

Electronic Supplementary Material (ESI) for Dalton Transactions.

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Supplementary information

Facile C-N Bond Cleavage of Primary Aliphatic Amines by (Salen)ruthenium(VI) Nitrido Complexes

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Materials. $[\text{Ru}^{\text{VI}}(\text{N})(\text{salchda})(\text{MeOH})](\text{PF}_6)$ **1**, 50% ^{15}N -labeled **1** (**Ru ^{15}N**) and ruthenium nitrido complexes with salchda ligands bearing various substituents were prepared by a literature method.¹ Benzylamine (99%, Aldrich), cyclohexylamine (99%, Aldrich), dichloromethane and 1,2-dichloroethane were purified according to literature procedures.²

Kinetics. Kinetic studies were carried out using either an Applied Photophysics SC20 stopped-flow spectrophotometer or an Agilent 8453 diode-array spectrophotometer. The temperatures of the solutions were maintained with a PolyScience digital temperature controller connected to a circulating water bath. The concentrations of primary amines were at least in 10-fold excess to that of **1**. The reaction progress was monitored by observing absorbance changes at 404, 362 and 400 nm. Pseudo-first-order rate constants, k_{obs} , were obtained by nonlinear least-square fits of A_t vs t according to the equation $A_t = A_\infty + (A_0 - A_\infty)\exp(-k_{\text{obs}}t)$, where A_0 and A_∞ are the initial and final absorbance, respectively.

Physical measurements. Infrared spectra were obtained from KBr plates using a Nicolet 360 FT-IR spectrophotometer. ^1H NMR spectra were recorded on a Bruker (400 MHz) FT NMR spectrometer. The chemical shifts (δ ppm) were reported with reference to tetramethylsilane (TMS). Electrospray ionization mass spectra (ESI/MS) were obtained on a PE SCIEX API 365 mass spectrometer. The analyte solution was continuously infused with a syringe pump at a constant flow rate of $5 \mu\text{L min}^{-1}$ into the pneumatically assisted electrospray probe with nitrogen as the nebulising gas. The declustering potential was typically set at 10–20 V. Cyclic voltammetry was performed on a CHI 660E instrument in CH_2Cl_2 using a glassy carbon working electrode, a saturated calomel reference electrode and a Pt wire counter electrode. Gas chromatographic analyses were performed on a HP5890 gas chromatograph with a DB-5MS column (30 m \times 0.25 mm i.d.) column. GC-MS measurements were carried out on a HP6890 gas chromatograph interfaced to a HP5973 mass-selective detector.

X-ray crystallography. Measurements were recorded on an Oxford Xcalibur, Sapphire 3, Gemini Ultra diffractometer with a mirror-monochromated Cu-K α radiation ($\lambda = 1.54178 \text{ \AA}$). Details of the intensity data collection and crystal data are given in Table S2. Absorption corrections were done by the multiscan method. The structures were resolved by the heavy-atom Patterson method or direct methods and refined by full-matrix least-squares using SHELX-97 and expanded using Fourier techniques.^{3,4} All non-hydrogen atoms were refined anisotropically. H atoms were generated by the program SHELXL-97. The positions of H atoms were calculated based on riding mode with thermal parameters equal to 1.2 times or 1.5 times that of the associated C atoms and 1.2 times that of the associated N atoms, all these were participated in the calculation of final R-indices. All calculations were performed using the teXsan crystallographic software.⁵

Computational details. DFT calculations have been performed to gain more insight into the mechanism of the reaction of **1** with benzylamine (PhCH_2NH_2) using the Gaussian 16 quantum chemistry software package.⁶ The potential energy profile of the reaction were calculated at the B3LYP-D3(BJ)/def2-TZVP level.⁷⁻¹¹ The solvent effect of dichloroethane was taken account by the Polarizable Continuum Model (PCM).^{12,13} The nature of all stationary points (minima and transition state structures) was confirmed by vibrational frequencies calculations.

Synthesis of $[\text{Ru}^{\text{III}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)_2]\text{PF}_6$ [2**] PF_6 .** Benzylamine (12 mg, 0.11 mmol) was added to a solution of **1** (41 mg, 0.0669 mmol) in $(\text{CH}_2\text{Cl})_2$ (20 mL) under argon. The mixture was stirred for 5 min under argon and then stirred for 5 min in air. The solution was then concentrated to 1 mL under vacuum followed by addition of diethyl ether to precipitate [**2**] PF_6 as a blue solid. Yield: 90 %. Anal. calcd. (found) for $\text{C}_{34}\text{H}_{38}\text{N}_4\text{O}_2\text{PF}_6\text{Ru}$: C, 52.31 (52.65); H, 4.91 (5.29); N, 7.18 (7.14). ESI/MS in acetone: m/z 636.

Synthesis of [Ru^{III}(salchda-Cl)(PhCH₂NH₂)₂]PF₆ [3]PF₆. Complex **3**PF₆ was prepared by a procedure similar to that for [2]PF₆ except that **1** with two chloro substituents on the salchda ligand was used. Yield: 87 %. Single crystals suitable for X-ray analysis were obtained by slow diffusion of n-pentane into a solution of [3]PF₆ in dichloromethane at room temperature. Anal. calcd. (found) for C₃₄H₃₆Cl₂N₄O₂PF₆Ru: C, 48.07 (48.31); H, 4.27 (4.46); N, 6.59 (6.53).

Determination of organic products by GC and GC-MS. In a typical reaction, deaerated benzylamine (12 mg, 0.11 mmol) was added to a deaerated solution of **1** (7 mg, 11.4 μmol) in CH₂Cl₂ (7 mL) and the mixture was stirred at room temperature under argon atmosphere for 1 min. The organic products were then analyzed by GC and GC-MS using chlorobenzene as internal standard. Bibenzyl and toluene were generated in 24% yield and 1.3% yield, respectively.

Following the similar procedure, deaerated cyclohexylamine (11 mg, 0.11 mmol) was added to a deaerated solution of **1** (4 mg, 6.5 μmol) in CH₂Cl₂ (4 mL) and the mixture was stirred at room temperature under argon atmosphere for 1 min. The organic products were then analyzed by GC and GC-MS using chlorobenzene as internal standard. Cyclohexane, cyclohexene and bicyclohexyl were generated in 34% yield, 5.4% yield and 2.8% yield, respectively.

Determination of N₂. In a typical reaction, a deaerated solution of **1**-¹⁵N (2 mg, 3.3 μmol) in CH₂Cl₂ (5 mL) was placed in a round bottom flask (total volume = ca. 6 mL) sealed with a septum under argon at room temperature. Degassed benzylamine (10 mg, 93 μmol) was added using a gastight syringe and the mixture was stirred for 10 min. 50 μL gas in the headspace was withdrawn and analyzed by GC-MS.

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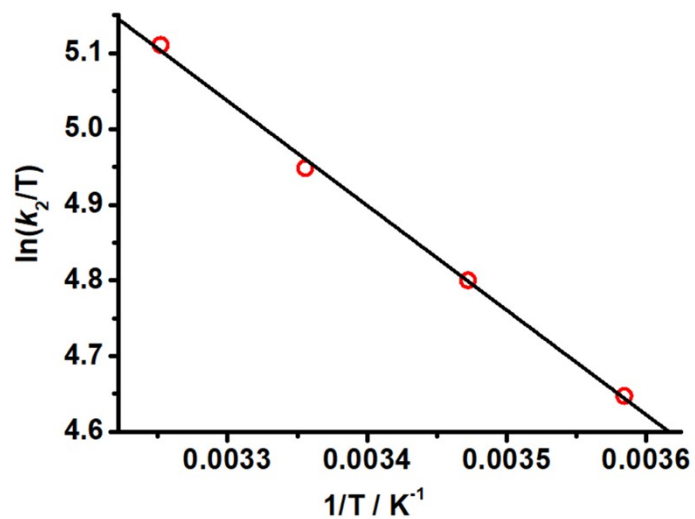


Fig. S1 Plot of $\ln(k_2/T)$ vs $1/T$ for the first step. Slope = $-(1.38 \pm 0.04) \times 10^3$; y-intercept = (9.60 ± 0.14) ; $r^2 = 0.997$.

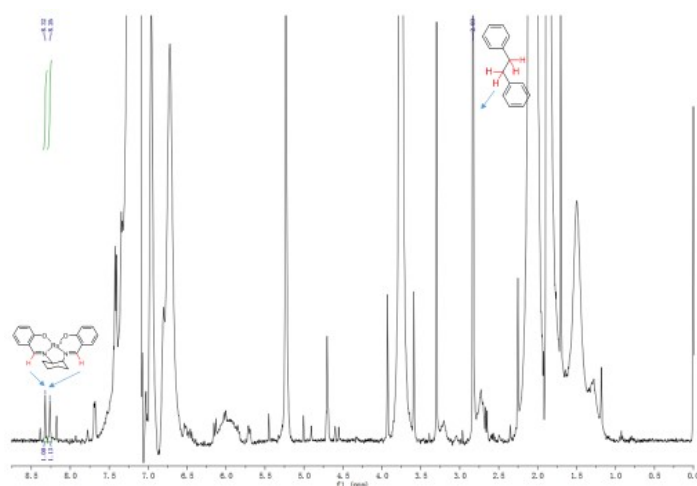


Fig. S2 ^1H NMR spectrum of the red solution obtained from the reaction of **1** (8.9 mg) with benzylamine (20 mg) in 1.5 ml CD_2Cl_2 .

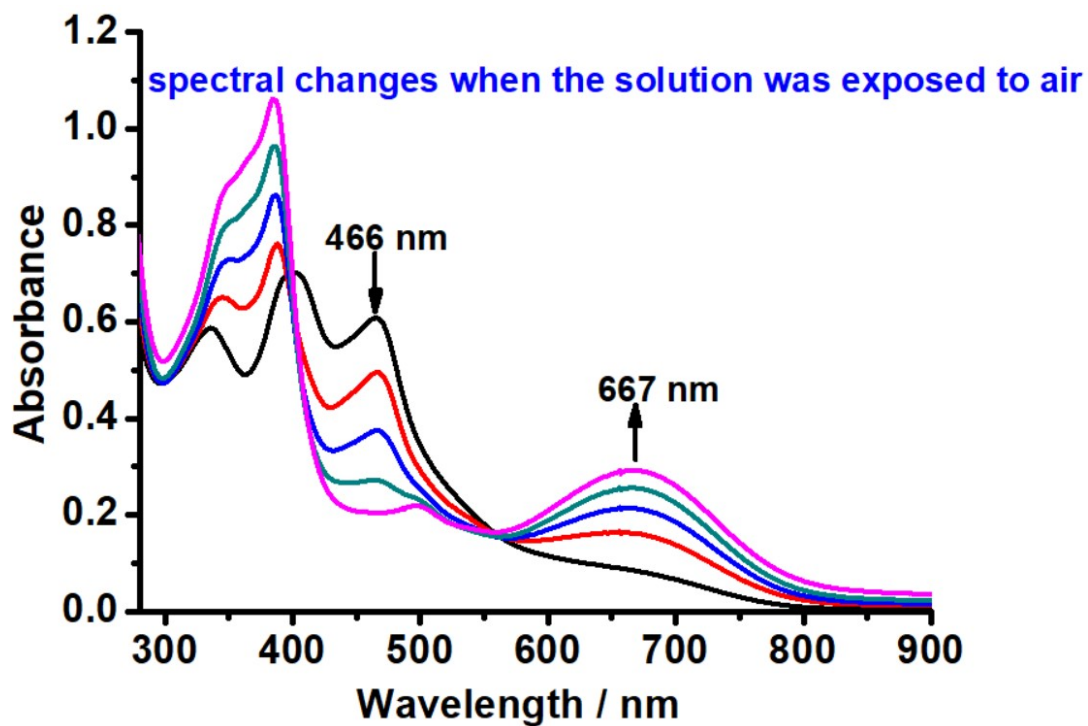


Figure S3 UV-Vis spectrophotometric changes when the final red solution was exposed to air. Reaction of **1** (6.52×10^{-5} M) with benzylamine (1.20×10^{-3} M) in 1,2-dichloroethane at 25 °C under argon.

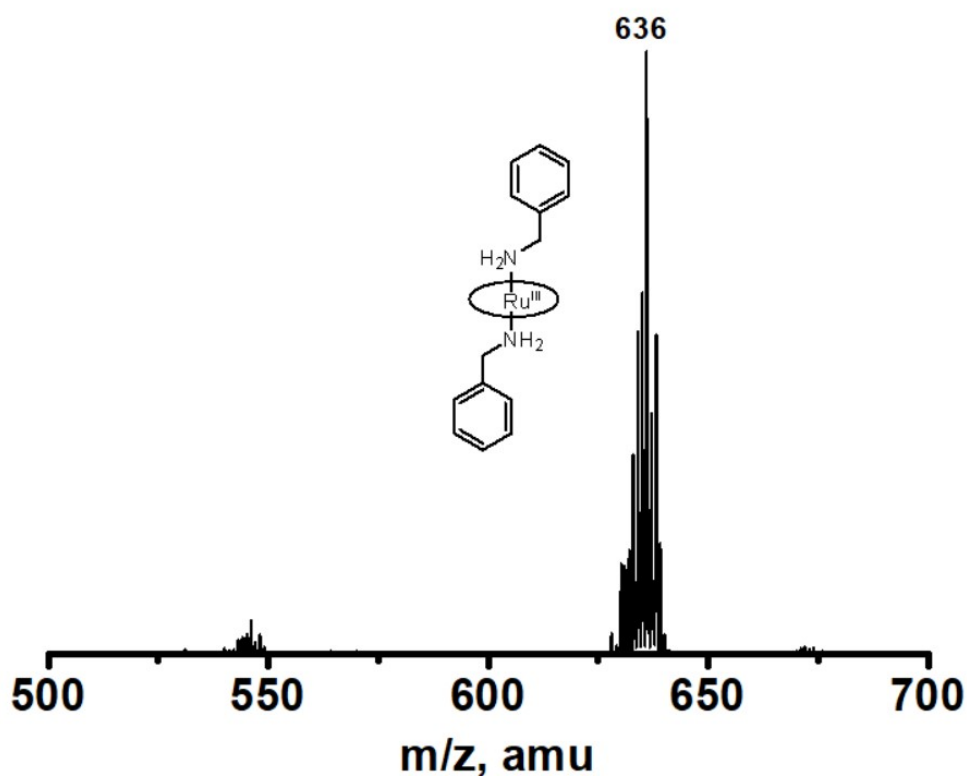


Fig. S4 ESI/MS spectrum of the red solution of the reaction of **1** with benzylamine under argon.

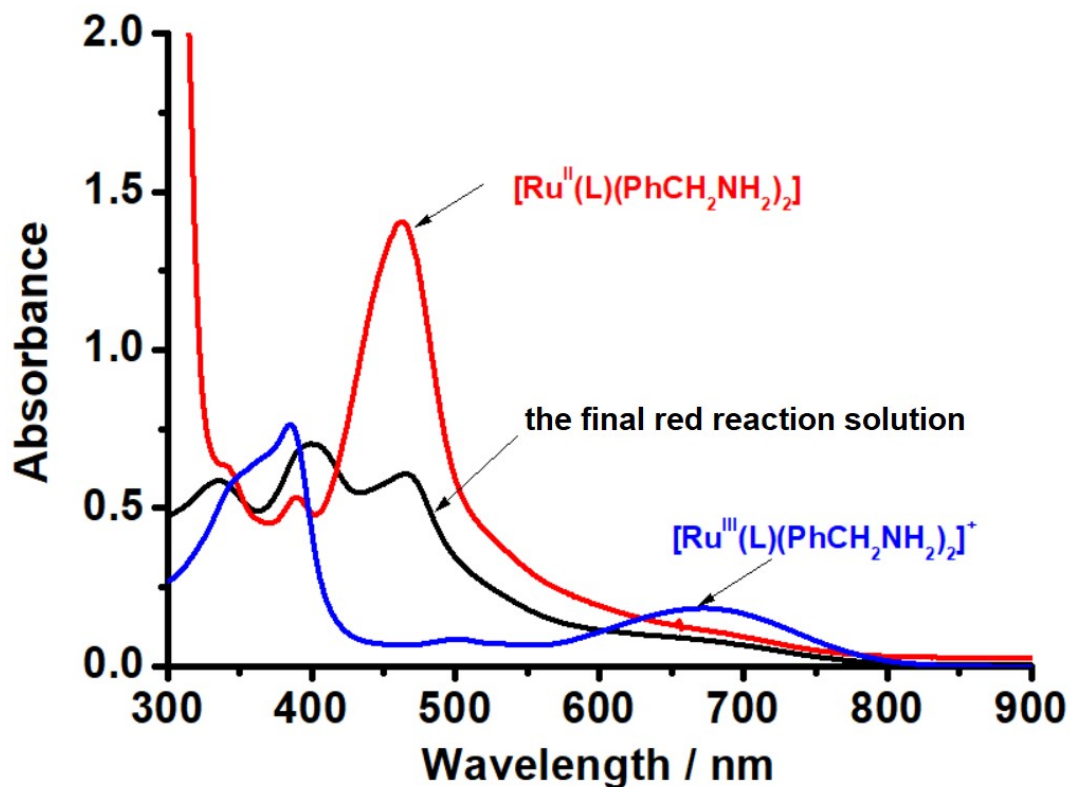


Fig. S5 UV-Vis Spectra of the final red solution, $[\text{Ru}^{\text{II}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)_2]$ and $[\text{Ru}^{\text{III}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)_2]^+$ in 1,2-dichloroethane with $[\text{Ru}] = 5.00 \times 10^{-5} \text{ M}$, respectively. The final spectrum contains some Ru(II) dinitrogen complex which makes the spectrum slightly different from that of pure $[\text{Ru}^{\text{II}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)_2]$.

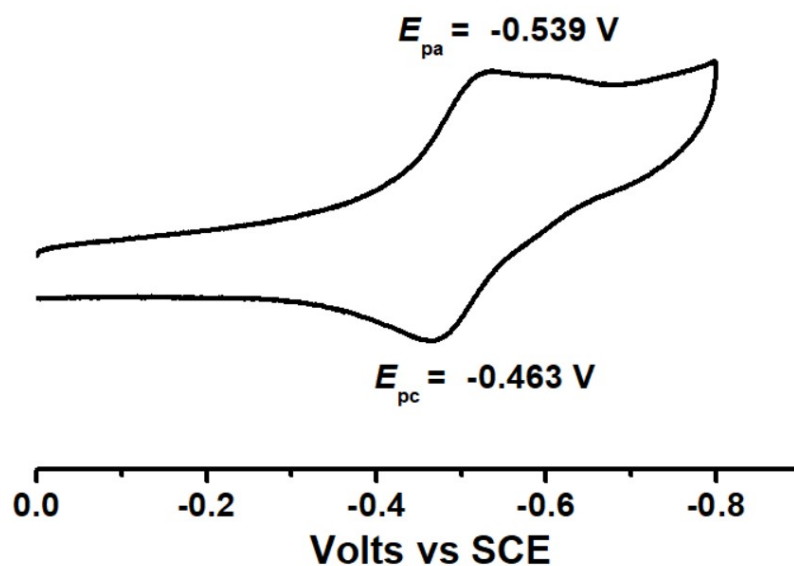


Fig. S6 Cyclic voltammogram of $[\mathbf{3}]\text{PF}_6$ in CH_2Cl_2 containing 0.1 M $t\text{Bu}_4\text{NPF}_6$.

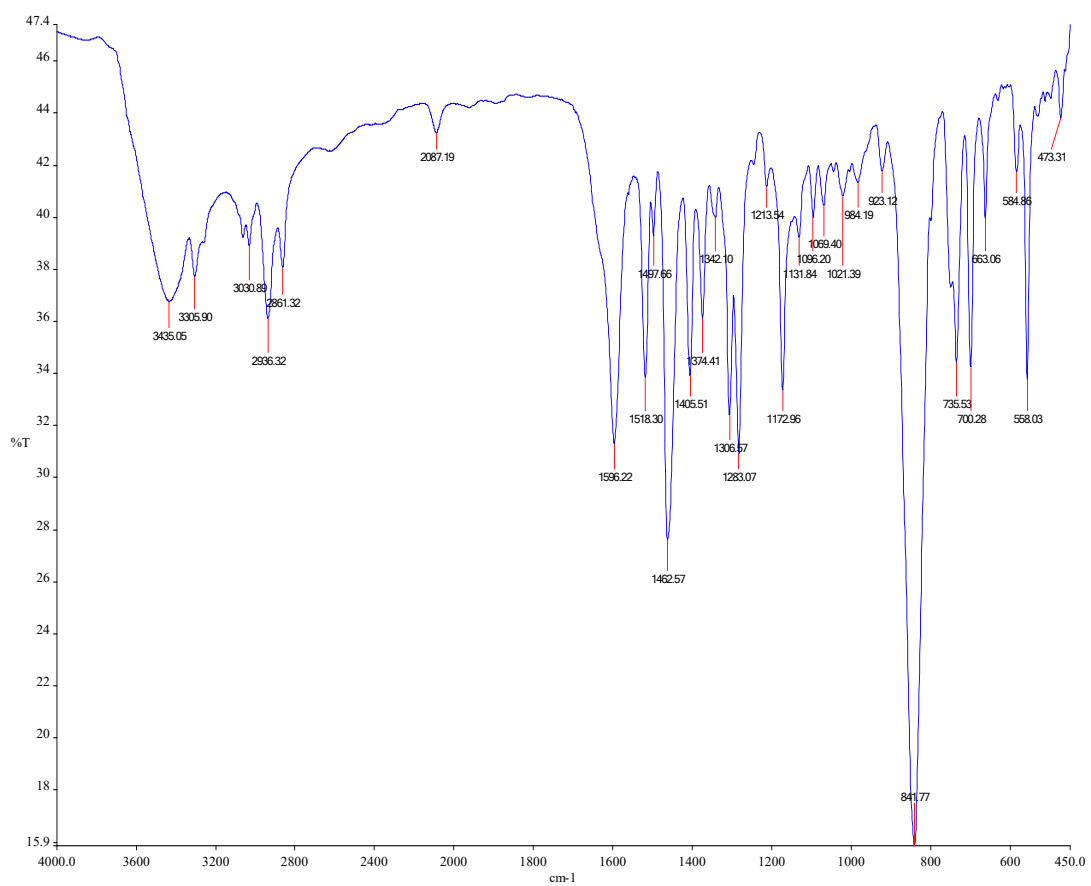


Fig. S7 IR spectrum of the solid obtained from the reaction of **1-Cl** with benzylamine in CH₂Cl₂ under Ar.

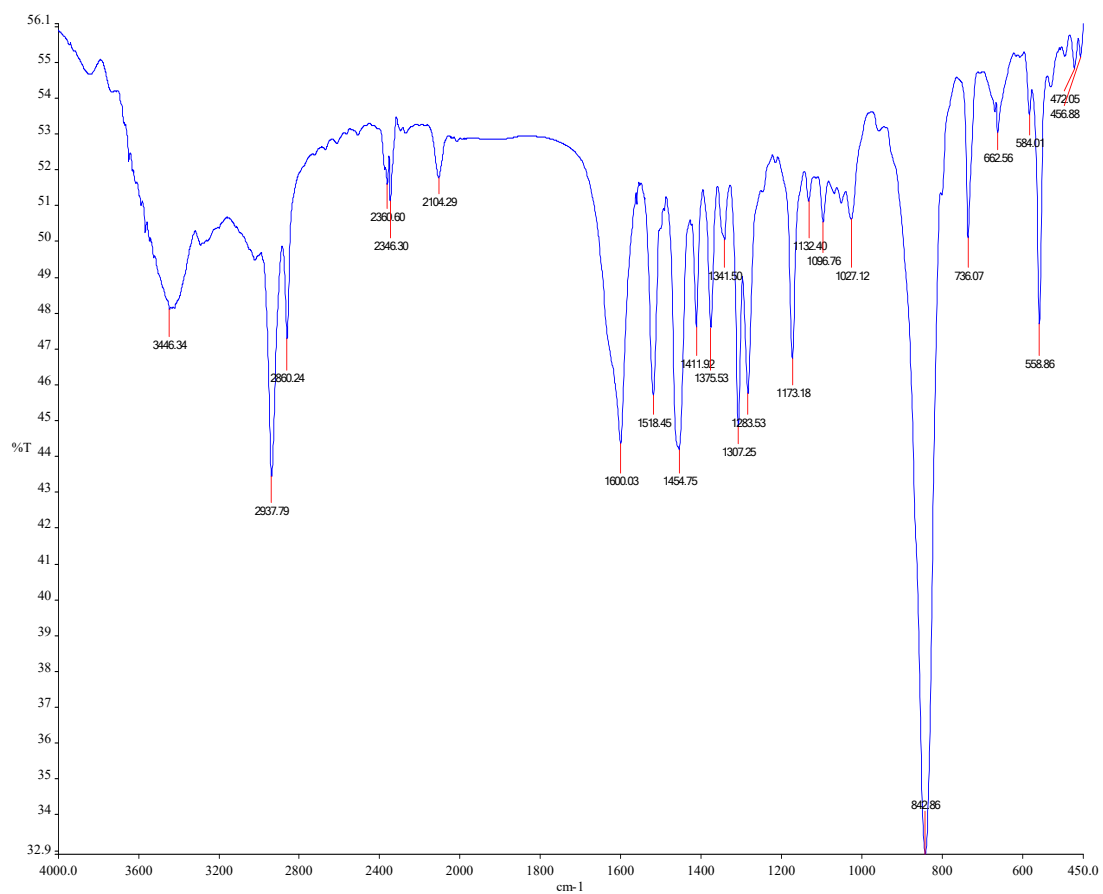


Fig. S8 IR spectrum of the solid obtained from the reaction of **1-Cl** with cyclohexylamine in CH₂Cl₂ under Ar.

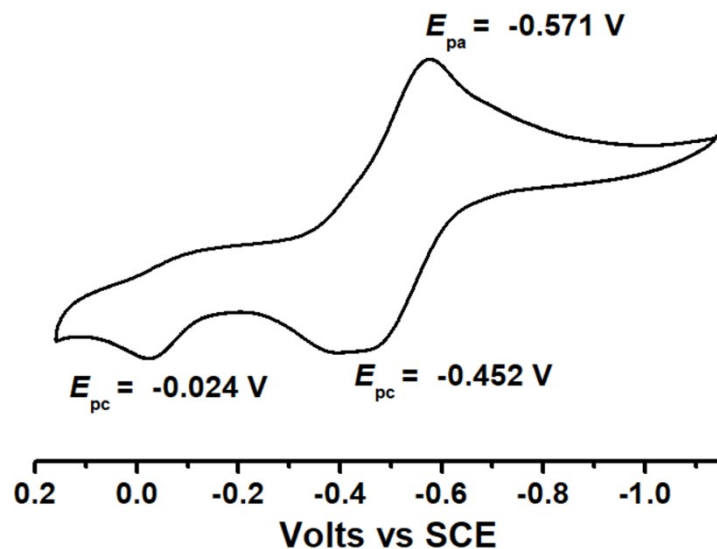


Fig. S9 Cyclic voltammogram recorded in CH_2Cl_2 containing 0.1 M $t\text{Bu}_4\text{NPF}_6$ for the reaction of **1-Cl** with benzyl amine under Ar. The presence of two oxidative waves at around -0.452 V is due to the formation of $[\text{Ru}^{\text{II}}(\text{salchda-Cl})(\text{PhCH}_2\text{NH}_2)]$ via partial dissociation of a benzyl amine ligand upon the reduction of $[\text{Ru}^{\text{III}}(\text{salchda-Cl})(\text{PhCH}_2\text{NH}_2)_2]^+$.

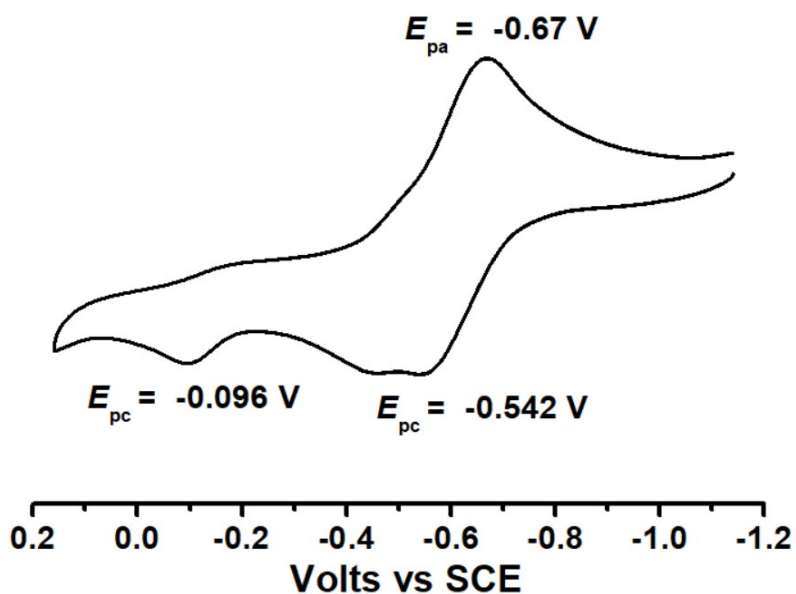


Fig. S10 Cyclic voltammogram recorded in CH_2Cl_2 containing 0.1 M $n\text{Bu}_4\text{NPF}_6$ for the reaction of **1** with benzyl amine under Ar. The presence of two oxidative waves around -0.542 V is due to the formation of $[\text{Ru}^{\text{II}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)]$ via partial dissociation of one benzyl amine ligand upon the reduction of $[\text{Ru}^{\text{III}}(\text{salchda})(\text{PhCH}_2\text{NH}_2)_2]^+$.

Table S1 Crystal data and structure refinement for **3PF₆**.

Empirical formula	C ₃₄ H ₃₆ Cl ₂ F ₆ N ₄ O ₂ PRu
Formula weight	849.61
Temperature/K	173(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	17.7212(2)
b/Å	16.1974(2)
c/Å	24.1947(3)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	6944.78(14)
Z	8
ρ _{calc} /g/cm ³	1.625
μ/mm ⁻¹	6.132
F(000)	3448.0
Crystal size/mm ³	0.35 × 0.11 × 0.03
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	7.308 to 136.486
Index ranges	-13 ≤ h ≤ 21, -19 ≤ k ≤ 18, -29 ≤ l ≤ 29
Reflections collected	32870
Independent reflections	6351 [R _{int} = 0.0322, R _{sigma} = 0.0235]
Data/restraints/parameters	6351/0/451
Goodness-of-fit on F ²	1.026
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0349, wR ₂ = 0.0864
Final R indexes [all data]	R ₁ = 0.0432, wR ₂ = 0.0926
Largest diff. peak/hole / e Å ⁻³	0.95/-0.66

Table S2 Selected bond lengths(Å) and bond angles(°) for **3**.

bond lengths			
Ru1–N1	1.978(2)	Ru1–N2	1.994(3)
Ru1–O1	1.999(2)	Ru1–O2	2.012(2)
Ru1–N3	2.111(3)	Ru1–N4	2.131(3)
bond angles			
N1–Ru1–N3	88.64(10)	N2–Ru1–N3	96.09(10)
O1–Ru1–N3	86.72(10)	O2–Ru1–N3	89.40(10)
N1–Ru1–N4	94.82(11)	N1–Ru1–N4	86.07(11)
O1–Ru1–N4	91.34(10)	O2–Ru1–N4	87.25(10)
N3–Ru1–N4	176.11(10)	O1–Ru1–O2	90.40(8)

Table S3 Second-order rate constants of the reactions between benzylamine and nitrido complexes with salchda ligands (L-X) bearing different substituents in (CH₂Cl)₂ at 25 °C under Ar.

L-X	$k_2 / \text{M}^{-1} \text{s}^{-1}$
MeO	$(3.30 \pm 0.16) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$
Me	$(2.14 \pm 0.07) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$
H	$(4.20 \pm 0.06) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$
Cl	$(5.08 \pm 0.05) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$
Br	$(3.68 \pm 0.21) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$

Table S4. Cartesian coordinates for the optimized geometries at B3LYP-D3(BJ)/def2-TZVP level.

[RuLN]⁺

Ru	-0.02739000	-0.51139700	0.55569500
N	-0.12897600	-0.46000900	2.13610600
N	-1.26373500	0.97386900	-0.12538000
N	1.35615900	0.93945000	0.16067100
O	-1.35366500	-1.88111100	-0.03353100
O	1.27037200	-1.92503700	0.04021800
C	-0.57581300	2.25682000	-0.45169500
C	-1.37688300	3.52038400	-0.15816800
C	0.74930900	2.28098900	0.31043500
H	-0.34567200	2.21328000	-1.52075100
C	-0.54716400	4.75363200	-0.53058700
H	-1.63917800	3.53857000	0.90328800
H	-2.30648500	3.53227000	-0.72573300
C	1.59828300	3.47079700	-0.10586300
H	0.51898000	2.37315400	1.37725400
C	0.81552000	4.76146800	0.15859500
H	-1.10602500	5.65278000	-0.26820800
H	-0.40787200	4.77400200	-1.61555600
H	2.53002100	3.48767000	0.46076800
H	1.85348400	3.39367000	-1.16667900
H	1.40407100	5.61467100	-0.18040500
H	0.67960100	4.88055300	1.23742200
C	-2.65395100	-1.68444400	-0.15412300
C	-3.26364200	-0.40550500	-0.29654300
C	-3.47451000	-2.82380400	-0.19219200
C	-4.66548500	-0.32340400	-0.46972200
C	-4.83956700	-2.70495700	-0.34466400
H	-3.00247200	-3.79149000	-0.09563700
C	-5.44962100	-1.44912400	-0.48175300
H	-5.11195400	0.65515900	-0.59137300
H	-5.44805000	-3.59990400	-0.36269200
H	-6.52039100	-1.37229500	-0.60440000
C	2.57431500	-1.77767000	-0.14368100
C	3.24812400	-0.52844000	-0.24215700
C	3.32493500	-2.95362600	-0.29471900
C	4.63921200	-0.51234300	-0.49264500
C	4.68368600	-2.90120200	-0.52973100
H	2.80465400	-3.89861800	-0.22508700
C	5.35543800	-1.67581000	-0.63015900
H	5.13574400	0.44641100	-0.57031000

H	5.23547700	-3.82571100	-0.64045300
H	6.41950400	-1.64785400	-0.81566000
C	-2.52542900	0.80626200	-0.37352100
C	2.59921200	0.73443500	-0.12736700
H	-3.08436200	1.67855800	-0.69774000
H	3.22247900	1.60585700	-0.30034400

[RuLN]⁰

Ru	-0.01438100	-0.54049100	0.41485200
N	-0.13287700	-0.43327300	2.07658500
N	-1.24304500	0.94466000	-0.20061100
N	1.37852200	0.91804600	0.22678700
O	-1.48691700	-1.96294600	0.12840300
O	1.32404600	-1.95805300	-0.06175100
C	-0.53621700	2.22048900	-0.48278900
C	-1.35091300	3.48794700	-0.24529400
C	0.74580900	2.23947600	0.36473400
H	-0.23172400	2.18471600	-1.53516200
C	-0.50353000	4.72897400	-0.53800200
H	-1.69596800	3.49905400	0.79288100
H	-2.23527300	3.50300400	-0.88189600
C	1.60205500	3.45321700	0.03702400
H	0.43822200	2.29737400	1.41501000
C	0.79606800	4.73442100	0.26338100
H	-1.08692100	5.62495300	-0.31922000
H	-0.27049100	4.75815100	-1.60717100
H	2.49353700	3.46407100	0.66599700
H	1.93564400	3.40214900	-1.00404400
H	1.40297200	5.60028300	-0.00644600
H	0.56666300	4.82933200	1.32920500
C	-2.74451500	-1.69648300	-0.04243600
C	-3.28661000	-0.38770300	-0.28514700
C	-3.65955000	-2.78168100	-0.02569000
C	-4.68335100	-0.24557300	-0.48185400
C	-5.00825300	-2.59661100	-0.20611800
H	-3.24996500	-3.76826200	0.14646000
C	-5.53997300	-1.31460600	-0.43551100
H	-5.07036400	0.74839600	-0.67225200
H	-5.67080600	-3.45285200	-0.17263300
H	-6.60256600	-1.17794500	-0.57978800
C	2.62434700	-1.78153700	-0.18765800
C	3.29179800	-0.52045600	-0.16719100
C	3.40943200	-2.93530400	-0.38784700

C	4.69075100	-0.48360400	-0.34543500
C	4.77755400	-2.86249100	-0.54550500
H	2.89665400	-3.88773500	-0.40820600
C	5.43571900	-1.62693300	-0.52442100
H	5.17986400	0.48316100	-0.33588300
H	5.34496400	-3.77373100	-0.68825700
H	6.50801700	-1.57130900	-0.65041300
C	-2.51141300	0.80116200	-0.42192100
C	2.62930100	0.74814000	-0.02267100
H	-3.06492300	1.67251200	-0.76020300
H	3.25893400	1.62314900	-0.15187500

Benzylamine (PhCH₂NH₂)

C	-2.31255900	0.34252000	-0.00024000
C	-1.36272700	1.35495800	0.00020300
C	-0.00430400	1.04439700	0.00050200
C	0.42409600	-0.27930800	0.00036900
C	-0.54089500	-1.29017700	-0.00011600
C	-1.89488300	-0.98650700	-0.00040600
H	-3.36789600	0.58271000	-0.00048900
H	-1.67507000	2.39171300	0.00030900
H	0.72279500	1.84582800	0.00080500
H	-0.22379800	-2.32724000	-0.00029200
H	-2.62645300	-1.78475100	-0.00080200
N	2.88860900	0.39857200	-0.00106400
H	2.78263800	0.99390900	0.81258000
H	2.78164400	0.99175100	-0.81616200
C	1.89491800	-0.66648000	0.00092200
H	2.08211000	-1.29859600	0.87347800
H	2.08189000	-1.30174600	-0.86938000

PhCH₂NH₃⁺

C	-2.35435800	0.35706300	-0.00821100
C	-1.39794800	1.36121300	0.00671700
C	-0.04311000	1.03922500	0.01741200
C	0.36274700	-0.29109600	0.01325300
C	-0.60447300	-1.29770200	-0.00453500
C	-1.95281400	-0.97609800	-0.01430100
H	-3.40652100	0.60802500	-0.01597600
H	-1.69796200	2.40040000	0.01059400

H	0.67225900	1.85110300	0.02896800
H	-0.29839800	-2.33662800	-0.01095900
H	-2.69172300	-1.76612900	-0.02809800
N	2.77164900	0.42298700	-0.03280200
H	2.68086100	1.04396000	0.77354000
H	2.63678100	0.98214500	-0.87766500
C	1.80505300	-0.72385100	0.03343500
H	2.04460700	-1.26882300	0.94514600
H	2.03539400	-1.36474700	-0.81553900
H	3.73257600	0.07725200	-0.04301600

TS1

Ru	-0.51510200	0.01031400	-0.22542700
N	0.16505400	0.16468700	1.39768500
N	-1.68125900	-1.63586800	-0.12299900
N	-2.23475300	0.93579000	0.32481200
O	1.13679500	-1.13285200	-0.91639400
O	0.09859100	1.57763800	-1.24031400
C	-3.11290500	-1.31962200	0.16511000
C	-3.89403800	-2.42210500	0.87174800
C	-3.14640000	-0.02012300	0.98764400
H	-3.58408000	-1.10977000	-0.80134700
C	-5.32973100	-1.96421500	1.14355200
H	-3.39038600	-2.67135600	1.81035400
H	-3.91975700	-3.32649200	0.26462600
C	-4.57467400	0.44690700	1.22139100
H	-2.68095000	-0.23489100	1.95552800
C	-5.37273800	-0.65360300	1.92471300
H	-5.85953600	-2.74727400	1.68805700
H	-5.85033100	-1.83635000	0.18949500
H	-4.57819900	1.35081300	1.83211900
H	-5.04410300	0.69431900	0.26452800
H	-6.40500600	-0.32612700	2.05652800
H	-4.96084600	-0.81141200	2.92614900
C	1.13815100	-2.43362700	-1.03699400
C	0.00024900	-3.27923400	-0.81749700
C	2.35200800	-3.05325100	-1.41613000
C	0.14190000	-4.67860600	-1.00754800
C	2.44760000	-4.41465200	-1.57634000
H	3.20687500	-2.41035700	-1.57853200
C	1.33325900	-5.24722300	-1.37365100
H	-0.72801900	-5.30370600	-0.84838300

H	3.39570500	-4.84961300	-1.86671300
H	1.41606700	-6.31657100	-1.50632500
C	-0.44471300	2.79329000	-1.19949500
C	-1.68315500	3.11493500	-0.57756600
C	0.26600700	3.81745200	-1.84568000
C	-2.14829400	4.44372400	-0.64171800
C	-0.21113600	5.11260300	-1.87365900
H	1.20332900	3.55731100	-2.31857000
C	-1.42941400	5.43694300	-1.26862700
H	-3.09890800	4.67497900	-0.17723500
H	0.36532100	5.88044800	-2.37342000
H	-1.80410600	6.45047200	-1.29659300
C	-1.30016100	-2.83854300	-0.43524600
C	-2.53662400	2.16191700	0.08594000
H	-2.05185100	-3.62160700	-0.40312600
H	-3.50991100	2.53257800	0.39172300
C	6.61246400	0.47548000	0.98858500
C	5.79585300	0.35608500	-0.13187400
C	4.43815100	0.62904600	-0.03382300
C	3.88612400	1.02100000	1.18668700
C	4.70839200	1.13816300	2.30524400
C	6.06830800	0.86836500	2.20618500
H	7.67141600	0.26705000	0.91112600
H	6.21781400	0.05638400	-1.08200900
H	3.80222400	0.54037000	-0.90623600
H	4.28544800	1.44715300	3.25324800
H	6.70180900	0.96753200	3.07764900
N	1.67915500	-0.02894900	1.44712300
H	1.89264100	-0.45767700	2.34757300
H	1.93753900	-0.66283100	0.67359800
C	2.41104100	1.27383600	1.28844700
H	2.14760000	1.89062300	2.14358900
H	2.01306700	1.72464400	0.38230900

INT1

Ru	0.49265900	-0.91508400	-0.53429400
N	0.36171700	0.04862000	0.94688800
N	2.07134200	-2.07218200	-0.12679600
N	-0.51924800	-2.42807100	0.32073400
O	1.65641200	0.48610000	-1.52463200
O	-0.98693900	-0.48790400	-1.73648100
C	1.69515700	-3.38857400	0.45346900

C	2.74308100	-4.02570100	1.35979700
C	0.37083800	-3.19351000	1.20792300
H	1.49879500	-4.05918400	-0.39055300
C	2.21927500	-5.34644800	1.93026300
H	2.98424200	-3.33112200	2.17020900
H	3.66379900	-4.21688900	0.80894300
C	-0.15973400	-4.51551800	1.74184200
H	0.57378000	-2.52659100	2.05289300
C	0.88542500	-5.16705700	2.65041100
H	2.96337100	-5.76593700	2.60908800
H	2.09714400	-6.06455400	1.11351100
H	-1.08224300	-4.35131700	2.30084000
H	-0.39565400	-5.18326000	0.90771500
H	0.51314700	-6.13059000	3.00165000
H	1.03048800	-4.54191400	3.53682200
C	2.95710400	0.46194600	-1.58469200
C	3.77873000	-0.59241100	-1.06374000
C	3.60962700	1.55173500	-2.21022600
C	5.18787900	-0.49185200	-1.19641300
C	4.97822600	1.61417900	-2.30686700
H	2.98560200	2.34315400	-2.60303100
C	5.78785900	0.58514200	-1.79408700
H	5.79409000	-1.29918300	-0.80415400
H	5.43796900	2.46953000	-2.78585100
H	6.86396200	0.64126100	-1.87681800
C	-2.22906600	-0.95307800	-1.63188000
C	-2.64081900	-1.99243000	-0.75387100
C	-3.19572000	-0.35684600	-2.45749600
C	-3.99771400	-2.37177100	-0.73964300
C	-4.52086500	-0.73832100	-2.40338900
H	-2.87021000	0.43195500	-3.12212400
C	-4.93468000	-1.75322200	-1.53651700
H	-4.29843800	-3.16758400	-0.06927900
H	-5.24379600	-0.23905800	-3.03536100
H	-5.97360100	-2.04782900	-1.49144500
C	3.29630500	-1.77776500	-0.43735600
C	-1.75173400	-2.72105300	0.11499900
H	4.06207700	-2.50982500	-0.19816000
H	-2.18025800	-3.58321700	0.61636300
C	2.78504800	5.98235000	0.97810800
C	3.54908500	4.93979700	0.46576400
C	3.20435700	3.62307100	0.74512500
C	2.09334300	3.33828400	1.53745900
C	1.33263000	4.38845700	2.05074500

C	1.67701300	5.70502800	1.77282900
H	3.05387300	7.00821600	0.76299400
H	4.41424000	5.15009900	-0.14920400
H	3.80024600	2.81373200	0.34325100
H	0.47126100	4.17435200	2.67129700
H	1.08402100	6.51414600	2.17841500
N	0.67460300	1.48383700	0.78703500
H	1.01386300	1.66000300	-0.16732800
H	-0.25488800	2.01781000	0.95309900
C	1.69767000	1.91228400	1.79027500
H	2.54392100	1.23624600	1.69013800
H	1.25054000	1.77211100	2.77191300
C	-6.85732100	2.00426800	0.46630800
C	-6.10473500	2.88525300	-0.30537500
C	-4.72227100	2.76137500	-0.35281400
C	-4.07281400	1.76106100	0.37073200
C	-4.83504300	0.88203100	1.13638800
C	-6.21936800	1.00132300	1.18676600
H	-7.93516600	2.09627900	0.49958100
H	-6.59700700	3.66219300	-0.87611800
H	-4.14201600	3.43967700	-0.96780700
H	-4.34118000	0.08803400	1.68333600
H	-6.79955500	0.30678000	1.78064800
N	-1.81681300	2.57200600	1.16996200
H	-2.12740000	2.51045800	2.13465300
H	-1.97587700	3.52907300	0.87208600
C	-2.57477500	1.62562600	0.32367100
H	-2.29228800	0.62248700	0.63731900
H	-2.21678200	1.75318900	-0.69748200

TS2

Ru	-0.73133400	-0.88378300	0.56507700
N	-0.44396100	0.09357200	-0.89136700
N	-2.50350800	-1.68586100	0.07328800
N	-0.01616600	-2.52555200	-0.34520500
O	-1.62375900	0.66205300	1.60830800
O	0.83118900	-0.74979800	1.75957800
C	-2.37333300	-3.03820200	-0.52590500
C	-3.51101300	-3.45708100	-1.45066600
C	-1.02414600	-3.08373200	-1.26122300
H	-2.31575000	-3.74638500	0.30838600
C	-3.23668000	-4.84337700	-2.03899300

H	-3.61106100	-2.71837700	-2.25169900
H	-4.45658500	-3.48070700	-0.90906800
C	-0.74681000	-4.47145500	-1.82064700
H	-1.08335400	-2.37091800	-2.09100000
C	-1.88593700	-4.90245100	-2.74708400
H	-4.03900100	-5.10757800	-2.72971100
H	-3.25753800	-5.58432500	-1.23366000
H	0.19457300	-4.47266400	-2.37229700
H	-0.64530500	-5.18639100	-0.99829300
H	-1.69490200	-5.91227200	-3.11359000
H	-1.90423000	-4.24659000	-3.62301800
C	-2.89818500	0.92794200	1.58956200
C	-3.89931500	0.09810600	0.98362300
C	-3.33271900	2.12001900	2.22037200
C	-5.25578800	0.50646000	1.04437600
C	-4.65654300	2.48618800	2.24161500
H	-2.57508000	2.73947800	2.68164200
C	-5.63966900	1.67660200	1.64629700
H	-6.00014700	-0.13642000	0.59054600
H	-4.94449400	3.41066400	2.72641900
H	-6.67987700	1.96914600	1.67020800
C	1.94766600	-1.45577400	1.64870700
C	2.14755100	-2.53554600	0.74230300
C	3.01179200	-1.09569700	2.49547100
C	3.39959100	-3.18410400	0.72412900
C	4.22970900	-1.74007700	2.43740600
H	2.84810700	-0.27639100	3.18264500
C	4.43543700	-2.79505500	1.54267500
H	3.53748900	-4.00726600	0.03354200
H	5.03258000	-1.41952400	3.08879400
H	5.39114100	-3.29784300	1.49555200
C	-3.65285800	-1.15457500	0.34604300
C	1.13929400	-3.05115200	-0.14936600
H	-4.54448900	-1.70660500	0.06339800
H	1.40054300	-3.96283700	-0.67749500
C	-1.02235500	6.44900200	-0.99395400
C	-1.95509400	5.67659600	-0.30993800
C	-2.03888900	4.31100100	-0.55136500
C	-1.18928700	3.70331200	-1.47566500
C	-0.26037600	4.48513600	-2.16134400
C	-0.17679000	5.85163300	-1.92268400
H	-0.95942400	7.51340000	-0.80954200
H	-2.62109800	6.13780300	0.40750800
H	-2.77071900	3.71448500	-0.02084900

H	0.39284900	4.02617400	-2.89345700
H	0.54337900	6.45006100	-2.46505900
N	-0.39525000	1.51717400	-0.69647300
H	-0.68373500	1.76021200	0.25802800
H	0.79192200	1.84847000	-0.87646800
C	-1.25610400	2.21852900	-1.69445700
H	-2.27333800	1.84483300	-1.58182800
H	-0.89018800	1.93519400	-2.67942000
C	7.10128600	1.14311300	-0.51292400
C	6.43792700	2.22584600	0.05798800
C	5.05421100	2.21171700	0.17205100
C	4.31630600	1.12096700	-0.28920600
C	4.98805800	0.04061700	-0.85520200
C	6.37408200	0.04923600	-0.96644700
H	8.18011700	1.15159000	-0.59748300
H	7.00021500	3.07614900	0.42142000
H	4.54595000	3.05134700	0.63209300
H	4.42379800	-0.81861800	-1.19519500
H	6.88466900	-0.79951500	-1.40260500
N	2.11509300	2.06758500	-1.05229200
H	2.37309500	1.91925200	-2.02454100
H	2.36048800	3.02586500	-0.81994700
C	2.81813300	1.10055100	-0.17178400
H	2.43890600	0.11473400	-0.42627500
H	2.50138300	1.31662300	0.84761100

INT2⁰

Ru	1.23052400	-0.54999200	-0.59119000
N	0.74118200	0.32367600	0.90620800
N	3.18497800	-0.58303100	-0.11396800
N	1.22767800	-2.33768800	0.30774000
O	1.42178300	1.20555800	-1.64889700
O	-0.49084200	-0.91874600	-1.57213100
C	3.60854000	-1.88908800	0.44014500
C	4.83986800	-1.85610200	1.33943200
C	2.40102400	-2.48179200	1.18593900
H	3.81409400	-2.54218800	-0.41595400
C	5.14676500	-3.25387600	1.88172300
H	4.65993600	-1.16161900	2.16590200
H	5.70544700	-1.48783300	0.78873900
C	2.70516000	-3.88190300	1.70102100
H	2.19926600	-1.82576600	2.04069400

C	3.94352700	-3.85868500	2.59982000
H	6.00356700	-3.20119200	2.55567900
H	5.43896000	-3.90455100	1.05142100
H	1.85451800	-4.26957700	2.26346000
H	2.87147600	-4.55619000	0.85506700
H	4.17157700	-4.87258400	2.93304100
H	3.72431800	-3.27331300	3.49839400
C	2.45834500	1.99322900	-1.55952200
C	3.70475600	1.64791500	-0.93937500
C	2.35111400	3.28599300	-2.13023200
C	4.75117200	2.60093700	-0.93681400
C	3.38619900	4.18979800	-2.08698200
H	1.41134600	3.53881800	-2.60394900
C	4.60807900	3.85251100	-1.48315600
H	5.69126700	2.31928100	-0.47746800
H	3.25625400	5.17030000	-2.52819500
H	5.42270700	4.56265800	-1.45518000
C	-1.17687700	-2.03600200	-1.49036900
C	-0.85346000	-3.14602900	-0.64824200
C	-2.33891600	-2.13893900	-2.28864500
C	-1.72621800	-4.25655700	-0.62386000
C	-3.17093000	-3.23428400	-2.22836300
H	-2.56792500	-1.30485200	-2.93915400
C	-2.87312500	-4.30975600	-1.38127800
H	-1.46902300	-5.08898700	0.02045100
H	-4.06366800	-3.25931700	-2.84045900
H	-3.52645700	-5.16964600	-1.33142900
C	4.01525700	0.37556100	-0.35271600
C	0.32953300	-3.24979900	0.16703500
H	5.05984700	0.23435600	-0.08943400
H	0.45600600	-4.19587900	0.68466400
C	-2.57423600	5.64572000	1.09193400
C	-1.48399300	5.51689400	0.23726000
C	-0.53495900	4.52757300	0.46255500
C	-0.66638200	3.65213100	1.54120400
C	-1.75427700	3.79771800	2.40122300
C	-2.70509200	4.78822700	2.17859200
H	-3.31250200	6.41726500	0.91747900
H	-1.37080000	6.18987800	-0.60255500
H	0.31762400	4.43742300	-0.19993900
H	-1.85219200	3.14215100	3.25850000
H	-3.54179500	4.89399300	2.85668500
N	0.03606700	1.46066200	0.73696400
H	0.03265100	1.80248300	-0.22941200

H	-1.73800600	1.08746900	1.07742500
C	0.31987400	2.53238700	1.72303900
H	1.34439900	2.88470800	1.57727400
H	0.24877800	2.08866100	2.71435600
C	-7.37264300	-0.92262700	0.15992400
C	-6.85181000	0.13502400	-0.57872500
C	-5.48403500	0.37573200	-0.57788100
C	-4.62780400	-0.43490000	0.16697200
C	-5.15513400	-1.49591600	0.90020400
C	-6.52289900	-1.73970100	0.89729100
H	-8.43754400	-1.11429700	0.15357400
H	-7.50921100	0.76519200	-1.16286600
H	-5.07996900	1.18844200	-1.16965300
H	-4.49117200	-2.14005000	1.46349300
H	-6.92345200	-2.56979700	1.46386800
N	-2.76608600	0.89298700	1.16682400
H	-2.97007100	0.60451400	2.12343900
H	-3.26359000	1.76793800	0.99694900
C	-3.15380100	-0.17459500	0.17578000
H	-2.59208200	-1.05958600	0.45635400
H	-2.78762700	0.16981200	-0.78661600

INT2+

Ru	0.80613300	0.65608300	-0.67662300
N	0.64009400	-0.15315200	0.94010700
N	0.33306700	2.55466000	-0.05383400
N	2.69289800	1.26377400	-0.23711900
O	-1.04812200	0.41545200	-1.47040500
O	1.48163900	-1.07743300	-1.62711300
C	1.54494600	3.38384400	0.19821800
C	1.37161900	4.53608500	1.18020000
C	2.69288500	2.46026600	0.64098600
H	1.82135100	3.79199500	-0.78060400
C	2.68082500	5.31907400	1.31026100
H	1.06844100	4.13649600	2.15266400
H	0.58521600	5.21223100	0.84567700
C	4.00032700	3.23706100	0.72866600
H	2.44058900	2.08164000	1.63884900
C	3.84864800	4.41513700	1.69478300
H	2.55636500	6.11126600	2.05018300
H	2.89859400	5.81011800	0.35682600
H	4.80558900	2.59094900	1.07811800
H	4.27712600	3.59529600	-0.26745700

H	4.77762100	4.98691600	1.71812000
H	3.69131100	4.02817600	2.70625700
C	-2.09300800	1.18283800	-1.21933700
C	-2.06044100	2.39059200	-0.45569700
C	-3.33231300	0.77257600	-1.74777300
C	-3.27057100	3.07274300	-0.21346200
C	-4.49725900	1.45845100	-1.47867900
H	-3.34652600	-0.12174400	-2.35649000
C	-4.47751300	2.61425500	-0.69205700
H	-3.23236600	3.98764100	0.36491100
H	-5.43463400	1.08623000	-1.87031200
H	-5.39242100	3.14737400	-0.47607100
C	2.72819200	-1.45362500	-1.64942900
C	3.83812000	-0.70770400	-1.11879100
C	3.01472500	-2.70327800	-2.25224800
C	5.13914800	-1.26519000	-1.20669900
C	4.29105900	-3.20418900	-2.31451400
H	2.17690200	-3.26074800	-2.64876800
C	5.37623300	-2.48595400	-1.78306900
H	5.96318500	-0.69544000	-0.79437000
H	4.46062200	-4.17034800	-2.77333400
H	6.37824000	-2.88847100	-1.83044800
C	-0.85813800	3.04086100	-0.00252200
C	3.75948000	0.56569700	-0.47304300
H	-0.99153800	4.05279900	0.36866300
H	4.71064600	0.96267500	-0.13087600
C	2.48391800	-4.97846700	1.08136800
C	1.16522300	-5.16378100	1.48000300
C	0.44618900	-4.10391300	2.02297100
C	1.04532300	-2.85703500	2.18067100
C	2.37270000	-2.68091800	1.78847500
C	3.08734500	-3.73424400	1.23651200
H	3.03949800	-5.79929800	0.64711400
H	0.69276300	-6.13019400	1.36191700
H	-0.58577300	-4.24521900	2.32036700
H	2.83947800	-1.71087300	1.89704000
H	4.10904500	-3.58087400	0.91576800
N	-0.19728500	-0.87456500	1.49935800
H	-1.18171300	-1.15305400	1.05400400
C	0.24781900	-1.67693900	2.67023800
H	-0.65428900	-1.98690100	3.19382200
H	0.83516800	-1.02452000	3.31272500
C	-7.61779400	-1.24150700	-0.47297300
C	-6.60232300	-2.03825000	-0.98383300

C	-5.31843300	-1.96855500	-0.44863600
C	-5.03423500	-1.09965100	0.59883100
C	-6.06266300	-0.30668800	1.11016900
C	-7.34322800	-0.37501400	0.58221300
H	-8.61433000	-1.29198900	-0.89172300
H	-6.80356300	-2.71496400	-1.80430600
H	-4.54005500	-2.59020500	-0.87089800
H	-5.85080900	0.38434600	1.91770700
H	-8.12671300	0.25282800	0.98676200
N	-2.55471700	-1.63680200	0.49939000
H	-2.52000100	-1.39092100	-0.48478500
H	-2.63969000	-2.64549900	0.56317300
C	-3.64943300	-0.95089700	1.19058400
H	-3.40207200	0.11207800	1.22652700
H	-3.65191700	-1.30106700	2.22518700

TS3

Ru	-0.77600500	0.65893700	0.66962500
N	-0.60975800	-0.14759700	-0.94715300
N	-0.31838900	2.55995100	0.04985200
N	-2.67018000	1.25614800	0.24607800
O	1.09023300	0.42359600	1.45361500
O	-1.43220600	-1.07840600	1.62427800
C	-1.53680500	3.38290300	-0.18917400
C	-1.37759600	4.54143200	-1.16622100
C	-2.68253600	2.45476800	-0.62765700
H	-1.80861500	3.78469700	0.79364900
C	-2.69215300	5.31736400	-1.28279500
H	-1.07896200	4.14883400	-2.14294200
H	-0.59273000	5.22036200	-0.83374800
C	-3.99505500	3.22436900	-0.70433000
H	-2.43440600	2.08105200	-1.62846500
C	-3.85676900	4.40840500	-1.66506900
H	-2.57762300	6.11498300	-2.01851300
H	-2.90658400	5.80103300	-0.32479000
H	-4.79841000	2.57488500	-1.05206700
H	-4.26825600	3.57612300	0.29511900
H	-4.78941600	4.97453500	-1.67956300
H	-3.70324000	4.02797900	-2.67962200
C	2.12538300	1.20308000	1.20032000
C	2.07830600	2.41301400	0.44070800
C	3.37216700	0.80310900	1.71993700
C	3.28134700	3.10579000	0.19283900

C	4.52975700	1.49927400	1.44567500
H	3.39791700	-0.09162900	2.32765200
C	4.49556600	2.65670200	0.66199900
H	3.23138200	4.02191300	-0.38283500
H	5.47232700	1.13403700	1.83156400
H	5.40432400	3.19865200	0.44182800
C	-2.67663200	-1.46041000	1.65906000
C	-3.79576800	-0.71990000	1.14052400
C	-2.95198700	-2.71111100	2.26534700
C	-5.09294900	-1.28294200	1.24267300
C	-4.22531700	-3.21814500	2.34122600
H	-2.10768800	-3.26488900	2.65341700
C	-5.31910800	-2.50493400	1.82150200
H	-5.92382600	-0.71682800	0.83902900
H	-4.38547100	-4.18504600	2.80194500
H	-6.31889900	-2.91162300	1.87937900
C	0.86827000	3.05621400	-0.00293100
C	-3.73065200	0.55484500	0.49405900
H	0.99237200	4.07194200	-0.36705900
H	-4.68789300	0.94799100	0.16437100
C	-2.53917000	-4.93302000	-1.08915500
C	-1.22600200	-5.13522600	-1.49767300
C	-0.49674300	-4.08386300	-2.04350600
C	-1.07942900	-2.82817000	-2.19443600
C	-2.40115800	-2.63527500	-1.79109700
C	-3.12620700	-3.68015500	-1.23663600
H	-3.10286700	-5.74714100	-0.65273200
H	-0.76593600	-6.10834800	-1.38557400
H	0.53084900	-4.23914700	-2.34917200
H	-2.85509400	-1.65848000	-1.89291100
H	-4.14282700	-3.51334700	-0.90671000
N	0.21183300	-0.87565400	-1.51288000
H	1.25041900	-1.20434700	-1.03535700
C	-0.26882300	-1.65886600	-2.68667700
H	0.61811500	-1.98241600	-3.22779100
H	-0.85452800	-0.99148000	-3.31573400
C	7.54508200	-1.31098200	0.47415200
C	6.51888700	-2.09090700	0.98925000
C	5.23651000	-2.00773000	0.45264000
C	4.96572200	-1.14103500	-0.60012600
C	6.00422700	-0.36440300	-1.11563500
C	7.28320900	-0.44720700	-0.58626200
H	8.54049400	-1.37237800	0.89398600
H	6.71029200	-2.76529500	1.81383600

H	4.45157700	-2.61803900	0.87914800
H	5.80233200	0.32475400	-1.92714300
H	8.07511900	0.16789200	-0.99372500
N	2.48021900	-1.62951800	-0.48770900
H	2.43652800	-1.34564200	0.48727900
H	2.54825400	-2.64174200	-0.51724800
C	3.58800300	-0.97966600	-1.20031700
H	3.35427000	0.08452500	-1.26209100
H	3.58116600	-1.36035500	-2.22368200

INT3

Ru	-0.69896000	0.19503100	-0.59690200
N	0.29414600	0.49211800	0.93652400
N	-0.28049700	-1.77204000	-0.60621600
N	-2.37966500	-0.42281100	0.35617500
O	0.98046600	0.62138900	-1.76863600
O	-1.52923300	2.06752800	-0.98639200
C	-1.41517000	-2.60689200	-0.12871800
C	-1.04865200	-3.97572200	0.43302000
C	-2.20261000	-1.78349100	0.90744700
H	-2.07289700	-2.74699300	-0.99433400
C	-2.30417600	-4.71663100	0.89943900
H	-0.35369600	-3.84662500	1.26832800
H	-0.54125100	-4.57604200	-0.32219000
C	-3.46365300	-2.51511300	1.34620400
H	-1.54945800	-1.65971800	1.77926700
C	-3.10705200	-3.89487000	1.90368800
H	-2.01831200	-5.67520800	1.33615900
H	-2.93110200	-4.94083500	0.03055300
H	-3.98675200	-1.94065300	2.11173700
H	-4.14267400	-2.61868100	0.49411400
H	-4.02051100	-4.42340400	2.18203500
H	-2.52301300	-3.77006500	2.82098700
C	1.96657800	-0.20744000	-1.93760600
C	1.94750000	-1.60113200	-1.58703600
C	3.15447700	0.29379200	-2.53048800
C	3.09479200	-2.38740600	-1.84592300
C	4.25090000	-0.50305600	-2.75288100
H	3.16790700	1.34438800	-2.78952900
C	4.23316300	-1.86505300	-2.40863500
H	3.05998200	-3.43762800	-1.58037400
H	5.14020200	-0.07297800	-3.19745500
H	5.09787500	-2.48933200	-2.58611100

C	-2.73119100	2.43306400	-0.63174800
C	-3.67677700	1.62144100	0.08301200
C	-3.14664700	3.74004700	-0.99083700
C	-4.94583000	2.16185800	0.39111500
C	-4.39114800	4.22927500	-0.66674300
H	-2.43488700	4.34876700	-1.53318300
C	-5.31239500	3.43812200	0.03502600
H	-5.64551400	1.53395600	0.93059600
H	-4.65891100	5.23761700	-0.95839300
H	-6.29039700	3.82278600	0.28912800
C	0.83143800	-2.29376000	-1.01605000
C	-3.45657200	0.26677100	0.51680300
H	0.95422700	-3.36949400	-0.93586700
H	-4.29656100	-0.19324800	1.02900100
C	5.80117600	2.10864100	1.43170200
C	5.59932600	1.54302100	2.68592700
C	4.34470100	1.05713900	3.03714600
C	3.27598200	1.14178500	2.14669200
C	3.48565100	1.70965900	0.89010500
C	4.74102400	2.18698700	0.53471000
H	6.77910400	2.47949900	1.15296900
H	6.42000500	1.47106100	3.38818100
H	4.19486900	0.60602200	4.01072100
H	2.67144700	1.76369900	0.18057400
H	4.89129000	2.61510900	-0.44796800
N	1.27373200	-0.04835700	1.40393000
C	1.90937600	0.64060200	2.54950300
H	2.00281300	-0.08902400	3.35428700
H	1.27131300	1.46213900	2.88854500

TS4

Ru	0.54181400	0.74938000	-0.45793000
N	0.49636100	0.34627500	1.34926400
N	1.68258200	-0.87786300	-0.80244300
N	-0.96884400	-0.50847300	-0.92611600
O	2.20897700	1.96563000	-0.24504100
O	-0.71210200	2.41047000	-0.55076100
C	0.90169200	-2.01120300	-1.36160700
C	1.47587100	-3.40248300	-1.11855700
C	-0.53516200	-1.91421600	-0.81736900
H	0.84881500	-1.83580700	-2.44259900
C	0.56859400	-4.47236800	-1.73123100
H	1.57602500	-3.56472600	-0.04097500

H	2.47178800	-3.48776500	-1.55359900
C	-1.43737000	-2.96012800	-1.45619300
H	-0.48888700	-2.11452300	0.25904500
C	-0.86604800	-4.35953900	-1.22237200
H	0.97334300	-5.46166700	-1.51011000
H	0.57554900	-4.36576900	-2.82076700
H	-2.43829500	-2.90232200	-1.02770300
H	-1.52765300	-2.76443000	-2.52924100
H	-1.50065100	-5.10122100	-1.71083500
H	-0.89102800	-4.57959700	-0.15027200
C	3.40939200	1.50485800	-0.03969900
C	3.81121700	0.13259300	-0.18459400
C	4.41389800	2.43313900	0.33761700
C	5.15985900	-0.21447300	0.05647200
C	5.71406000	2.05086800	0.57179400
H	4.11098500	3.46680100	0.44373400
C	6.10436800	0.70977100	0.43487100
H	5.44482000	-1.25316800	-0.06560000
H	6.44319000	2.79626300	0.86573200
H	7.12719100	0.41088700	0.61810400
C	-1.97991600	2.35670800	-0.84120900
C	-2.71219900	1.16988400	-1.18608000
C	-2.70434400	3.57740800	-0.83220100
C	-4.08564400	1.27926400	-1.49769100
C	-4.04444200	3.63860500	-1.13487200
H	-2.15346800	4.47121500	-0.56913200
C	-4.75677600	2.47847600	-1.47595600
H	-4.62040700	0.37029600	-1.74819300
H	-4.55313000	4.59473500	-1.10769100
H	-5.81046300	2.52678900	-1.71359000
C	2.95709300	-0.94149600	-0.61467000
C	-2.17808900	-0.16445800	-1.20590600
H	3.46451700	-1.88212400	-0.80843100
H	-2.89115400	-0.94053600	-1.46614400
C	-3.76692400	-1.40015000	1.54483200
C	-3.53226400	-0.06006200	1.83658300
C	-2.42056900	0.30704700	2.57817400
C	-1.52841200	-0.66179900	3.06476000
C	-1.77471500	-2.01003200	2.75405700
C	-2.88224800	-2.37384800	2.00585300
H	-4.63016700	-1.68494300	0.95760300
H	-4.20608300	0.70018400	1.46603700
H	-2.23129000	1.35243200	2.78636400
H	-1.08456800	-2.76789500	3.10436700

H	-3.05759600	-3.41704800	1.77592600
N	0.97247200	0.06999400	2.36402200
C	-0.31144300	-0.26599100	3.72847100
H	-0.28492400	0.71232000	4.19126500
H	0.24388300	-1.02769800	4.25929300

INT4

Ru	0.00441700	-0.55174800	-0.05642800
N	-0.18151800	-0.60720000	1.76411900
N	-1.31399800	0.96726500	-0.26527400
N	1.35432900	0.94966200	0.04212700
O	-1.47636100	-1.96704200	-0.41204100
O	1.48149800	-1.99793500	-0.21867700
C	-0.63166200	2.26243100	-0.49922700
C	-1.44040300	3.51478500	-0.18279400
C	0.69613700	2.25264900	0.28090900
H	-0.37332900	2.27550100	-1.56492200
C	-0.61778200	4.77025800	-0.48053100
H	-1.73593000	3.49688800	0.87069600
H	-2.35464300	3.53742200	-0.77617300
C	1.52040600	3.49423500	-0.03615100
H	0.44321700	2.26545900	1.34774800
C	0.71544200	4.76102200	0.26195200
H	-1.19549900	5.65635400	-0.21172300
H	-0.43327800	4.82938500	-1.55793300
H	2.43553100	3.50248100	0.55658200
H	1.81503000	3.47466800	-1.09002200
H	1.30546300	5.63887500	-0.00726400
H	0.53182700	4.82289900	1.33923400
C	-2.74703500	-1.70936800	-0.29303900
C	-3.32797600	-0.39712400	-0.21045500
C	-3.64168000	-2.81034300	-0.26711700
C	-4.73232100	-0.27409000	-0.10878000
C	-5.00260000	-2.64630600	-0.15481300
H	-3.20493400	-3.79851700	-0.33234100
C	-5.56804900	-1.36460400	-0.07090800
H	-5.15078800	0.72457500	-0.05930100
H	-5.64329900	-3.51954200	-0.13107700
H	-6.63832000	-1.23772400	0.01504900
C	2.75826600	-1.74158700	-0.20746800
C	3.35214200	-0.43516700	-0.12159400
C	3.64467500	-2.84545000	-0.30464300

C	4.76174500	-0.32279300	-0.14064400
C	5.01095300	-2.69064600	-0.31725700
H	3.19667300	-3.82870300	-0.36750700
C	5.59021700	-1.41509000	-0.23458200
H	5.19042200	0.67050600	-0.07462400
H	5.64468600	-3.56622500	-0.39020400
H	6.66459200	-1.29446400	-0.24378000
C	-2.59589400	0.83856000	-0.28985700
C	2.63406100	0.80625600	-0.01129100
H	-3.20685200	1.73072600	-0.39428700
H	3.25810700	1.69404200	0.03734800
N	-0.29537900	-0.64739100	2.87228700

PhCH₂•

C	1.83203800	0.00017200	0.00012100
C	1.12892200	-1.20774400	-0.00011800
C	-0.25094800	-1.21472300	-0.00008600
C	-0.99136300	-0.00018600	0.00005300
C	-0.25123400	1.21465400	-0.00015900
C	1.12860000	1.20792300	0.00008500
H	2.91385700	0.00011300	0.00023700
H	1.67088000	-2.14504600	-0.00015900
H	-0.79052700	-2.15384900	-0.00025200
H	-0.79125500	2.15351100	-0.00039500
H	1.67019600	2.14541800	0.00008500
C	-2.39189500	-0.00007700	0.00030500
H	-2.94896400	-0.92695800	0.00026000
H	-2.94890800	0.92669700	-0.00098500