431000	H	5.280950000	13.406231000	7.611749000
C	13.531680000	16.217860000	2.271241000	H	7.386411000	12.147429000	8.053764000
H	14.594606000	16.031701000	2.401568000	C	4.538770000	10.986773000	1.154699000
C	12.699562000	15.189488000	1.829579000	C	4.496531000	9.607937000	0.906961000
H	13.115956000	14.210513000	1.609953000	C	3.459168000	11.776339000	0.726584000
N	6.608649000	12.454028000	1.039611000	C	3.412467000	9.032347000	0.241315000
C	6.174872000	13.805951000	0.849438000	C	2.380360000	11.204566000	0.051763000
C	5.526763000	14.169924000	-0.334207000	C	2.352464000	9.829634000	-0.193321000
C	6.425331000	14.782304000	1.825804000	H	5.319558000	8.978597000	1.233209000
C	5.123333000	15.493590000	-0.534773000	H	3.451491000	12.844543000	0.918989000
C	6.021294000	16.098816000	1.611778000	H	3.401121000	7.960945000	0.060780000
C	5.362928000	16.464027000	0.433576000	H	1.557614000	11.834626000	-0.275589000

H	1.507622000	9.383830000	-0.711515000				

TS-rotation (in Figure S20)

Ru	8.281551000	12.128791000	0.055514000	C	5.014353000	14.557431000	0.757782000
N	9.054543000	13.861328000	-0.752194000	C	7.272925000	15.124077000	1.372208000
N	7.971682000	11.864641000	-1.832960000	C	4.659293000	15.904513000	0.831504000
C	8.082266000	12.978871000	-2.669156000	C	6.903112000	16.466759000	1.453944000
N	9.826203000	12.118579000	1.265102000	C	5.598667000	16.873399000	1.174697000
C	9.924621000	11.192306000	2.327770000	C	9.646058000	9.031961000	3.536797000
C	7.564415000	9.199514000	-0.659699000	C	8.619922000	8.509426000	4.335132000
C	8.531480000	9.366226000	1.345934000	C	10.964962000	8.667981000	3.856780000
C	8.787816000	14.055354000	-2.078046000	C	8.897712000	7.667583000	5.413995000
C	10.133457000	14.631834000	-0.403969000	C	11.235429000	7.825393000	4.931192000
N	8.054467000	10.090926000	0.280306000	C	10.211011000	7.302908000	5.740521000
C	7.391218000	10.808600000	-2.540667000	H	7.588589000	8.770925000	4.113970000
C	10.453609000	15.476070000	-1.532794000	H	11.782742000	9.039957000	3.245919000
H	11.253815000	16.202017000	-1.561157000	H	8.065542000	7.299170000	6.003667000
C	10.741484000	11.784864000	3.337647000	H	12.270498000	7.564777000	5.134986000
H	10.957931000	11.334175000	4.295236000	C	10.555903000	6.372326000	6.916574000
C	10.860019000	14.379537000	0.776723000	C	11.478332000	7.118315000	7.910289000
C	12.922003000	17.506850000	1.445513000	H	11.738022000	6.465734000	8.752887000
H	12.774425000	18.583232000	1.475849000	H	12.412548000	7.439049000	7.437363000
C	11.166809000	13.010065000	2.887875000	H	10.982781000	8.010012000	8.311007000
H	11.796507000	13.710665000	3.417644000	C	11.287497000	5.117729000	6.381820000
C	11.998857000	15.276848000	1.122534000	H	11.545598000	4.444975000	7.208947000
C	9.332605000	9.915042000	2.374124000	H	10.654049000	4.564305000	5.679101000
C	7.201648000	9.528491000	-1.987026000	H	12.215907000	5.376752000	5.862008000
C	8.248002000	7.970348000	1.123848000	C	9.302758000	5.906579000	7.682451000
H	8.528129000	7.165286000	1.787979000	H	8.615928000	5.345104000	7.038774000
C	7.102892000	11.310668000	-3.844022000	H	9.597691000	5.245605000	8.505196000
H	6.614080000	10.747590000	-4.626730000	H	8.752879000	6.749141000	8.117391000
C	7.668458000	7.869374000	-0.110075000	H	4.250056000	13.833286000	0.514843000
H	7.386692000	6.963443000	-0.627342000	H	8.280676000	14.823415000	1.624849000
C	7.373706000	8.137410000	-4.078617000	H	5.318769000	17.917672000	1.238465000
H	8.267480000	8.694779000	-4.343226000	C	3.221996000	16.294552000	0.603229000
C	11.840499000	16.673412000	1.157885000	F	3.107782000	17.580967000	0.207578000
H	10.864722000	17.105051000	0.971112000	F	2.640567000	15.523243000	-0.342343000
C	9.619022000	15.117349000	-2.566981000	F	2.484671000	16.158779000	1.728073000
H	9.629631000	15.500877000	-3.579026000	C	7.937545000	17.498487000	1.811652000
C	7.531895000	12.631239000	-3.922217000	F	8.622742000	17.913958000	0.715182000
H	7.460217000	13.282991000	-4.783367000	F	7.386624000	18.599757000	2.364681000
C	10.618829000	13.241475000	1.589532000	F	8.850385000	17.017817000	2.683386000
C	5.108054000	6.673348000	-3.381346000	C	5.810708000	11.813691000	1.668043000
H	4.220834000	6.108822000	-3.105816000	C	5.302688000	12.483004000	2.937976000
C	6.702546000	8.443441000	-2.881519000	H	6.440540000	10.981948000	2.009526000
C	5.781745000	6.381792000	-4.569109000	H	5.933537000	13.318659000	3.226403000
H	5.426132000	5.587189000	-5.219628000	C	4.190829000	12.297643000	3.807189000
C	6.917711000	7.117231000	-4.913633000	C	3.034119000	11.495290000	3.582436000
H	7.456328000	6.891961000	-5.830413000	C	4.228016000	13.024755000	5.039827000
C	5.563940000	7.692626000	-2.544536000	C	2.018165000	11.419019000	4.527180000
H	5.030579000	7.925271000	-1.628951000	C	3.211721000	12.936414000	5.976256000
C	14.183177000	16.965623000	1.700575000	C	2.093917000	12.126753000	5.731955000
H	15.023907000	17.616827000	1.924489000	H	2.922416000	10.956198000	2.653094000
C	14.357063000	15.580281000	1.661624000	H	5.090545000	13.655287000	5.242182000
H	15.337151000	15.147538000	1.844836000	H	1.147264000	10.803181000	4.316659000
C	13.277784000	14.745926000	1.374732000	H	3.283985000	13.501328000	6.902046000
H	13.424440000	13.671065000	1.325088000	H	1.293558000	12.057481000	6.463116000
N	6.722544000	12.768695000	0.945435000	C	4.804154000	11.089705000	0.751974000
C	6.337523000	14.148894000	0.997637000	C	4.382687000	11.565174000	-0.495166000

C	4.334947000	9.832837000	1.167954000	H	4.699148000	9.409081000	2.100768000
C	3.447705000	10.855960000	-1.255685000	H	3.132533000	11.253057000	-2.216599000
C	3.397845000	9.124687000	0.416840000	H	3.037788000	8.163462000	0.774583000
C	2.933139000	9.645814000	-0.794013000	H	2.201221000	9.099813000	-1.382765000
H	4.804376000	12.475179000	-0.905234000				

TS-*cis* (in Figure S20)

Ru	8.457106000	11.961873000	0.124213000	C	12.512242000	15.280365000	2.662589000
N	9.124311000	13.741105000	-0.411840000	H	12.981816000	14.309440000	2.535357000
N	7.958745000	11.985053000	-1.787026000	N	6.740924000	12.474121000	1.020403000
C	8.245756000	13.139333000	-2.500441000	C	5.982232000	13.540375000	0.435606000
N	9.704363000	11.980699000	1.693492000	C	4.857886000	13.299882000	-0.360963000
C	9.859040000	10.928191000	2.578818000	C	6.440790000	14.857407000	0.585919000
C	7.788080000	9.183561000	-0.891110000	C	4.203753000	14.366201000	-0.985627000
C	8.746270000	9.144542000	1.167338000	C	5.782014000	15.910177000	-0.039891000
C	8.908061000	14.128178000	-1.724018000	C	4.653239000	15.675024000	-0.828538000
C	9.940773000	14.631144000	0.229592000	C	9.712825000	8.578371000	3.387341000
N	8.349013000	9.961702000	0.122037000	C	8.694620000	7.879560000	4.049302000
C	7.540799000	10.990046000	-2.626807000	C	11.038422000	8.273423000	3.739812000
C	10.216020000	15.687959000	-0.719858000	C	8.985428000	6.920841000	5.022899000
H	10.834244000	16.554610000	-0.529835000	C	11.323098000	7.316755000	4.710137000
C	10.525999000	11.445985000	3.744738000	C	10.305656000	6.614119000	5.379416000
H	10.779416000	10.874762000	4.626847000	H	7.657179000	8.089264000	3.801576000
C	10.434206000	14.376286000	1.536181000	H	11.852233000	8.787816000	3.236119000
C	11.335847000	17.792098000	2.935126000	H	8.157040000	6.414495000	5.506365000
H	10.870277000	18.768968000	3.038093000	H	12.364718000	7.110560000	4.941591000
C	10.787454000	12.779079000	3.524559000	C	10.666309000	5.561241000	6.443259000
H	11.291786000	13.454559000	4.201465000	C	11.478939000	6.230441000	7.577377000
C	11.200073000	15.473527000	2.194829000	H	11.752595000	5.489783000	8.338919000
C	9.407399000	9.600625000	2.339088000	H	12.404020000	6.682114000	7.204181000
C	7.387199000	9.651852000	-2.175268000	H	10.894843000	7.019545000	8.064846000
C	8.382355000	7.794502000	0.820976000	C	11.519300000	4.445431000	5.793157000
H	8.568881000	6.921378000	1.430230000	H	11.792988000	3.689851000	6.539952000
C	7.488592000	11.567437000	-3.951628000	H	10.964817000	3.945309000	4.990807000
H	7.194427000	11.043313000	-4.850726000	H	12.445656000	4.839626000	5.362382000
C	7.788171000	7.822154000	-0.416148000	C	9.418605000	4.908929000	7.068089000
H	7.408759000	6.972015000	-0.965144000	H	8.811926000	4.388337000	6.318461000
C	7.605485000	7.548219000	-3.569081000	H	9.724954000	4.169402000	7.816705000
H	8.596241000	7.394638000	-3.151514000	H	8.782698000	5.645776000	7.572028000
C	10.626566000	16.750746000	2.335681000	H	4.505629000	12.291447000	-0.522690000
H	9.615831000	16.922899000	1.976246000	H	7.319748000	15.044361000	1.187676000
C	9.582835000	15.375875000	-1.910048000	H	4.140736000	16.495450000	-1.316868000
H	9.621683000	15.947364000	-2.828368000	C	2.963679000	14.087551000	-1.793674000
C	7.919919000	12.880033000	-3.868589000	F	2.750957000	15.031858000	-2.734032000
H	8.036938000	13.572424000	-4.692446000	F	3.032347000	12.892691000	-2.420638000
C	10.297725000	13.127745000	2.215283000	F	1.859563000	14.055147000	-1.009795000
C	5.086598000	7.967256000	-4.688221000	C	6.328903000	17.308467000	0.080777000
H	4.103719000	8.137390000	-5.120196000	F	7.156346000	17.612413000	-0.941209000
C	6.856824000	8.667502000	-3.165399000	F	5.339906000	18.230717000	0.074606000
C	5.837804000	6.854435000	-5.071409000	F	7.032305000	17.478988000	1.225072000
H	5.445457000	6.154930000	-5.804774000	C	6.158564000	11.560538000	2.047894000
C	7.100214000	6.650454000	-4.509976000	C	6.644950000	12.605283000	2.970508000
H	7.699151000	5.795141000	-4.812129000	H	6.840410000	10.711678000	2.097639000
C	5.592313000	8.864844000	-3.747092000	H	7.670373000	12.446469000	3.284531000
H	5.004047000	9.729489000	-3.451706000	C	6.019095000	13.777007000	3.538619000
C	12.634216000	17.581840000	3.403797000	C	4.696388000	14.212580000	3.284166000
H	13.186661000	18.393389000	3.869956000	C	6.813395000	14.545112000	4.426259000
C	13.220230000	16.321998000	3.262287000	C	4.196371000	15.352596000	3.904984000
H	14.236097000	16.151196000	3.609367000	C	6.303918000	15.677435000	5.049255000

C	4.991588000	16.086215000	4.790882000	C	3.160010000	9.584564000	0.803447000
H	4.067703000	13.663936000	2.594268000	C	2.629774000	10.433473000	2.998879000
H	7.837207000	14.234149000	4.617171000	C	2.266600000	9.696157000	1.873192000
H	3.179961000	15.672875000	3.694461000	H	5.103329000	10.096414000	0.037116000
H	6.930456000	16.247017000	5.729438000	H	4.147791000	11.631763000	3.940173000
H	4.592689000	16.974615000	5.272312000	H	2.898160000	8.990613000	-0.067705000
C	4.755025000	11.001399000	1.968233000	H	1.952541000	10.508317000	3.845325000
C	4.398865000	10.219710000	0.856344000	H	1.301551000	9.198780000	1.832910000
C	3.869293000	11.078757000	3.049262000				

TS-*trans* (in Figure S20)

Ru	8.284260000	11.921760000	0.429746000	C	12.826876000	17.595078000	3.138143000
N	8.927584000	13.709937000	-0.217461000	H	13.431749000	18.410170000	3.526630000
N	7.813129000	11.841294000	-1.476347000	C	13.383724000	16.325802000	2.966040000
C	8.018106000	12.979608000	-2.242387000	H	14.428494000	16.151023000	3.210117000
N	9.712811000	11.972550000	1.825555000	C	12.607913000	15.279660000	2.466935000
C	9.997609000	10.930264000	2.702712000	H	13.053301000	14.301407000	2.312822000
C	7.638264000	9.078581000	-0.478223000	N	6.513850000	12.566935000	1.107154000
C	8.750201000	9.105727000	1.490235000	C	5.955868000	13.732933000	0.477596000
C	8.678640000	14.019667000	-1.533312000	C	5.123531000	13.621911000	-0.642576000
C	9.796929000	14.609808000	0.323945000	C	6.316102000	15.002925000	0.938063000
N	8.210655000	9.899822000	0.494054000	C	4.646871000	14.774607000	-1.270407000
C	7.323348000	10.820338000	-2.255029000	C	5.839211000	16.147024000	0.299833000
C	10.045437000	15.615239000	-0.688404000	C	4.996116000	16.042936000	-0.806040000
H	10.692216000	16.473791000	-0.571784000	C	10.018039000	8.592824000	3.563376000
C	10.784524000	11.474711000	3.771762000	C	9.108580000	7.828896000	4.309289000
H	11.134611000	10.922736000	4.632214000	C	11.385527000	8.364236000	3.795312000
C	10.416755000	14.376869000	1.578016000	C	9.540943000	6.889552000	5.248921000
C	11.489855000	17.810513000	2.798616000	C	11.811955000	7.427226000	4.732568000
H	11.047239000	18.795377000	2.923836000	C	10.903445000	6.664537000	5.487389000
C	10.990049000	12.809058000	3.515905000	H	8.042094000	7.965447000	4.149465000
H	11.541721000	13.503544000	4.133432000	H	12.120142000	8.922507000	3.221976000
C	11.255972000	15.477467000	2.133326000	H	8.790636000	6.330460000	5.797509000
C	9.553206000	9.591613000	2.552683000	H	12.880664000	7.283386000	4.868224000
C	7.179672000	9.502392000	-1.753777000	C	11.419568000	5.637481000	6.510347000
C	8.428549000	7.733838000	1.183229000	C	12.283705000	6.357793000	7.573021000
H	8.727050000	6.875681000	1.768371000	H	12.667757000	5.637471000	8.305786000
C	7.169174000	11.358200000	-3.580996000	H	13.143564000	6.865641000	7.123620000
H	6.801040000	10.809562000	-4.437131000	H	11.696039000	7.109983000	8.111974000
C	7.736961000	7.721030000	0.000368000	C	12.281419000	4.576562000	5.784529000
H	7.370182000	6.849055000	-0.522213000	H	12.664708000	3.839994000	6.501415000
C	7.342653000	7.385120000	-3.136312000	H	11.692200000	4.042501000	5.030319000
H	8.366421000	7.261569000	-2.795508000	H	13.141518000	5.026827000	5.277908000
C	10.712873000	16.764676000	2.299142000	C	10.273931000	4.908104000	7.238147000
H	9.675950000	16.943501000	2.030390000	H	9.639052000	4.347887000	6.542128000
C	9.357892000	15.247544000	-1.827679000	H	10.688715000	4.190842000	7.955367000
H	9.367889000	15.755785000	-2.783330000	H	9.637571000	5.603242000	7.798044000
C	7.596403000	12.677933000	-3.569071000	H	4.869735000	12.646377000	-1.036081000
H	7.636561000	13.349144000	-4.417299000	H	6.988874000	15.085047000	1.784449000
C	10.352751000	13.137270000	2.272876000	H	4.628160000	16.931923000	-1.303157000
C	4.733964000	7.727458000	-4.059556000	C	3.701533000	14.637151000	-2.434957000
H	3.717281000	7.868783000	-4.417463000	F	3.760560000	15.705741000	-3.259333000
C	6.599228000	8.490178000	-2.688306000	F	3.966804000	13.537232000	-3.169920000
C	5.480869000	6.628036000	-4.487038000	F	2.416964000	14.532303000	-2.018687000
H	5.050443000	5.909508000	-5.179494000	C	6.287178000	17.488216000	0.813976000
C	6.788045000	6.462511000	-4.024265000	F	7.603154000	17.700081000	0.573536000
H	7.382833000	5.617956000	-4.362604000	F	5.608261000	18.508009000	0.251465000
C	5.288942000	8.650106000	-3.171471000	F	6.123472000	17.580406000	2.155618000
H	4.705454000	9.505668000	-2.842222000	C	5.581983000	11.637344000	1.841120000

C	5.802567000	12.595548000	2.937339000	H	8.343978000	12.063076000	7.597106000
H	6.136269000	10.711319000	1.976111000	C	4.202889000	11.345794000	1.302895000
H	5.256964000	13.528872000	2.856618000	C	4.046731000	10.267668000	0.417654000
C	6.555726000	12.420728000	4.149528000	C	3.076691000	12.096052000	1.662484000
C	7.085841000	11.178801000	4.562696000	C	2.793258000	9.959433000	-0.109742000
C	6.698889000	13.533622000	5.014269000	C	1.820844000	11.785794000	1.136756000
C	7.722453000	11.056711000	5.792987000	C	1.676786000	10.720778000	0.246729000
C	7.335093000	13.406398000	6.241476000	H	4.913847000	9.673686000	0.139375000
C	7.847115000	12.164959000	6.636363000	H	3.169847000	12.923552000	2.359617000
H	6.998761000	10.311666000	3.917684000	H	2.689900000	9.121453000	-0.793542000
H	6.292783000	14.495530000	4.710514000	H	0.956177000	12.377366000	1.424409000
H	8.128811000	10.094787000	6.090271000	H	0.699343000	10.481323000	-0.162789000
H	7.432634000	14.269958000	6.893055000				

P-*cis* (in Figure S20)

Ru	8.390057000	11.861722000	0.093802000	C	6.894795000	5.984133000	-3.721077000
N	8.896004000	13.619495000	-0.737474000	H	7.527967000	5.156394000	-4.029967000
N	7.764596000	11.609383000	-1.742694000	C	5.291477000	8.125374000	-2.939756000
C	7.847231000	12.690111000	-2.610405000	H	4.663687000	8.956674000	-2.630217000
N	9.812239000	12.110730000	1.455299000	C	13.074750000	17.757954000	1.924561000
C	10.089066000	11.196990000	2.469025000	H	13.727671000	18.588324000	2.180203000
C	7.756108000	8.940065000	-0.465962000	C	13.590282000	16.463970000	1.820941000
C	8.874828000	9.211377000	1.478769000	H	14.649455000	16.283914000	1.986291000
C	8.531428000	13.810406000	-2.044982000	C	12.752013000	15.398240000	1.494202000
C	9.783884000	14.576539000	-0.342245000	H	13.160458000	14.396525000	1.397960000
N	8.337417000	9.866650000	0.392392000	N	6.531949000	12.426040000	0.932435000
C	7.262403000	10.500740000	-2.384525000	C	6.289970000	13.848986000	0.896434000
C	9.931326000	15.494945000	-1.454888000	C	5.637091000	14.447407000	-0.181094000
H	10.570501000	16.366983000	-1.467394000	C	6.838736000	14.644939000	1.909515000
C	10.880447000	11.882410000	3.451476000	C	5.514467000	15.838131000	-0.229014000
H	11.230971000	11.455314000	4.380387000	C	6.706180000	16.029254000	1.848820000
C	10.483563000	14.470837000	0.887711000	C	6.038777000	16.637446000	0.783087000
C	11.715099000	17.976815000	1.695362000	C	10.066962000	9.001933000	3.648596000
H	11.301478000	18.978421000	1.779310000	C	9.123586000	8.380574000	4.478556000
C	11.103660000	13.164571000	3.003584000	C	11.423749000	8.786816000	3.944731000
H	11.669522000	13.932539000	3.512163000	C	9.514015000	7.589568000	5.561521000
C	11.379735000	15.602915000	1.264227000	C	11.808176000	7.997506000	5.025026000
C	9.641040000	9.847973000	2.491985000	C	10.865675000	7.379385000	5.865761000
C	7.215754000	9.228999000	-1.750228000	H	8.064626000	8.518285000	4.274294000
C	8.576401000	7.804228000	1.334528000	H	12.182620000	9.237621000	3.311397000
H	8.884175000	7.026465000	2.019109000	H	8.739687000	7.138913000	6.172876000
C	6.962194000	10.918762000	-3.726781000	H	12.869999000	7.857029000	5.209300000
H	6.546046000	10.287835000	-4.500667000	C	11.336682000	6.519734000	7.052482000
C	7.887788000	7.643206000	0.161396000	C	12.188095000	7.387218000	8.010231000
H	7.533235000	6.711557000	-0.256720000	H	12.539530000	6.787002000	8.858617000
C	7.435234000	7.018530000	-2.956231000	H	13.068424000	7.803378000	7.509324000
H	8.485088000	6.997837000	-2.678258000	H	11.601745000	8.224558000	8.405796000
C	10.876650000	16.911341000	1.365897000	C	12.194930000	5.343439000	6.528459000
H	9.819796000	17.090536000	1.200297000	H	12.542519000	4.722900000	7.363802000
C	9.160396000	15.020501000	-2.497299000	H	11.615321000	4.707091000	5.849963000
H	9.080054000	15.447557000	-3.488875000	H	13.077739000	5.694811000	5.984299000
C	7.321040000	12.257654000	-3.859976000	C	10.159710000	5.933494000	7.855539000
H	7.249322000	12.853093000	-4.761283000	H	9.532139000	5.277801000	7.241049000
C	10.454188000	13.324604000	1.734282000	H	10.544447000	5.335063000	8.689217000
C	4.750310000	7.090313000	-3.703731000	H	9.523042000	6.718810000	8.278876000
H	3.701841000	7.122902000	-3.988809000	H	5.255093000	13.849069000	-0.994409000
C	6.640901000	8.103871000	-2.549753000	H	7.383615000	14.186880000	2.725271000
C	5.549999000	6.015281000	-4.096425000	H	5.953078000	17.716477000	0.731294000
H	5.129507000	5.209309000	-4.691951000	C	4.762608000	16.470627000	-1.371256000

F	5.183307000	17.729665000	-1.612828000	H	4.057671000	13.604399000	2.498428000
F	4.898569000	15.765077000	-2.514240000	H	6.809248000	11.023523000	4.576904000
F	3.436131000	16.540523000	-1.108163000	H	3.278458000	14.498015000	4.645261000
C	7.245764000	16.887998000	2.962027000	H	6.008369000	11.911712000	6.735528000
F	7.778783000	18.037084000	2.481430000	H	4.234813000	13.661476000	6.784056000
F	6.270238000	17.246498000	3.828302000	C	4.022326000	11.638102000	0.340365000
F	8.201795000	16.260144000	3.673095000	C	3.786372000	11.798924000	-1.037555000
C	5.428093000	11.385762000	0.797636000	C	2.923499000	11.525914000	1.201905000
C	6.054856000	11.612027000	2.136090000	C	2.487422000	11.916726000	-1.527189000
H	5.849529000	10.525325000	0.285491000	C	1.620612000	11.632296000	0.706987000
H	6.807614000	10.868749000	2.378069000	C	1.398990000	11.842137000	-0.653195000
C	5.485511000	12.230056000	3.373514000	H	4.624913000	11.816324000	-1.729861000
C	4.489676000	13.221858000	3.415046000	H	3.079752000	11.338218000	2.257748000
C	6.024486000	11.775765000	4.589593000	H	2.325246000	12.054907000	-2.592428000
C	4.046037000	13.729353000	4.635673000	H	0.780414000	11.544061000	1.390168000
C	5.575869000	12.280466000	5.809849000	H	0.385614000	11.929805000	-1.034960000
C	4.583668000	13.260748000	5.836472000				

P-*trans* (in Figure S20)

Ru	8.219548000	11.947961000	0.640831000	H	3.678059000	7.806549000	-4.193982000
N	8.868910000	13.721226000	-0.064926000	C	6.506349000	8.445563000	-2.382865000
N	7.740086000	11.821540000	-1.267239000	C	5.423096000	6.538818000	-4.159829000
C	7.954200000	12.930151000	-2.065830000	H	5.006277000	5.803406000	-4.842770000
N	9.678987000	12.022356000	1.995263000	C	6.711461000	6.372527000	-3.647120000
C	10.009863000	10.989633000	2.871037000	H	7.306354000	5.510454000	-3.937688000
C	7.537829000	9.088408000	-0.183169000	C	5.216877000	8.606588000	-2.919375000
C	8.706697000	9.151632000	1.749423000	H	4.635680000	9.482379000	-2.644722000
C	8.622029000	13.990294000	-1.388626000	C	12.822355000	17.680302000	3.123662000
C	9.744080000	14.633837000	0.441471000	H	13.429306000	18.507324000	3.482531000
N	8.135466000	9.928771000	0.759472000	C	13.392938000	16.419690000	2.933596000
C	7.231756000	10.784791000	-2.009335000	H	14.450001000	16.263993000	3.133591000
C	9.990707000	15.609440000	-0.598540000	C	12.614569000	15.357651000	2.473192000
H	10.642321000	16.467768000	-0.510181000	H	13.069551000	14.386206000	2.304771000
C	10.861696000	11.540017000	3.883957000	N	6.226630000	12.630532000	1.116437000
H	11.256744000	10.993984000	4.728627000	C	5.811049000	13.836314000	0.432372000
C	10.398145000	14.418224000	1.682324000	C	5.224170000	13.784989000	-0.834007000
C	11.468768000	17.871991000	2.839978000	C	6.077986000	15.069794000	1.026952000
H	11.015554000	18.850203000	2.978627000	C	4.889518000	14.975009000	-1.482516000
C	11.063813000	12.869351000	3.599678000	C	5.760114000	16.251595000	0.359079000
H	11.656642000	13.565417000	4.176133000	C	5.156966000	16.212938000	-0.897046000
C	11.246905000	15.531716000	2.196839000	C	10.103160000	8.660571000	3.743861000
C	9.559174000	9.650412000	2.763845000	C	9.261019000	7.901844000	4.567613000
C	7.076350000	9.481259000	-1.467292000	C	11.485729000	8.433337000	3.856568000
C	8.367387000	7.774771000	1.483521000	C	9.773516000	6.962922000	5.466336000
H	8.679243000	6.928754000	2.079067000	C	11.991922000	7.499036000	4.755604000
C	7.079970000	11.282072000	-3.351562000	C	11.151456000	6.737184000	5.586020000
H	6.698097000	10.714080000	-4.188722000	H	8.187438000	8.053129000	4.507073000
C	7.638594000	7.740283000	0.324943000	H	12.168321000	8.990587000	3.221049000
H	7.250172000	6.859094000	-0.165381000	H	9.073863000	6.406560000	6.080990000
C	7.248415000	7.316505000	-2.771315000	H	13.068420000	7.356480000	4.799781000
H	8.259333000	7.192025000	-2.395077000	C	11.756010000	5.715037000	6.564814000
C	10.689659000	16.810607000	2.378064000	C	12.684667000	6.447210000	7.563303000
H	9.639806000	16.969659000	2.149416000	H	13.129007000	5.732836000	8.267554000
C	9.300391000	15.206412000	-1.725126000	H	13.503524000	6.965286000	7.053039000
H	9.308164000	15.683721000	-2.696648000	H	12.127444000	7.192863000	8.142218000
C	7.523737000	12.596472000	-3.381924000	C	12.578160000	4.667265000	5.777099000
H	7.563722000	13.243100000	-4.248787000	H	13.018655000	3.933396000	6.463399000
C	10.361026000	13.188937000	2.391841000	H	11.944717000	4.128461000	5.063214000
C	4.679154000	7.662385000	-3.795402000	H	13.396078000	5.129311000	5.214518000

C	10.677669000	4.967433000	7.372683000	C	7.249199000	12.972720000	4.358847000
H	9.999698000	4.402698000	6.722405000	C	6.741786000	10.493955000	5.533457000
H	11.155289000	4.252673000	8.052463000	C	7.850086000	12.640385000	5.571049000
H	10.076434000	5.651363000	7.982644000	C	7.593231000	11.401674000	6.163703000
H	5.038914000	12.832603000	-1.313198000	H	5.484012000	10.112683000	3.827250000
H	6.557433000	15.109506000	1.998829000	H	7.449252000	13.941536000	3.909139000
H	4.907427000	17.131507000	-1.414412000	H	6.532937000	9.532252000	5.993291000
C	4.184955000	14.930998000	-2.814065000	H	8.517434000	13.348743000	6.052399000
F	4.579974000	15.942955000	-3.617606000	H	8.055946000	11.145599000	7.112644000
F	4.407509000	13.775263000	-3.470057000	C	3.803766000	11.520388000	0.854748000
F	2.844387000	15.052206000	-2.663475000	C	3.467429000	10.418924000	0.051204000
C	6.140752000	17.562815000	0.992844000	C	2.828489000	12.498953000	1.099198000
F	7.464847000	17.813107000	0.857933000	C	2.192654000	10.302607000	-0.502137000
F	5.481162000	18.603317000	0.445356000	C	1.555429000	12.385039000	0.541200000
F	5.880331000	17.564939000	2.320765000	C	1.233670000	11.288264000	-0.261202000
C	5.177751000	11.553592000	1.434512000	H	4.212734000	9.650916000	-0.137840000
C	5.633266000	12.473988000	2.500125000	H	3.054250000	13.357500000	1.724246000
H	5.679008000	10.592227000	1.412644000	H	1.950817000	9.441113000	-1.118167000
H	4.956640000	13.304483000	2.696742000	H	0.812980000	13.153177000	0.738064000
C	6.402239000	12.060923000	3.713008000	H	0.240203000	11.201405000	-0.692087000
C	6.153178000	10.819340000	4.310273000				

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