Electronic Supplementary Material (ESI) for Chemical Science.

Regiodivergent Synthesis of Pyrazino-Indolines *vs.* Triazocines *via* α-Imino Carbenes Addition to Imidazolidines

Alejandro Guarnieri-Ibáñez,[a] Adiran de Aguirre,[a] Céline Besnard,[b] Amalia I. Poblador-Bahamonde *[a] and Jérôme Lacour *[a]

[a] *University of Geneva, Department of Organic Chemistry, Quai Ernest Ansermet 30, CH-1211 Geneva 4, Switzerland*
[b] *Laboratory of Crystallography, University of Geneva, quai Ernest Ansermet 24, CH-1211 Genève 4, Switzerland*

amalia.pobladorbahamonde@unige.ch
jerome.lacour@unige.ch

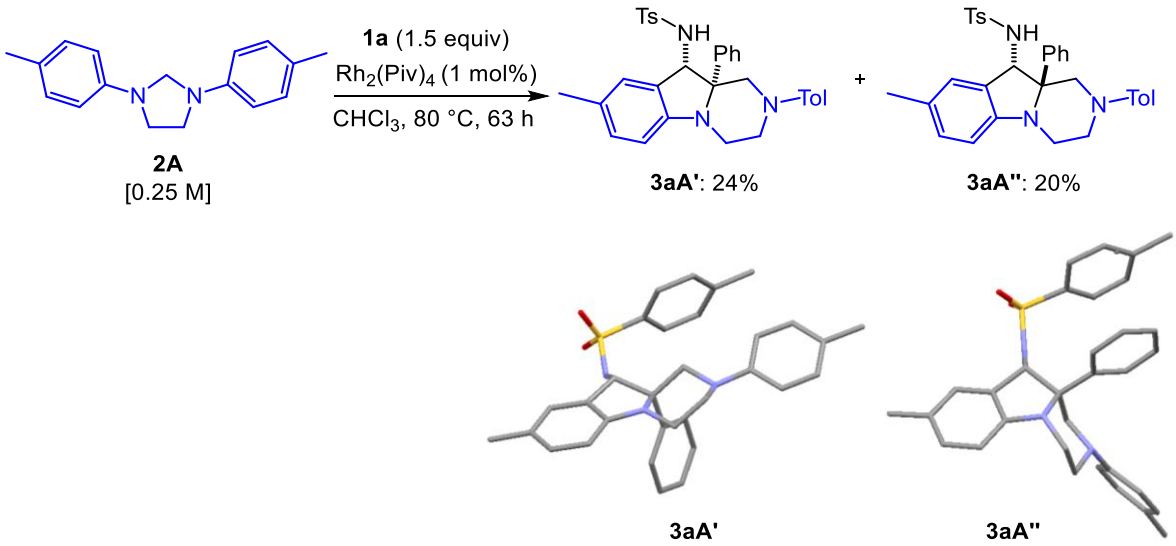
Supporting Information

Table of Contents

1. General remarks

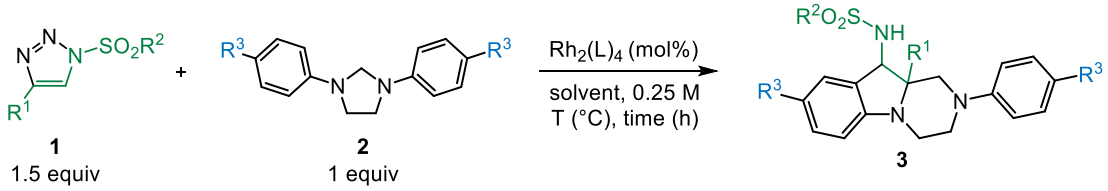
Unless otherwise stated, reagents were purchased from commercial sources and used without further purification. NMR spectra were recorded on 400 or 500 MHz spectrometer at 20 °C. ^{1}H-NMR: chemical shifts are given in ppm relative to Me_4Si with solvent resonances used as internal standards ($CDCl_3$ δ = 7.26 ppm or CD_2Cl_2 δ = 5.32 ppm). Data were reported as follows: chemical shift (δ) in ppm on the δ scale, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublet, td = triplet of doublets, q = quartet and m = multiplet), coupling constant (Hz) and integration. ^{13}C-NMR: chemicals shifts were given in ppm relative to Me_4Si with solvent resonances used as internal standards ($CDCl_3$ δ = 77.16 ppm or CD_2Cl_2 δ = 53.84 ppm). IR spectra were recorded using an ATR sampler and are reported in wave numbers (cm^{-1}). Melting points (Mp) were measured in open capillary tubes and were uncorrected. Electrospray mass spectra (ESI) were obtained by the department of Mass Spectrometry of the University of Geneva. Flash column chromatography was performed with silica gel 40 - 63 µm or alumina (neutral Brockmann I, 50 - 200 µm). Imidazolidines were synthesized following reported procedures.[1]

2. Scheme S1. Initial experiment and X-ray structures



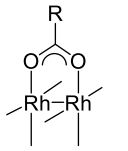
Top: reactivity of the *N*-tosyl-4-phenyl-1,2,3-triazole **1a** with imidazolidine **2A**.
Bottom: Stick views of the crystal structures of **3aA'** and **3aA''**. H-atoms are omitted for clarity.

3. Optimization of the reaction conditions

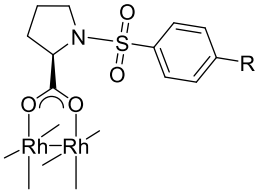


Entry	Catalyst	Cat. Loading	Solvent	T (°C)	Time	Conversion[a]	Yield[a]	dr[a]
1	-	-	$CHCl_3$	80 °C	40 h	-	-	-
2	$Rh_2(Piv)_4$	1 mol%	$CHCl_3$	80 °C	63 h	84%	44%	1.2:1
3	$Rh_2(Piv)_4$	2 mol%	$CHCl_3$	80 °C	63 h	95%	53%	1.3:1
4	$Rh_2(Piv)_4$	3 mol%	$CHCl_3$	80 °C	40 h	>99%	69%	1.6:1
5	$Rh_2(Piv)_4$	5 mol%	$CHCl_3$	80 °C	40 h	>99%	76%	2.2:1
6	$Rh_2(esp)_2$	3 mol%	$CHCl_3$	80 °C	40 h	97%	68%	1.3:1
7	Rh_2(*S*-TCPTTL)$_4$	3 mol%	$CHCl_3$	80 °C	40 h	>99%	74%	1.2:1
8	$Rh_2(Oct)_4$	3 mol%	$CHCl_3$	80 °C	40 h	80%	28%	2.1:1
9	Rh_2(*R*-DOSP)$_4$	3 mol%	$CHCl_3$	80 °C	40 h	84%	29%	1.9:1
10	Rh_2(*S*-PTTL)$_4$	3 mol%	$CHCl_3$	80 °C	40 h	51%	-	-
11	$Rh_2(TFA)_4$	3 mol%	$CHCl_3$	80 °C	40 h	84%	-	-
12	Rh_2(*S*-PTAD)$_4$	3 mol%	$CHCl_3$	80 °C	40 h	70%	-	-
13	$Rh_2(Piv)_4$	3 mol%	CH_2Cl_2	80 °C	40 h	>99%	80%	3.4:1
14	$Rh_2(Piv)_4$	3 mol%	Toluene	80 °C	40 h	>99%	76%	2.8:1
15	$Rh_2(Piv)_4$	3 mol%	Chlorobenzene	80 °C	40 h	>99%	80%	2.5:1
16	$Rh_2(Piv)_4$	3 mol%	1,2-DCE	80 °C	40 h	>99%	78%	2.3:1
17	$Rh_2(Piv)_4$	3 mol%	*n*-Bu_2O	80 °C	40 h	86%	59%	2.7:1
18	$Rh_2(Piv)_4$	3 mol%	Toluene	60 °C	40 h	97%	75%	3.4:1
19	$Rh_2(Piv)_4$	3 mol%	Toluene	100 °C	40 h	>99%	71%	2.6:1
20	$Rh_2(Piv)_4$	3 mol%	Toluene	120 °C	40 h	>99%	66%	2.3:1
21	$Rh_2(Piv)_4$	3 mol%	CH_2Cl_2	60 °C	40 h	>99%	78%	3.3:1
22	$Rh_2(Piv)_4$	3 mol%	CH_2Cl_2	100 °C	40 h	>99%	77%	2.9:1
23[b]	**$Rh_2(Piv)_4$**	**3 mol%**	**CH_2Cl_2**	**80 °C**	**14 h**	**>99%**	**78%**	**3.6:1**

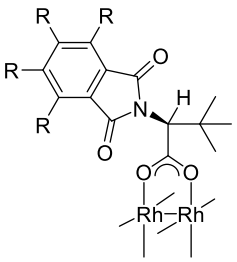
(a) Determined by ^{1}H-NMR spectroscopy using 1,3,5-trimethoxybenzene as reference. (b) Optimized conditions.



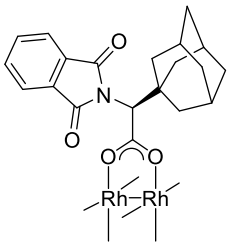
R = *n*-C_7H_{15} : $Rh_2(Oct)_4$
R = *t*-Bu : $Rh_2(Piv)_4$
R = CF_3 : $Rh_2(TFA)_4$



R = *n*-$C_{12}H_{25}$: Rh_2(*R*-DOSP)$_4$



R = H : Rh_2(*S*-PTTL)$_4$
R = Cl : Rh_2(*S*-TCPTTL)$_4$



Rh_2(*S*-PTAD)$_4$

4. General procedure I: synthesis of *N*-sulfonyl-1,2,3-triazoles

Important note: *Sulfonyl azides are potentially explosive materials and must be handled with caution.*
Azide synthesis: Following the reported procedure,[2] to a stirred solution of sulfonyl chloride (1.0 equiv) in water/acetone mixture (1:2, 0.2 M), NaN_3 (1.3 equiv) was slowly added at 0 °C. The resulting solution was stirred at room temperature for 12 h. The residue was suspended in Et_2O, the layers were separated and the aqueous phase was extracted three times with Et_2O. The organic layers were combined, dried over $MgSO_4$, filtered and concentrated under reduced pressure. The desired azide was obtained sufficiently pure to be used without any further purification.

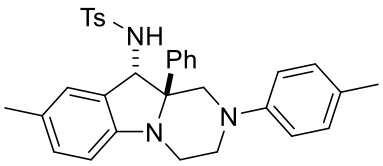
Caution: *Care should be taken to protect the reaction mixture from light at each step of the synthesis of the triazoles.*
Triazole synthesis: Following the reported procedure,[3] 0.05 equiv of copper(I) thiophene-2-carboxylate (CuTC) and 1 equiv of the corresponding sulfonyl azide were diluted in toluene (0.2 M). Then 1.3 equiv of the corresponding alkyne was added and the solution was stirred at room temperature overnight and protected from light. The mixture was diluted with saturated NH_4Cl_{aq} and extracted three times with EtOAc. The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude material was purified by column chromatography or by precipitations to afford the desired product. Products of type **1** were then stored at -20 °C.

5. General procedure II: synthesis of compounds 3 and 4

In a 2 mL screw-cap vial equipped with a magnetic stirring bar, $Rh_2(Piv)_4$ (3.66 mg, 0.006 mmol, 3 mol%), *N*-sulfonyltriazole **1** (0.3 mmol, 1.5 equiv) and the corresponding imidazolidine **2** (0.2 mmol, 1 equiv) were dissolved in 0.8 mL of anhydrous CH_2Cl_2 (0.25 M). After 14 h hours stirring at 80 °C, the solution was concentrated under reduced pressure and the residue was purified by column chromatography.

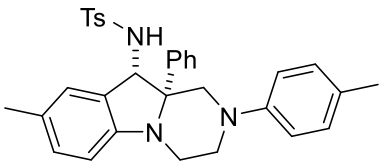
Analysis data for compounds 3

Compound 3aA'' (minor dia):



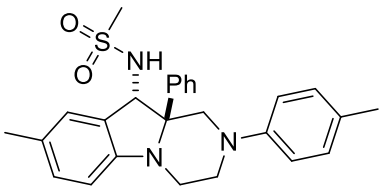
Following general procedure II, compound **3aA''** is obtained as a white solid (18 mg, 17% yield) starting from triazole **1a** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 201-203 °C; **Rf =** 0.57 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.45-7.38 (m, 2H), 7.25-7.20 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 7.01-6.95 (m, 1H), 6.79 (d, *J* = 8.5 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 1H), 6.44 (s, 1H), 4.91 (d, *J* = 9.7 Hz, 1H), 4.78 (d, *J* = 9.7 Hz, 1H), 3.93 (d, *J* = 12.3 Hz, 1H), 3.62-3.52 (m, 1H), 3.31 (ddd, *J* = 14.0, 12.0, 3.8 Hz, 1H), 3.12-3.01 (m, 2H), 2.86 (td, *J* = 11.7, 3.5 Hz, 1H), 2.42 (s, 3H), 2.26 (s, 3H), 2.15 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.8 (C), 147.2 (C), 143.7 (C), 142.2 (C), 137.6 (C), 130.4 (CH), 130.2 (C), 129.9 (2xCH), 129.8 (2xCH), 128.6 (2xCH), 128.0 (C), 127.3 (2xCH), 127.1 (CH), 127.0 (C), 126.9 (2xCH), 125.3 (CH), 117.3 (2xCH), 107.7 (CH), 72.9 (C), 67.1 (CH), 50.6 (CH_2), 47.0 (CH_2), 41.5 (CH_2), 21.7 (CH_3), 20.7 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3279, 2922, 2803, 1617, 1516, 1486, 1440, 1330, 1157, 1091, 808, 693, 659 cm^{-1}; **HR-MS (ESI):** m/z = 524.2371 $[M+H]^+$ (calculated for $C_{32}H_{34}N_3O_2S$ m/z = 524.2366).

Compound 3aA' (major dia):



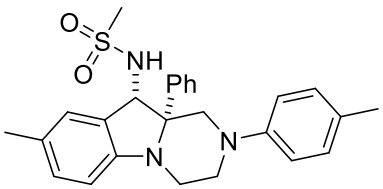
Following general procedure II, compound **3aA'** is obtained as a white solid (64 mg, 61% yield) starting from triazole **1a** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 178-180 °C; **Rf =** 0.50 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.50 (d, *J* = 8.3 Hz, 1H), 7.34-7.22 (m, 7H), 7.06-6.98 (m, 3H), 6.72 (d, *J* = 4.5 Hz, 2H), 6.68 (s, 1H), 6.50 (d, *J* = 8.0 Hz, 1H), 4.60 (d, *J* = 9.6 Hz, 1H), 4.25 (d, *J* = 9.6 Hz, 1H), 3.92 (d, *J* = 12.3 Hz, 1H), 3.66-3.55 (m, 1H), 3.34 (ddd, *J* = 13.7, 12.0, 3.7 Hz, 1H), 3.16-3.06 (m, 1H), 2.91 (d, *J* = 12.4 Hz, 1H), 2.82 (td, *J* = 11.7, 3.4 Hz, 1H), 2.46 (s, 3H), 2.25 (s, 3H), 2.18 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.7 (C), 147.6 (C), 143.4 (C), 138.5 (C), 137.1 (C), 130.5 (CH), 130.3 (C), 129.73 (2xCH), 129.72 (2xCH), 129.1 (2xCH), 127.9 (C), 127.8 (C), 127.8 (2xCH), 127.7 (CH), 127.2 (2xCH), 127.1 (CH), 117.5 (2xCH), 107.3 (CH), 72.0 (C), 62.2 (CH), 55.9 (CH_2), 47.7 (CH_2), 41.3 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3290, 2921, 1734, 1616, 1513, 1492, 1448, 1336, 1157, 1090, 1041, 909, 809, 701, 659 cm^{-1}; **HR-MS (ESI):** m/z = 524.2369 $[M+H]^+$ (calculated for $C_{32}H_{34}N_3O_2S$ m/z = 524.2366).

Compound 3bA'' (minor dia):



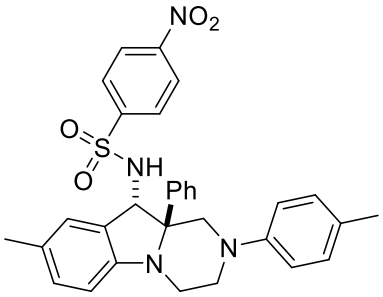
Following general procedure II, compound **3bA''** is obtained as a white solid (10 mg, 11% yield) starting from triazole **1a** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 98-100 °C; **Rf =** 0.43 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.75-7.68 (m, 2H), 7.45-7.37 (m, 2H), 7.36-7.29 (m, 1H), 7.12-7.02 (m, 4H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.54 (d, *J* = 8.4 Hz, 1H), 5.01 (d, *J* = 10.3 Hz, 1H), 4.66 (d, *J* = 10.1 Hz, 1H), 4.00 (d, *J* = 12.2 Hz, 1H), 3.62 (d, *J* = 13.2 Hz, 1H), 3.43-3.30 (m, 1H), 3.13-3.00 (m, 2H), 2.90 (td, *J* = 11.8, 3.3 Hz, 1H), 2.61 (s, 3H), 2.29 (s, 3H), 2.27 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.8 (C), 146.9 (C), 142.1 (C), 130.7 (C), 130.6 (CH), 129.9 (2xCH), 129.0 (2xCH), 128.6 (C), 127.9 (CH), 127.21 (2xCH), 127.17 (C), 125.1 (CH), 117.8 (2xCH), 108.3 (CH), 73.4 (C), 67.9 (CH), 49.4 (CH_2), 47.2 (CH_2), 41.8 (CH_3), 41.7 (CH_2), 20.9 (CH_3), 20.6 (CH_3)ppm; **IR (neat):** 3271, 2924, 1618, 1514, 1488, 1447, 1327, 1249, 1141, 1118, 975, 809, 702 cm^{-1}; **HR-MS (ESI):** m/z = 448.2048 $[M+H]^+$ (calculated for $C_{26}H_{30}N_3O_2S$ m/z = 448.2053).

Compound 3bA' (major dia):



Following general procedure II, compound **3bA'** is obtained as a brownish solid (42 mg, 47% yield) starting from triazole **1b** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 93-95 °C; **Rf =** 0.34 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.64-7.56 (m, 2H), 7.49-7.41 (m, 2H), 7.37-7.30 (m, 1H), 7.18 (s, 1H), 7.11-7.06 (m, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 6.80 (d, *J* = 8.5 Hz, 2H), 6.59 (d, *J* = 8.1 Hz, 1H), 4.67 (d, *J* = 8.7 Hz, 1H), 4.16-4.04 (m, 2H), 3.71-3.61 (m, 1H), 3.46-3.33 (m, 1H), 3.14-3.05 (m, 1H), 2.99 (d, *J* = 12.6 Hz, 1H), 2.85 (td, *J* = 11.9, 3.2 Hz, 1H), 2.29 (s, 3H), 2.25 (s, 3H), 2.24 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.7 (C), 147.8 (C), 138.1 (C), 130.9 (CH), 130.5 (C), 129.8 (2xCH), 129.1 (2xCH), 128.7 (C), 128.39 (C), 128.35 (2xCH), 128.0 (CH), 127.3 (CH), 117.6 (2xCH), 108.8 (CH), 72.1 (C), 62.5 (CH), 54.1 (CH_2), 47.3 (CH_2), 41.9 (CH_3), 41.6 (CH_2), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3272, 2926, 1617, 1513, 1492, 1448, 1323, 1149, 974, 909, 808, 702 cm^{-1}; **HR-MS (ESI):** m/z = 448.2061 $[M+H]^+$ (calculated for $C_{26}H_{30}N_3O_2S$ m/z = 448.2053).

Compound 3cA'' (minor dia):

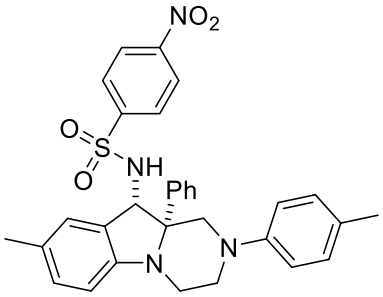


Following general procedure II, compound **3cA''** is obtained as a yellowish solid (9 mg, 8% yield) starting from triazole **1c** and imidazolidine **2A** (50 mg, 0.2 mmol).

Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1) followed by washing with pentane/Et_2O.

M.p. = 190-192 °C; **Rf =** 0.61 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.11 (d, *J* = 8.9 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 2H), 7.40-7.32 (m, 2H), 7.24-7.12 (m, 3H), 7.10-7.01 (m, 3H), 6.84-6.74 (m, 3H), 6.50 (d, *J* = 8.0 Hz, 1H), 5.04 (s, 2H), 3.77 (d, *J* = 12.0 Hz, 1H), 3.54 (d, *J* = 14.1 Hz, 1H), 3.27-3.16 (m, 1H), 3.09-2.97 (m, 2H), 2.86 (td, *J* = 11.8, 3.3 Hz, 1H), 2.27 (s, 3H), 2.24 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.1 (C), 149.7 (C), 146.9 (C), 146.1 (C), 141.8 (C), 130.8 (CH), 129.9 (2xCH), 128.7 (2xCH), 128.6 (C), 128.3 (2xCH), 127.4 (CH), 127.0 (2xCH), 126.4 (C), 125.1 (CH), 124.4 (2xCH), 117.7 (2xCH), 108.3 (CH), 72.9 (C), 68.0 (CH), 49.4(CH_2), 47.2 (CH_2), 41.5 (CH_2), 20.9 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3252, 2803, 1611, 1528, 1488, 1443, 1338, 1309, 1159, 1091, 808, 736 cm^{-1}; **HR-MS (ESI):** m/z = 555.2061 $[M+H]^+$ (calculated for $C_{31}H_{31}N_4O_4S$ m/z 555.2061).

Compound 3cA' (major dia):

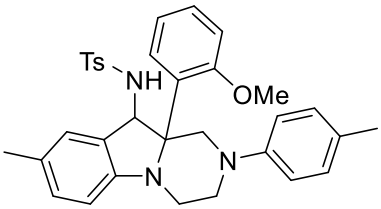


Following general procedure II, compound **3cA''** is obtained as an orange solid (60 mg, 55% yield) starting from triazole **1c** and imidazolidine **2A** (50 mg, 0.2 mmol).

Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1) followed by washing with pentane/Et_2O.

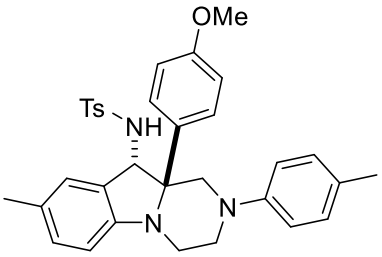
M.p. = 103-105 °C; **Rf =** 0.50 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.19 (d, *J* = 8.6 Hz, 2H), 7.65-7.57 (m, 2H), 7.40-7.26 (m, 5H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 2H), 6.95 (s, 1H), 6.73 (d, *J* = 8.2 Hz, 2H), 6.57 (d, *J* = 8.0 Hz, 1H), 4.57 (d, *J* = 9.5 Hz, 1H), 4.53 (d, *J* = 9.5 Hz, 1H), 3.89 (d, *J* = 12.4 Hz, 1H), 3.63 (d, *J* = 14.0 Hz, 1H), 3.42-3.28 (m, 1H), 3.05 (d, *J* = 10.3 Hz, 1H), 2.96 (d, *J* = 12.4 Hz, 1H), 2.82 (td, *J* = 11.8, 3.2 Hz, 1H), 2.24 (s, 3H), 2.23 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.8 (C), 149.5 (C), 147.7 (C), 147.1 (C), 137.2 (C), 131.1 (CH), 130.7 (C), 129.8 (2xCH), 129.2 (2xCH), 128.6 (C), 128.0 (2xCH), 127.9 (CH), 127.7 (C), 127.6 (2xCH), 127.2 (CH), 124.2 (2xCH), 117.7 (2xCH), 108.7 (CH), 72.1 (C), 62.4 (CH), 54.8 (CH_2), 47.3 (CH_2), 41.6 (CH_2), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3290, 2922, 1615, 1526, 1492, 1346, 1309, 1161, 909, 809, 733 cm^{-1}; **HR-MS (ESI):** m/z = 555.2060 $[M+H]^+$ (calculated for $C_{31}H_{31}N_4O_4S$ m/z = 555.2061).

Compound 3dA (both dia):



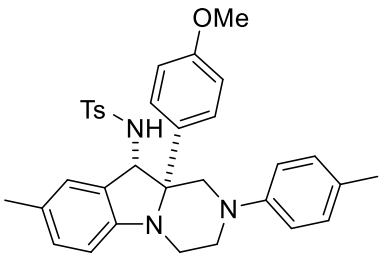
Following general procedure II, compound **3dA** is obtained as a brownish solid (65 mg, 58% yield) starting from triazole **1d** and imidazolidine **2A** (51 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 157-159 °C; **Rf =** 0.35 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$,** inseparable mixture of diastereoisomers (dr 1:1)): δ [7.64 (*dia A*) and 7.45 (*dia B*) (d, *J* = 8.0 Hz, 2H)], 7.61-7.53 (*dia B*, m, 1H), 7.32-7.27 (*dia B*, m, 1H), 7.24-7.12 (m, 6H, aromatics), 7.05-6.92 (m, 7H, aromatics), 6.88 (*dia A*, dd, *J* = 8.3, 1.2 Hz, 1H), 6.83 (*dia B*, d, *J* = 8.1 Hz, 1H), 6.80-6.72 (*dia A*, m, 3H), 6.67-6.48 (*dia B*, m, 4H), 6.45 (*dia A*, d, *J* = 8.0 Hz, 1H), 6.21 (*dia A*, s, 1H), [5.14 (*dia A*) and 4.84 (*dia B*) (d, *J* = 9.1 Hz, 1H)], 4.80-4.68 (*dia A* and *dia B*, m, 2H), 4.30 (*dia A*, d, *J* = 12.8 Hz, 1H), 4.14 (*dia B*, s, 1H), [3.84 (*dia A*) and 3.69 (*dia B*), s, 3H)], 3.74-3.58 (*dia A* and *dia B*, m, 3H), 3.48-3.36 (*dia A*, m, 2H), 3.21-3.16 (*dia A*, m, 1H), 3.06 (*dia B*, d, *J* = 11.3 Hz, 1H), 2.98 (*dia A*, td, *J* = 11.4, 4.3 Hz, 1H), 2.85-2.72 (*dia B*, m, 2H), [2.42 (*dia B*) and 2.41 (*dia A*) (s, 3H)], [2.25 (*dia A*) and 2.20 (*dia B*) (s, 3H)], [2.10 (*dia B*) and 2.07 (*dia A*) (s, 3H)] ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** inseparable mixture of diastereoisomers (dr 1:1)): δ [158.2 (*dia A*) and 157.3 (*dia B*) (C)], [149.9 (*dia B*) and 149.4 (*dia A*) (C)], [147.34 (*dia B*) and 147.29 (*dia A*) (C)], [143.34 (*dia A*) and 142.8 (*dia B*) (C)], [139.6 (*dia B*) and 138.5 (*dia A*) (C)], [130.3 (*dia B*) and [130.1 (*dia A*) (CH)], 129.8 (*dia B*, CH), [129.71 (*dia A*) and 129.52 (*dia B*) (2xCH)], [129.7 (*dia A*) and 129.47 (*dia B*) 2xCH), 129.56 (*dia A*, CH), 129.4 (*dia B*, CH), [129.19 (*dia A*) and 129.11 (*dia B*) (C)], [129.16 (*dia A*) and 129.07 (*dia B*) (C)], 128.7 (*dia A*, CH), 128.0 (*dia A*, C), 127.6 (*dia B*, CH), [127.3 (*dia A*) and 127.07 (*dia B*) (2xCH)], [127.11 (*dia A*,) and 127.0 (*dia B*) (C)], 126.0 (*dia A*; CH), [120.9 (*dia B*) and 120.4 (*dia A*) (CH)], [116.9 (*dia B*) and 116.6 (*dia A*) (2xCH)], [112.0 (*dia A*) and 111.6 (*dia B*) (CH)], [109.0 (*dia B*) and 106.7 (*dia A*) (CH)], [73.3 (*dia B*) and 71.7 (*dia A*) (C)], [63.5 (d*ia A*) and 59.8 (*dia B*) (CH)], [55.5 (*dia A*) and 55.0 (*dia B*) (CH_3)], [54.4 (*dia B*) and 51.6 (*dia A*) (CH_2)], [47.1 (*dia A*) and 46.1 (*dia B*) (CH_2)], [42.6 (*dia B*) and 41.2 (*dia A*) (CH_2)], [21.63 (*dia A*) and 21.60 (*dia B*) (CH_3)], [20.69 (*dia A*) and 20.69 (*dia B*) (CH_3)], [20.6 (*dia B*) and 20.5 (*dia A*) (CH_3)] ppm;
IR (neat): 2938, 1617, 1600, 1490, 1450, 1431, 1329, 1234, 1161, 1055, 1030, 909, 815, 755 cm^{-1};
HR-MS (ESI): m/z = 554.2457 $[M+H]^+$ (calculated for $C_{33}H_{36}N_3O_3S$ m/z = 554.2472).

Compound 3eA'' (minor dia):



Following general procedure II, compound **3eA''** is obtained as a brownish solid (19 mg, 17% yield) starting from triazole **1e** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 170-172 °C; **Rf =** 0.47 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.8 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 6.49-6.42 (m, 2H), 4.90 (d, *J* = 9.6 Hz, 1H), 4.78 (d, *J* = 9.7 Hz, 1H), 3.88 (d, *J* = 12.2 Hz, 1H), 3.80 (s, 3H), 3.59-3.49 (m, 1H), 3.34-3.23 (m, 1H), 3.10-2.99 (m, 2H), 2.84 (td, *J* = 11.7, 3.4 Hz, 1H), 2.42 (s, 3H), 2.26 (s, 3H), 2.16 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 158.7 (C), 149.8 (C), 147.0 (C), 143.7 (C), 137.4 (C), 133.8 (C), 130.4 (CH), 130.2 (C), 129.82 (2xCH), 129.76 (2xCH), 128.05 (2xCH), 127.99 (C), 127.2 (2xCH), 127.1 (C), 125.2 (CH), 117.4 (2xCH), 113.9 (2xCH), 107.8 (CH), 72.6 (C), 67.1 (CH), 55.3 (CH_3), 50.2 (CH_2), 47.0 (CH_2), 41.4 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3261, 2925, 1613, 1513, 1486, 1443, 1330, 1249, 1154, 1091, 1043, 807, 658 cm^{-1}; **HR-MS (ESI):** m/z = 554.2471 $[M+H]^+$ (calculated for $C_{33}H_{36}N_3O_3S$ m/z = 554.2472).

Compound 3eA' (major dia):

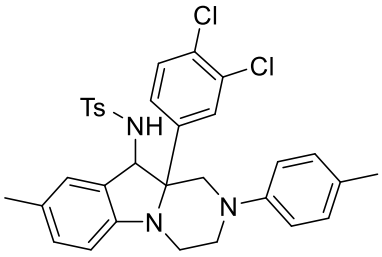


Following general procedure II, compound **3eA'** is obtained as a brownish solid (79 mg, 71% yield) starting from triazole **1e** and imidazolidine **2A** (50 mg, 0.2 mmol).

Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).

M.p. = 102-104 °C; **Rf =** 0.32 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.52 (d, *J* = 8.3 Hz, 2H), 7.26-7.22 (m, 2H), 7.15 (d, *J* = 8.3 Hz, 2H), 7.07-6.96 (m, 3H), 6.80 (d, *J* = 9.1 Hz, 2H), 6.76-6.67 (m, 3H), 6.48 (d, *J* = 8.0 Hz, 1H), 4.57 (d, *J* = 9.4 Hz, 1H), 4.29 (d, *J* = 9.4 Hz, 1H), 3.86 (d, *J* = 12.4 Hz, 1H), 3.80 (s, 3H), 3.64-3.53 (m, 1H), 3.38-3.25 (m, 1H), 3.15-3.07 (m, 1H), 2.88 (d, *J* = 12.3 Hz, 1H), 2.80 (td, *J* = 11.7, 3.4 Hz, 1H), 2.46 (s, 3H), 2.25 (s, 3H), 2.18 (s, 3H)ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 158.9 (C), 149.6 (C), 147.5 (C), 143.4 (C), 138.3 (C), 130.4 (CH), 130.3 (C), 129.69 (4xCH), 128.9 (2xCH), 128.6 (C), 127.9 (C), 127.8 (C), 127.2 (2xCH), 127.1 (CH), 117.5 (2xCH), 114.4 (2xCH), 107.2 (CH), 71.6 (C), 62.1 (CH), 55.8 (CH_2), 55.3 (CH_3), 47.7 (CH_2), 41.1 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3289, 2923, 1614, 1512, 1493, 1444, 1335, 1247, 1157, 1093, 1031, 909, 809, 658 cm^{-1}; **HR-MS (ESI):** m/z = 554.2473 $[M+H]^+$ (calculated for $C_{33}H_{36}N_3O_3S$ m/z = 554.2472).

Compound 3fA (both dia):

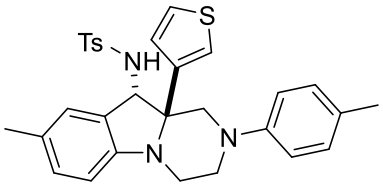


Following general procedure II, compound **3fA** is obtained as a brownish solid (79 mg, 67% yield) starting from triazole **1f** and imidazolidine **2A** (50 mg, 0.2 mmol).

Purification: column chromatography (SiO_2, pentane/EtOAc, 8.5:1.5).

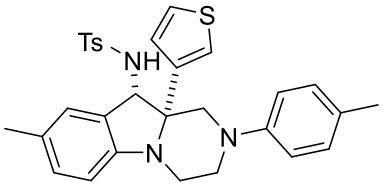
M.p. = 180-182 °C; **Rf =** 0.36 (SiO_2, pentane/EtOAc, 8.5:1.5); **^{1}H NMR (400 MHz, $CDCl_3$**, inseparable mixture of diastereoisomers (dr 1:3.2)): δ [7.54 (minor) and 7.44 (major) (d, *J* = 8.3 Hz, 2H)], 7.50 (minor, s, 1H), 7.40-7.34 (m, 1H, aromatics), 7.28-7.22 (m, 3.3H, aromatics), 7.19 (minor, d, *J* = 8.1 Hz, 2H), 7.16-7.09 (m, 1H, aromatics), 7.08-7.00 (m, 4H, aromatics), 6.78 (minor, d, *J* = 8.5 Hz, 2H), 6.75-6.69 (m, 3H, aromatics), 6.64-6.61 (minor, m, 1H), [6.54 (major) and 6.48 (minor) (d, *J* = 8.1 Hz, 1H)], 4.87 (minor, s, 2H), 4.58 (major, d, *J* = 9.7 Hz, 1H), 4.34 (major, d, *J* = 9.7 Hz, 1H), 3.83-3.72 (major and minor, m, 1H), [3.66-3.58 (major) and 3.58-3.51 (minor) (m, 1H)], [3.34-3.23 (major) and 3.22-3.16 (minor) (m, 1H)], 3.11-2.99 (m, 1.6H), 2.91 (major, d, *J* = 12.6 Hz, 1H), 2.88-2.74 (m, 1H), [2.47 (major) and 2.45 (minor) (s, 3H)], [2.27 (minor) and 2.25 (major) (s, 3H)], 2.2 (major and minor, s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$**, inseparable mixture of diastereoisomers (dr 1:3.2)): δ [149.6 (minor) and 149.4 (major) (C)], [147.3 (major) and 146.6 (minor) (C)], [144.3 (minor) and 143.7 (major), (C)], [142.7 (minor) and 138.32 (major) (C)], [138.28 (major) and 137.0 (minor) (C)], [132.9 (major) and 132.6 (minor) (C)], [131.6 (major) and 131.3 (minor) (C)], [130.9 (major) and 130.47 (minor) (CH)], [130.9 (major) (C)], [130.6 (major) and 130.1 (minor) (CH)], [130.6 (major) and 129.2 (minor) (CH)], [129.91 (minor) and 129.84 (major) (2xCH)], [129.86 (minor) and 129.76 (major) (2xCH)], [128.9 (major) and 128.8 (minor) (C)], [127.8 (major) (C)], [127.4 (major) and 126.6 (minor) (CH)], [127.2 (major) and 125.3 (minor) (CH)], [127.1 (minor) and 126.8 (major) (2xCH)], [117.80 (major) and 117.78 (minor) (2xCH)], [108.4 (major) and 108.2 (minor) (CH)], [72.7 (minor) and 71.5 (major) (C)], [67.0 (minor) and 62.2 (major) (CH)], [55.0 (major) and 49.7 (minor) (CH_2)], [47.7 (major) and 47.3 (minor) (CH_2)], [41.6 (minor) and 41.5 (major) (CH_2)], [21.78 (minor) and 21.76 (major) (CH_3)], [20.78 (minor) and 20.75 (major) (CH_3)], [20.64 (minor) and 20.62 (major) (CH_3)] ppm; **IR (neat):** 3266, 2918, 1618, 1517, 1494, 1446, 1338, 1207, 1158, 1092, 909, 808, 794, 658 cm^{-1}; **HR-MS (ESI):** m/z = 592.1602 $[M+H]^+$ (calculated for $C_{32}H_{32}Cl_2N_3O_2S$ m/z = 592.1587).

Compound 3gA'' (minor dia):



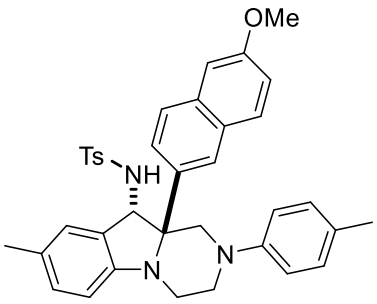
Following general procedure II, compound **3gA''** is obtained as a white solid (15 mg, 14% yield) starting from triazole **1g** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 194-196°C; **Rf =** 0.53 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.24-7.17 (m, 3H), 7.14-7.01 (m, 4H), 6.98 (d, *J* = 8.1 Hz, 1H), 6.76 (d, *J* = 8.1 Hz, 2H), 6.53 (s, 1H), 6.44 (d, *J* = 7.9 Hz, 1H), 4.99 (d, *J* = 9.5 Hz, 1H), 4.77 (d, *J* = 9.6 Hz, 1H), 3.74 (d, *J* = 12.1 Hz, 1H), 3.54 (d, *J* = 14.4 Hz, 1H), 3.37-3.24 (m, 1H), 3.08 (d, *J* = 11.0 Hz, 1H), 3.03 (d, *J* = 12.1 Hz, 1H), 2.82 (td, *J* = 11.8, 3.3 Hz, 1H), 2.43 (s, 3H), 2.27 (s, 3H), 2.17 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.7 (C), 146.8 (C), 143.7 (C), 143.6 (C), 137.6 (C), 130.4 (CH), 130.1 (C), 129.9 (2xCH), 129.8 (2xCH), 128.2 (C), 127.3 (C), 127.2 (2xCH), 126.7 (CH), 125.7 (CH), 125.3 (2xCH), 123.0 (2xCH), 117.2 (2xCH), 107.8 (CH), 71.0 (C), 66.2 (CH), 51.2 (CH_2), 46.8 (CH_2), 41.6 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3271, 2920, 1618, 1514, 1490, 1441, 1330, 1158, 1092, 909, 809, 664 cm^{-1}; **HR-MS (ESI):** m/z = 530.1937 $[M+H]^+$ (calculated for $C_{30}H_{32}N_3O_2S_2$ m/z = 530.1931).

Compound 3gA' (major dia):



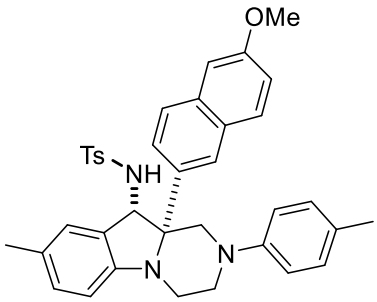
Following general procedure II, compound **3gA''** is obtained as a white solid (72 mg, 68% yield) starting from triazole **1g** and imidazolidine **2A** (50 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 207-209 °C; **Rf =** 0.46 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.63 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.25-7.23 (m, 1H), 7.08-6.94 (m, 4H), 6.80 (d, *J* = 5.0 Hz, 1H), 6.74-6.64 (m, 3H), 6.43 (d, *J* = 8.0 Hz, 1H), 4.66 (d, *J* = 9.7 Hz, 1H), 4.37 (d, *J* = 9.7 Hz, 1H), 3.75 (d, *J* = 12.0 Hz, 1H), 3.59-3.50 (m, 1H), 3.28 (td, *J* = 12.5, 3.5 Hz, 1H), 3.23-3.16 (m, 1H), 2.88 (d, *J* = 12.0 Hz, 1H), 2.80 (td, *J* = 11.6, 3.5 Hz, 1H), 2.47 (s, 3H), 2.26 (s, 3H), 2.18 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 149.5 (C), 147.2 (C), 143.6 (C), 139.1 (C), 138.5 (C), 130.3 (CH), 130.1 (C), 129.83 (2xCH), 129.76 (2xCH), 127.93 (C), 127.86 (C), 127.32 (2xCH), 127.28 (CH), 126.7 (CH), 126.5 (CH), 123.9 (CH), 117.3 (2xCH), 106.6 (CH), 70.9 (C), 62.2 (CH), 57.0 (CH_2), 48.0 (CH_2), 41.0 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3371, 2841, 1614, 1513, 1492, 1340, 1160, 911, 816, 722 cm^{-1}; **HR-MS (ESI):** m/z = 530.1918 $[M+H]^+$ (calculated for $C_{30}H_{32}N_3O_2S_2$ m/z = 530.1931).

Compound 3hA'' (minor dia):



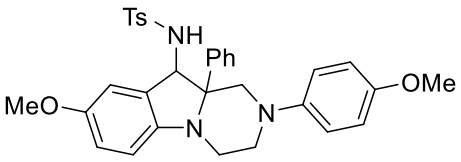
Following general procedure II, compound **3hA''** is obtained as a brownish solid (19 mg, 16% yield) starting from triazole **1h** and imidazolidine **2A** (51 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 166-168 °C; **Rf =** 0.36 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (500 MHz, $CDCl_3$):** δ 7.66-7.63 (m, 1H), 7.63-7.58 (m, 2H), 7.56-7.52 (m, 1H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.14-7.09 (m, 2H), 7.07 (d, *J* = 8.2 Hz, 2H), 7.04-7.00 (m, 1H), 6.86 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 6.68 (s, 1H), 6.50 (d, *J* = 7.9 Hz, 1H), 5.07 (d, *J* = 9.8 Hz, 1H), 4.87 (d, *J* = 9.9 Hz, 1H), 3.97 (d, *J* = 12.3 Hz, 1H), 3.94 (s, 3H), 3.62-3.54 (m, 1H), 3.33-3.22 (m, 1H), 3.12 (d, *J* = 12.4 Hz, 1H), 3.07-3.00 (m, 1H), 2.87 (td, *J* = 11.7, 3.3 Hz, 1H), 2.28 (s, 3H), 2.21 (s, 3H), 2.20 (s, 3H) ppm; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 157.8 (C), 149.8 (C), 147.0 (C), 143.5 (C), 137.2 (C), 136.9 (C), 133.9 (C), 130.4 (CH), 130.3 (C), 130.0 (CH), 129.8 (2xCH), 129.5 (2xCH), 128.8 (C), 128.3 (C), 127.3 (CH), 127.2 (C), 127.0 (2xCH), 126.3 (CH), 125.4 (CH), 125.3 (CH), 118.7 (CH), 117.4 (2xCH), 107.9 (CH), 105.6 (CH), 72.9 (C), 67.1 (CH), 55.5 (CH_3), 49.7 (CH_2), 47.0 (CH_2), 41.6 (CH_2), 21.6 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3269, 2921, 1605, 1513, 1486, 1439, 1328, 1215, 1156, 1092, 1027, 808, 666 cm^{-1}; **HR-MS (ESI):** m/z = 604.2618 $[M+H]^+$ (calculated for $C_{37}H_{38}N_3O_3S$ m/z = 604.2628).

Compound 3hA' (major dia):



Following general procedure II, compound **3hA'** is obtained as a white solid (66 mg, 55% yield) starting from triazole **1h** and imidazolidine **2A** (51 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).
M.p. = 111-113 °C; **Rf =** 0.25 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.65 (d, *J* = 8.6 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.44-7.27 (m, 3H), 7.17-7.08 (m, 2H), 7.07-6.93 (m, 5H), 6.90-6.79 (m, 1H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.55 (d, *J* = 8.0 Hz, 1H), 4.64 (d, *J* = 9.4 Hz, 1H), 4.36 (d, *J* = 9.4 Hz, 1H), 3.97 (d, *J* = 12.7 Hz, 1H) 3.94 (s, 3H), 3.64 (d, *J* = 13.5 Hz, 1H), 3.46-3.28 (m, 1H), 3.07 (d, *J* = 10.9 Hz, 1H), 2.98 (d, *J* = 12.4 Hz, 1H), 2.83 (td, *J* = 11.7, 3.3 Hz, 1H), 2.37 (s, 3H), 2.25 (s, 3H), 2.22 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 158.1 (C), 149.7 (C), 147.6 (C), 143.1 (C), 138.2 (C), 134.0 (C), 132.3 (C), 130.6 (CH), 130.3 (C), 130.0 (CH), 129.7 (2xCH), 129.5 (2xCH), 129.1 (C), 128.2 (C), 128.1 (C), 127.6 (CH), 127.3 (CH), 127.0 (CH), 126.9 (2xCH), 126.0 (CH), 118.9 (CH), 117.6 (2xCH), 107.7 (CH), 105.6 (CH), 71.9 (C), 62.3 (CH), 55.5 (CH_3),55.4 (CH_2), 47.7 (CH_2), 41.5 (CH_2), 21.7 (CH_3), 20.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 3290, 2922, 1606, 1513, 1492, 1335, 1265, 1212, 1157, 1034, 808, 664 cm^{-1}; **HR-MS (ESI):** m/z = 604.2642 $[M+H]^+$ (calculated for $C_{37}H_{38}N_3O_3S$ m/z = 604.2628).

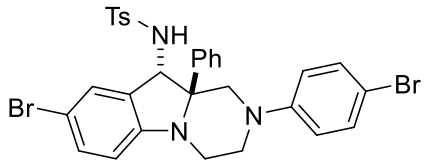
Compound 3aB (both dia):



Following general procedure II, compound **3aB** is obtained as a brownish solid (100 mg, 90% yield) starting from triazole **1a** and imidazolidine **2B** (56 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8:2).

M.p. = 134-136 °C; **Rf =** 0.43 (SiO_2, pentane/EtOAc, 7:3); **^{1}H NMR (400 MHz, $CDCl_3$,** inseparable mixture of diastereoisomers (dr 1:3)): δ [7.56 (*minor*) and 7.48 (*major*) (d, *J* = 8.3 Hz, 2H)], 7.36-7.28 (m, 5.6H, aromatics), 7.25-7.21 (m, 2.6H, aromatics), 7.19-7.14 (m, 1H, aromatics), 6.85-6.76 (m, 6.6H, aromatics), 6.56-6.51 (m, 3H, aromatics), 6.49 (*minor*, d, J = 8.6 Hz, 1H), 6.29-6.25 (*minor*, m, 1H), [4.90 (*minor*) and 4.54 (*major*) (d, *J* = 9.7 Hz, 1H)], [4.84 (*minor*) and 4.30 (*major*) (d, *J* = 9.7 Hz, 1H)], [3.85 (*minor*) and 4.83 (*major*) (d, *J* = 12.3 Hz, 1H)], [3.76 (*minor*) and 3.74 (*major*) (s, 3H)], [3.62 (*minor*) and 3.65 (*major*) (s, 3H)], 3.61-3.50 (m, 1H), 3.42-3.28 (m, 1H), [3.04 (*minor*) and 2.91 (*major*) (d, *J* = 12.3 Hz, 1H)], 3.02-2.94 (m, 1H), 2.85-2.76 (m, 1H), [2.40 (*minor*) and 2.43 (*major*) (s, 3H)] ppm; **^{13}C NMR (100 MHz, $CDCl_3$**, inseparable mixture of diastereoisomers (dr 1:3)): δ [154.53 (*major*) and 154.52 (*minor*) (C)], [153.3 (*minor*) and 153.2 (*major*) (C)], [146.2 (*minor*) and 146.1 (*major*) (C)], [144.0 (*major*) and 143.7 (*minor*) (C)], [143.39 (*minor*) and 143.37 (*major*) (C)], [142.0 (*minor*) and 138.5 (*major*) (C)], [137.6 (*minor*) and 137.3 (*major*) (C)], [129.9 (*minor*) and 129.8 (*major*) (2xCH)], [129.1 (*major*) and 128.6 (*minor*) (2xCH)], [128.9 (*major*) and 128.0 (*minor*) (C)], [127.8 (*major*) and 127.7 (*minor*) (2xCH)], [127.6 (*minor*) and 126.9 (*major*) (CH)], [127.19 (*minor*) and 127.16 (*major*) (2xCH)], [119.4 (*major*) and 119.3 (*minor*) (2xCH)], [116.3 (*major*) and 115.9 (*minor*) (CH)], [114.6 (*minor*) and 114.50 (*major*) (2xCH)], [112.2 (*major*) and 110.7 (*minor*) (CH)], [108.6 (*minor*) and 108.4 (*major*) (CH)], [73.21 (*minor*) and 72.24 (*major*) (C)], [67.1 (*minor*) and 62.2 (*major*) (CH)], [56.8 (*major*) and 51.5 (*minor*) (CH_2)], [56.1 (*major*) and 56.1 (*minor*) (CH_3)], [55.71 (*minor*) and 55.67 (*major*) (CH_3)], [48.1 (*major*) and 47.6 (*minor*) (CH_2)], [41.8 (*minor*) and 41.6 (*major*) (CH_2)], [21.7 (*major*) and 21.6 (*minor*) (CH_3)] ppm; **IR (neat):** 2929, 1490, 1448, 1340, 1240, 1212, 1159, 1092, 1028, 915, 842, 812, 698, 660 cm^{-1}; **HR-MS (ESI):** m/z 556.2267 $[M+H]^+$ (calculated for $C_{32}H_{34}N_3O_4S$ m/z = 556.2265).

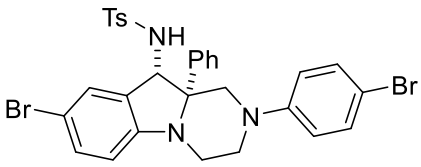
Compound 3aC'' (minor dia):



Following general procedure II, compound **3aC''** is obtained as a yellowish solid (22 mg, 17% yield) starting from triazole **1a** and imidazolidine **2C** (76 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).

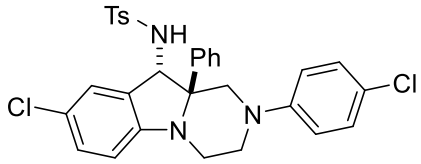
M.p. = 170-172 °C; **Rf =** 0.44 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.41-7.35 (m, 2H), 7.32 (d, *J* = 8.9 Hz, 2H), 7.28-7.21 (m, 6H), 6.74 (d, *J* = 8.9 Hz, 2H), 6.47-6.40 (m, 2H), 4.85 (d, *J* = 9.7 Hz, 1H), 4.79 (d, *J* = 9.7 Hz, 1H), 4.00 (d, *J* = 12.5 Hz, 1H), 3.63-3.53 (m, 1H), 3.44-3.31 (m, 1H), 3.19 (d, *J* = 12.6 Hz, 1H), 3.16-3.08 (m, 1H), 2.88 (td, *J* = 11.6, 3.7 Hz, 1H), 2.45 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.5 (C), 148.4 (C), 144.3 (C), 141.4 (C), 137.3 (C), 132.9 (CH), 132.1 (2xCH), 130.2 (2xCH), 128.9 (2xCH), 128.7 (C), 127.9 (CH), 127.6 (CH), 127.2 (2xCH), 126.5 (2xCH), 118.5 (2xCH), 112.9 (C), 109.9 (C), 109.1 (CH), 73.0 (C), 66.3 (CH), 50.8 (CH_2), 46.6 (CH_2), 41.3 (CH_2), 21.8 (CH_3) ppm; **IR (neat):** 3270, 2807, 1599, 1493, 1468, 1444, 1328, 1304, 1153, 1089, 808, 664 cm^{-1}; **HR-MS (ESI):** m/z = 652.0258 $[M+H]^+$ (calculated for $C_{30}H_{28}Br_2N_3O_2S$ m/z = 652.0264).

Compound 3aC' (major dia):



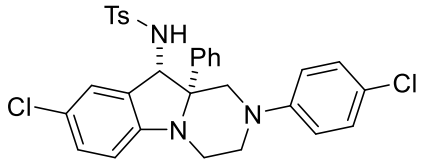
Following general procedure II, compound **3aC'** is obtained as a yellowish solid (91 mg, 69% yield) starting from triazole **1a** and imidazolidine **2C** (76 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1). **M.p. =** 110-112 °C; **Rf =** 0.33 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.38-7.26 (m, 8H), 7.24-7.17 (m, 2H), 6.72-6.70 (m, 1H), 6.68 (d, *J* = 9.0 Hz, 2H), 6.45 (d, *J* = 8.4 Hz, 1H), 4.66 (d, *J* = 9.8 Hz, 1H), 4.23 (d, *J* = 9.8 Hz, 1H), 4.02 (d, *J* = 12.4 Hz, 1H), 3.63-3.55 (m, 1H), 3.39-3.29 (m, 1H), 3.21-3.14 (m, 1H), 2.96 (d, *J* = 12.5 Hz, 1H), 2.84 (td, *J* = 11.6, 3.6 Hz, 1H), 2.48 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.5 (C), 148.7 (C), 144.0 (C), 138.2 (C), 136.0 (C), 132.9 (CH), 132.1 (2xCH), 130.0 (2xCH), 129.5 (C), 129.3 (2xCH), 129.1 (CH), 128.2 (CH), 127.7 (2xCH), 127.2 (2xCH), 118.7 (2xCH), 113.1 (C), 109.7 (C), 108.5 (CH), 72.3 (C), 61.9 (CH), 55.8 (CH_2), 47.3 (CH_2), 40.9 (CH_2), 21.8 (CH_3)ppm; **IR (neat):** 3288, 2925, 1594, 1476, 1336, 1219, 1157, 1080, 909, 810, 662 cm^{-1}; **HR-MS (ESI):** m/z = 652.0267 $[M+H]^+$ (calculated for $C_{30}H_{28}Br_2N_3O_2S$ m/z = 652.0264).

Compound 3aD'' (minor dia):



Following general procedure II, compound **3aD''** is obtained as a yellowish solid (20 mg, 18% yield) starting from triazole **1a** (3 equiv) and imidazolidine **2D** (58 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1). **M.p. =** 224-226 °C; **Rf =** 0.49 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.42-7.35 (m, 2H), 7.30-7.21 (m, 5H), 7.19 (d, *J* = 8.9 Hz, 2H), 7.13 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.79 (d, *J* = 8.9 Hz, 2H), 6.48 (d, *J* = 8.4 Hz, 1H), 6.39 (s, 1H), 4.84 (d, *J* = 9.7 Hz, 1H), 4.79 (d, *J* = 9.8 Hz, 1H), 4.00 (d, *J* = 13.2 Hz, 1H), 3.63-3.53 (m, 1H), 3.44-3.31 (m, 1H), 3.18 (d, *J* = 12.5 Hz, 1H), 3.15-3.06 (m, 1H), 2.88 (td, *J* = 11.6, 3.7 Hz, 1H), 2.44 (s, 3H)ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.1 (C), 148.0 (C), 144.2 (C), 141.5 (C), 137.3 (C), 130.1 (2xCH), 130.1 (CH), 129.2 (2xCH), 128.9 (2xCH), 128.3 (C), 127.5 (CH), 127.2 (2xCH), 126.6 (2xCH), 125.6 (C), 125.1 (CH), 123.1 (C), 118.1 (2xCH), 108.5 (CH), 73.0 (C), 66.3 (CH), 50.9 (CH_2), 46.7 (CH_2), 41.3 (CH_2), 21.7 (CH_3) ppm; **IR (neat):** 3269, 2807, 1599, 1496, 1469, 1444, 1329, 1243, 1212, 1154, 1091, 900, 809, 658 cm^{-1}; **HR-MS (ESI):** m/z = 564.1271 $[M+H]^+$ (calculated for $C_{30}H_{28}Cl_2N_3O_2S$ m/z = 564.1274).

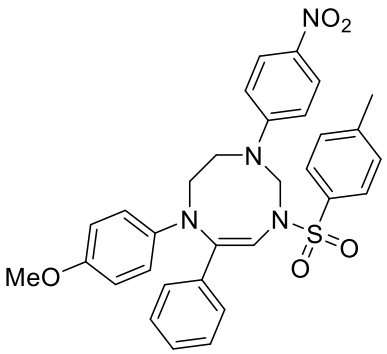
Compound 3aD' (major dia):



Following general procedure II, compound **3aD''** is obtained as a yellowish solid (63 mg, 56% yield) starting from triazole **1a** (3 equiv) and imidazolidine **2D** (58 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1). **M.p. =** 154-156 °C; **Rf =** 0.36 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.37-7.27 (m, 5H), 7.24-7.19 (m, 2H), 7.19-7.12 (m, 3H), 6.73 (d, *J* = 9.0 Hz, 2H), 6.68-6.63 (m, 1H), 6.49 (d, *J* = 8.4 Hz, 1H), 4.65 (d, *J* = 9.8 Hz, 1H), 4.23 (d, *J* = 9.8 Hz, 1H), 4.02 (d, *J* = 12.4 Hz, 1H), 3.63-3.54 (m, 1H), 3.42-3.30 (m, 1H), 3.21-3.12 (m, 1H), 2.97 (d, *J* = 12.4 Hz, 1H), 2.84 (td, *J* = 11.7, 3.6 Hz, 1H), 2.47 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.1 (C), 148.3 (C), 143.9 (C), 138.2 (C), 136.1 (C), 130.0 (CH), 129.9 (2xCH), 129.3 (2xCH), 129.2 (2xCH), 129.1 (C), 128.1 (CH), 127.7 (2xCH), 127.2 (2xCH), 126.4 (CH), 125.8 (C), 123.0 (C), 118.4 (2xCH), 107.9 (CH), 72.3 (C), 61.9 (CH), 56.0 (CH_2), 47.4 (CH_2), 41.0 (CH_2), 21.7 (CH_3) ppm; **IR (neat):** 3351, 2823, 1597, 1493, 1337, 1226, 1159, 1051, 909, 818, 659 cm^{-1}; **HR-MS (ESI):** m/z = 564.1278 $[M+H]^+$ (calculated for $C_{30}H_{28}Cl_2N_3O_2S$ m/z = 564.1274).

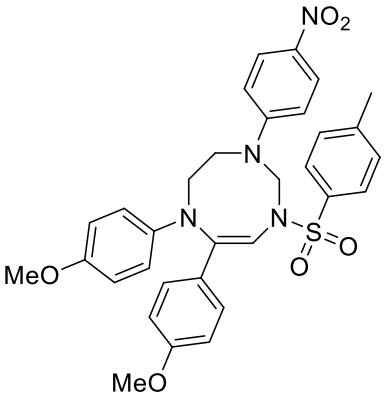
Analysis data for compounds 4

Compound 4aE:



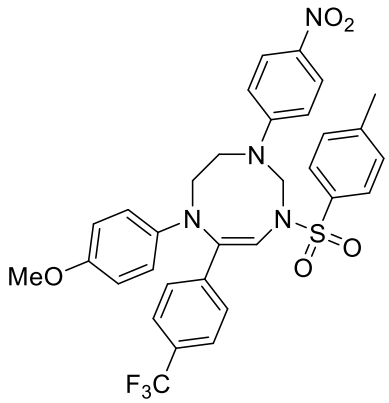
Following general procedure II, compound **4aE** is obtained as an orange solid (65 mg, 57% yield) starting from triazole **1a** and imidazolidine **2E** (59 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 7:3).
M.p. = 181-183 °C; **Rf =** 0.47 (SiO_2, pentane/EtOAc, 6:4); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.15 (d, *J* = 9.3 Hz, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.26-7.18 (m, 5H), 7.16-7.08 (m, 2H), 6.92 (d, *J* = 9.4 Hz, 2H), 6.84 (s, 1H), 6.49 (d, *J* = 9.1 Hz, 2H), 6.37 (d, *J* = 9.1 Hz, 2H), 5.26 (s, 2H), 3.70 (s, 3H), 3.69-3.56 (m, 4H), 2.45 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 152.1 (C), 150.8 (C), 144.4 (C), 139.8 (C), 139.5 (C), 137.1 (C), 136.5 (C), 130.4 (C), 130.1 (2xCH), 128.8 (2xCH), 128.2 (CH), 126.9 (2xCH), 126.11 (2xCH), 126.08 (2xCH), 119.2 (CH), 115.3 (2xCH), 113.3 (2xCH), 112.5 (2xCH), 65.0 (CH_2), 55.8 (CH_3), 47.3 (CH_2), 46.4 (CH_2), 21.7 (CH_3) ppm; **IR (neat):** 1595, 1508, 1383, 1315, 1292, 1220, 1151, 1108, 998, 924, 815, 764, 748, 665 cm^{-1}; **HR-MS (ESI):** m/z = 571.2041 $[M+H]^+$ (calculated for $C_{31}H_{31}N_4O_5S$ m/z = 571.2010).

Compound 4eE:



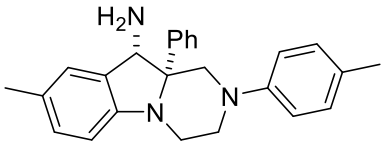
Following general procedure II, compound **4eE** is obtained as an orange solid (67 mg, 56% yield) starting from triazole **1e** and imidazolidine **2E** (59 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 7:3) followed by recrystallization with CH_2Cl_2, Et_2O and pentane.
M.p. = 138-140 °C; **Rf =** 0.48 (SiO_2, pentane/EtOAc, 6:4); **^{1}H NMR (400 MHz, CD_2Cl_2):** δ 8.11 (d, *J* = 9.4 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 9.4 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 6.68 (s, 1H), 6.50 (d, *J* = 9.1 Hz, 2H), 6.39 (d, *J* = 9.1 Hz, 2H), 5.22 (s, 2H), 3.74 (s, 3H), 3.68 (s, 3H), 3.65-3.58 (m, 4H), 2.45 (s, 3H) ppm; **^{13}C NMR (100 MHz, CD_2Cl_2):** δ 160.3 (C), 152.6 (C), 151.6 (C), 145.0 (C), 140.1 (C), 139.7 (C), 137.5 (C), 131.3 (C), 130.5 (2xCH), 129.4 (C), 127.9 (2xCH), 127.2 (2xCH), 126.2 (2xCH), 117.7 (CH), 115.5 (2xCH), 114.5 (2xCH), 114.2 (2xCH), 112.9 (2xCH), 65.5 (CH_2), 56.0 (CH_3), 55.8 (CH_3), 47.7 (CH_2), 46.9 (CH_2), 21.9 (CH_3) ppm; **IR (neat):** 1594, 1505, 1316, 1228, 1158, 1109, 1033, 994, 831, 815, 747, 657 cm^{-1}; **HR-MS (ESI):** m/z = 601.2139 $[M+H]^+$ (calculated for $C_{32}H_{33}N_4O_6S$ m/z = 601.2116).

Compound 4iE:



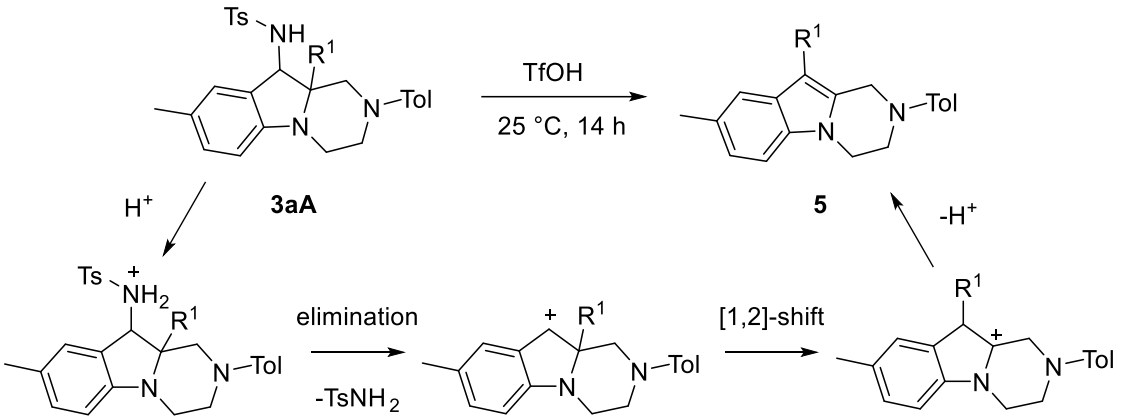
Following general procedure II, compound **4iE** is obtained as an orange solid (46 mg, 36% yield) starting from triazole **1i** and imidazolidine **2E** (60 mg, 0.2 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 7:3) followed by recrystallization with CH_2Cl_2, Et_2O and pentane.
M.p. = 147-149 °C; **Rf =** 0.47 (SiO_2, pentane/EtOAc, 6:4); **^{1}H NMR (400 MHz, CD_2Cl_2):** δ 8.12 (d, *J* = 9.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.1 Hz, 2H), 7.32-7.24 (m, 4H), 6.97 (s, 1H), 6.95 (d, *J* = 9.4 Hz, 2H), 6.51 (d, *J* = 9.2 Hz, 2H), 6.38 (d, *J* = 9.1 Hz, 2H), 5.25 (s, 2H), 3.68 (s, 3H), 3.66-3.59 (m, 4H), 2.45 (s, 3H) ppm; **^{13}C NMR (100 MHz, CD_2Cl_2):** δ 152.9 (C), 151.4 (C), 145.3 (C), 141.3 (C), 140.0 (C), 139.7 (C), 137.3 (C), 130.6 (2xCH), 129.9 (q, *J* = 32.4 Hz, C), 129.4 (C), 127.2 (2xCH), 126.6 (2xCH), 126.3 (2xCH), 126.0 (q, *J* = 3.8 Hz, 2xCH), 124.8 (q, *J* = 271.8 Hz, CF_3), 121.8 (CH), 115.7 (2xCH), 114.1 (2xCH), 113.0 (2xCH), 65.4 (CH_2), 56.0 (CH_3), 47.9 (CH_2), 46.7 (CH_2), 21.9 (CH_3) ppm; **^{19}F NMR (282 MHz, CD_2Cl_2):** δ -62.83 ppm; **IR (neat):** 1595, 1506, 1321, 1225, 1152, 1109, 1067, 999, 921, 833, 814, 744, 672 cm^{-1}; **HR-MS (ESI):** m/z = 639.1911 $[M+H]^+$ (calculated for $C_{32}H_{30}F_3N_4O_5S$ m/z = 639.1884).

6. Synthesis of 3A



In a 25 mL two-neck flask under N_2 atmosphere, sodium (69 mg, 3 mmol, 20 equiv; washed free of oil in hexane) was added to a stirred suspension of naphthalene (385 mg, 3 mmol, 20 equiv) in 7 mL of tetrahydrofuran at 25 °C. The resulting green suspension was stirred at 25 °C for 4 h and cooled down to -78 °C. Then, a solution of hexahydropyrazino[1,2-*a*]indole **3aA'** (79 mg, 0.15 mmol, 1 equiv) in tetrahydrofuran (7 mL) was slowly added to the green solution. The dark-green solution was stirred at -78 °C for 30 min and at 25 °C for 15 h. Then, the mixture was cooled down at -78 °C and 2 mL of water were added. The reaction mixture was extracted with CH_2Cl_2 (3×10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography to afford amine **3A** as a white solid (43 mg, 78% yield).
M.p. = 53-55 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.58 (d, *J* = 7.7 Hz, 2H), 7.50-7.41 (m, 2H), 7.37-7.29 (m, 1H), 7.19-7.14 (m, 1H), 7.09-7.04 (m, 1H), 7.03-6.98 (m, 2H), 6.77 (d, *J* = 8.5 Hz, 2H), 6.61 (d, *J* = 8.1 Hz, 1H), 3.93 (dd, *J* = 12.5, 1.6 Hz, 1H), 3.86 (s, 1H), 3.75-3.62 (m, 1H), 3.75-3.62 (m, 1H), 3.48 (ddd, *J* = 14.2, 12.1, 3.6 Hz, 1H), 3.07 (ddt, *J* = 11.3, 3.5, 1.7 Hz, 1H), 2.93 (d, *J* = 12.5 Hz, 1H), 2.87 (td, *J* = 11.8, 3.2 Hz, 1H), 2.29 (s, 3H) 2.24 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 150.1 (C), 147.8 (C), 138.8 (C), 131.9 (C), 130.1 (C), 129.9 (CH), 129.7 (2xCH), 129.1 (2xCH), 128.0 (C), 127.6 (CH), 127.43 (CH), 127.35 (2xCH), 117.64 (2xCH), 108.7 (CH), 73.8 (C), 61.8 (CH), 55.4 (CH_2), 47.2 (CH_2), 41.9 (CH_2), 20.9 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2922, 1615. 1512, 1490, 1448, 1358, 1249, 1222, 1206, 1098, 1037, 981, 804, 701 cm^{-1}; **HR-MS (ESI):** 370.2291 $[M+H]^+$ (calculated for $C_{25}H_{28}N_3$ m/z = 370.2278).

7. Scheme S2. Mechanistic rationale for the formation of 5

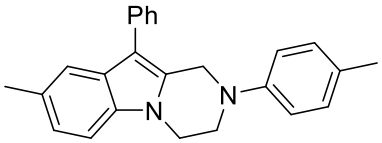


Tetrahydropyrazino[1,2-*a*]indole of type **5** are probably formed through protonation and elimination of $TsNH_2$ followed by a 1,2-shift of the aryl group (R^1) and a final proton loss.

8. General Procedure III: synthesis of tetrahydropyrazino[1,2-*a*]indoles 5

In a 2 mL screw-cap vial equipped with a magnetic stirring bar, 0.1 mmol of 1,2,3,4-tetrahydropyrazino[1,2-*a*]indoles **3** (as single or mixture of diastereoisomers) and 2.3 mmol (23 equiv) of triflic acid were added. The mixture was stirred at 25 °C during 14 h. Then, few milliliters of water were carefully added on the crude reaction mixture followed by the addition of $NaHCO_3$. The aqueous mixture was extracted with CH_2Cl_2 (3 x 20 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography.

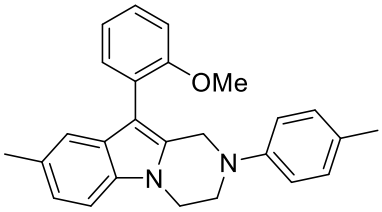
Compound 5aA:



Following general procedure III, compound **5aA** is obtained as an orange solid (43 mg, 82% yield) starting from hexahydropyrazino[1,2-*a*]indole **3aA** (52 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8.5:1.5).

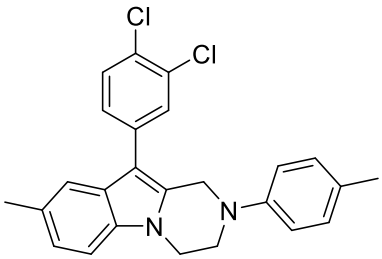
M.p. = 149-151 °C; **Rf =** 0.64 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.59 (m, 1H), 7.55-7.45 (m, 4H), 7.34-7.28 (m, 1H), 7.23 (d, *J* = 8.2 Hz, 1H), 7.12-7.04 (m, 3H), 6.92 (d, *J* = 8.5 Hz, 2H), 4.62 (s, 2H), 4.21 (t, *J* = 5.6 Hz, 2H), 3.77 (t, *J* = 5.6 Hz, 2H), 2.46 (s, 3H), 2.27 (s, 3H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 148.0 (C), 135.2 (C), 134.7 (C), 130.7 (C), 130.4 (C), 130.0 (2xCH), 129.9 (C), 129.1 (2xCH), 128.8 (2xCH), 127.4 (C), 125.8 (CH), 123.0 (CH), 119.0 (CH), 117.6 (2xCH), 111.7 (C), 108.6 (CH), 48.4 (CH_2), 48.1 (CH_2), 41.7 (CH_2), 21.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2922, 1598, 1546, 1512, 1454, 1365, 1230, 1150, 1114, 946, 818, 764, 704 cm^{-1}; **HR-MS (ESI):** m/z = 353.2024 $[M+H]^+$ (calculated for $C_{25}H_{25}N_2$ m/z = 353.2013).

Compound 5dA:



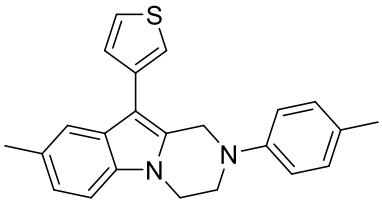
Following general procedure III, compound **5dA** is obtained as an orange solid (33 mg, 87% yield) starting from hexahydropyrazino[1,2-*a*]indole **3dA** (55 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 78-80 °C; **Rf =** 0.41 (SiO_2, pentane/EtOAc, 9:1); **^{1}H NMR (500 MHz, $CDCl_3$):** δ 7.48 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.37-7.31 (m, 2H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.09 (td, *J* = 7.4, 1.1 Hz, 1H), 7.07-7.04 (m, 3H), 7.02 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.91 (d, *J* = 8.6 Hz, 2H), 4.46 (s, 2H), 4.18 (t, *J* = 5.6 Hz, 2H), 3.84 (s, 3H), 3.82-3.77 (m, 2H), 2.42 (s, 3H), 2.26 (s, 3H) ppm; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 157.1 (C), 148.0 (C), 134.6 (C), 132.1 (CH), 131.6 (C), 130.0 (C), 129.9 (2xCH), 129.4 (C), 128.1 (C), 127.9 (CH), 123.6 (C), 122.6 (CH), 120.8 (CH), 119.1 (CH), 117.5 (2xCH), 111.3 (CH), 108.5 (CH), 107.3 (C), 55.5 (CH_3), 48.3 (CH_2), 48.0 (CH_2), 41.3 (CH_2), 21.7 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2919, 1615, 1514, 1452, 1372, 1238, 1025, 791, 751, 645 cm^{-1}; **HR-MS (ESI):** m/z = 383.2116 $[M+H]^+$ (calculated for $C_{26}H_{26}N_2O$ m/z = 383.2123).

Compound 5fA:



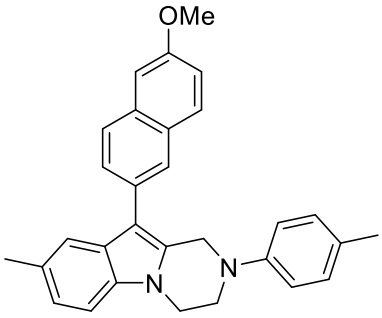
Following general procedure III, compound **5fA** is obtained as an orange solid (37 mg, 88% yield) starting from hexahydropyrazino[1,2-*a*]indole **3fA** (59 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 76-78 °C; **Rf =** 0.51 (SiO_2, pentane/EtOAc, 9:1); **^{1}H NMR (500 MHz, $CDCl_3$):** δ 7.58 (d, *J* = 2.1 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.50-7.46 (m, 1H), 7.33 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.23 (d, *J* = 8.3 Hz, 1H), 7.12-7.05 (m, 3H), 6.91 (d, *J* = 8.6 Hz, 2H), 4.57 (s, 2H), 4.20 (t, *J* = 5.6 Hz, 2H), 3.77 (t, *J* = 5.6 Hz, 2H), 2.47 (s, 3H), 2.28 (s, 3H) ppm; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 147.8 (C), 135.5 (C), 134.7 (C), 132.8 (C), 131.3 (C), 130.74 (C), 130.72 (CH), 130.5 (CH), 130.4 (C), 130.1 (2xCH), 129.5 (C), 128.2 (CH), 126.9 (C), 123.5 (CH), 118.4 (CH), 117.6 (2xCH), 109.4 (C), 108.8 (CH), 48.3 (CH_2), 48.1 (CH_2), 41.7 (CH_2), 21.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2919, 1591, 1513, 1485, 1452, 1369, 1230, 1114, 1026, 792 cm^{-1}; **HR-MS (ESI):** m/z = 421.1238 $[M+H]^+$ (calculated for $C_{25}H_{23}Cl_2N_2$ m/z = 421.1206).

Compound 5gA:



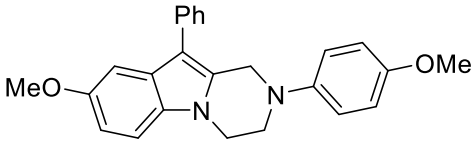
Following general procedure III, compound **5gA** is obtained as an orange solid (28 mg, 77% yield) starting from hexahydropyrazino[1,2-*a*]indole **3gA** (53 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 112-114 °C; **Rf =** 0.64 (SiO_2, pentane/EtOAc, 9:1); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.60-7.54 (m, 1H), 7.47 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.39 (dd, *J* = 4.9, 1.3 Hz, 1H), 7.25 (d, *J* = 1.4 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 1H), 7.10 (d, *J* = 8.1 Hz, 2H), 7.06 (dd, *J* = 8.2, 1.6 Hz, 1H), 6.94 (d, *J* = 8.5 Hz, 2H), 4.63 (s, 2H), 4.19 (t, *J* = 5.6 Hz, 2H),3.76 (t, *J* = 5.6 Hz, 2H), 2.48 (s, 3H), 2.28 (s, 3H) ppm; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 148.0 (C), 135.3 (C), 134.5 (C), 130.7 (C), 130.4 (C), 130.0 (2xCH), 129.8 (C), 128.3 (CH), 127.4 (C), 125.5 (CH), 123.0 (CH), 120.2 (CH), 119.1 (CH), 117.5 (2xCH), 108.6 (CH), 106.7 (C), 48.2 (CH_2), 48.2 (CH_2), 41.7 (CH_2), 21.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2916, 1614, 1512, 1486, 1451, 1372, 1217, 1157, 866, 790 cm^{-1}; **HR-MS (ESI):** m/z = 359.1595 $[M+H]^+$ (calculated for $C_{23}H_{23}N_2S$ m/z = 359.1582).

Compound 5hA:



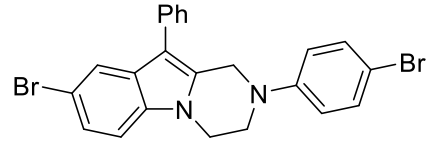
Following general procedure III, compound **5hA** is obtained as an orange solid (37 mg, 86% yield) starting from hexahydropyrazino[1,2-*a*]indole **3hA** (60 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 9:1).
M.p. = 110-112 °C; **Rf =** 0.42 (SiO_2, pentane/EtOAc, 9:1); **^{1}H NMR (500 MHz, $CDCl_3$):** δ 7.85 (d, *J* = 8.5 Hz, 1H), 7.83-7.82 (m, 1H), 7.79 (d, *J* = 8.7 Hz, 1H), 7.67 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.61-7.57 (m, 1H), 7.25-7.16 (m, 3H), 7.10-7.03 (m, 3H), 6.91 (d, *J* = 8.7 Hz, 2H), 4.67 (s, 2H), 4.23 (t, *J* = 5.6 Hz, 2H), 3.96 (s, 3H), 3.80 (t, *J* = 5.6 Hz, 2H), 2.47 (s, 3H), 2.26 (s, 3H) ppm; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 157.6 (C), 148.0 (C), 134.7 (C), 133.0 (C), 130.8 (C), 130.5 (C), 130.4 (C), 130.0 (2xCH), 129.9 (C), 129.5 (C), 129.4 (CH), 128.4 (CH), 127.6 (C), 127.1 (2xCH), 123.1 (CH), 119.1 (CH), 118.9 (CH), 117.6 (2xCH), 111.7 (C), 108.7 (CH), 105.9 (CH), 55.5 (CH_3), 48.3 (CH_2), 48.2 (CH_2), 41.7 (CH_2), 21.8 (CH_3), 20.6 (CH_3) ppm; **IR (neat):** 2921, 1606, 1513, 1482, 1453, 1373, 1267, 1203, 1158, 1031, 853, 807 cm^{-1}; **HR-MS (ESI):** m/z = 433.2284 $[M+H]^+$ (calculated for $C_{30}H_{29}N_2O$ m/z = 433.2280).

Compound 5aB:



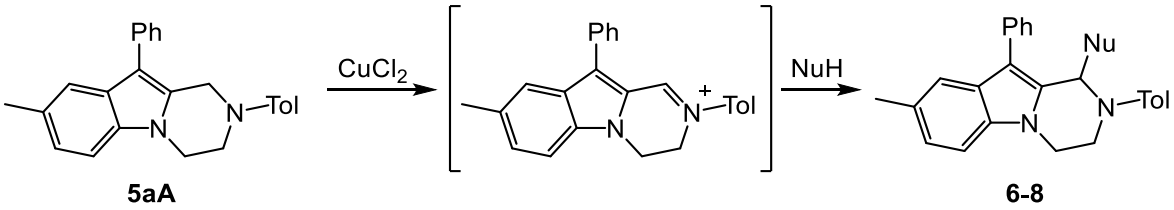
Following general procedure III, compound **5aB** is obtained as an orange solid (30 mg, 78% yield) starting from hexahydropyrazino[1,2-*a*]indole **3aB** (55 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8.5:1.5).
M.p. = 139-141 °C; **Rf =** 0.39 (SiO_2, pentane/EtOAc, 8:2); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.54-7.45 (m, 4H), 7.34-7.28 (m, 1H), 7.25-7.22 (m, 2H), 6.98 (d, *J* = 9.1 Hz, 2H), 6.90 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.84 (d, *J* = 9.0 Hz, 2H), 4.55 (s, 2H), 4.19 (t, *J* = 5.6 Hz, 2H), 3.85 (s, 3H), 3.76 (s, 3H), 3.70 (t, *J* = 5.6 Hz, 2H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 155.1 (C), 154.7 (C), 144.4 (C), 135.2 (C), 131.6 (C), 131.4 (C), 128.89 (2xCH), 128.88 (2xCH), 127.4 (C), 125.8 (CH), 119.7 (2xCH), 114.7 (2xCH), 111.8 (C), 111.5 (CH), 109.7 (CH), 101.3 (CH), 56.1 (CH_3), 55.7 (CH_3), 49.2 (CH_2), 49.1 (CH_2), 41.8 (CH_2).ppm; **IR (neat):** 2923, 1599, 1513, 1482, 1438, 1298, 1252, 1213, 1160, 1032, 762, 705 cm^{-1}; **HR-MS (ESI):** m/z = 385.1922 $[M+H]^+$ (calculated for $C_{25}H_{25}N_2O_2$ m/z =385.1916).

Compound 5aC:



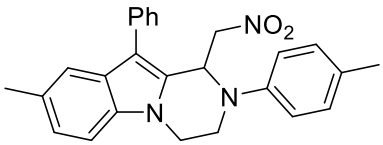
Following general procedure III, compound **5aC** is obtained as an orange solid (37 mg, 77% yield) starting from hexahydropyrazino[1,2-*a*]indole **3aC** (65 mg, 0.1 mmol).
Purification: column chromatography (SiO_2, pentane/EtOAc, 8.5:1.5).
M.p. = 111-113 °C; **Rf =** 0.43 (SiO_2, pentane/EtOAc, 9:1); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.86 (d, *J* = 1.8 Hz, 1H), 7.53-7.44 (m, 4H), 7.38-7.29 (m, 4H), 7.20 (d, *J* = 8.7 Hz, 1H), 6.84 (d, *J* = 9.0 Hz, 2H), 4.64 (s, 2H), 4.21 (t, *J* = 5.6 Hz, 2H), 3.81 (t, *J* = 5.6 Hz, 2H) ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 148.8 (C), 134.9 (C), 134.1 (C), 132.3 (2xCH), 130.9 (C), 129.1 (2xCH), 128.9 (2xCH), 128.7 (C), 126.5 (CH), 124.5 (CH), 121.9 (CH), 118.6 (2xCH), 114.0 (C), 113.1 (C), 112.1 (C), 110.4 (CH), 47.6 (CH_2), 47.2 (CH_2), 41.6 (CH_2) ppm; **IR (neat):** 2923, 1598, 1491, 1447, 1370, 1341, 1211, 1157, 1080, 769, 703 cm^{-1}; **HR-MS (ESI):** m/z = 482.9890 $[M+H]^+$ (calculated for $C_{23}H_{19}Br_2N_2$ m/z = 482.9896).

9. Postfunctionalizations of 5aA *via* oxidative C-C bond formation



5aA **6-8**

Synthesis of 6



In a 5 mL screw-cap vial equipped with a magnetic stirring bar, tetrahydropyrazino[1,2-*a*]indole **5aA** (35 mg, 0.1 mmol, 1 equiv) and $CuCl_2$ (13 mg, 1 equiv) were dissolved in a 1:1 mixture of $MeNO_2$/THF (2 mL). After 3 h stirring at 25 °C, DIPEA (19 µL, 1.1 equiv) was added and the mixture was stirred at 25 °C during 2 h more. The residue was purified by a short silica gel chromatography (pentane/EtOAc, 8:2) to afford **6** as a yellowish solid (38 mg, 92% yield).

M.p. = 112-114 °C;

Rf = 0.74 (SiO_2, pentane/EtOAc, 8:2);

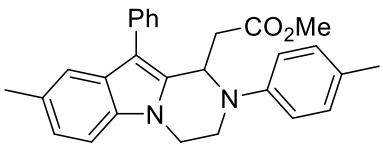
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58-7.49 (m, 4H), 7.47-7.43 (m, 1H), 7.37 (tt, *J* = 6.7, 1.7 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 1H), 7.12-7.06 (m, 3H), 6.99 (d, *J* = 8.6 Hz, 2H), 6.07 (dd, *J* = 10.7, 4.5 Hz, 1H), 4.71 (dd, *J* = 12.4, 10.8 Hz, 1H), 4.28 (dd, *J* = 12.4, 4.5 Hz, 1H), 4.11-4.00 (m, 2H), 3.96-3.82 (m, 2H), 2.44 (s, 3H), 2.28 (s, 3H) ppm;

^{13}C NMR (126 MHz, $CDCl_3$): δ 146.7 (C), 134.9 (C), 134.1 (C), 131.8 (C), 130.5 (C), 130.2 (2xCH), 129.4 (2xCH), 129.0 (2xCH), 127.2 (C), 127.1 (CH), 126.6 (C), 124.1 (CH), 119.5 (2xCH), 119.1 (CH), 113.4 (C), 108.8 (CH), 75.8 (CH_2), 54.5 (CH), 43.7 (CH_2), 38.2 (CH_2), 21.7 (CH_3), 20.7 (CH_3) ppm;

IR (neat): 2922, 2854, 1604, 1553, 1512, 1455, 1374, 1297, 1199, 1150, 1112, 1022, 795, 732, 700 cm^{-1};

HR-MS (ESI): m/z = 412.2022 $[M+H]^+$ (calculated for $C_{26}H_{26}N_3O_2$ m/z = 412.2025).

Synthesis of 7



In a 5 mL screw-cap vial equipped with a magnetic stirring bar, tetrahydropyrazino[1,2-*a*]indole **5aA** (35 mg, 0.1 mmol, 1 equiv) and $CuCl_2$ (13 mg, 1 equiv) were dissolved in THF (1 mL). After 16 h stirring at 25 °C, 1-tert-butyldimethylsilyloxy-1-methoxyethene (43 µL, 2 equiv) was added and the mixture was stirred at 25 °C. After 3 h, another extra equivalent of 1-tert-butyldimethylsilyloxy-1-methoxyethene (21 µL) was added to the mixture and it was stirred at 25 °C during 3 h more. The residue was purified by a short silica gel chromatography (pentane/EtOAc, 9:1) to afford **7** as a yellowish solid (31 mg, 73% yield).

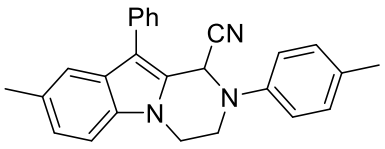
M.p. = 70-72 °C;

Rf = 0.50 (SiO_2, pentane/EtOAc, 9:1);

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.57-7.51 (m, 2H), 7.51-7.45 (m, 2H), 7.44-7.40 (m, 1H), 7.33 (ddt, *J* = 7.6, 6.9, 1.4 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.06 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.01 (d, *J* = 8.6 Hz, 2H), 5.83 (dd, *J* = 9.8, 5.0 Hz, 1H), 4.14-4.03 (m, 2H), 3.93-3.83 (m, 2H), 3.43 (s, 3H), 2.86 (dd, *J* = 14.9, 9.8 Hz, 1H), 2.54 (dd, *J* = 14.9, 5.0 Hz, 1H), 2.43 (s, 3H), 2.27 (s, 3H) ppm;

^{13}C NMR (126 MHz, $CDCl_3$): δ 170.9 (C), 147.0 (C), 134.9 (C), 134.6 (C), 131.9 (C), 130.1 (C), 130.0 (2xCH), 129.9 (C), 129.4 (2xCH), 129.0 (2xCH), 127.6 (C), 126.5 (CH), 123.4 (CH), 118.9 (CH), 118.04 (2xCH), 112.07 (C), 108.6 (CH), 52.7 (CH) , 51.7 (CH_3), 42.3 (CH_2), 39.4 (CH_2), 38.9 (CH_2), 21.6 (CH_3), 20.6 (CH_3).ppm;
IR (neat): 2922, 1736, 1603, 1513, 1485, 1434, 1367, 1260, 1228, 1170, 1111, 1014, 972, 794, 700 cm^{-1};
HR-MS (ESI): m/z = 425.2232 $[M+H]^+$ (calculated for $C_{28}H_{29}N_2O_2$ m/z = 425.2229).

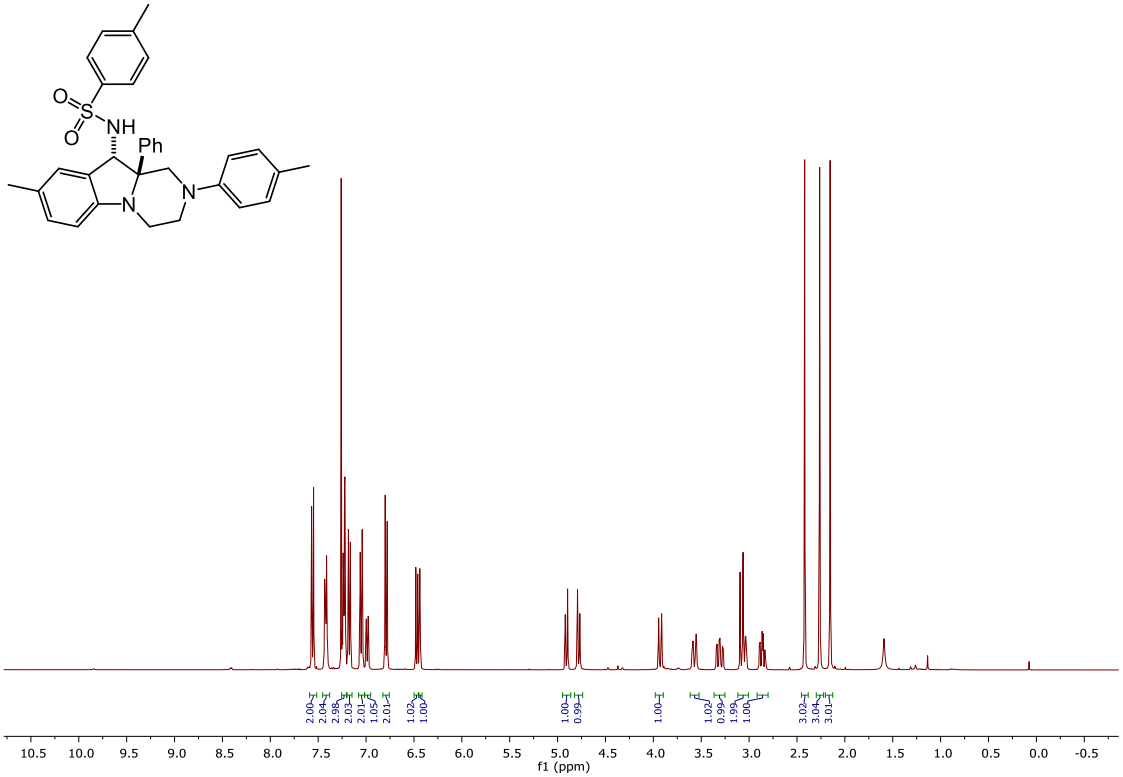
Synthesis of 8



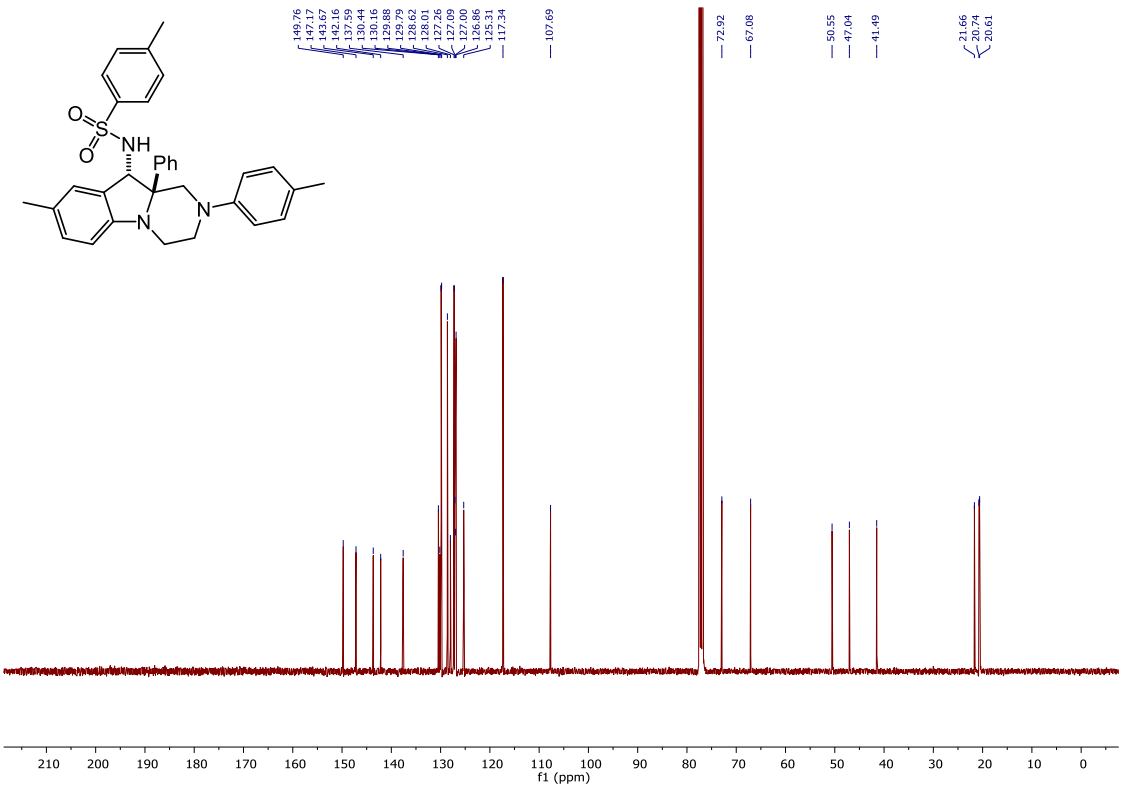
In a 5 mL screw-cap vial equipped with a magnetic stirring bar, tetrahydropyrazino[1,2-*a*]indole **5aA** (35 mg, 0.1 mmol, 1 equiv) and $CuCl_2$ (13 mg, 1 equiv) were dissolved in THF (1 mL). After 16 h stirring at 25 °C, a solution of NaCN (7 mg, 1.5 equiv) in MeOH (0.3 mL) was added and the mixture was stirred at 25 °C. After 3 h, another solution of NaCN (7 mg, 1.5 equiv) in MeOH (0.3 mL) was added to the mixture and it was stirred at 25 °C during 3 h more. The residue was diluted with CH_2Cl_2 and washed three times with saturated NH_4Claq. The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure to afford **8** as a yellowish solid (35 mg, 93% yield).
M.p. = 149-151 °C;
Rf = 0.80 (SiO_2, pentane/EtOAc, 8:2);
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.63-7.58 (m, 2H), 7.56-7.50 (m, 3H), 7.41-7.36 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.20-7.14 (m, 3H), 7.02 (d, *J* = 8.7 Hz, 2H), 5.61 (d, *J* = 1.4 Hz, 1H), 4.42 (ddd, *J* = 11.2, 4.0, 1.7 Hz, 1H), 4.10 (td, *J* = 11.3, 5.5 Hz, 1H), 3.95-3.80 (m, 2H), 2.47 (s, 3H), 2.31 (s, 3H) ppm;
^{13}C NMR (126 MHz, $CDCl_3$): δ 145.7 (C), 135.3 (C), 133.5 (C), 130.7 (C), 130.4 (2xCH), 129.5 (2xCH), 129.2 (2xCH), 127.5 (C), 127.00 (CH), 126.99 (C), 124.9 (CH), 124.4 (C), 119.8 (CH), 119.6 (2xCH), 116.2 (C), 114.9 (C), 109.3 (CH), 51.0 (CH), 44.7 (CH_2), 42.4 (CH_2), 21.7 (CH_3), 20.8 (CH_3) ppm;
IR (neat): 2920, 2856, 1511, 1453, 1360, 1300, 1220, 1146, 1115, 951, 907, 872, 801, 699 cm^{-1};
HR-MS (ESI): m/z = 378.1988 $[M+H]^+$ (calculated for $C_{26}H_{24}N_3$ m/z = 378.1970).

10. NMR spectra of new compounds

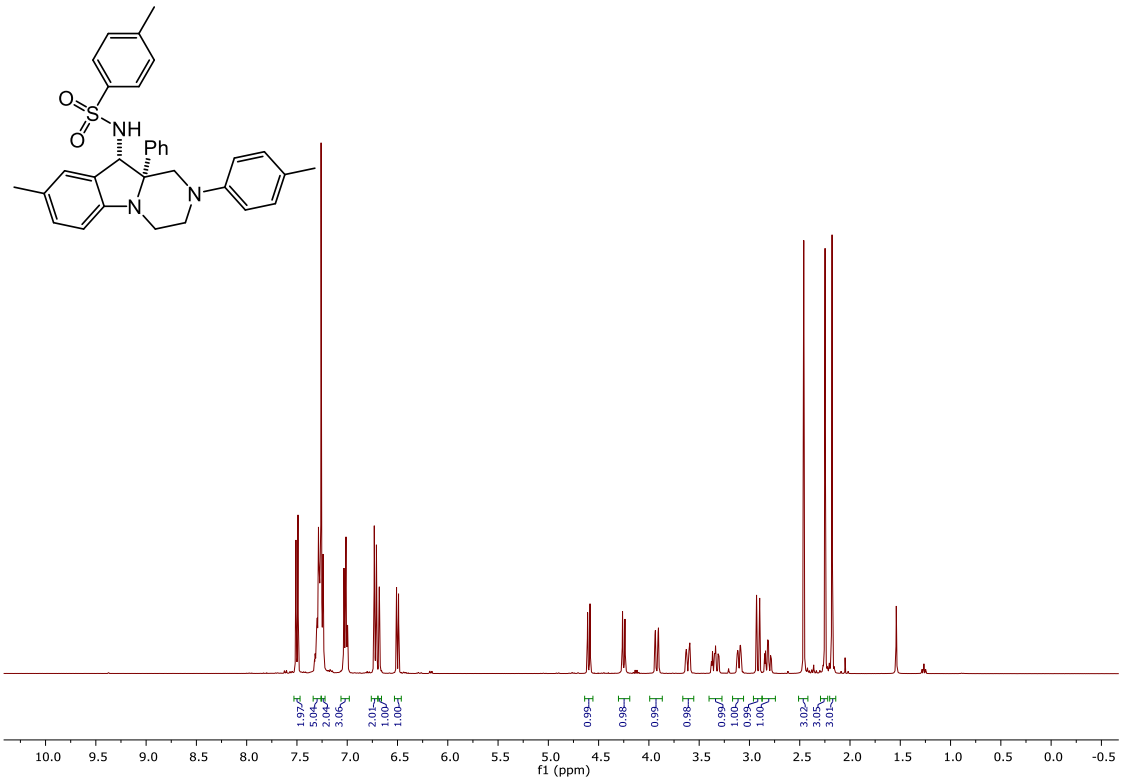
Compound 3aA'' ^{1}H NMR ($CDCl_3$, 400 MHz)



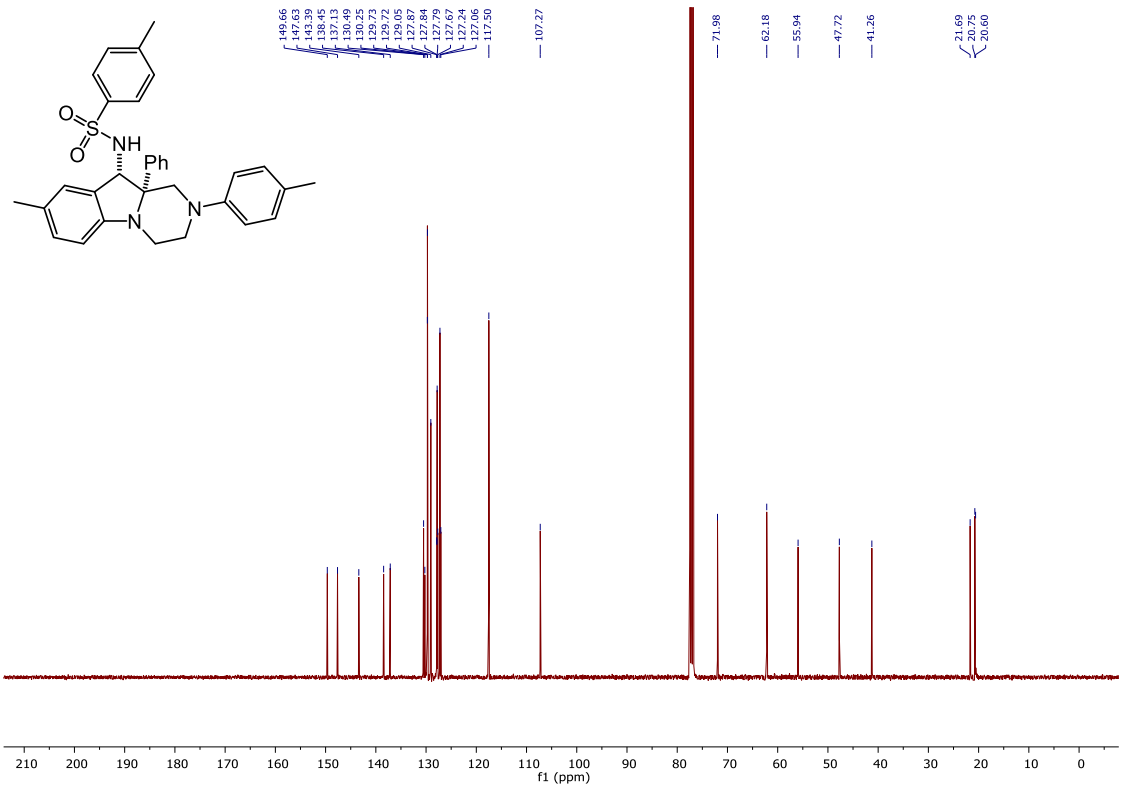
Compound 3aA'' ^{13}C NMR ($CDCl_3$, 100 MHz)



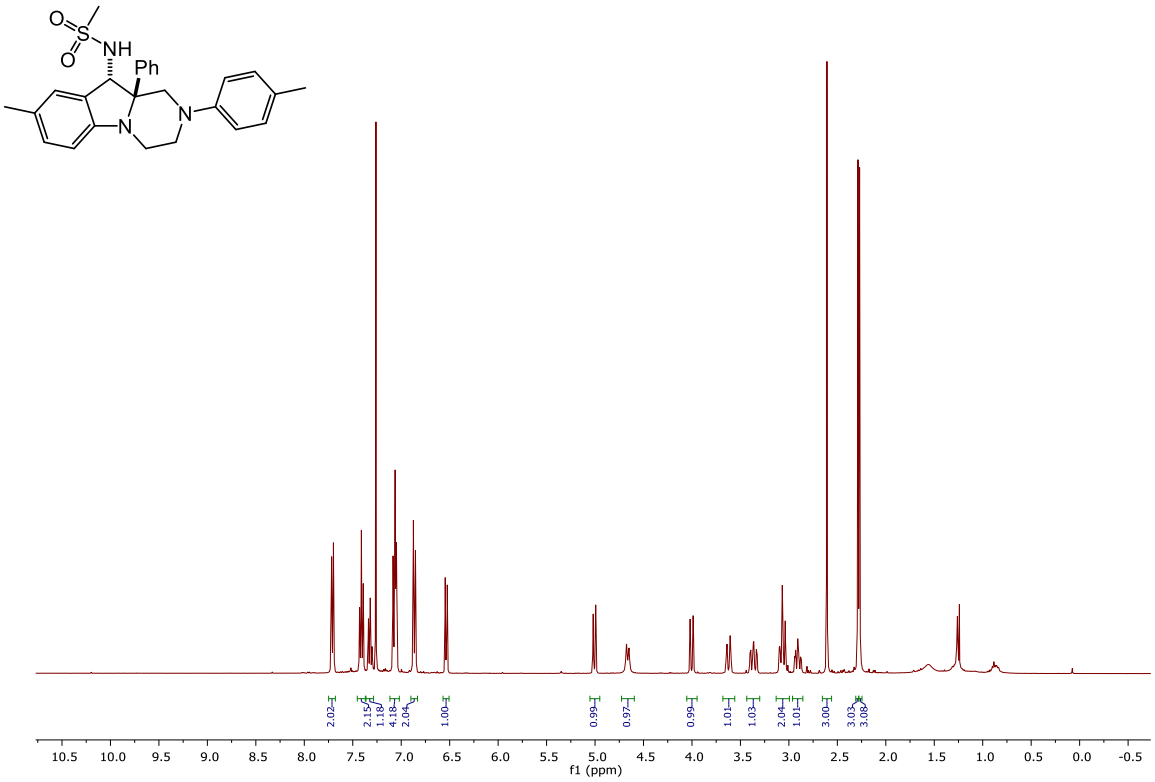
Compound 3aA' ^{1}H NMR ($CDCl_3$, 400 MHz)



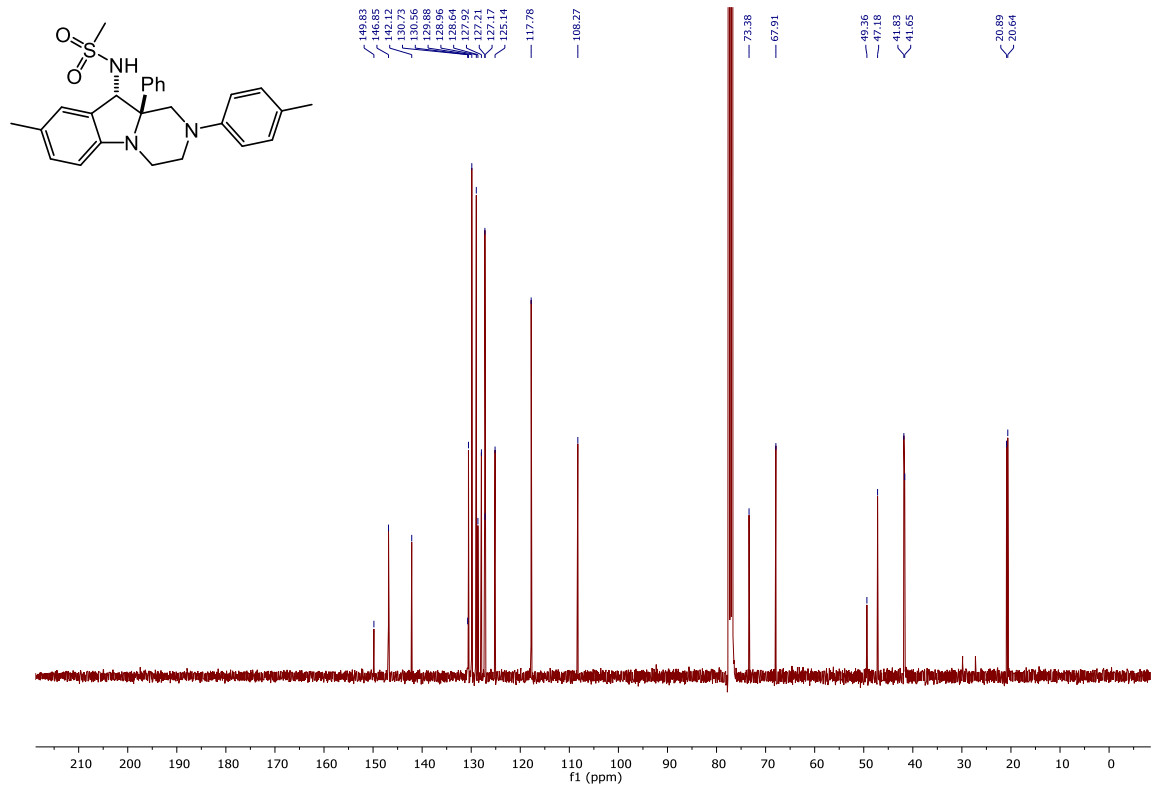
Compound 3aA' ^{13}C NMR ($CDCl_3$, 100 MHz)



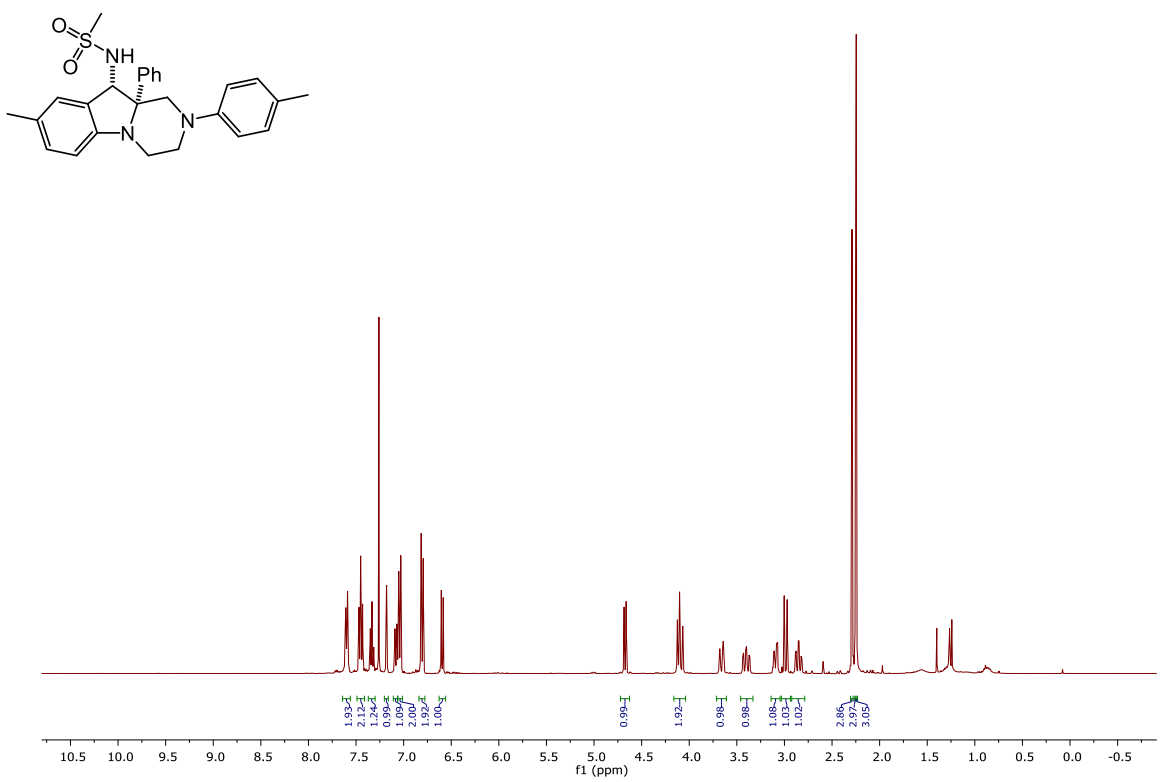
Compound 3bA'' ^{1}H NMR ($CDCl_3$, 400 MHz)



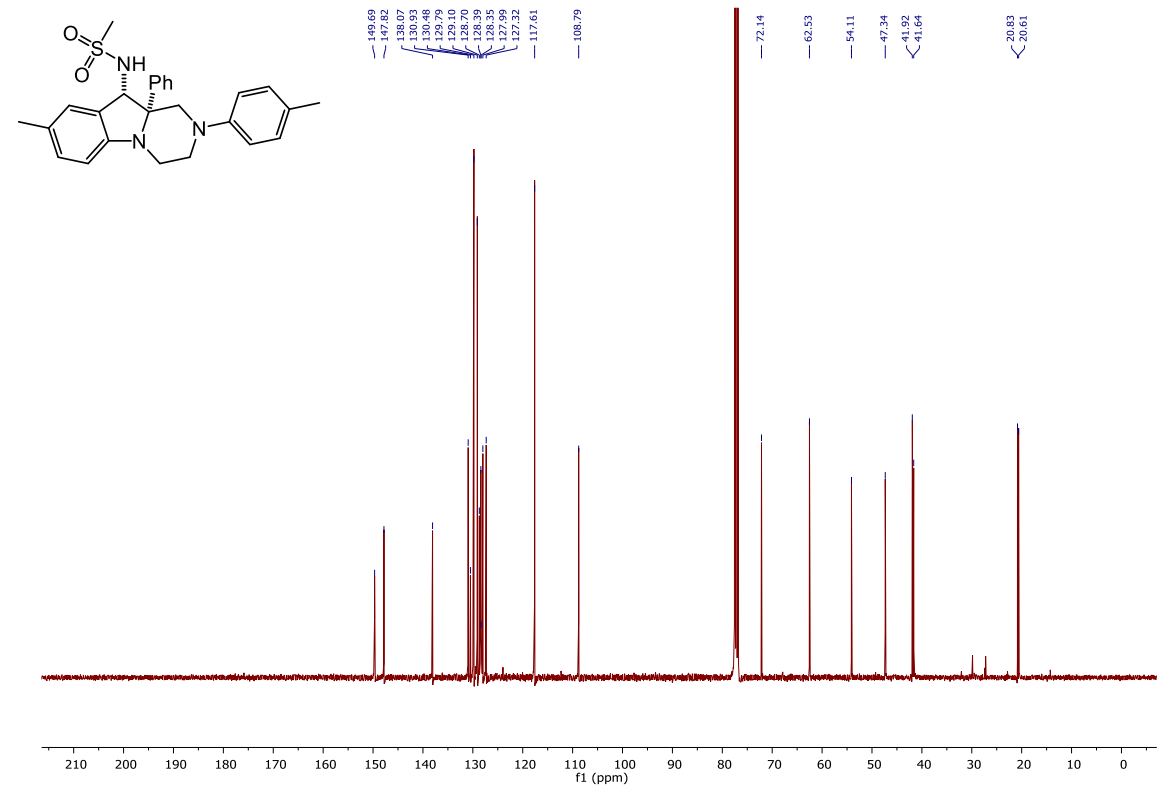
Compound 3bA'' ^{13}C NMR ($CDCl_3$, 100 MHz)



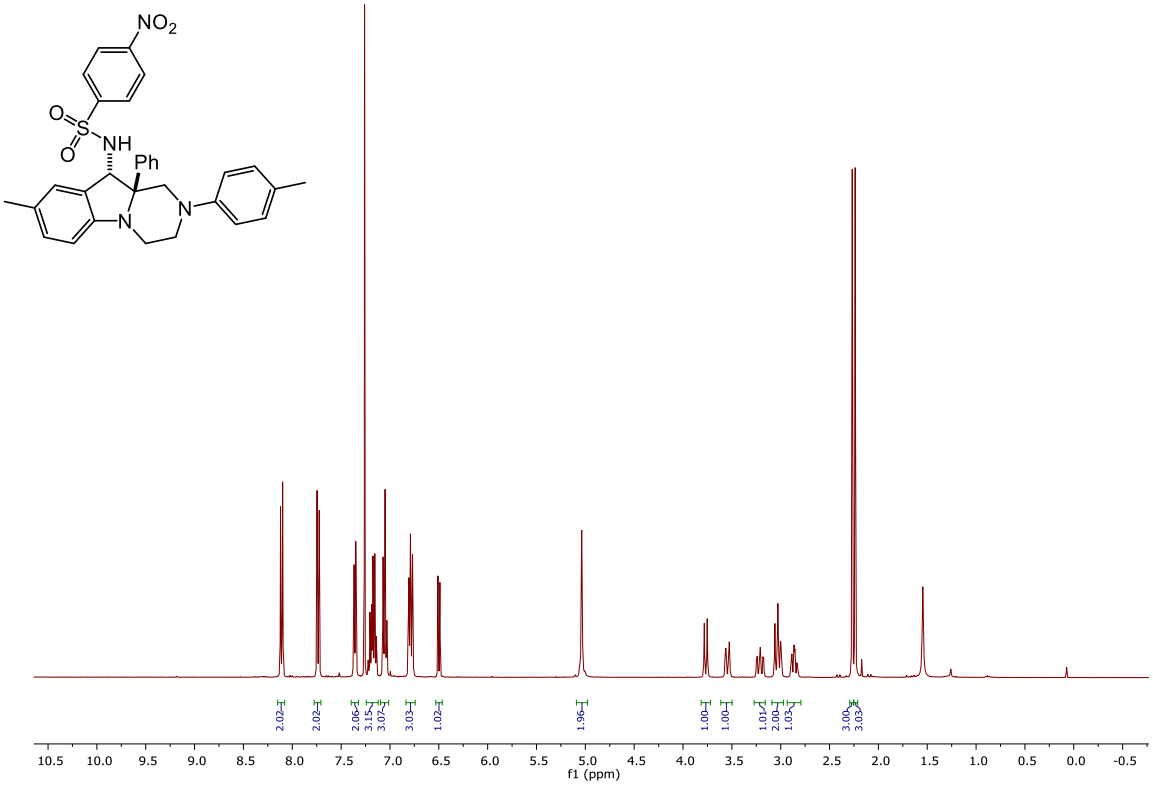
Compound 3bA' ^{1}H NMR ($CDCl_3$, 400 MHz)



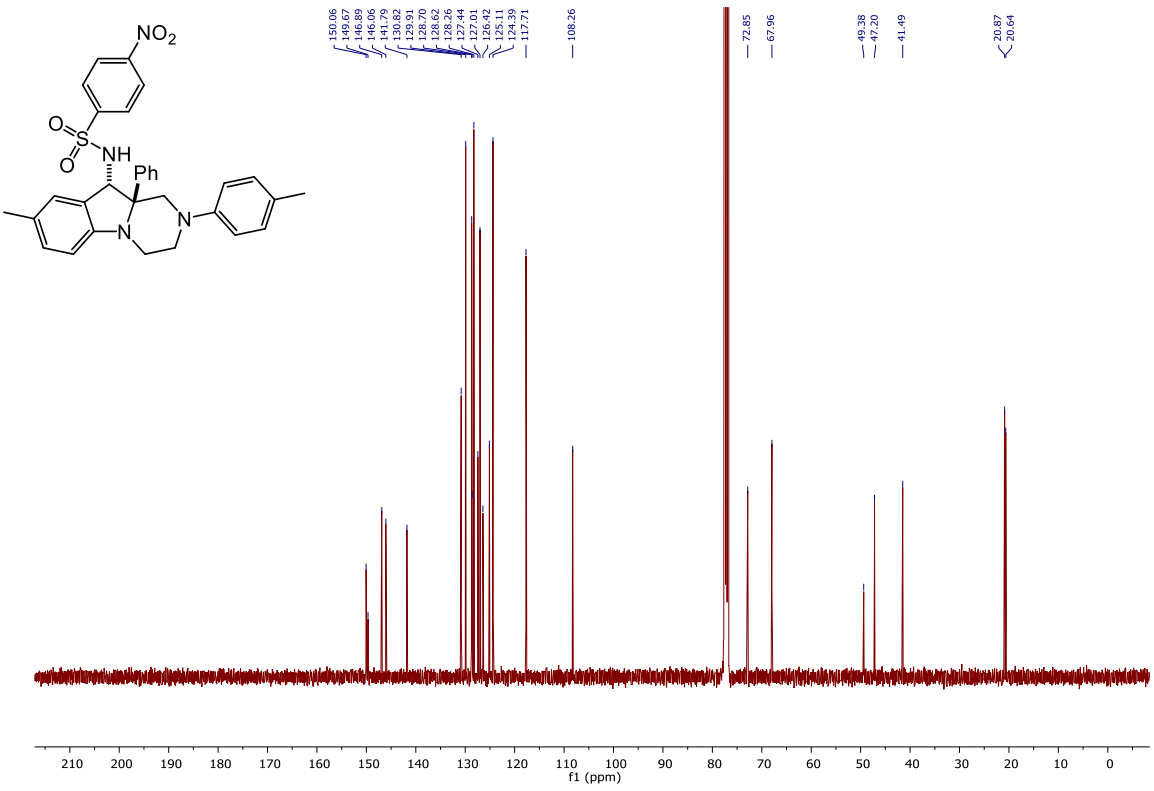
Compound 3bA' ^{13}C NMR ($CDCl_3$, 100 MHz)



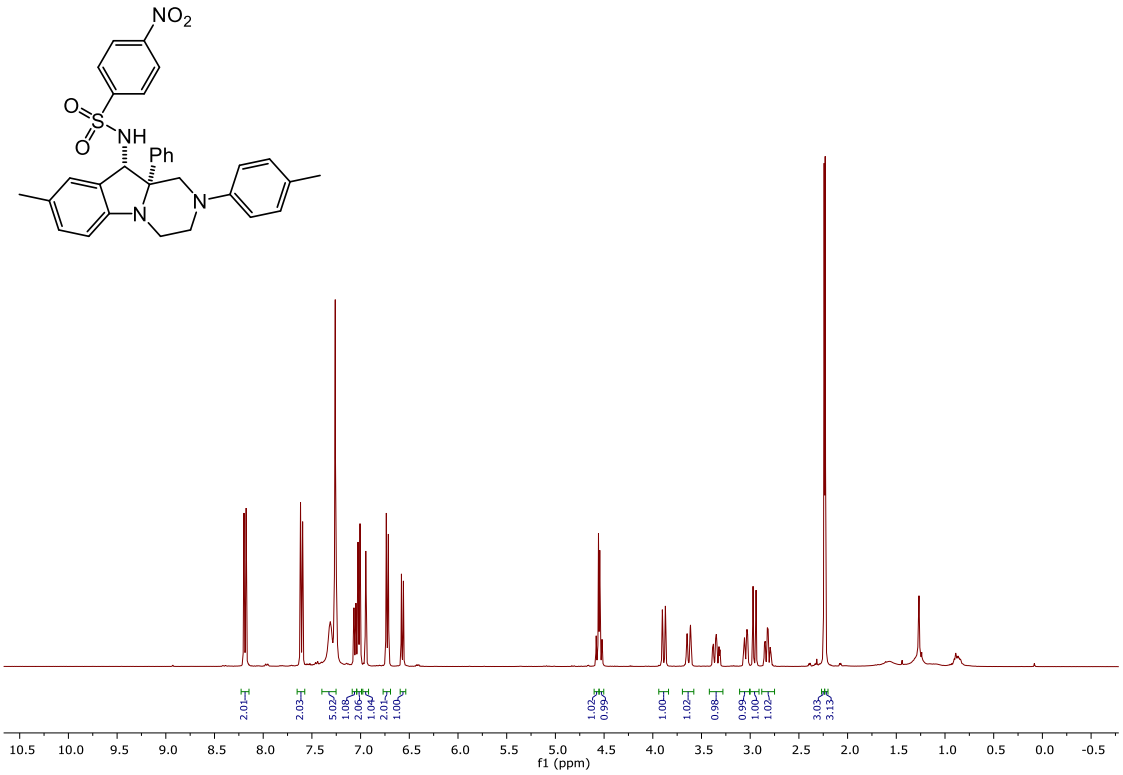
Compound 3cA'' ^{1}H NMR ($CDCl_3$, 400 MHz)



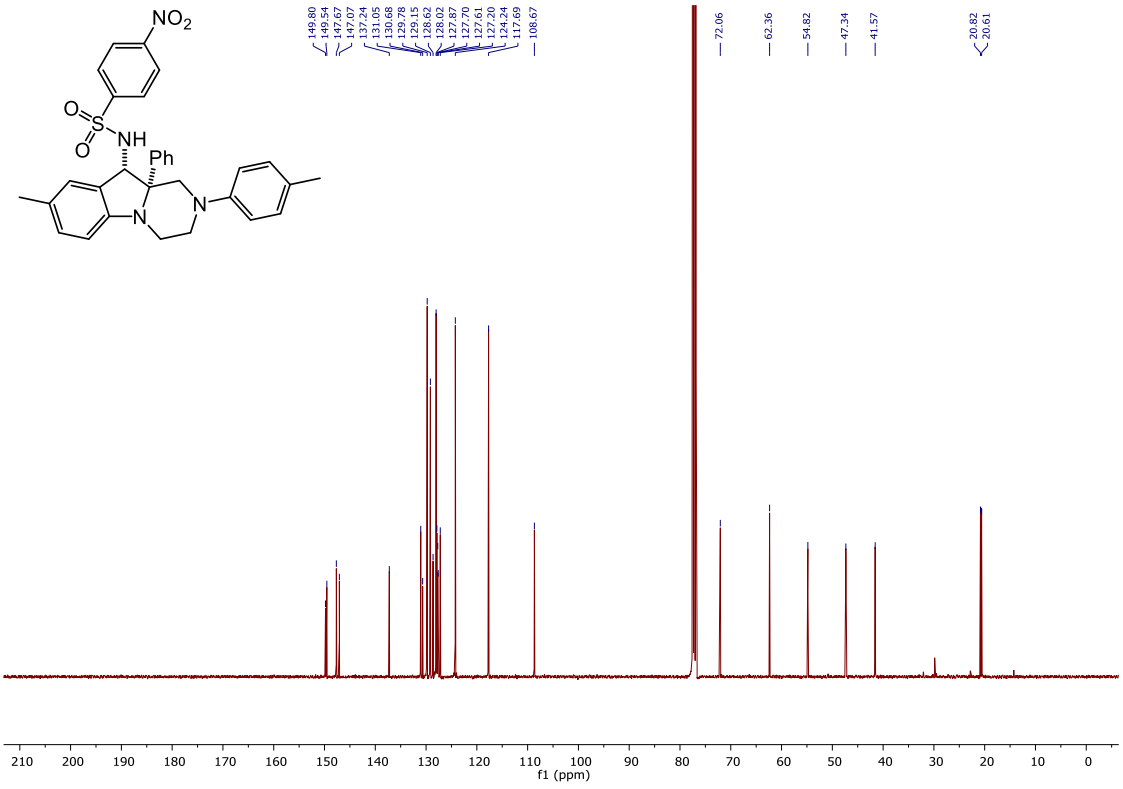
Compound 3cA'' ^{13}C NMR ($CDCl_3$, 100 MHz)



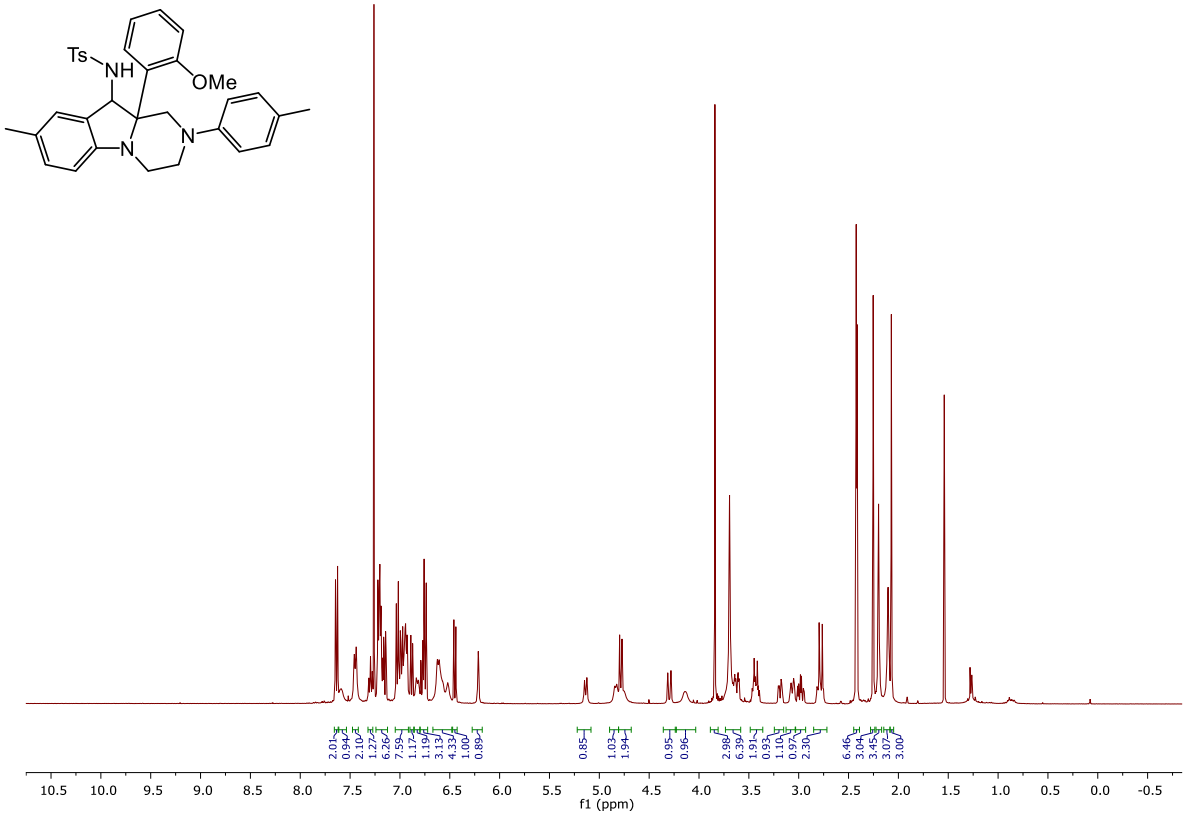
Compound 3cA' ^{1}H NMR ($CDCl_3$, 400 MHz)



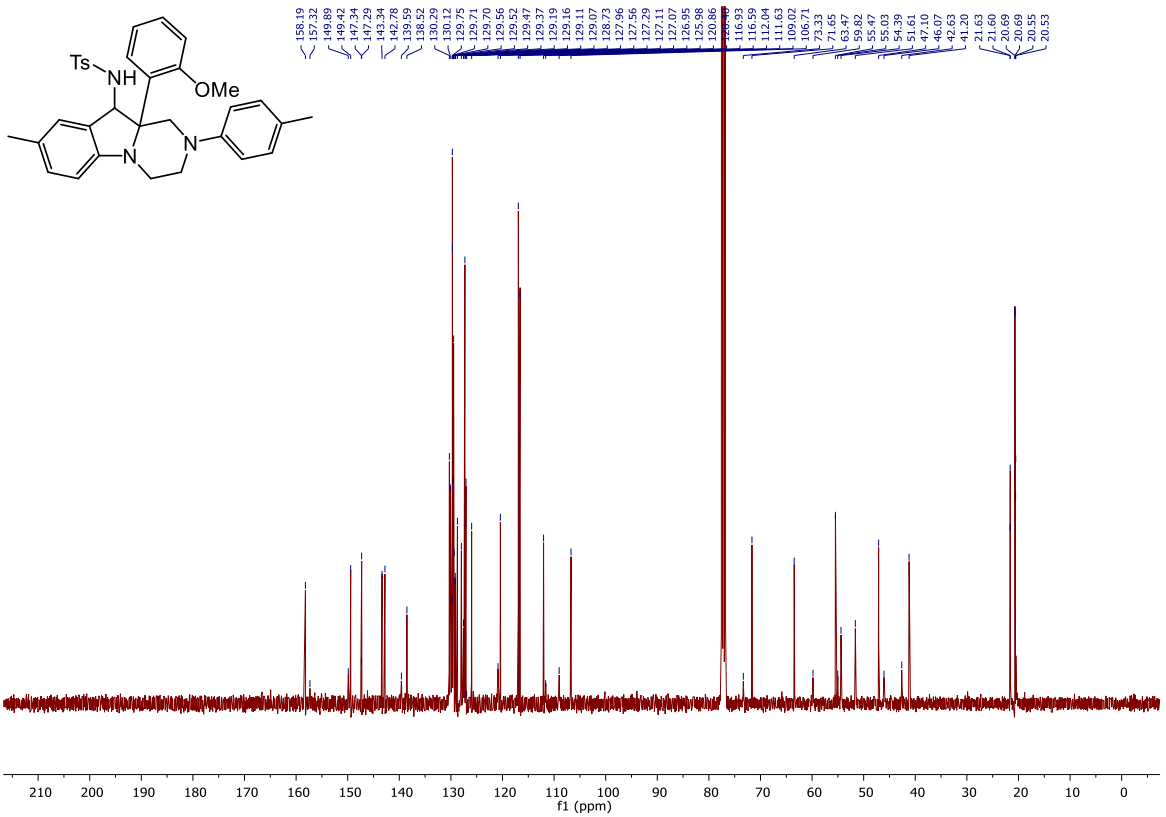
Compound 3cA' ^{13}C NMR ($CDCl_3$, 100 MHz)



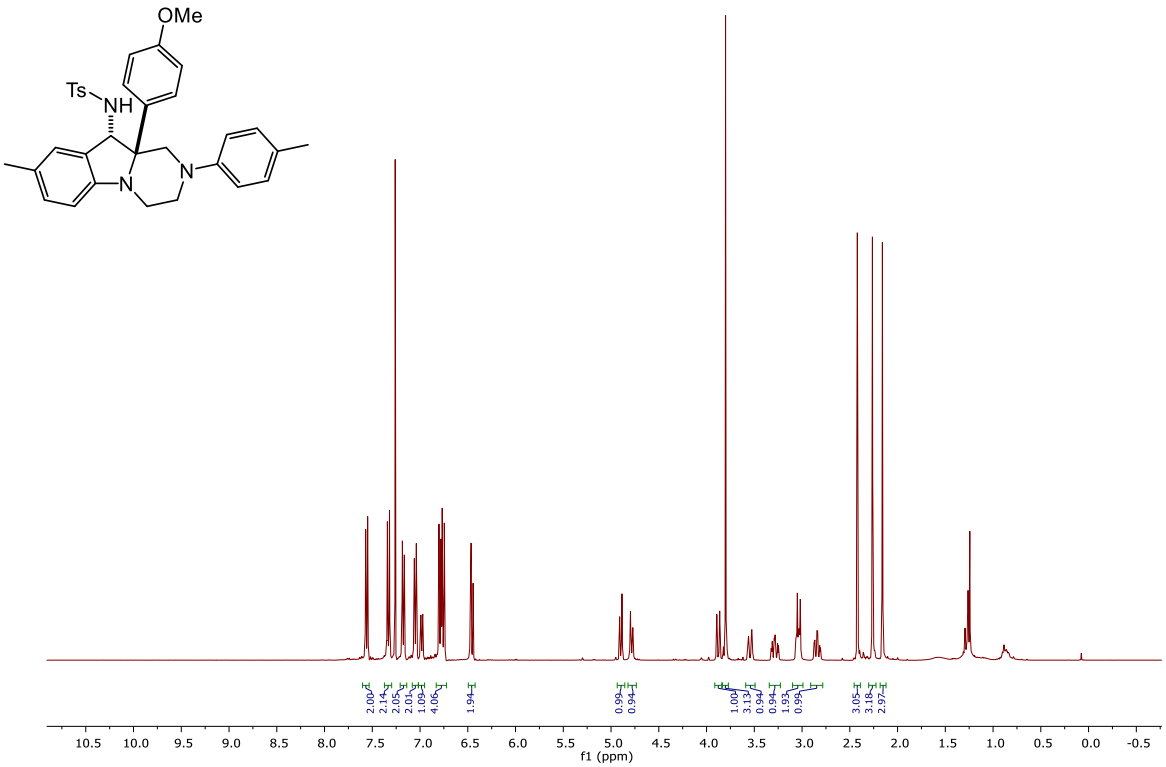
Compound 3dA ^{1}H NMR ($CDCl_3$, 400 MHz)



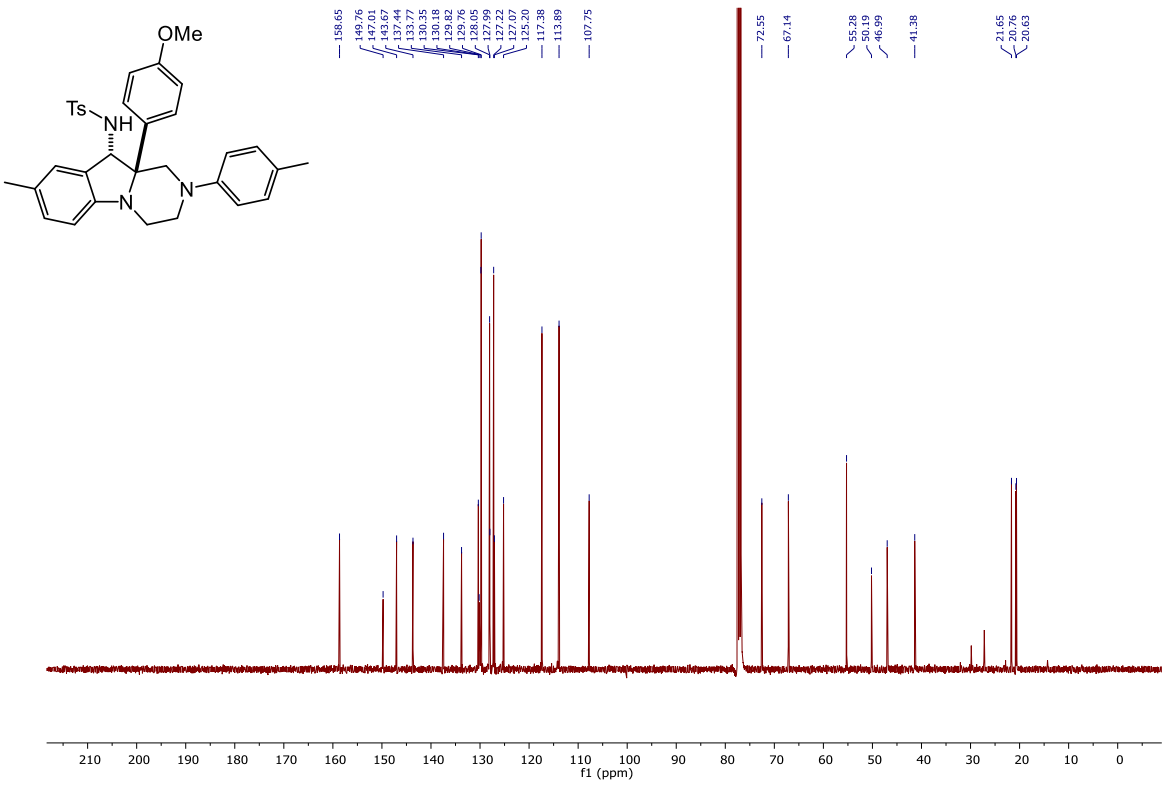
Compound 3dA ^{13}C NMR ($CDCl_3$, 100 MHz)



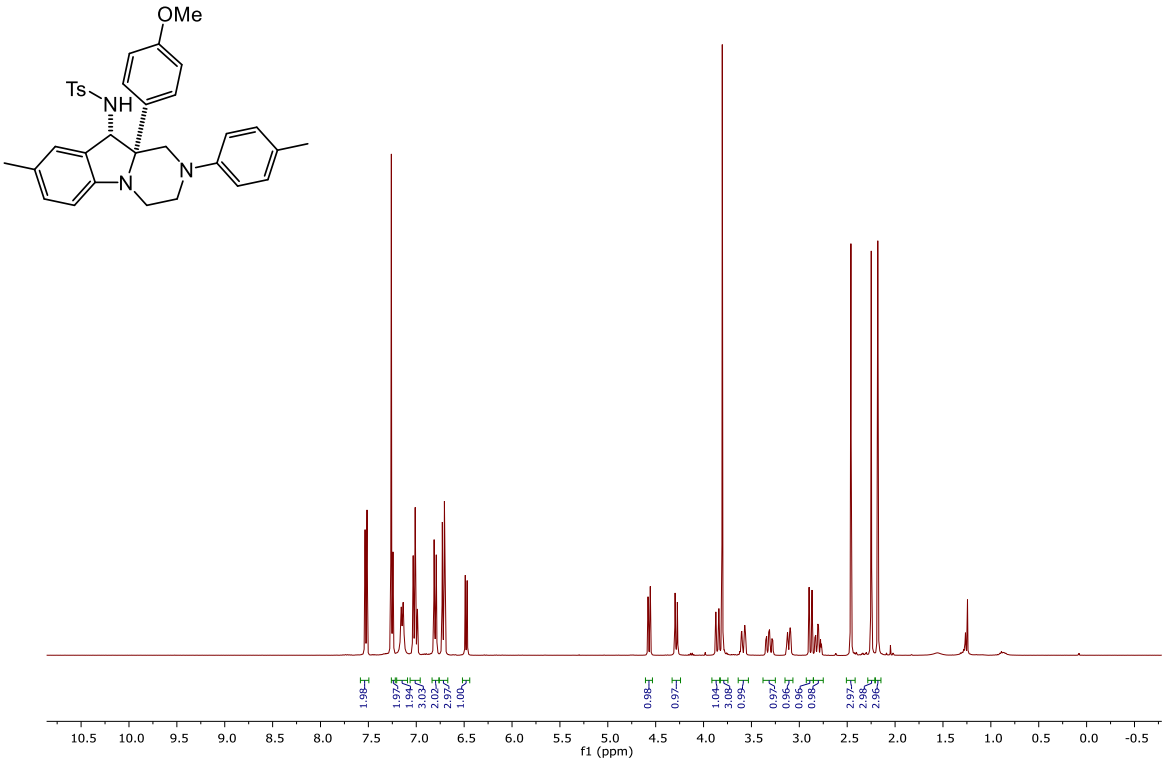
Compound 3eA'' ^{1}H NMR ($CDCl_3$, 400 MHz)



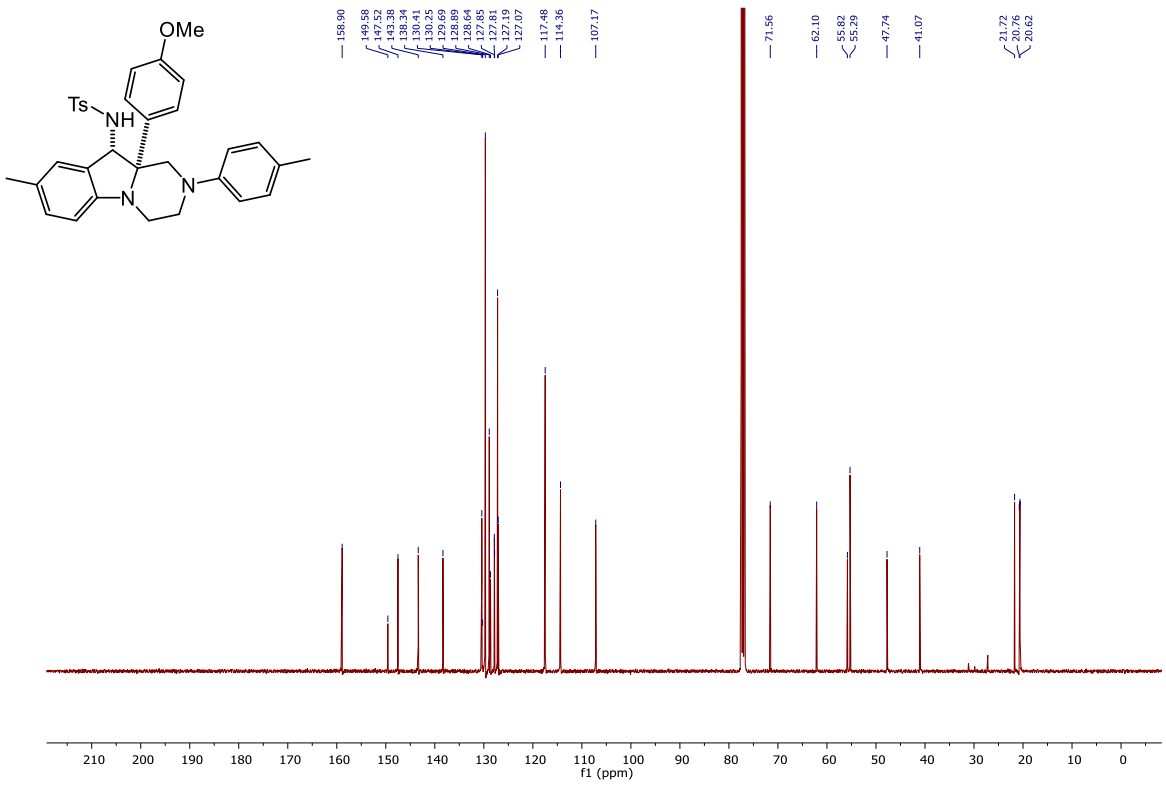
Compound 3eA'' ^{13}C NMR ($CDCl_3$, 100 MHz)



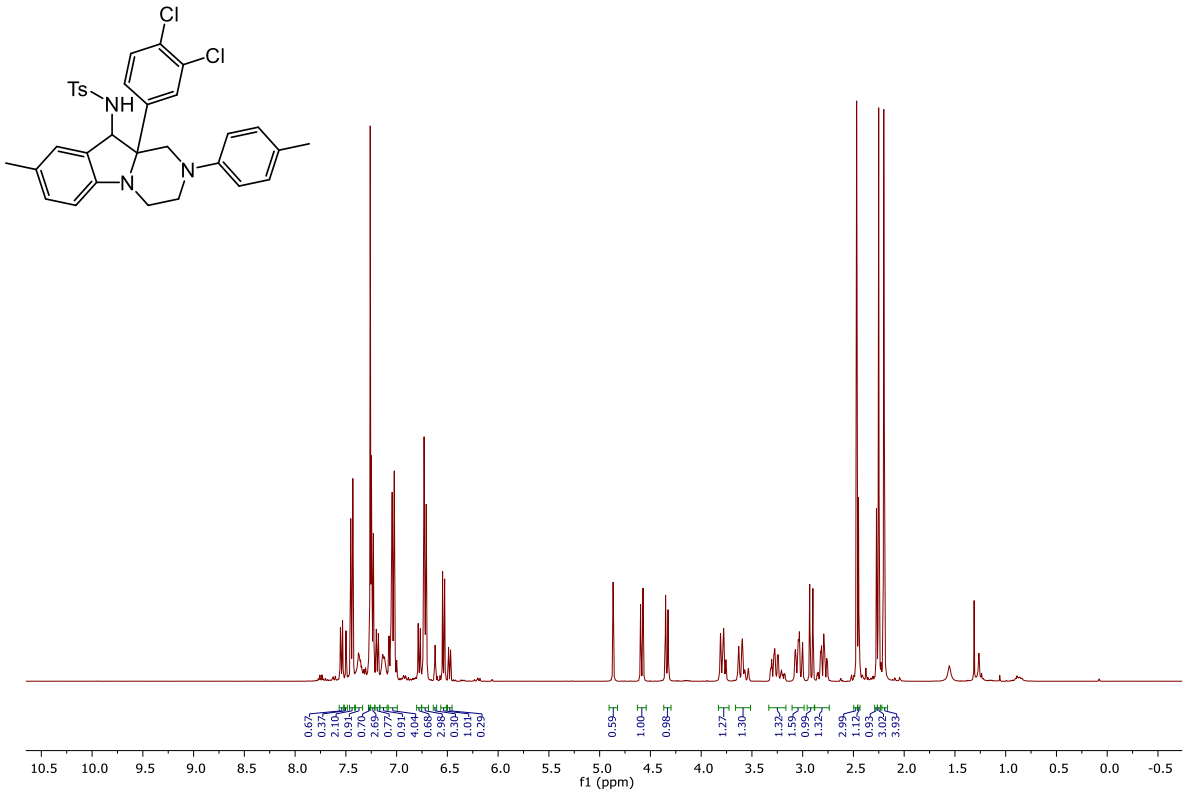
Compound 3eA' ^{1}H NMR ($CDCl_3$, 400 MHz)



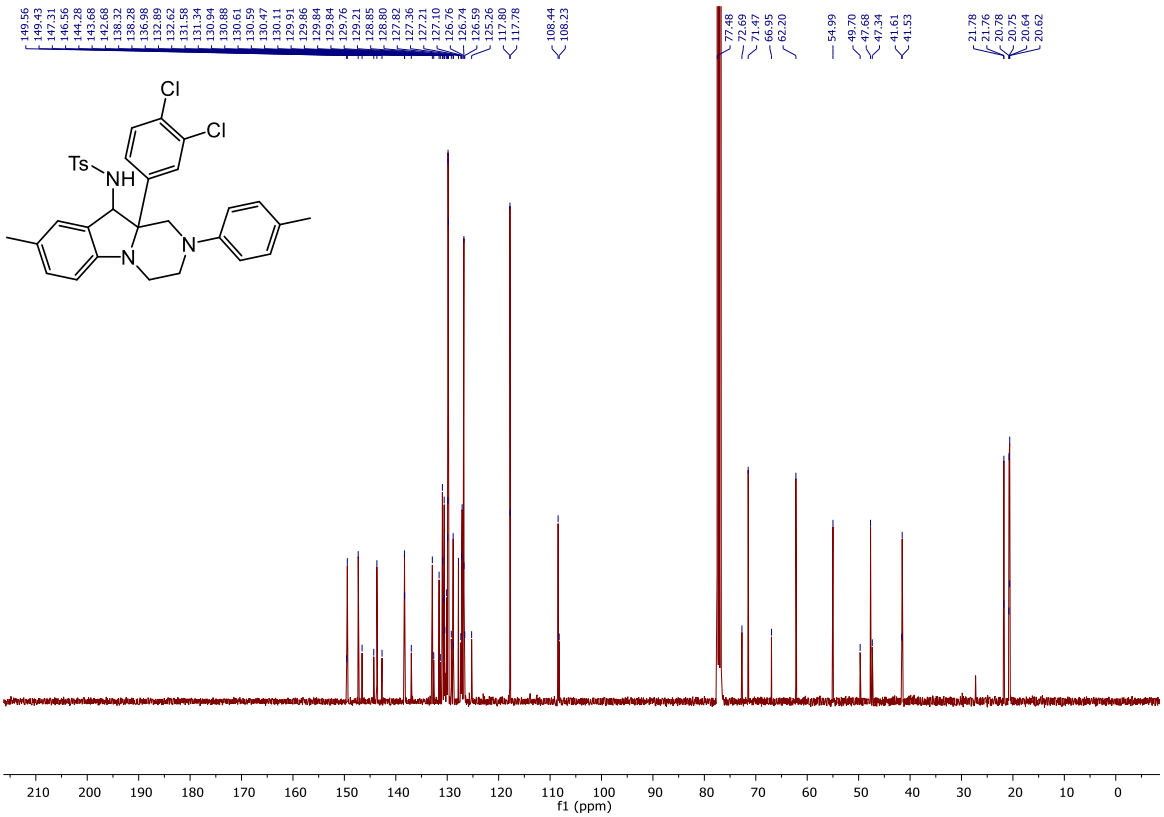
Compound 3eA' ^{13}C NMR ($CDCl_3$, 100 MHz)



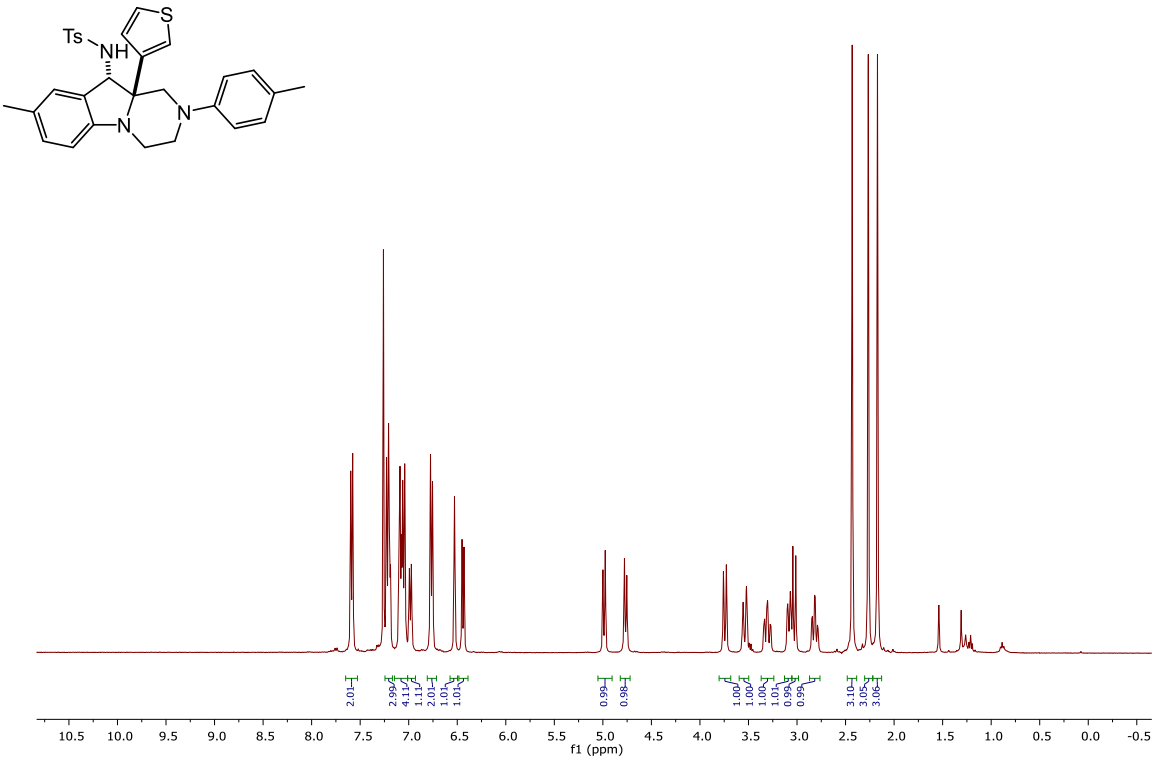
Compound 3fA ^{1}H NMR ($CDCl_3$, 400 MHz)



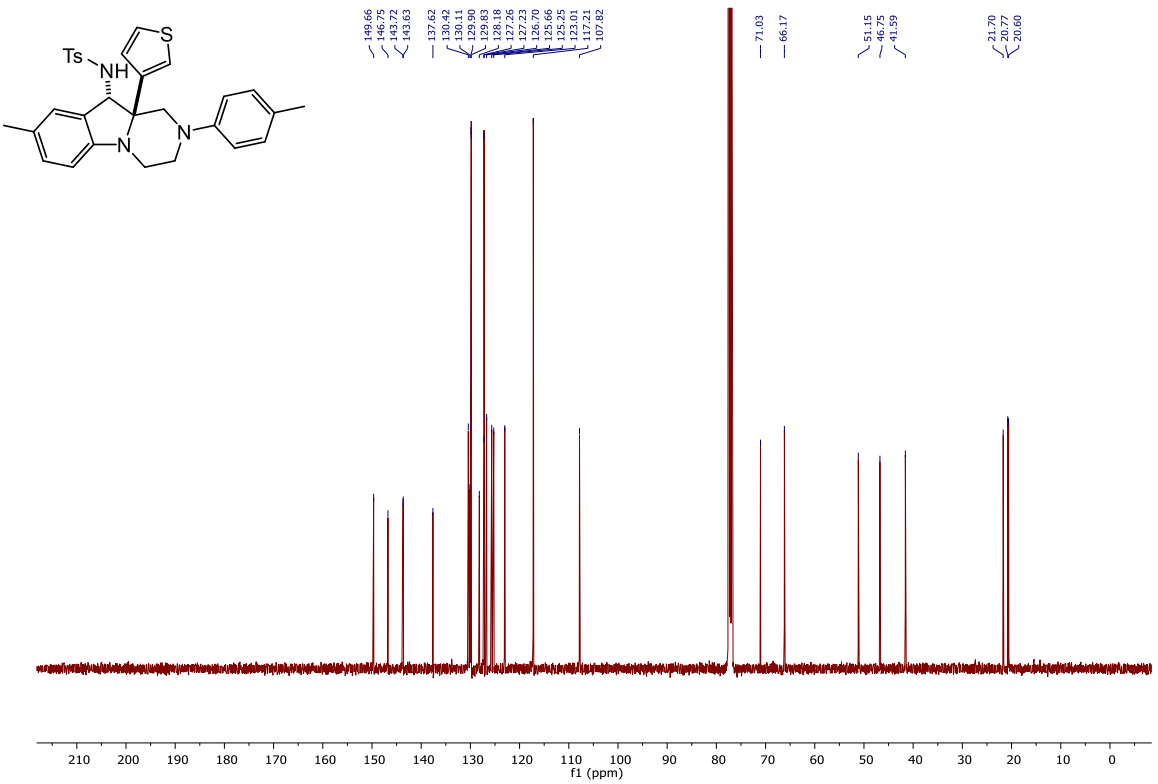
Compound 3fA ^{13}C NMR ($CDCl_3$, 100 MHz)



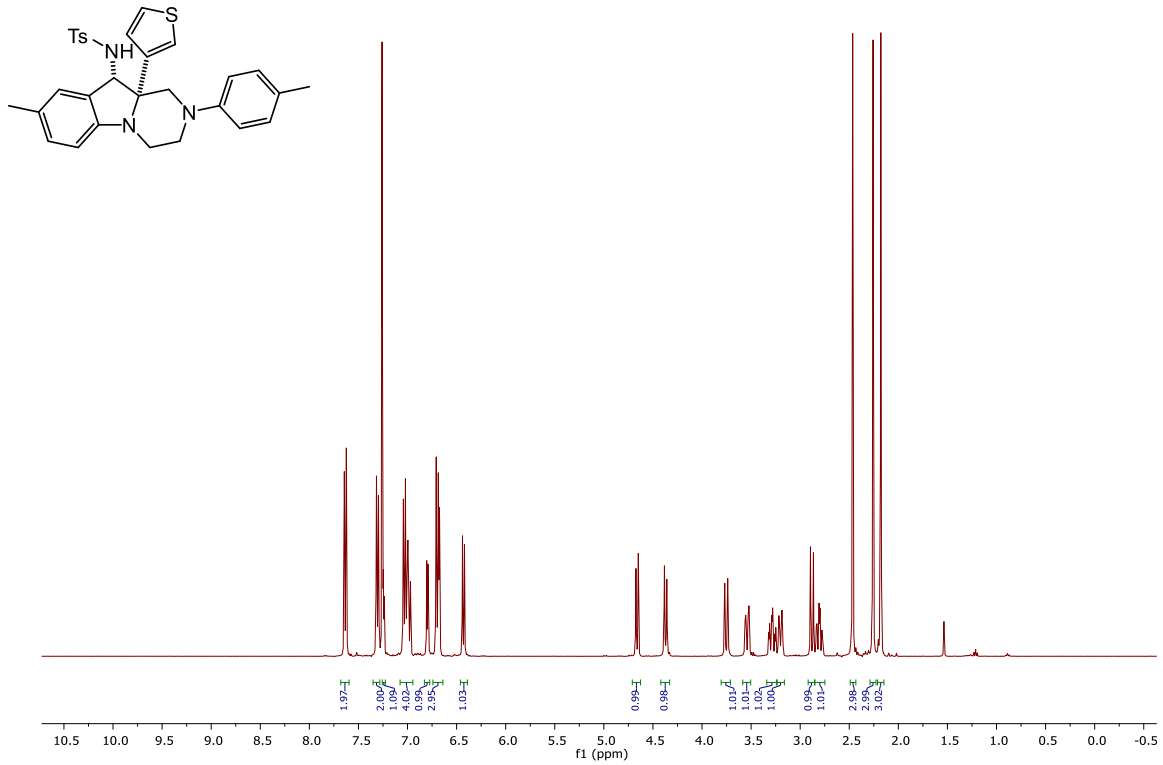
Compound 3gA'' ^{1}H NMR ($CDCl_3$, 400 MHz)



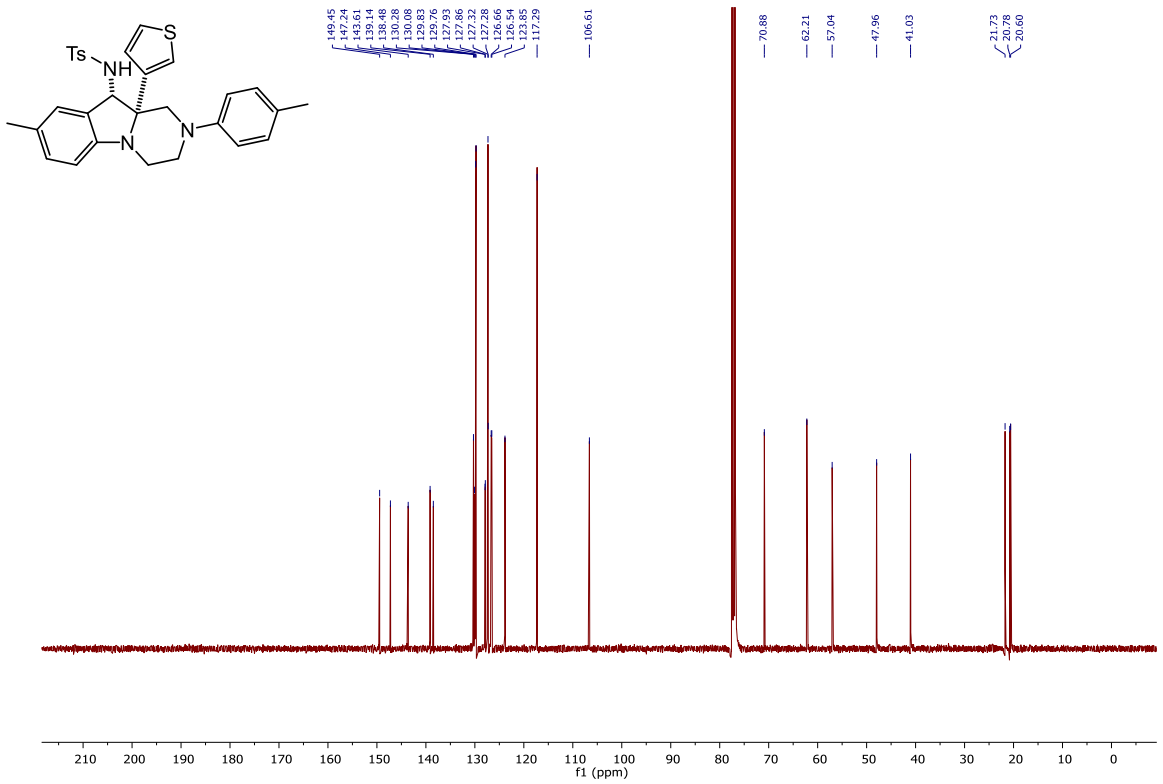
Compound 3gA'' ^{13}C NMR ($CDCl_3$, 100 MHz)



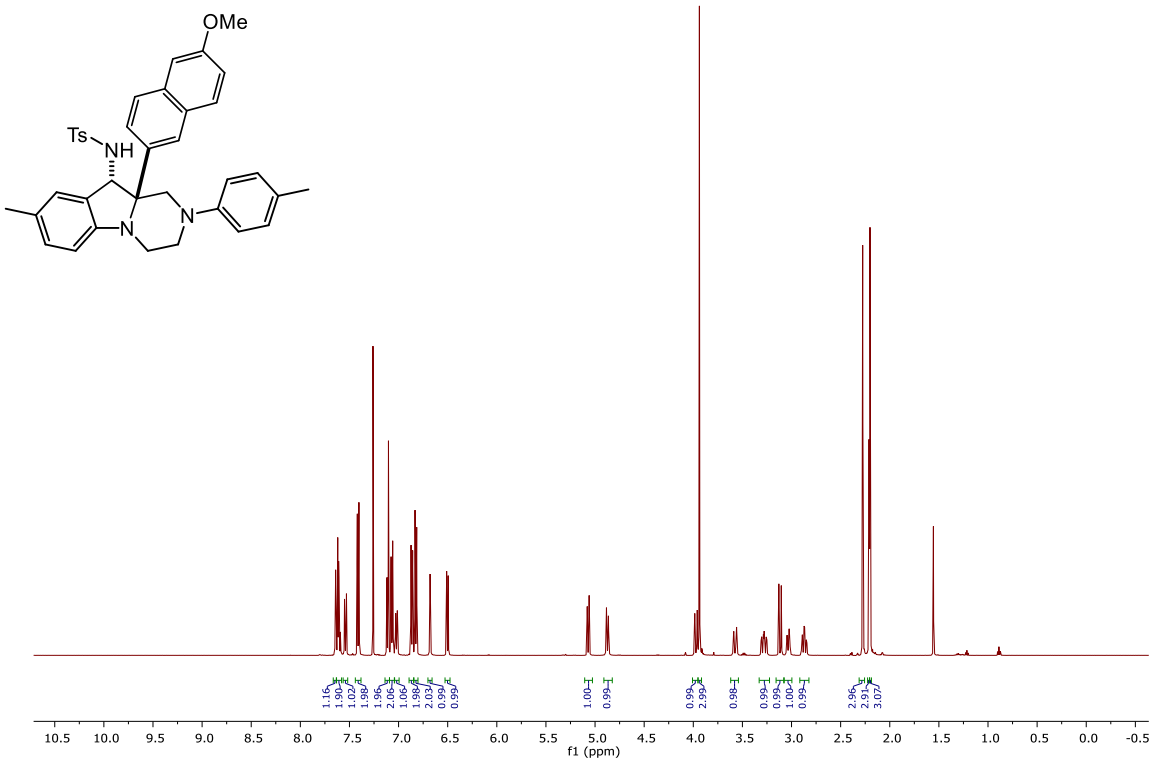
Compound 3gA' ^{1}H NMR ($CDCl_3$, 400 MHz)



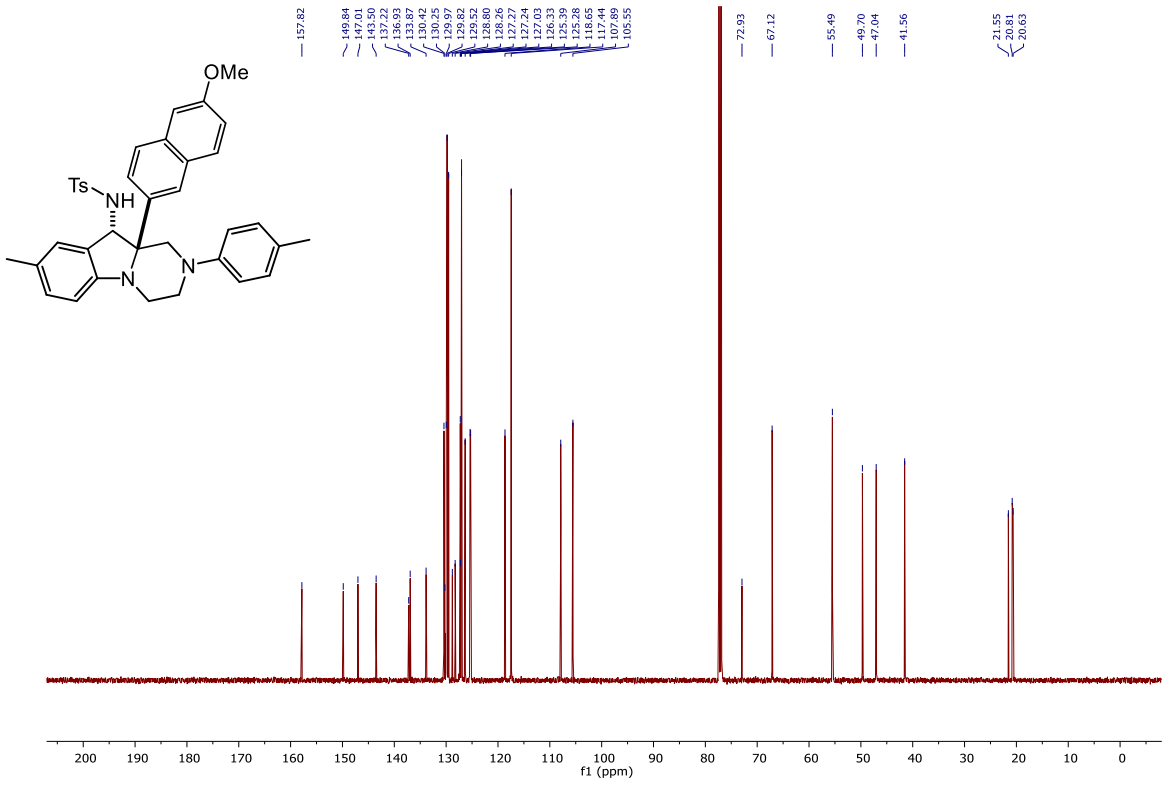
Compound 3gA' ^{13}C NMR ($CDCl_3$, 100 MHz)



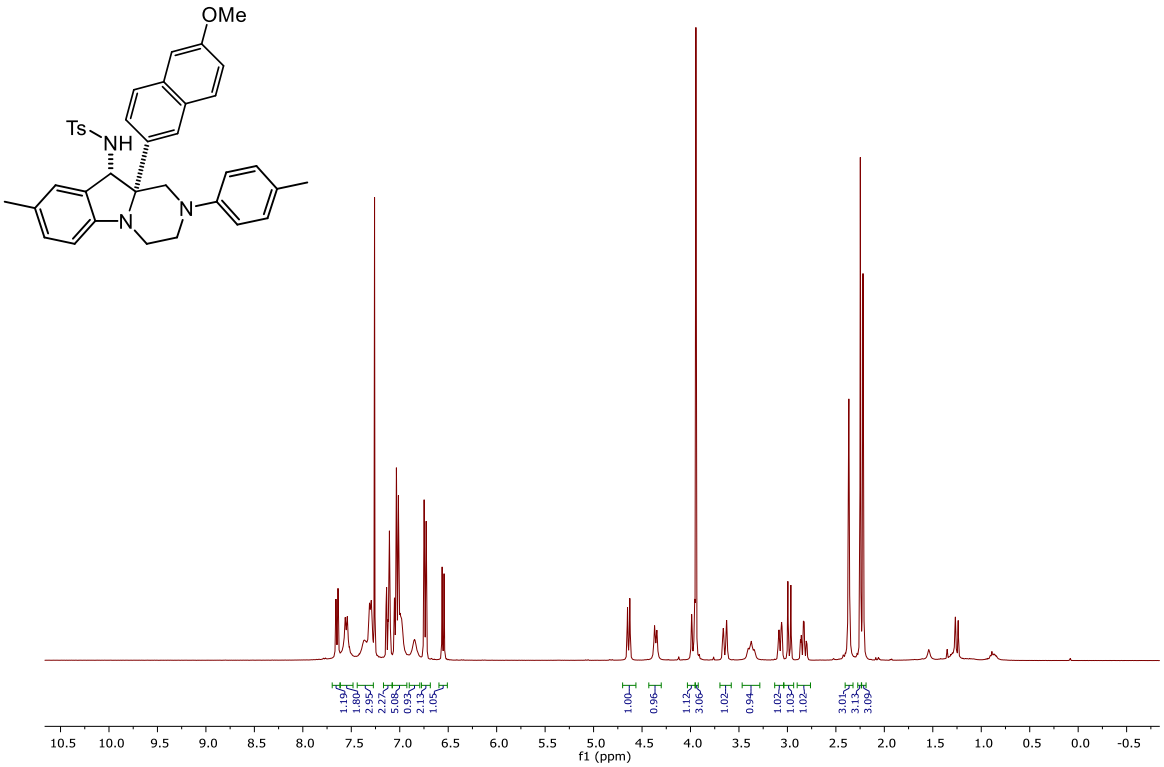
Compound 3hA'' ^{1}H NMR ($CDCl_3$, 500 MHz)



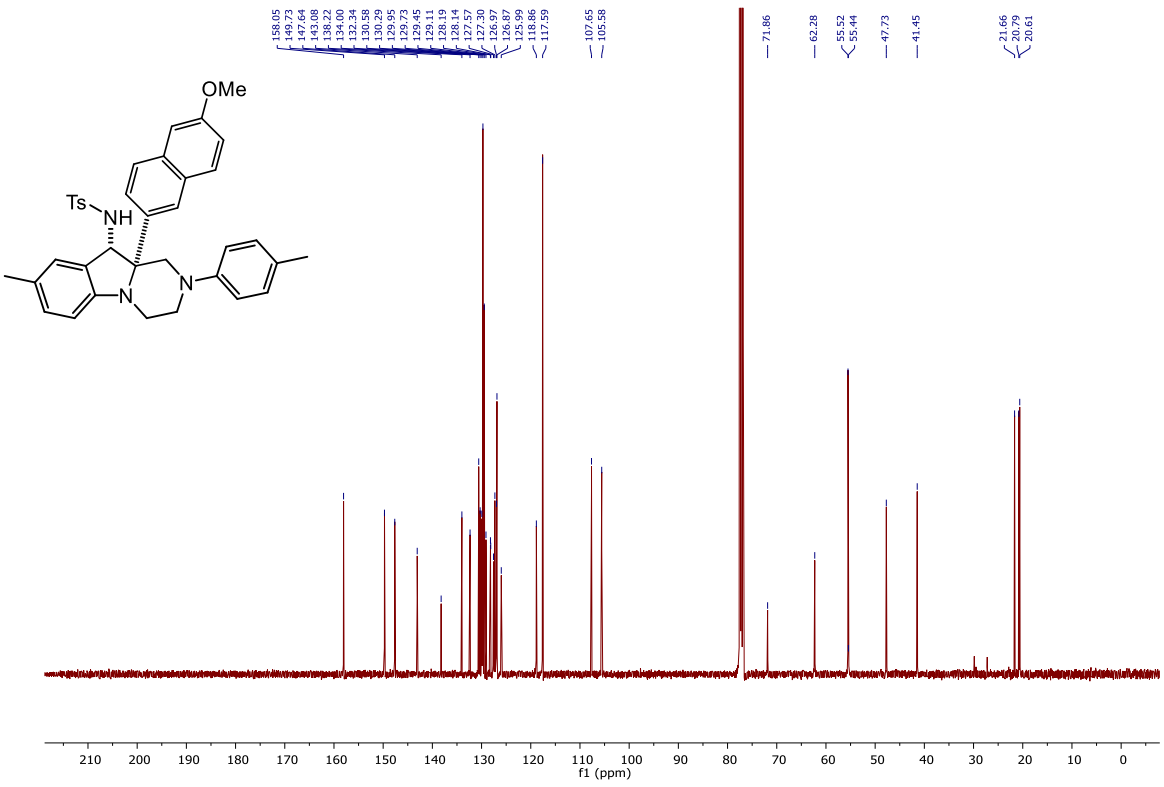
Compound 3hA'' ^{13}C NMR ($CDCl_3$, 126 MHz)



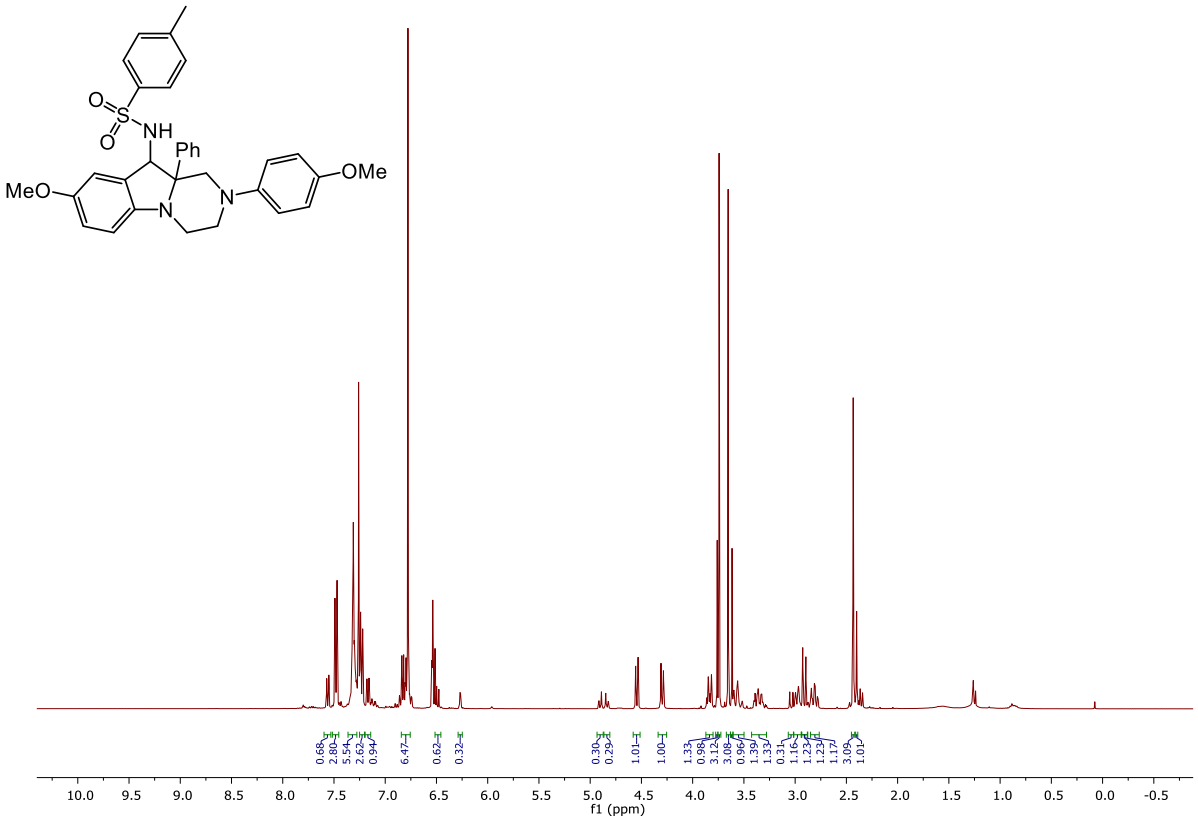
Compound 3hA' ^{1}H NMR ($CDCl_3$, 400 MHz)



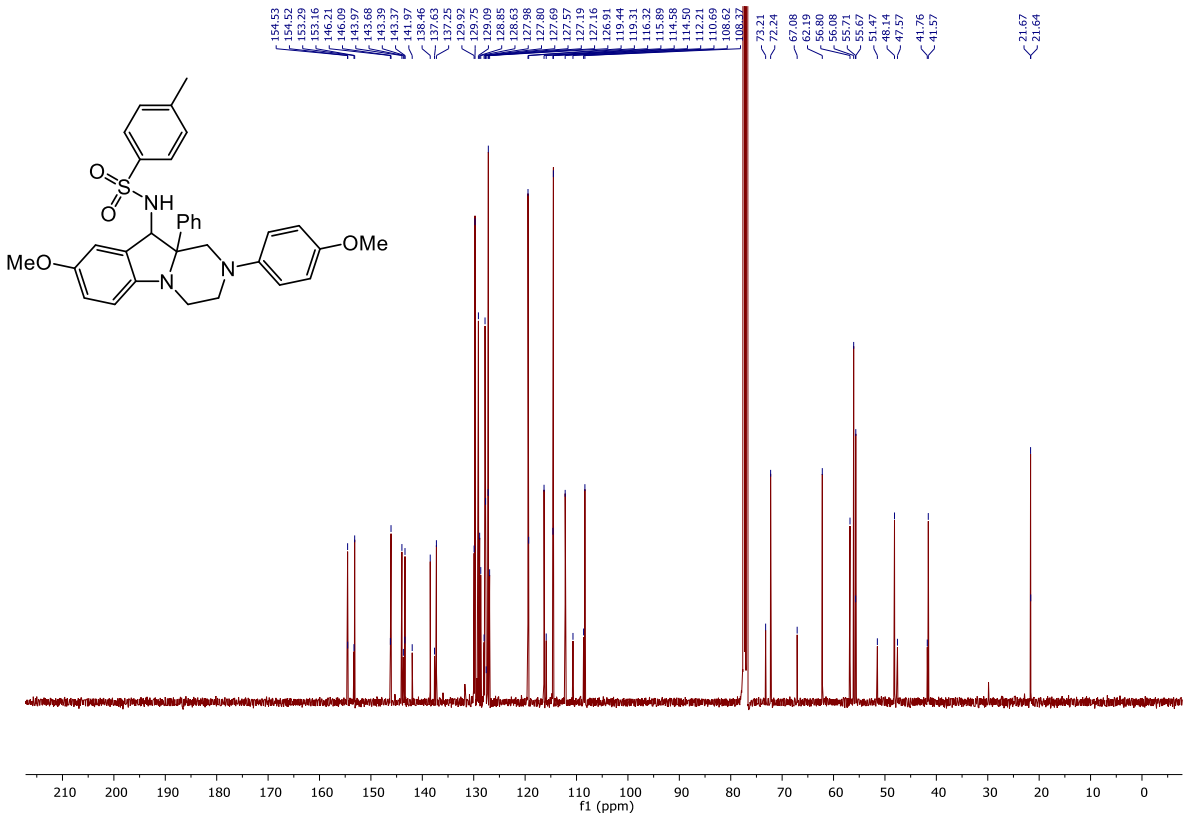
Compound 3hA' ^{13}C NMR ($CDCl_3$, 100 MHz)



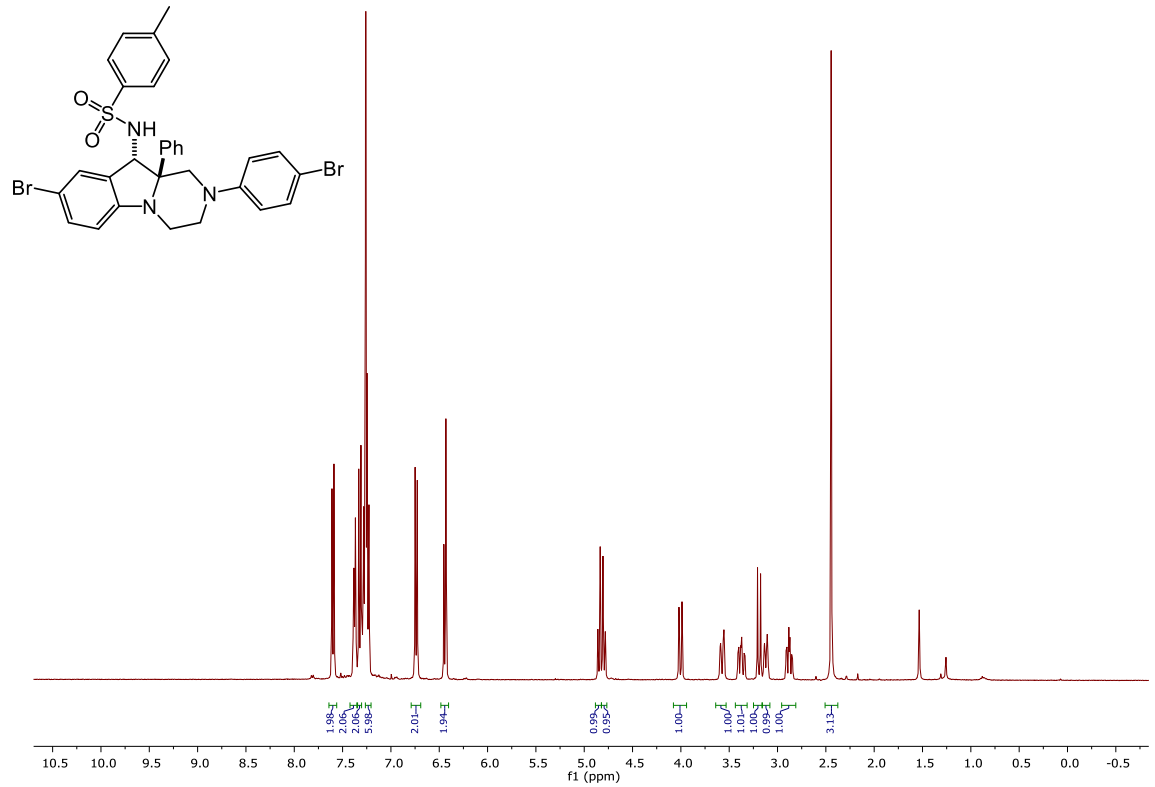
Compound 3aB ^{1}H NMR ($CDCl_3$, 400 MHz)



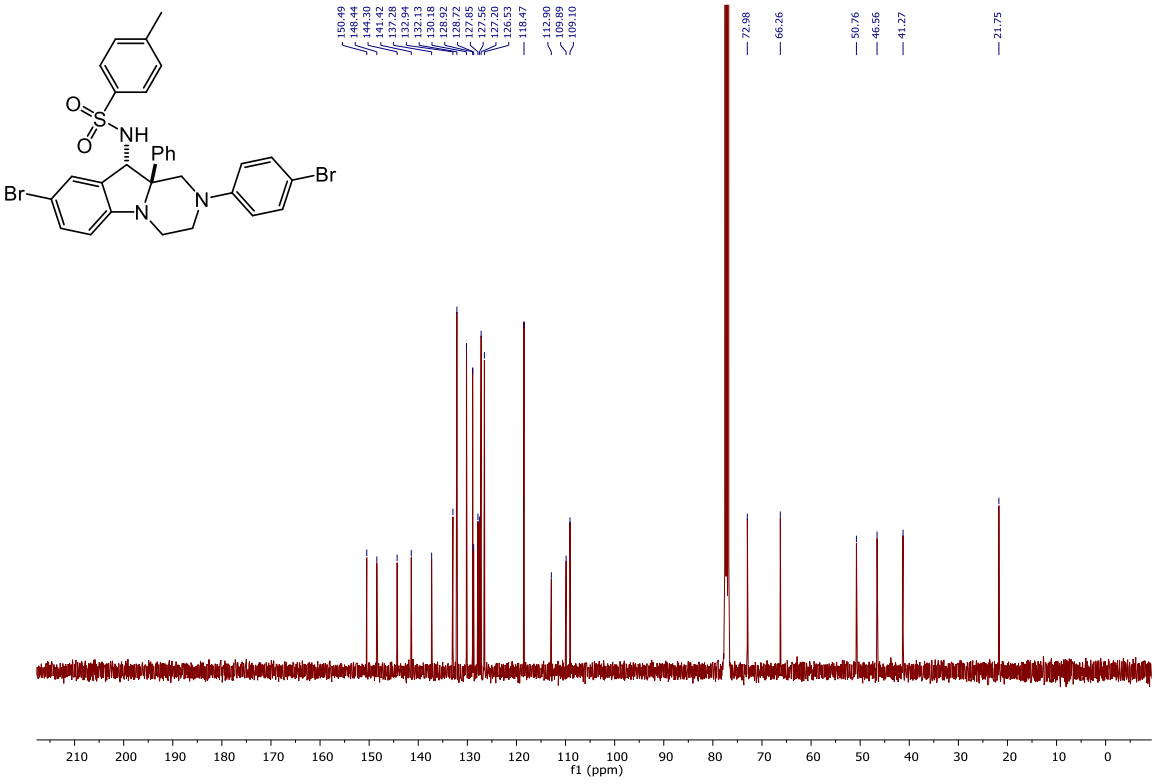
Compound 3aB ^{13}C NMR ($CDCl_3$, 100 MHz)



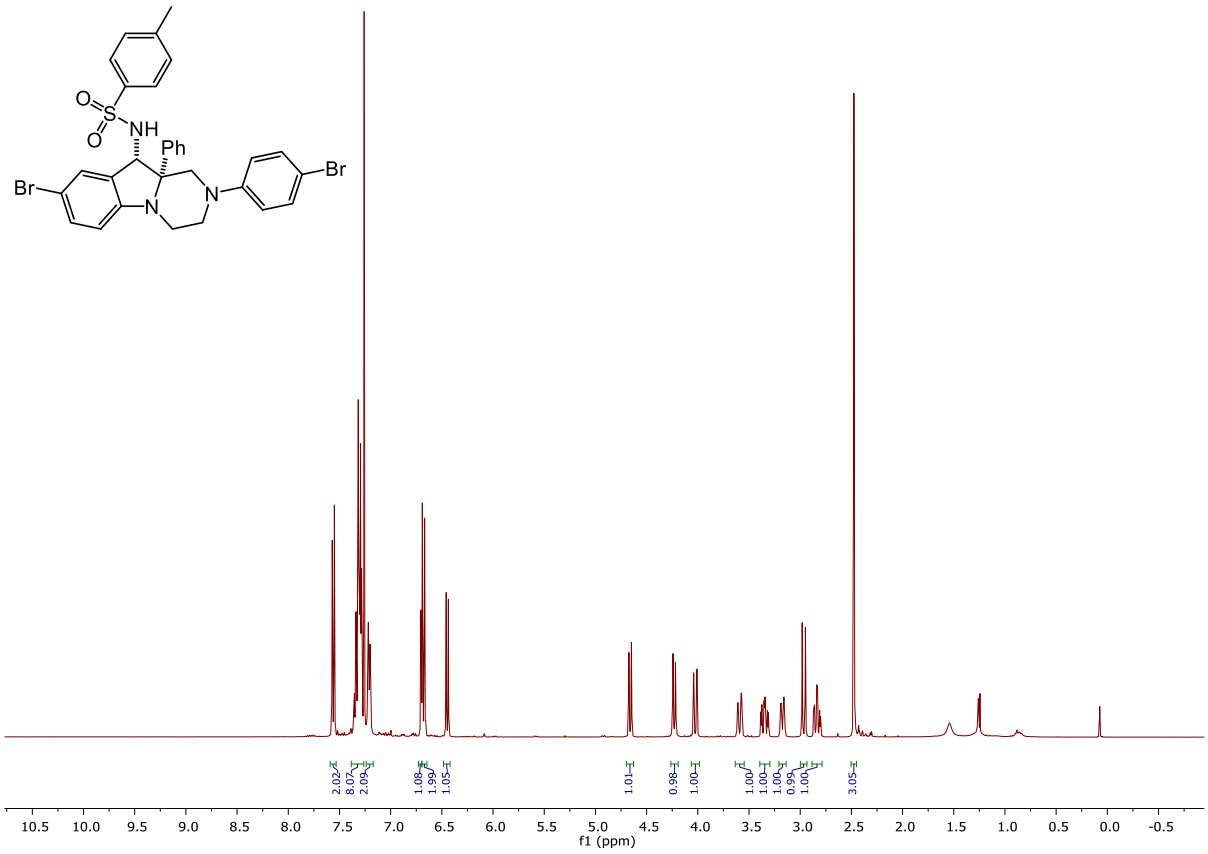
Compound 3aC'' ^{1}H NMR ($CDCl_3$, 400 MHz)



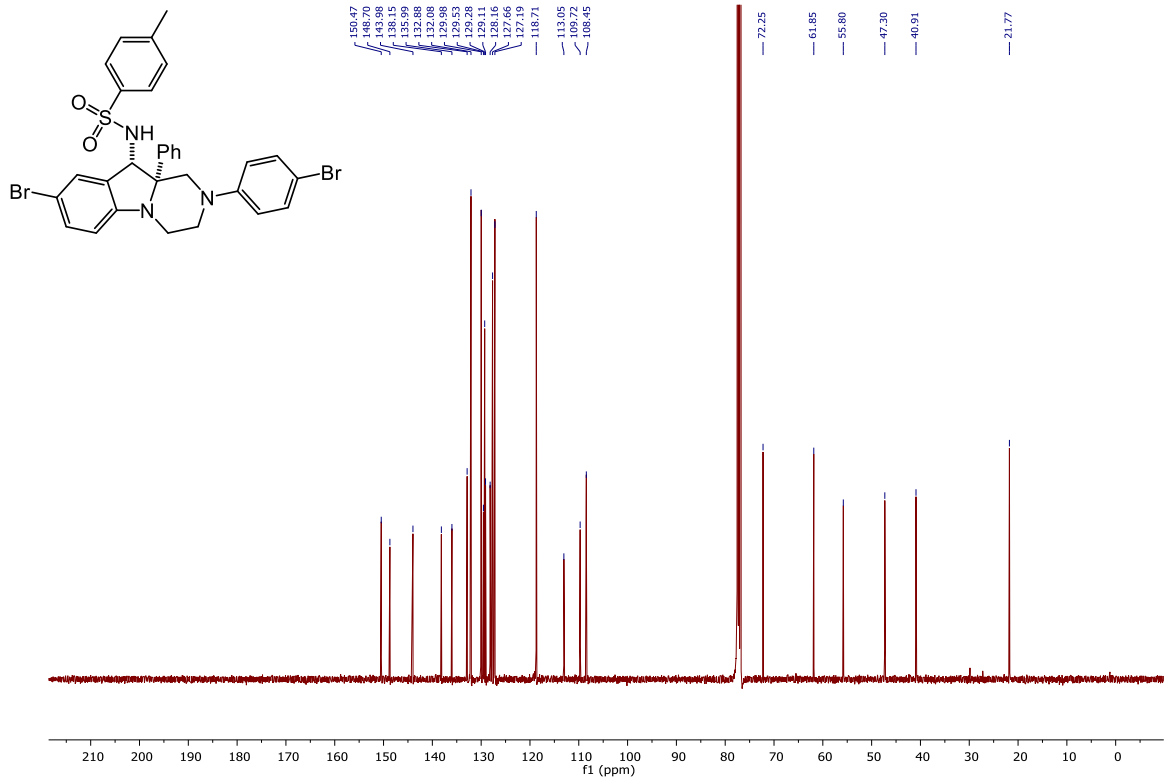
Compound 3aC'' ^{13}C NMR ($CDCl_3$, 100 MHz)



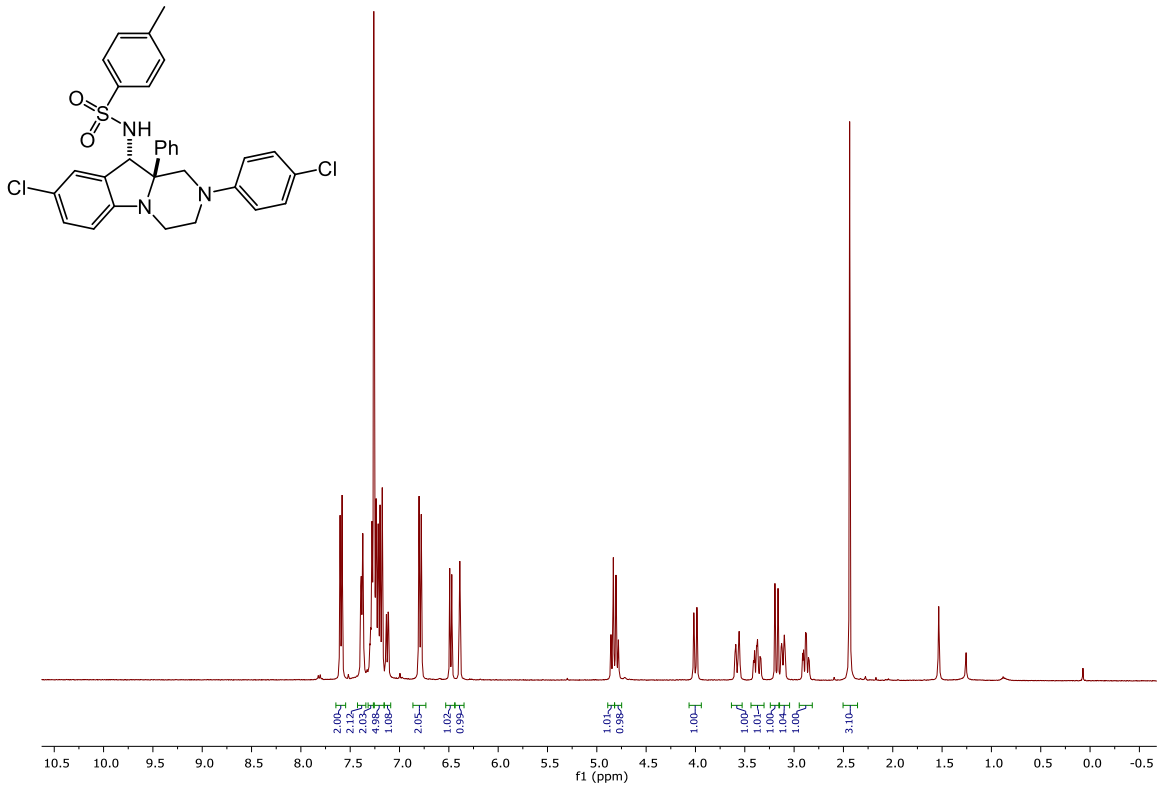
Compound 3aC' ^{1}H NMR ($CDCl_3$, 400 MHz)



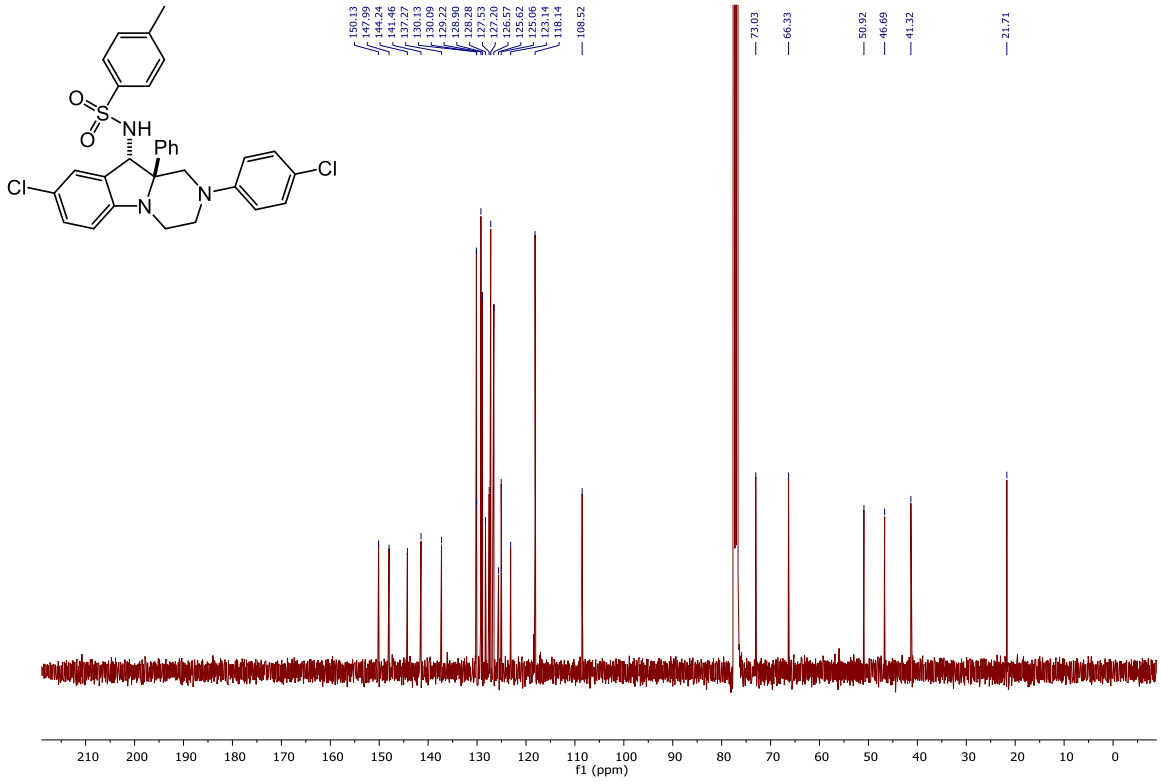
Compound 3aC' ^{13}C NMR ($CDCl_3$, 100 MHz)



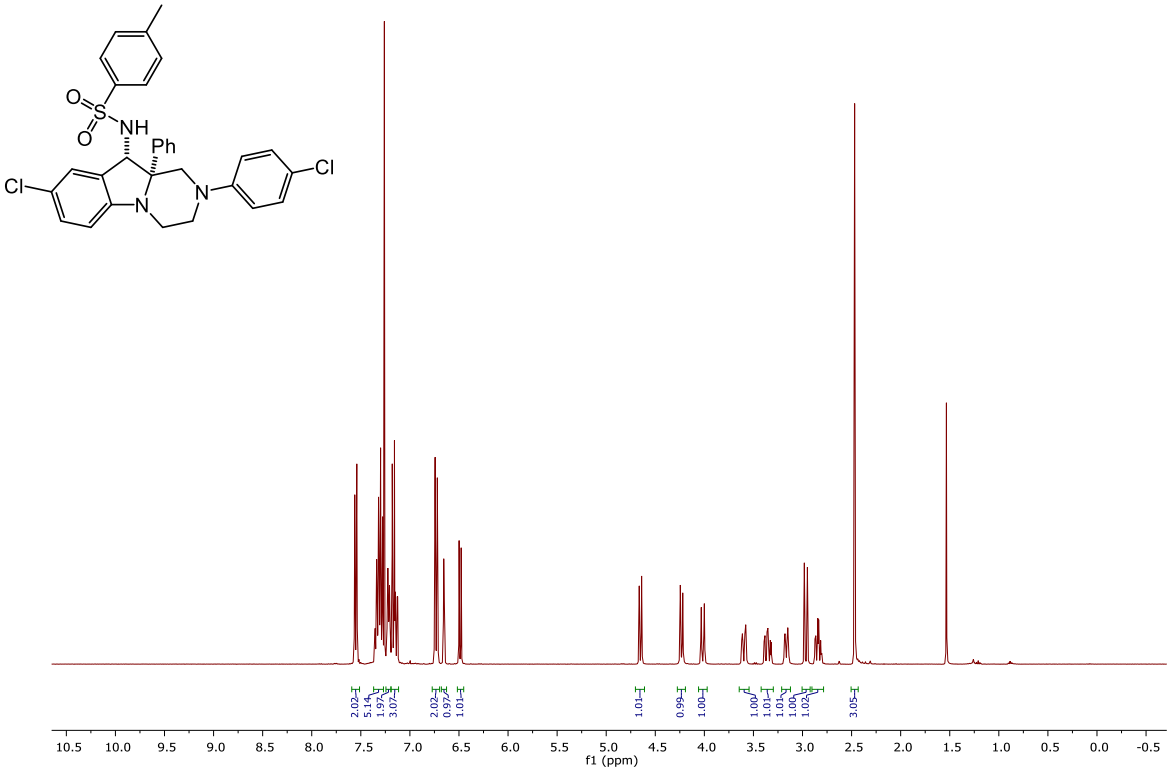
Compound 3aD'' ^{1}H NMR ($CDCl_3$, 400 MHz)



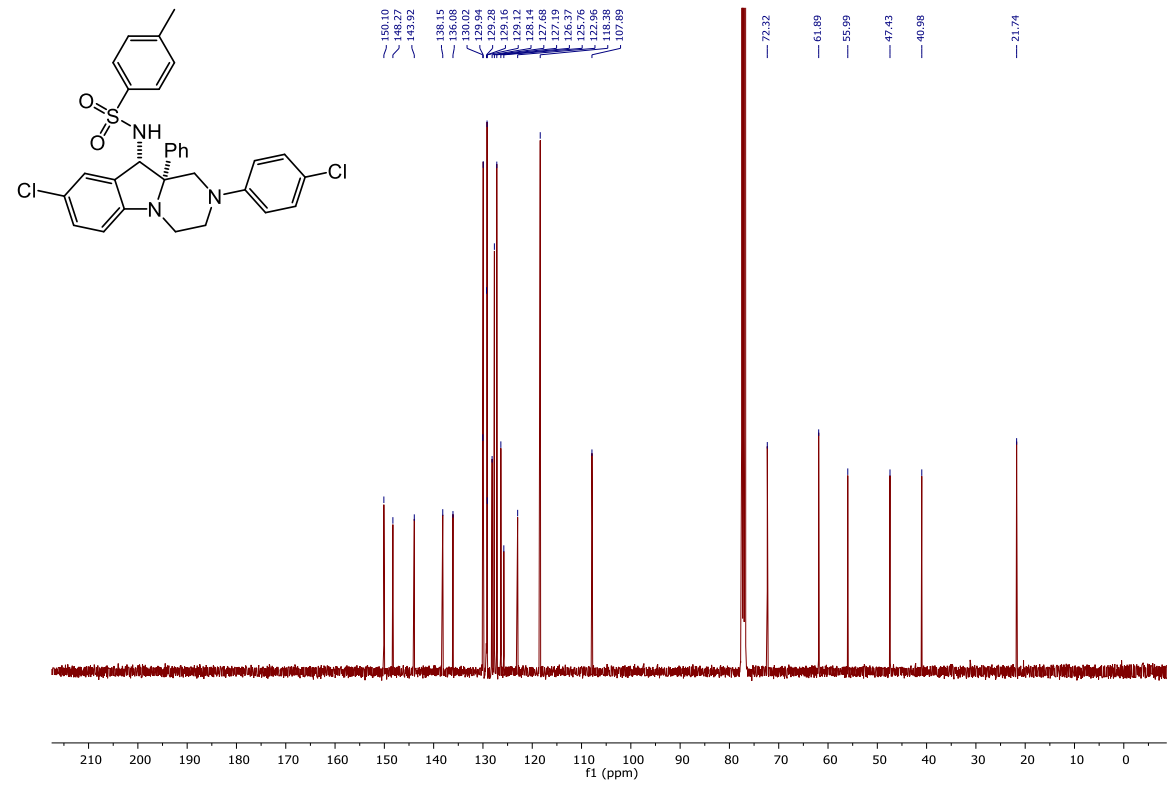
Compound 3aD'' ^{13}C NMR ($CDCl_3$, 100 MHz)



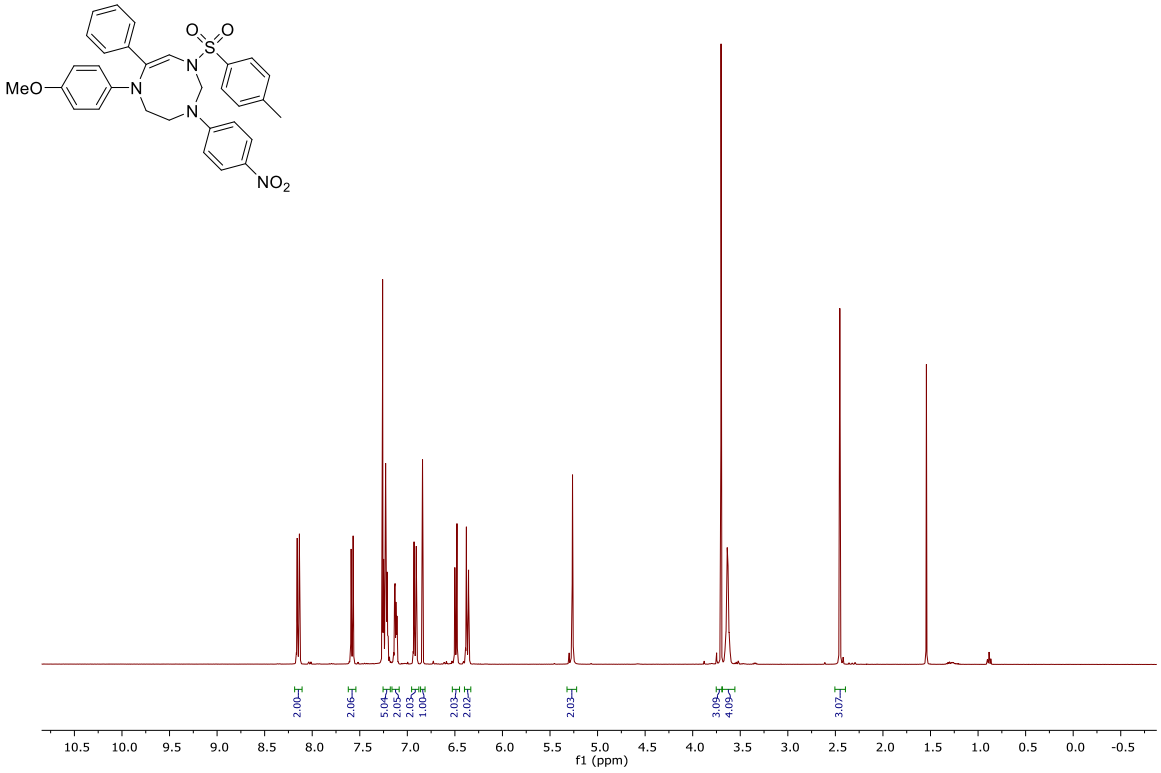
Compound 3aD' ^{1}H NMR ($CDCl_3$, 400 MHz)



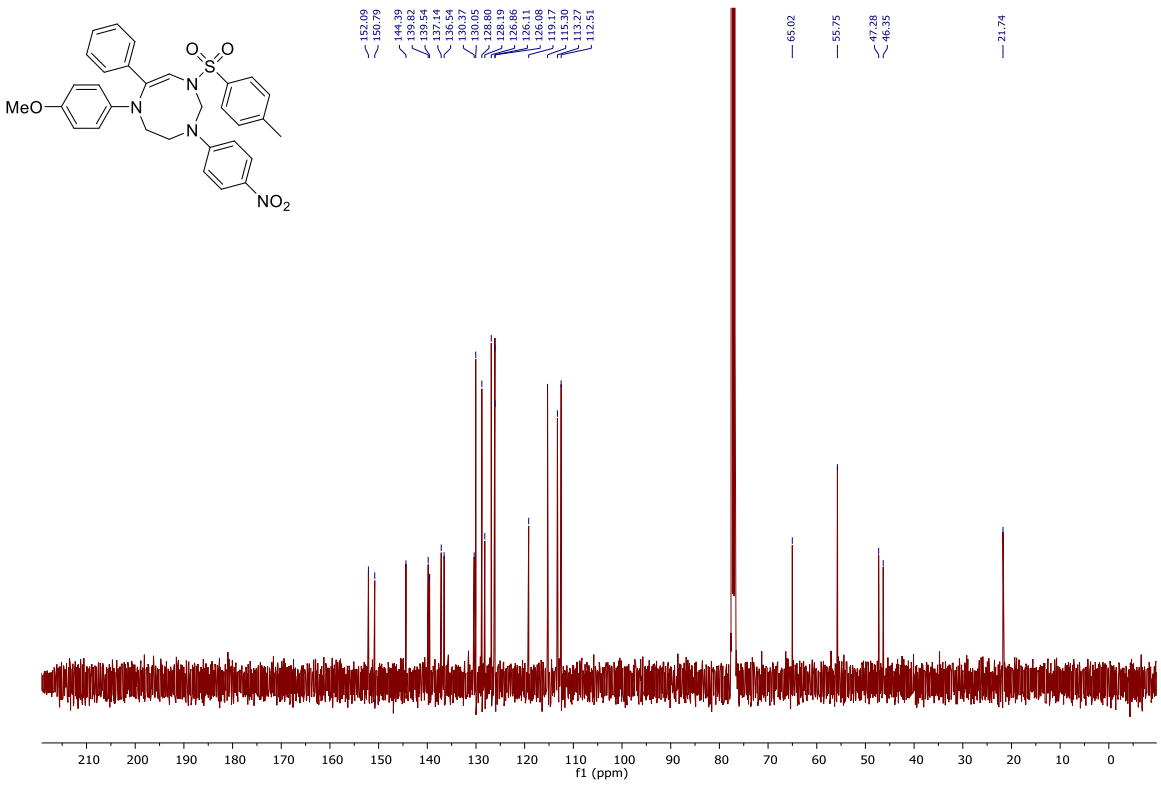
Compound 3aD' ^{13}C NMR ($CDCl_3$, 100 MHz)



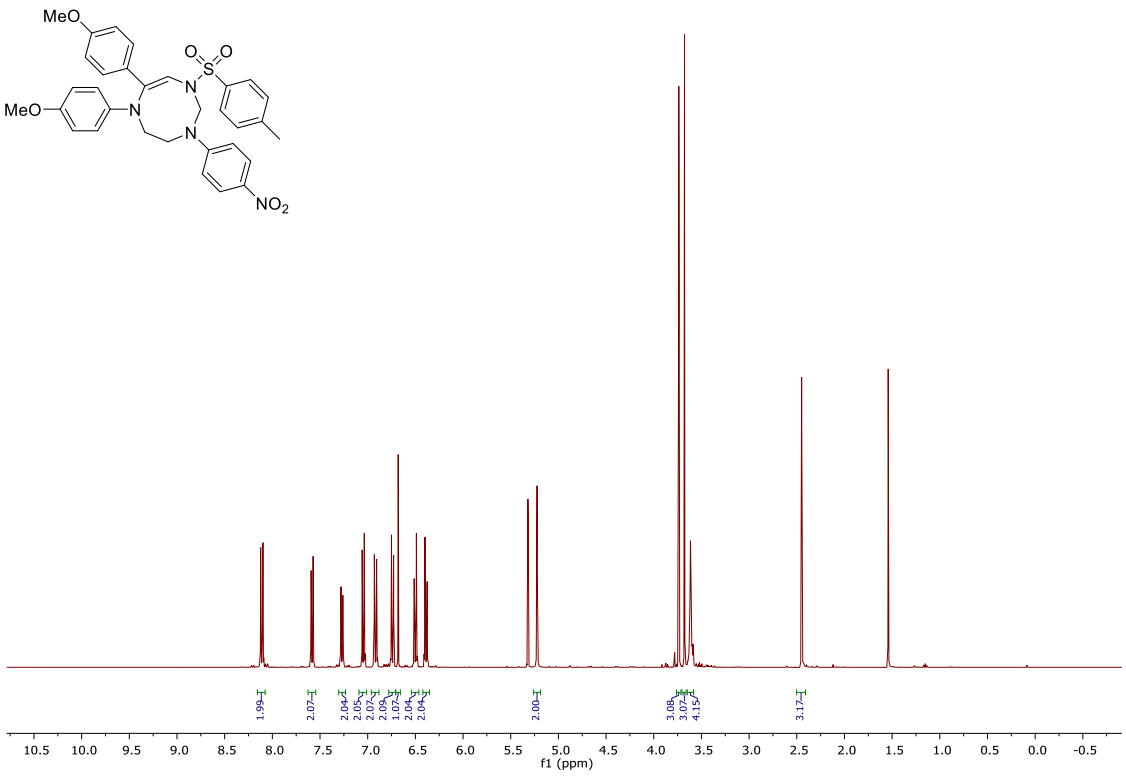
Compound 4aE ^{1}H NMR ($CDCl_3$, 400 MHz)



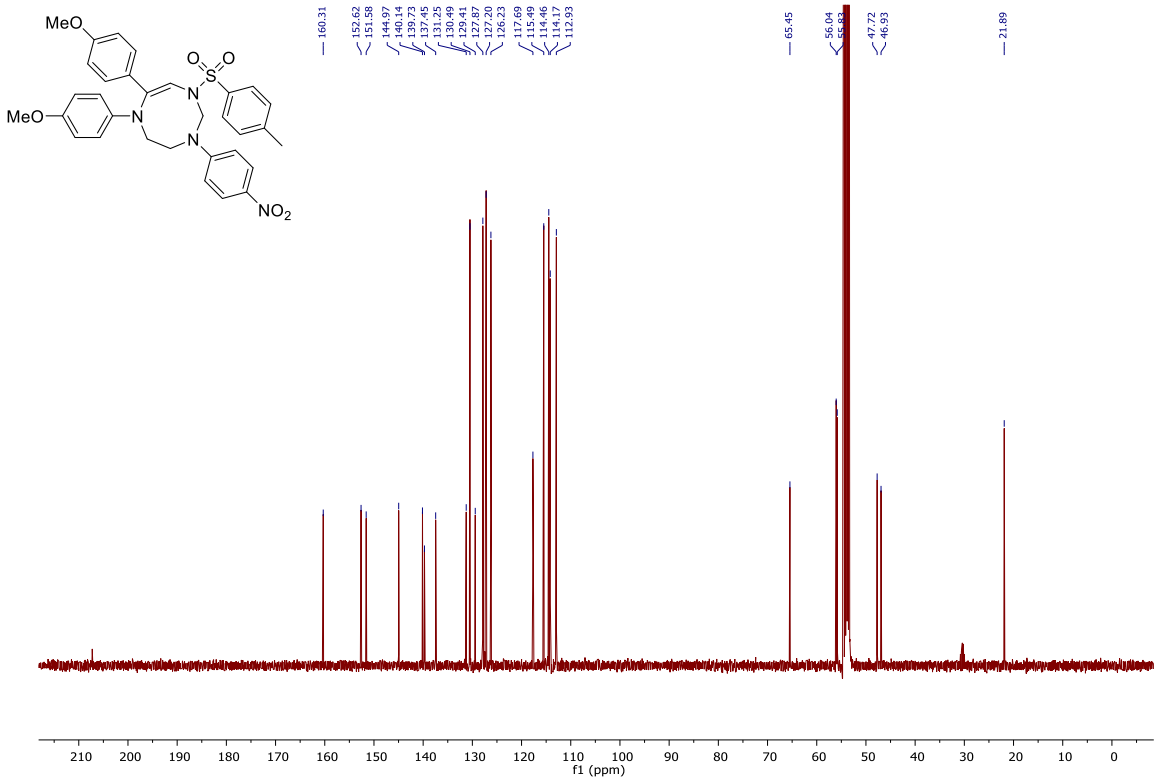
Compound 4aE ^{13}C NMR ($CDCl_3$, 100 MHz)



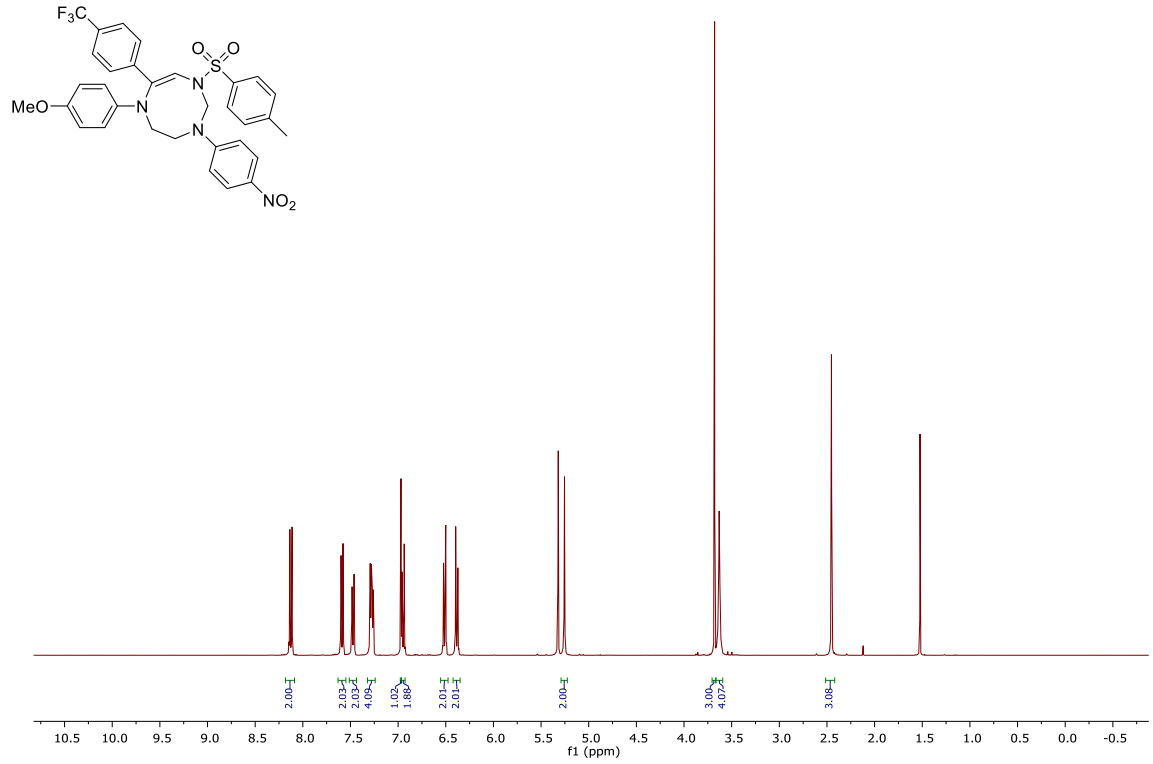
Compound 4eE ^{1}H NMR (CD_2Cl_2, 400 MHz)



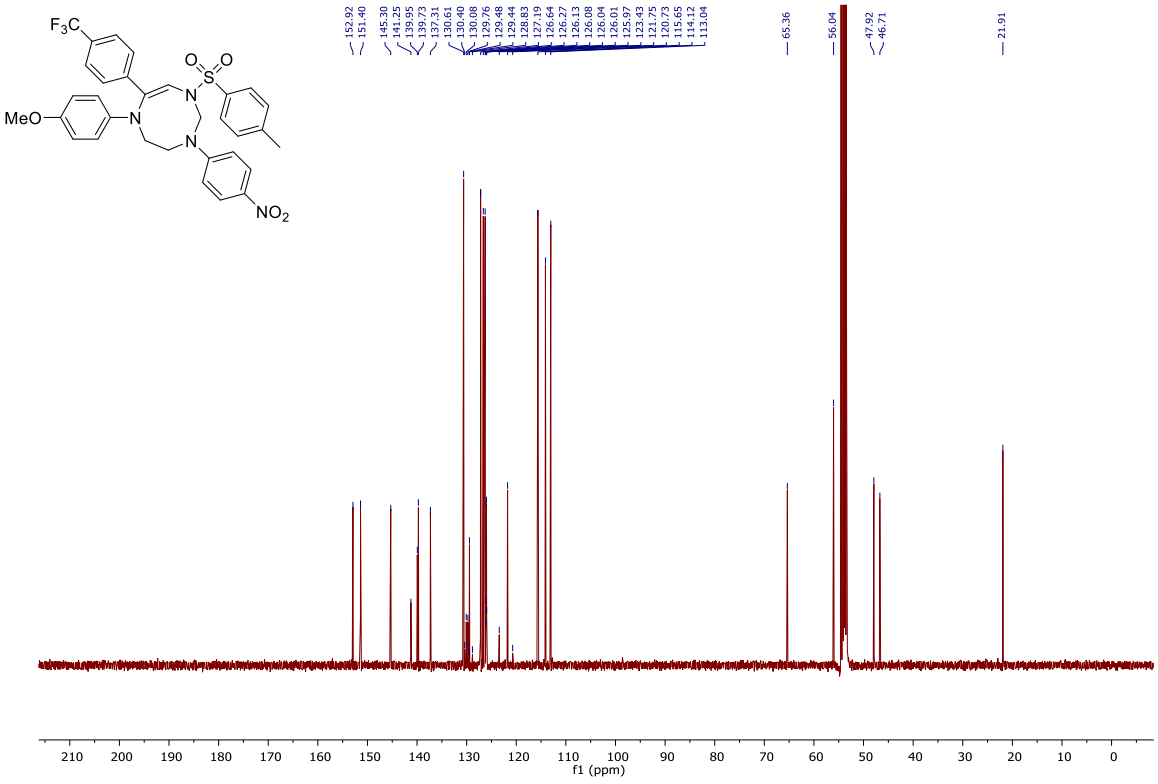
Compound 4eE ^{13}C NMR (CD_2Cl_2, 100 MHz)



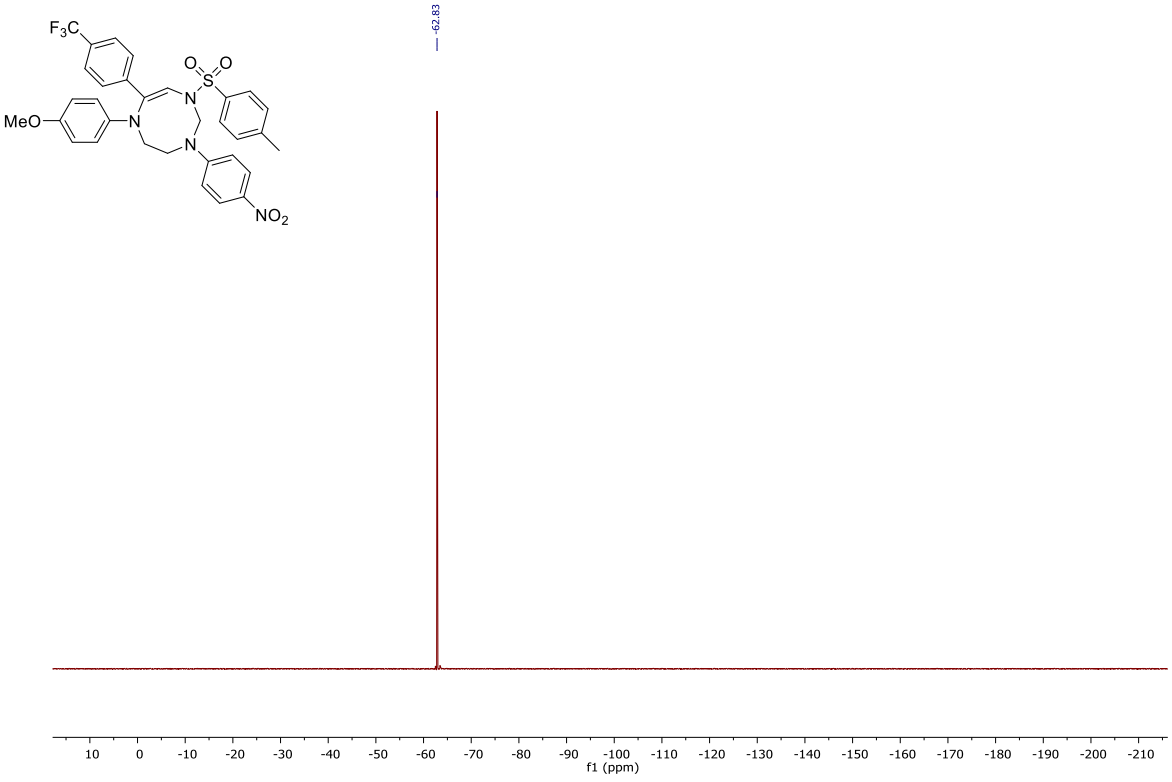
Compound 4iE ^{1}H NMR (CD_2Cl_2, 400 MHz)



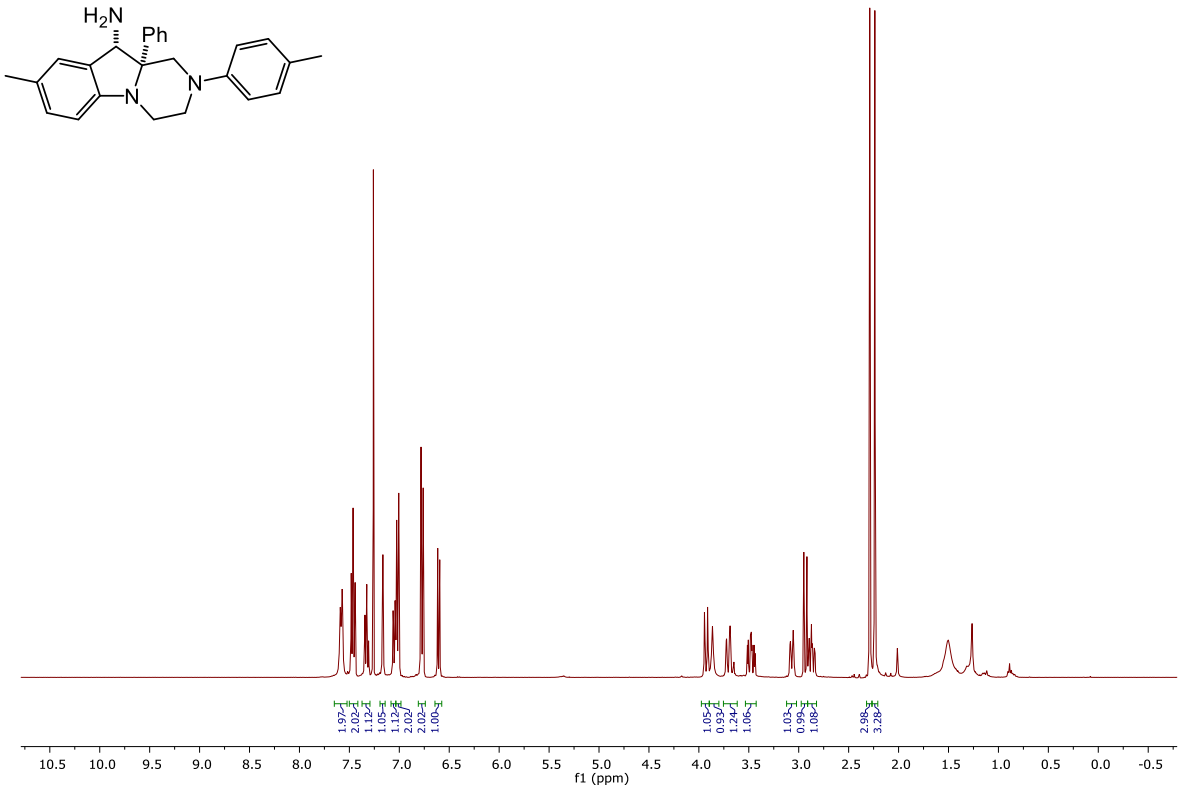
Compound 4iE ^{13}C NMR (CD_2Cl_2, 100 MHz)



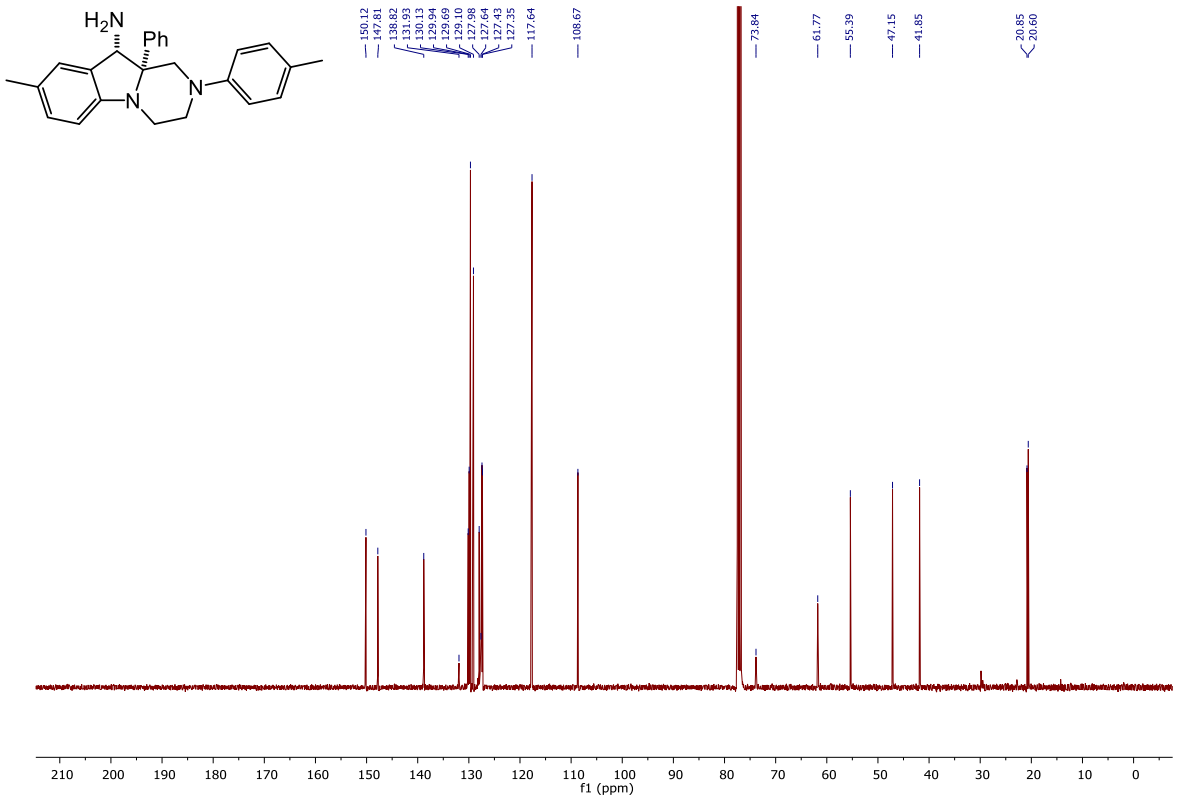
Compound 4iE ^{19}F NMR (CD_2Cl_2, 282 MHz)



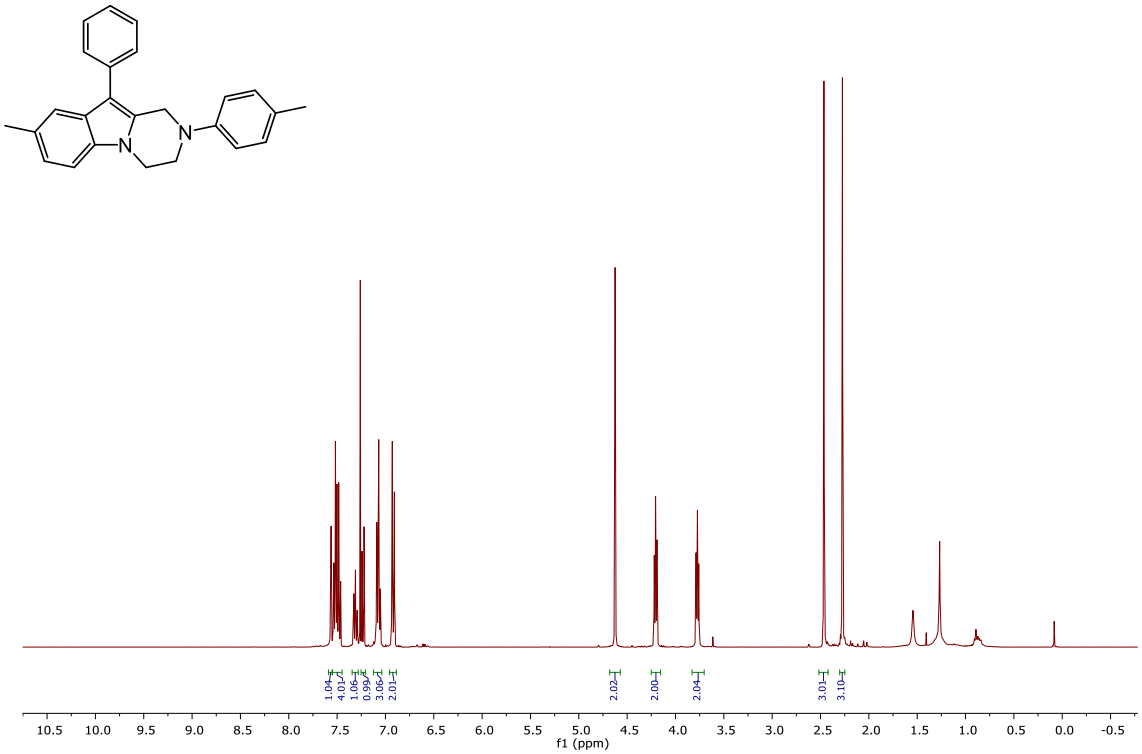
Compound 3A ^{1}H NMR ($CDCl_3$, 400 MHz)



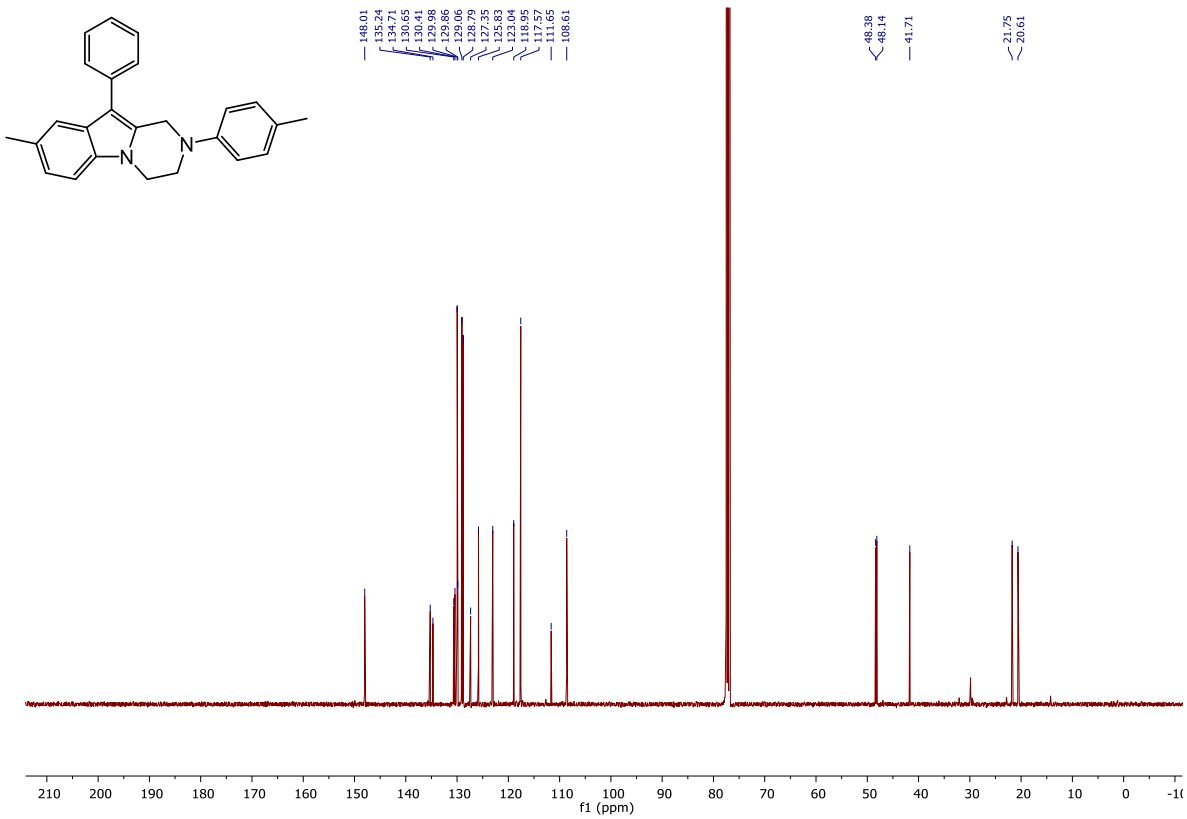
Compound 3A ^{13}C NMR ($CDCl_3$, 100 MHz)



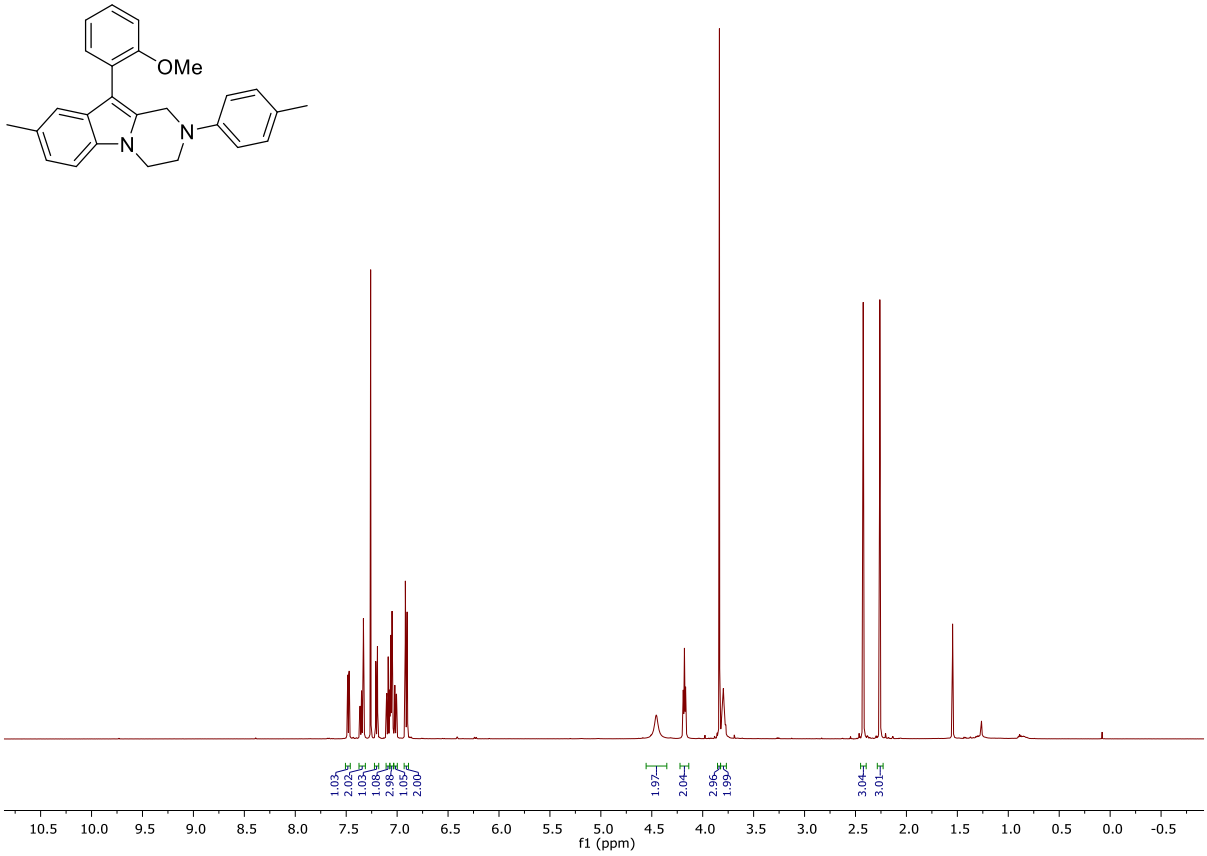
Compound 5aA ^{1}H NMR ($CDCl_3$, 400 MHz)



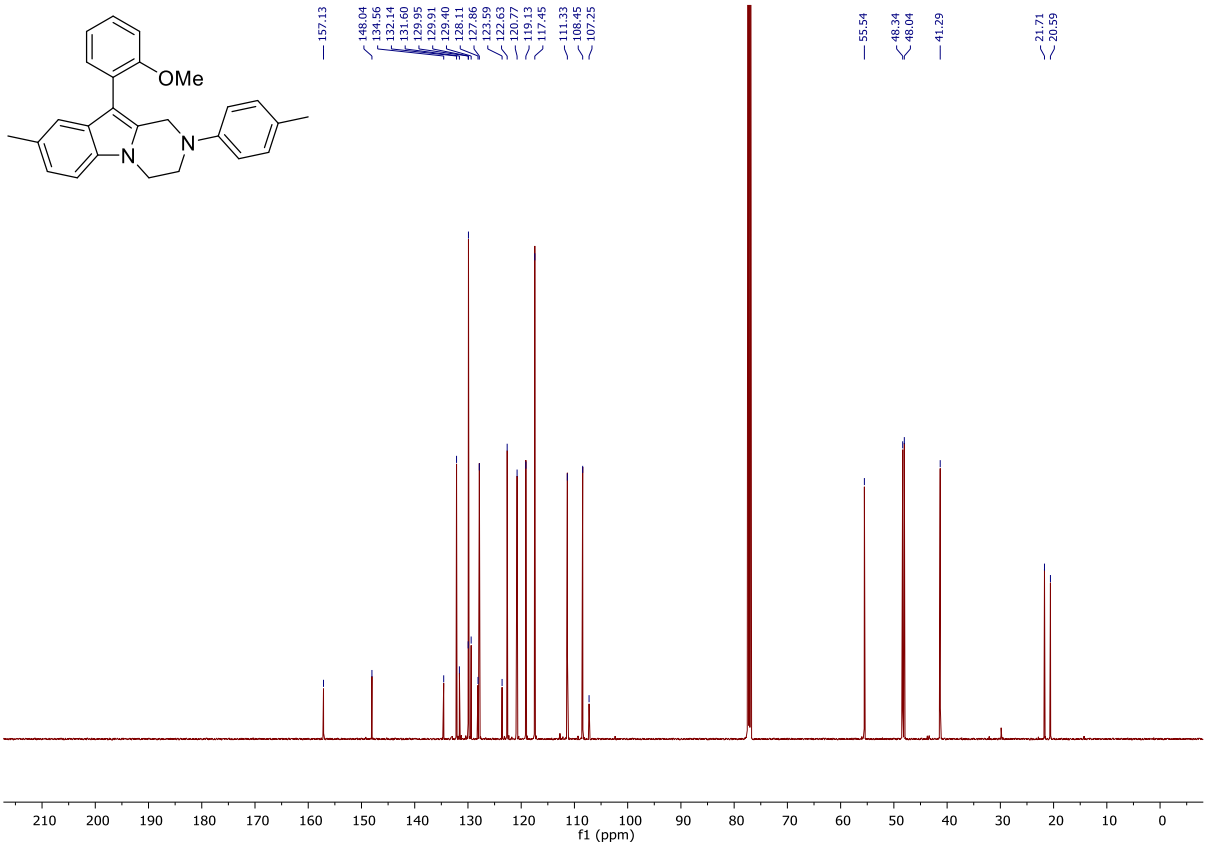
Compound 5aA ^{13}C NMR ($CDCl_3$, 100 MHz)



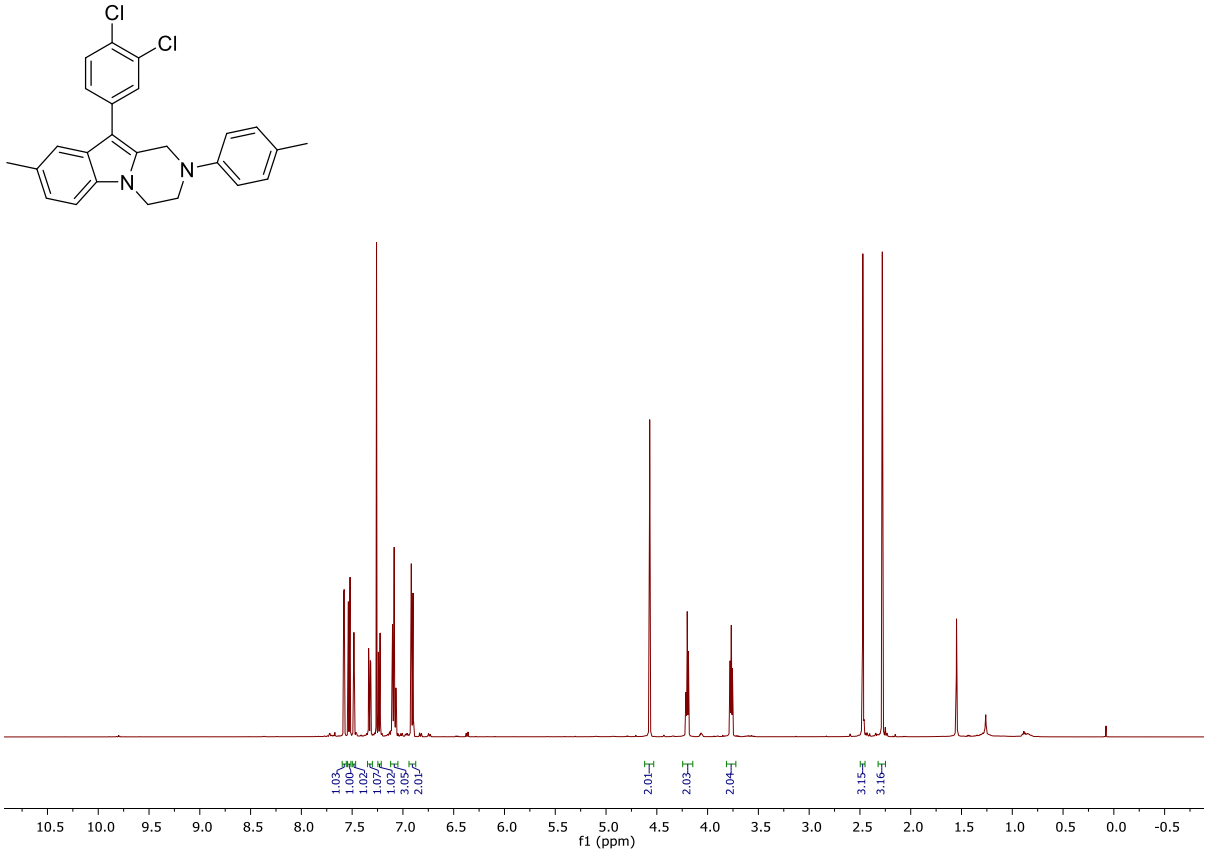
Compound 5dA ^{1}H NMR ($CDCl_3$, 500 MHz)



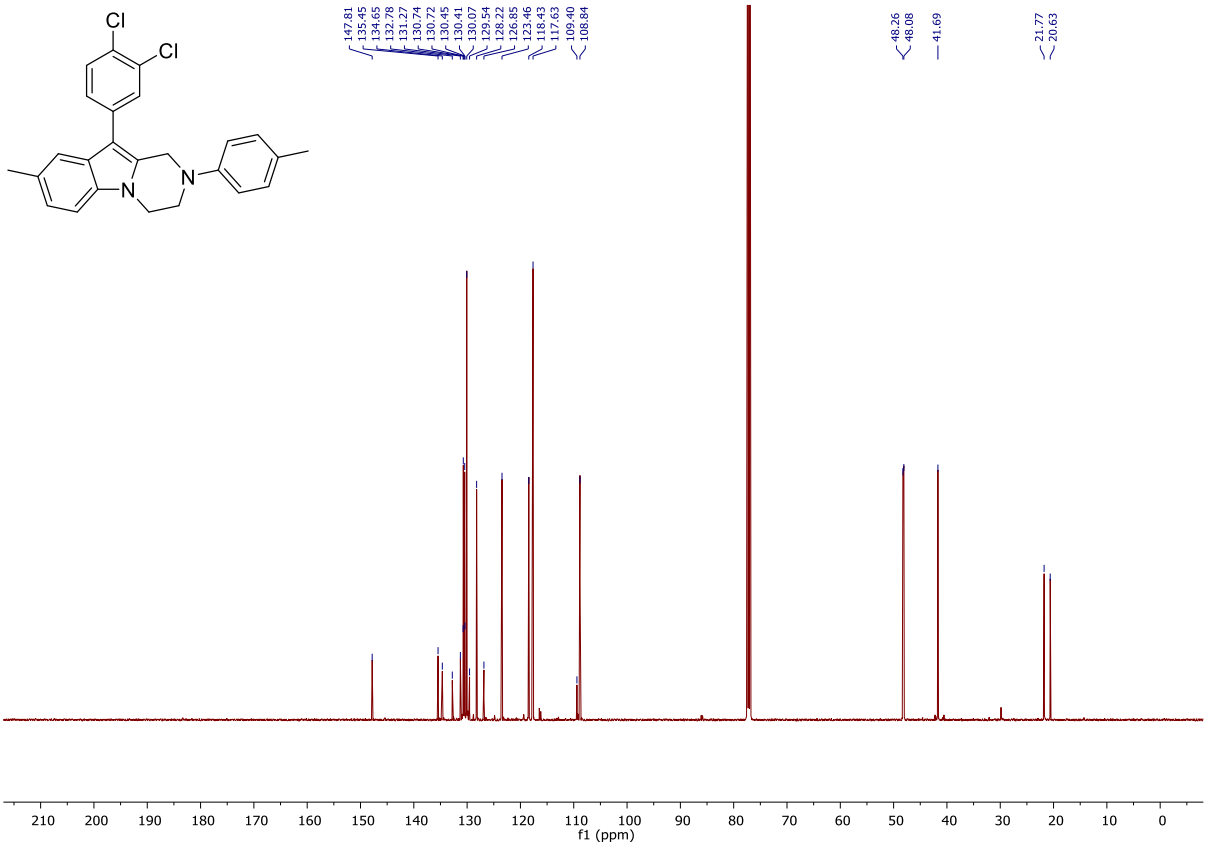
Compound 5dA ^{13}C NMR ($CDCl_3$, 126 MHz)



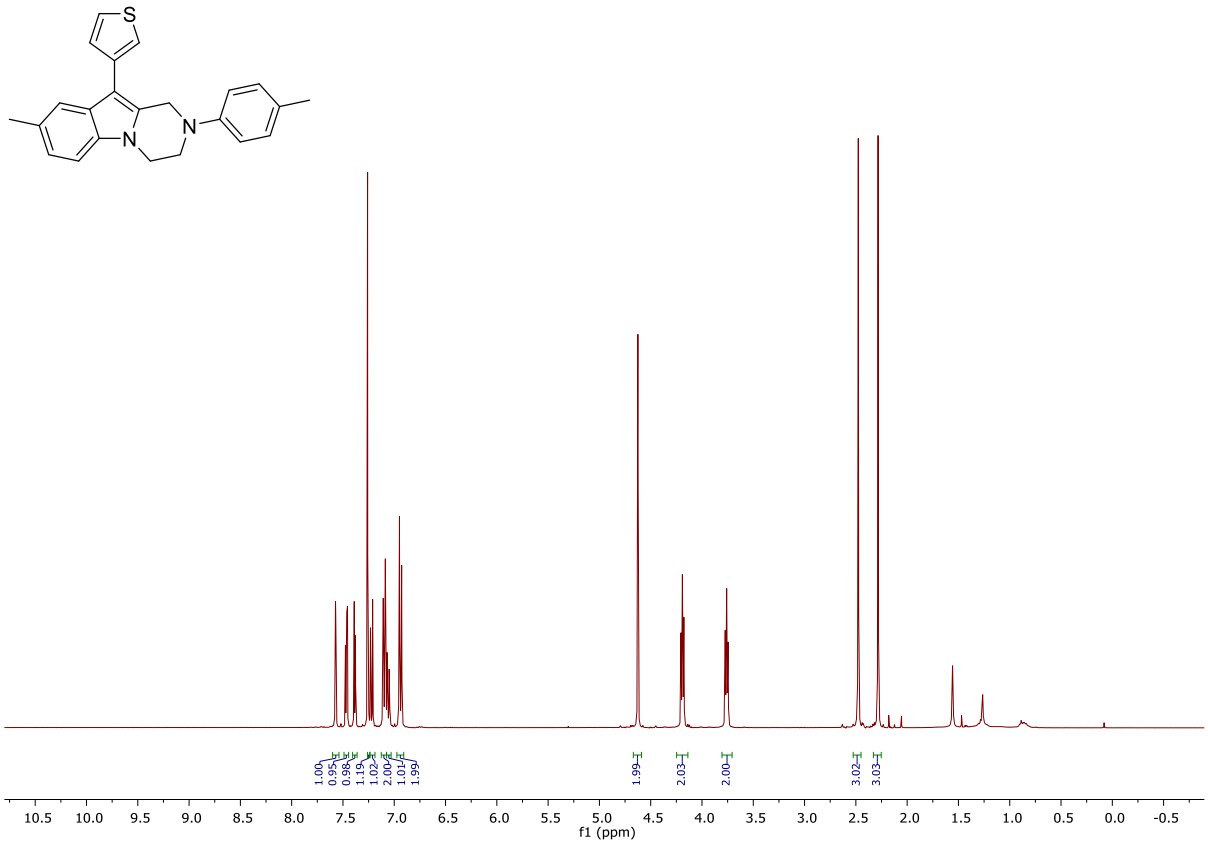
Compound 5fA ^{1}H NMR ($CDCl_3$, 500 MHz)



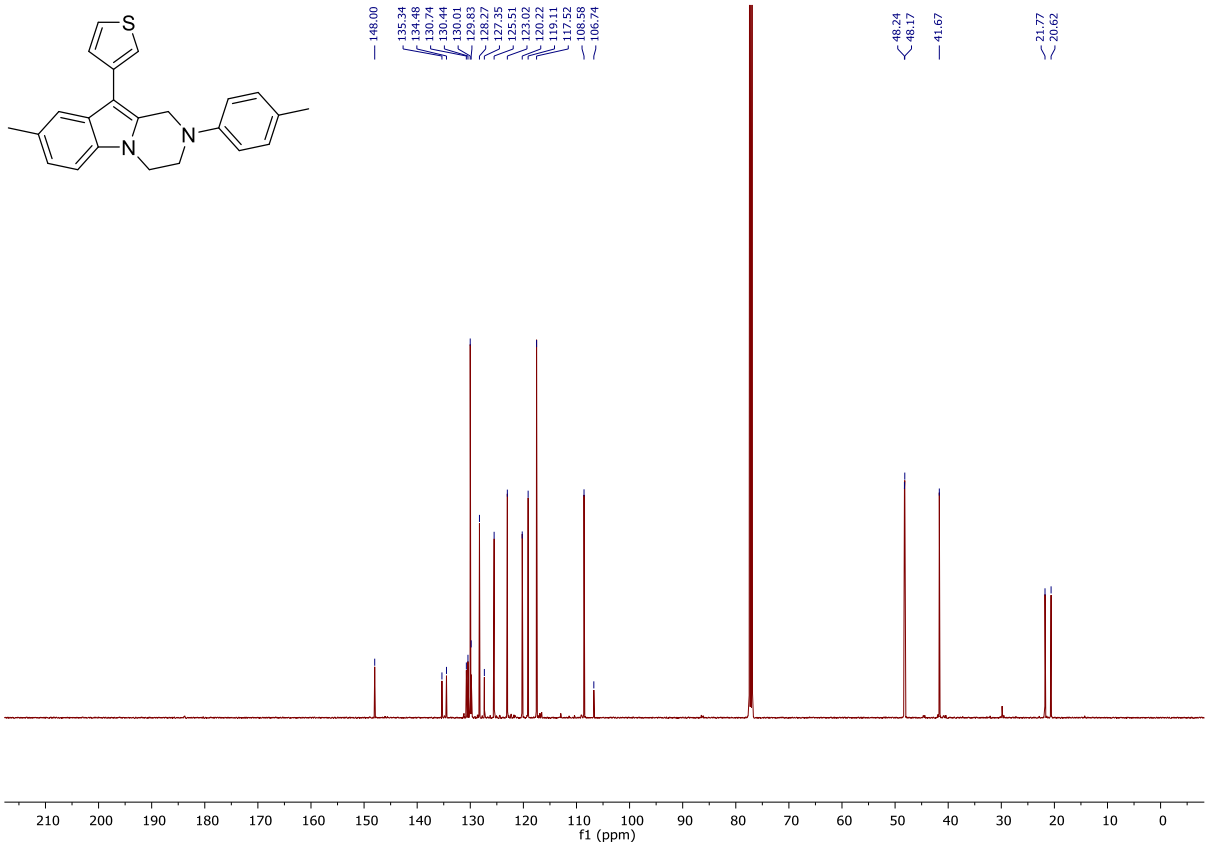
Compound 5fA ^{13}C NMR ($CDCl_3$, 126 MHz)



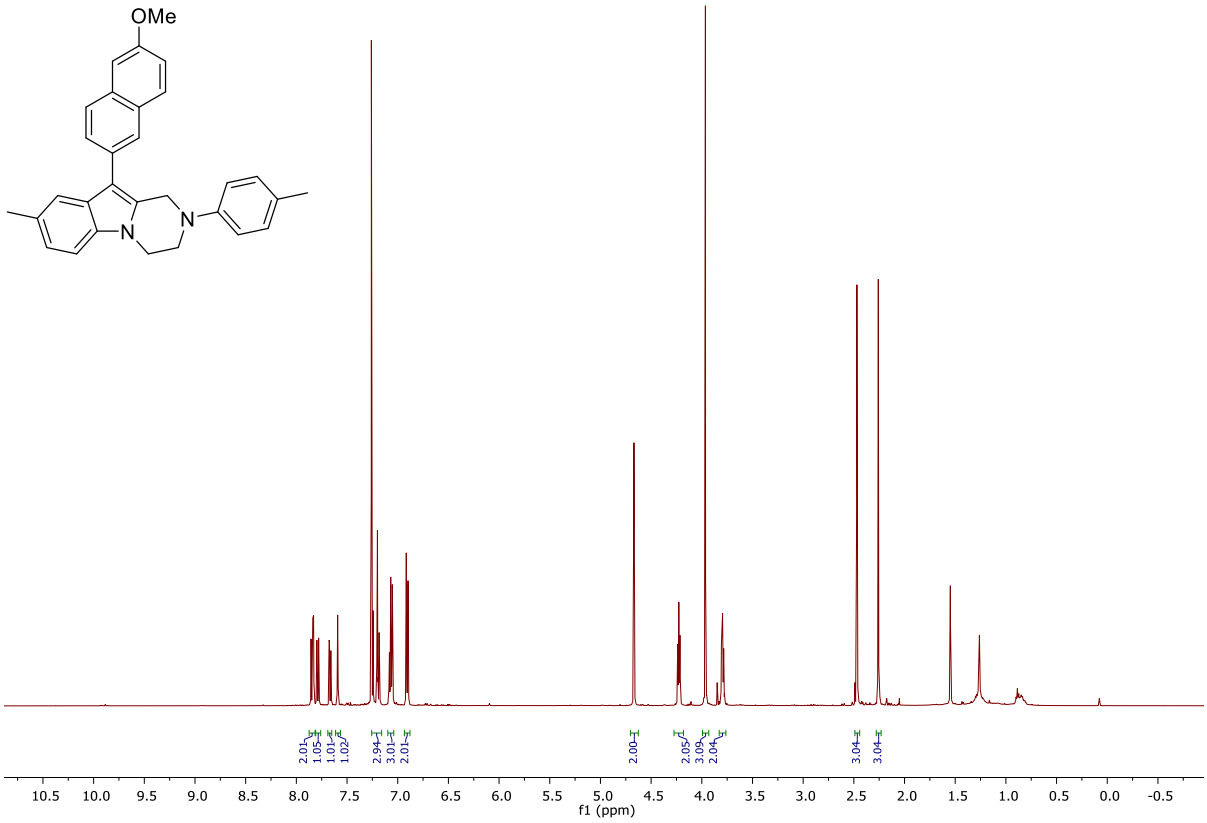
Compound 5gA ^{1}H NMR ($CDCl_3$, 400 MHz)



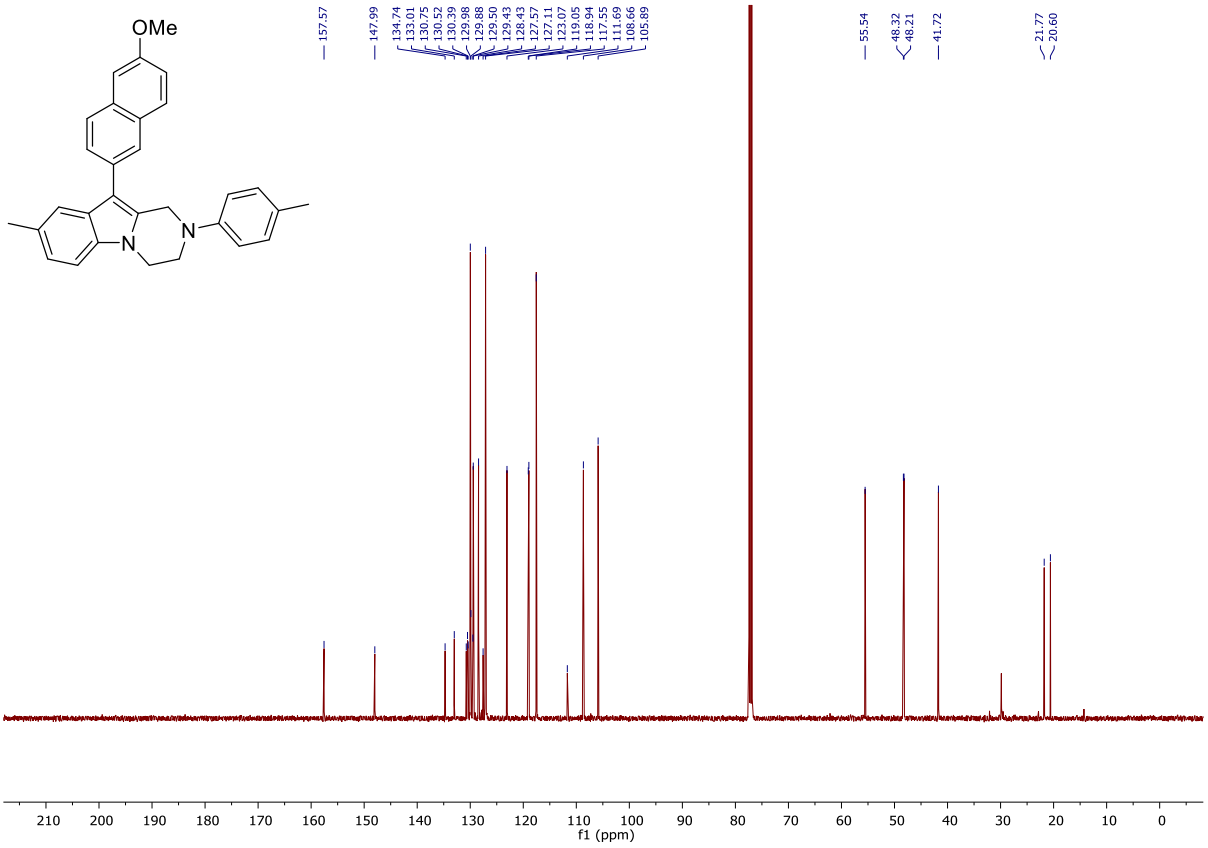
Compound 5gA ^{13}C NMR ($CDCl_3$, 126 MHz)



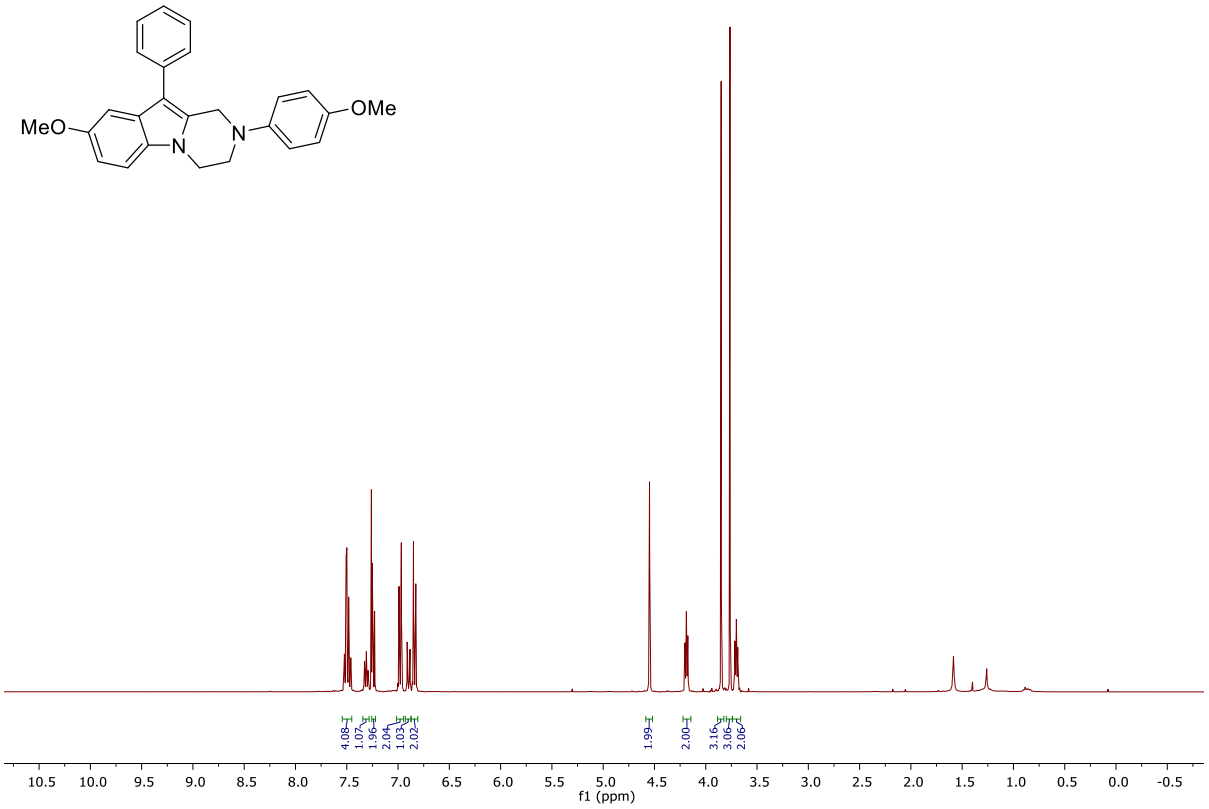
Compound 5hA ^{1}H NMR ($CDCl_3$, 500 MHz)



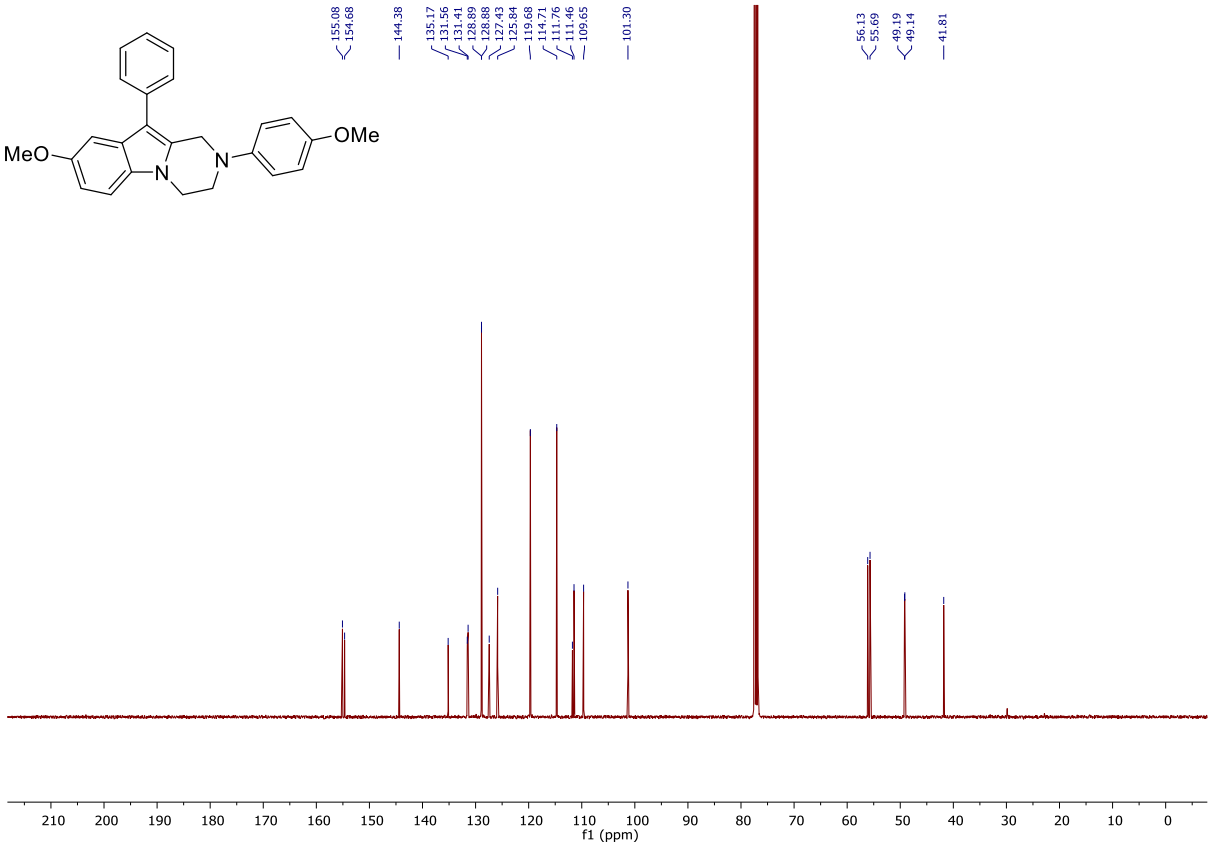
Compound 5hA ^{13}C NMR ($CDCl_3$, 126 MHz)



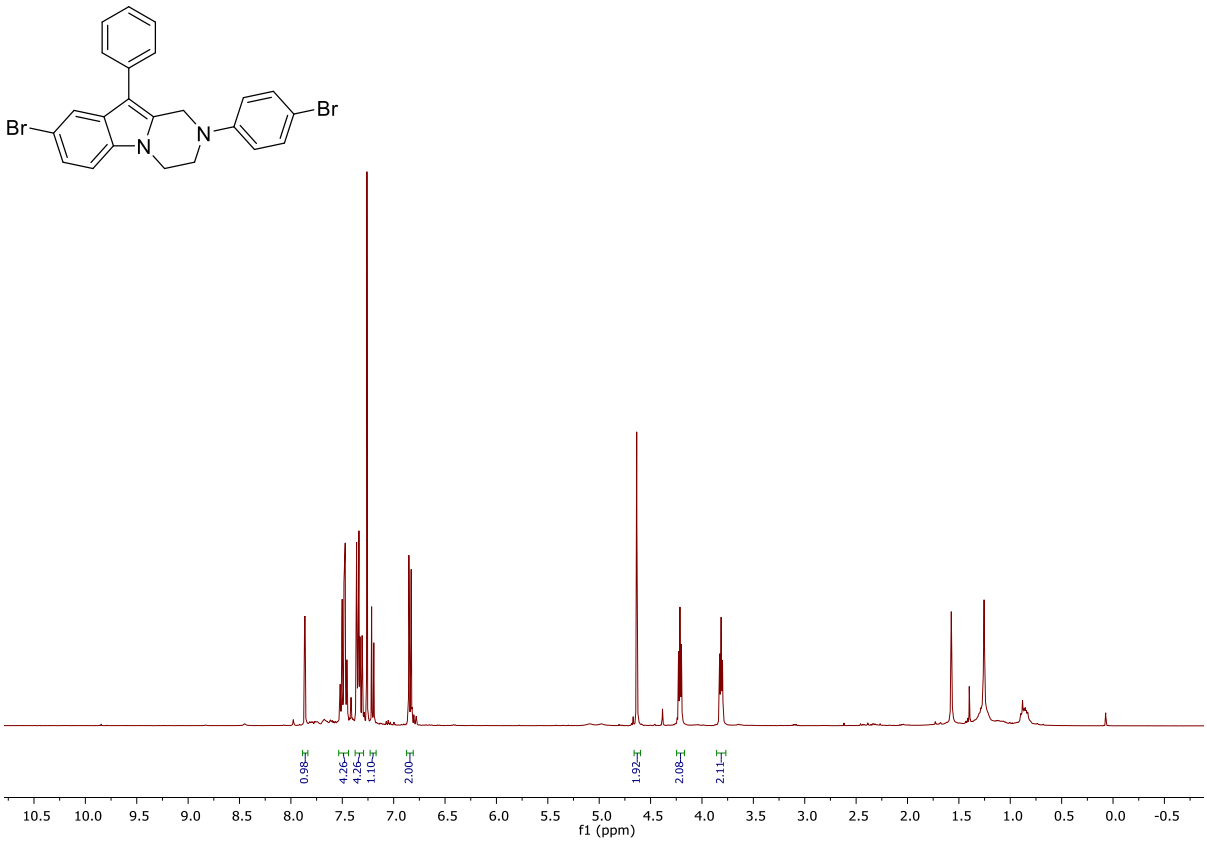
Compound 5aB ^{1}H NMR ($CDCl_3$, 400 MHz)



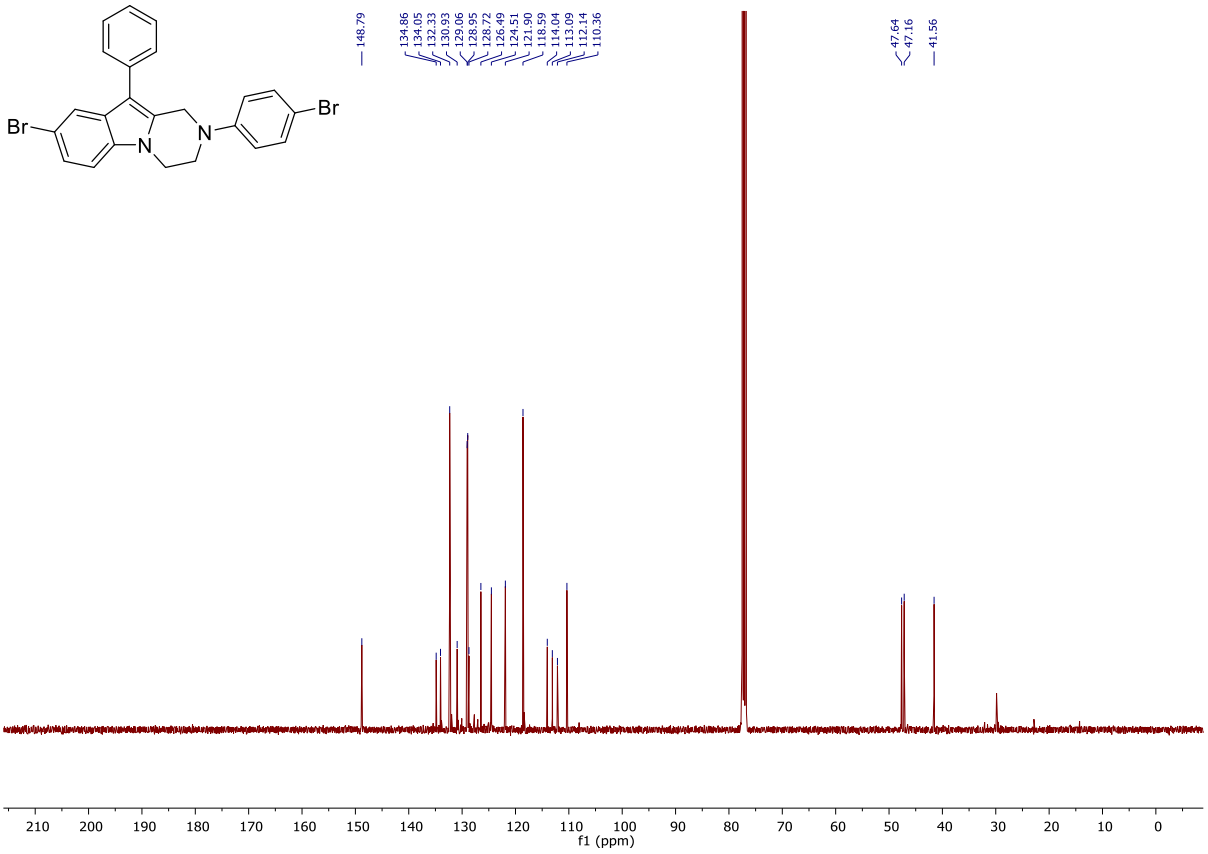
Compound 5aB ^{13}C NMR ($CDCl_3$, 100 MHz)



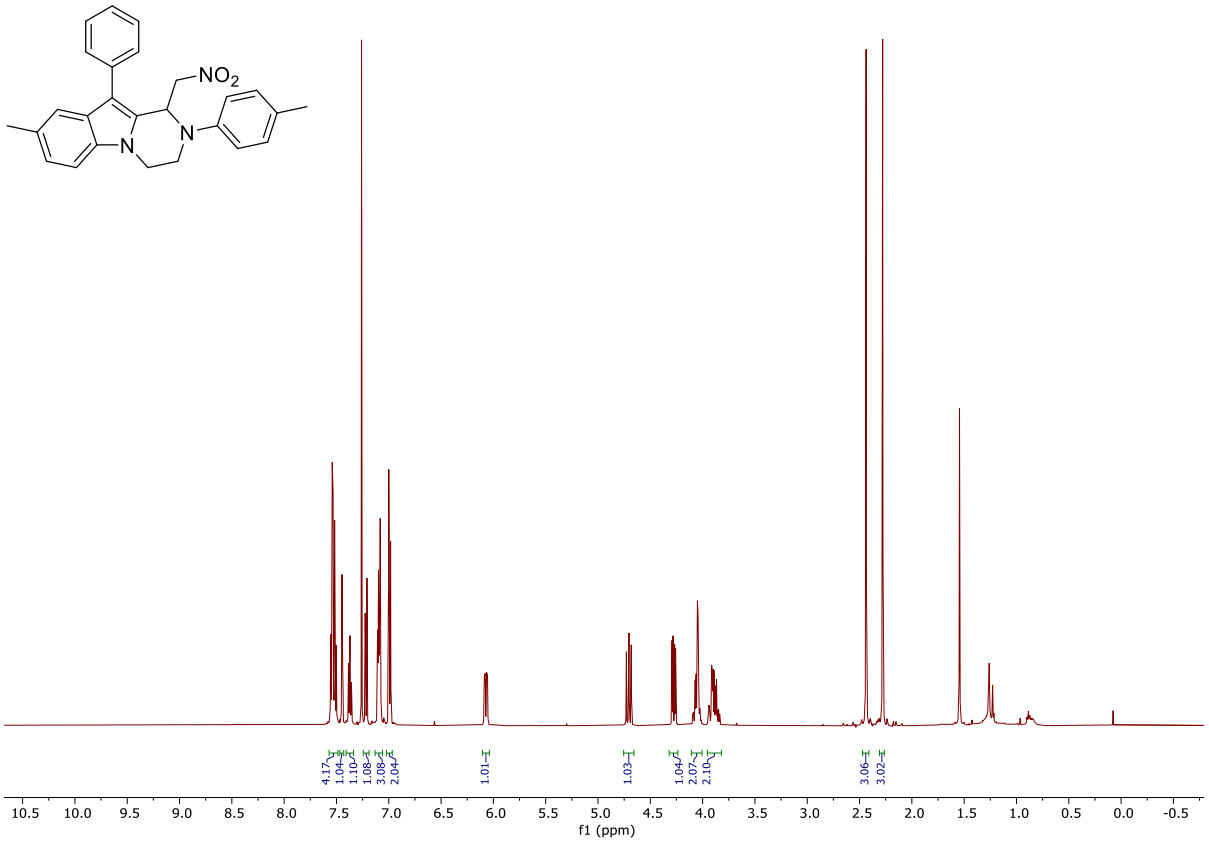
Compound 5aC ^{1}H NMR ($CDCl_3$, 400 MHz)



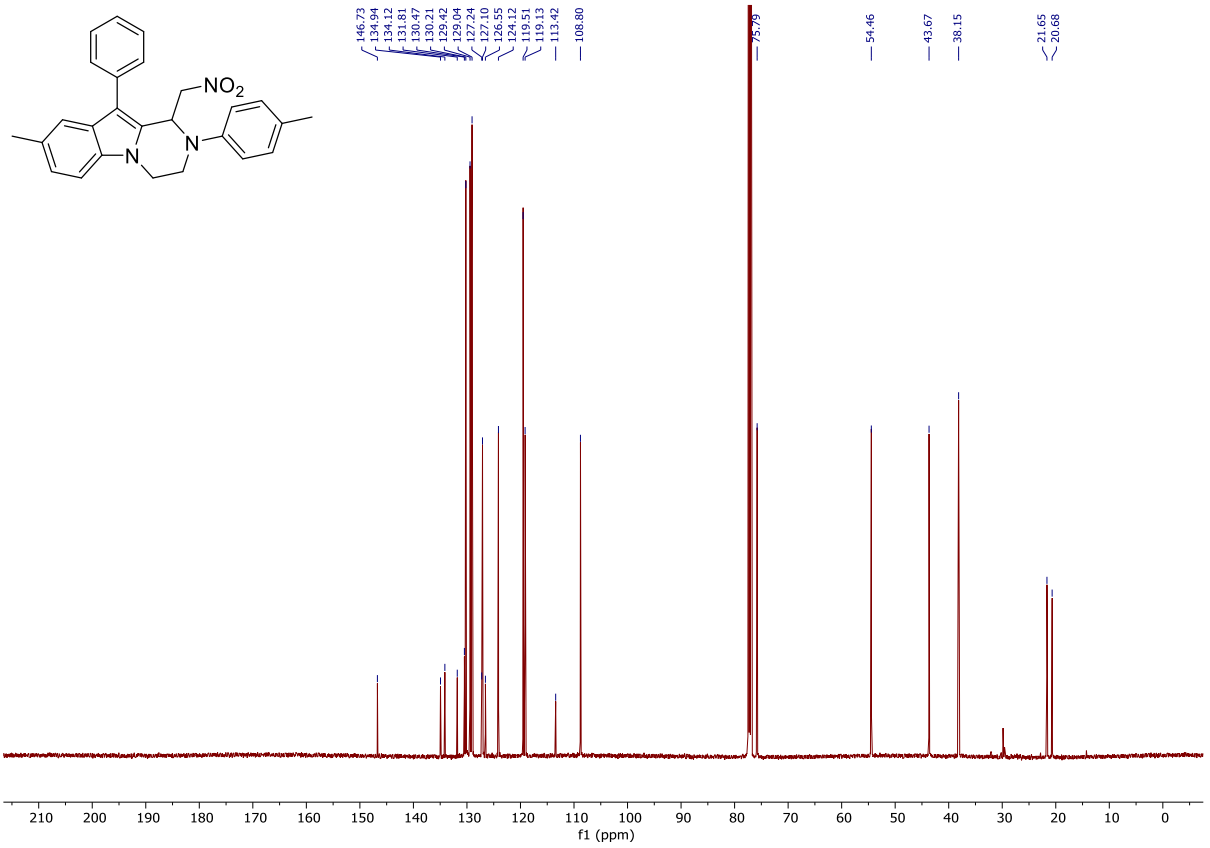
Compound 5aC ^{13}C NMR ($CDCl_3$, 100 MHz)



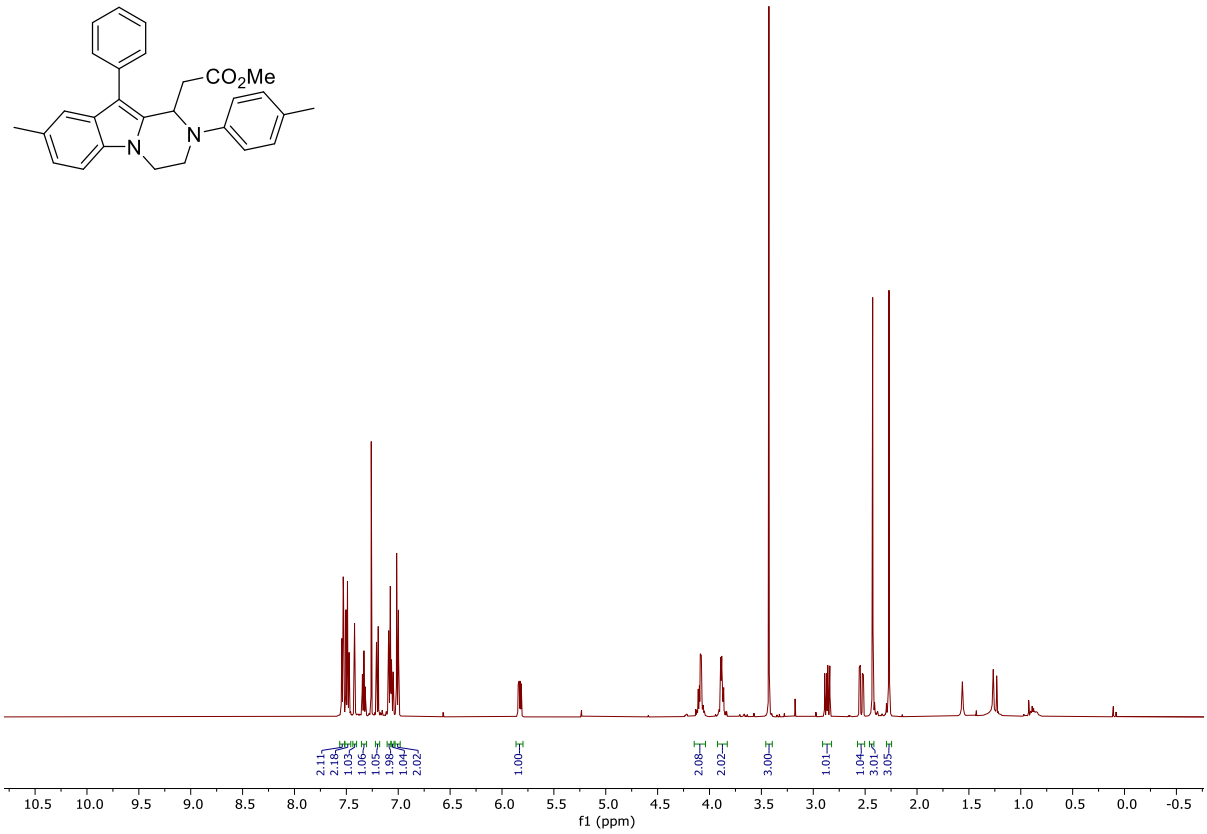
Compound 6 ^{1}H NMR ($CDCl_3$, 500 MHz)



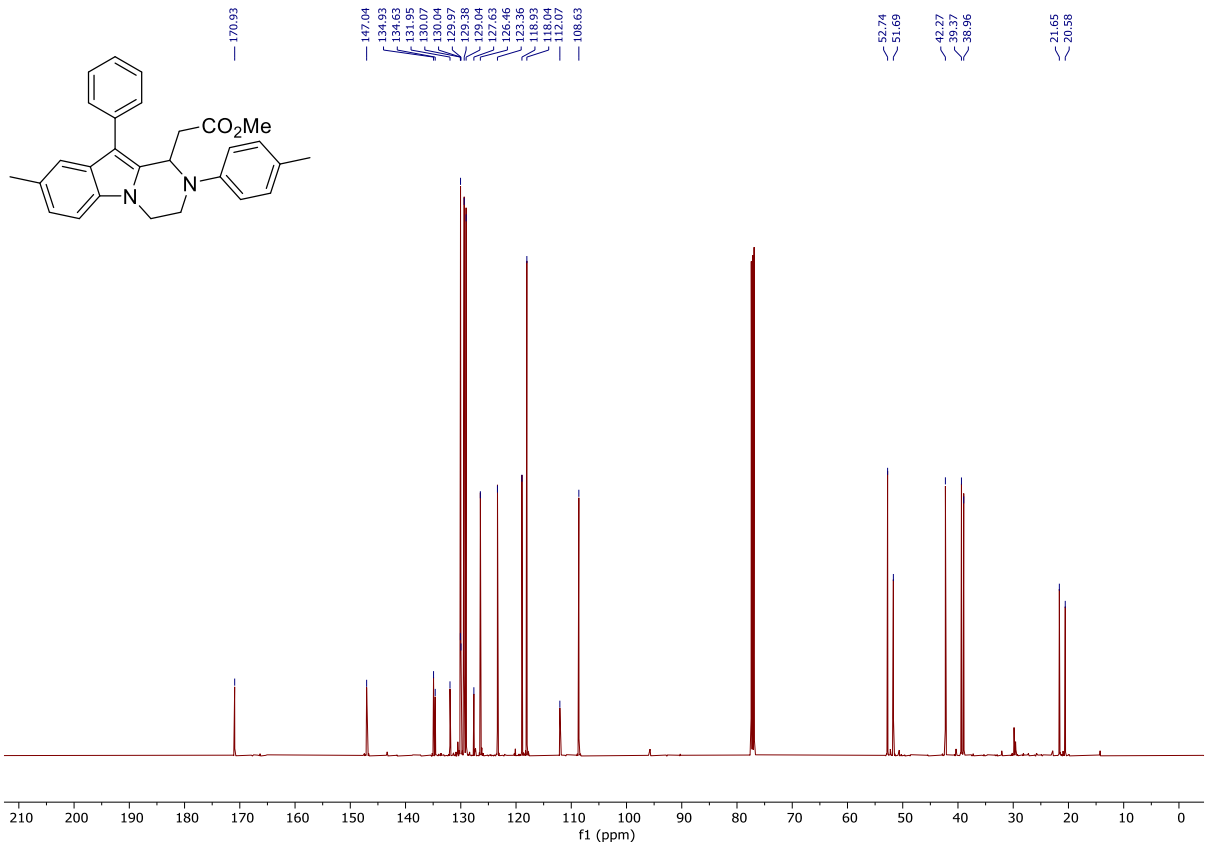
Compound 6 ^{13}C NMR ($CDCl_3$, 126 MHz)



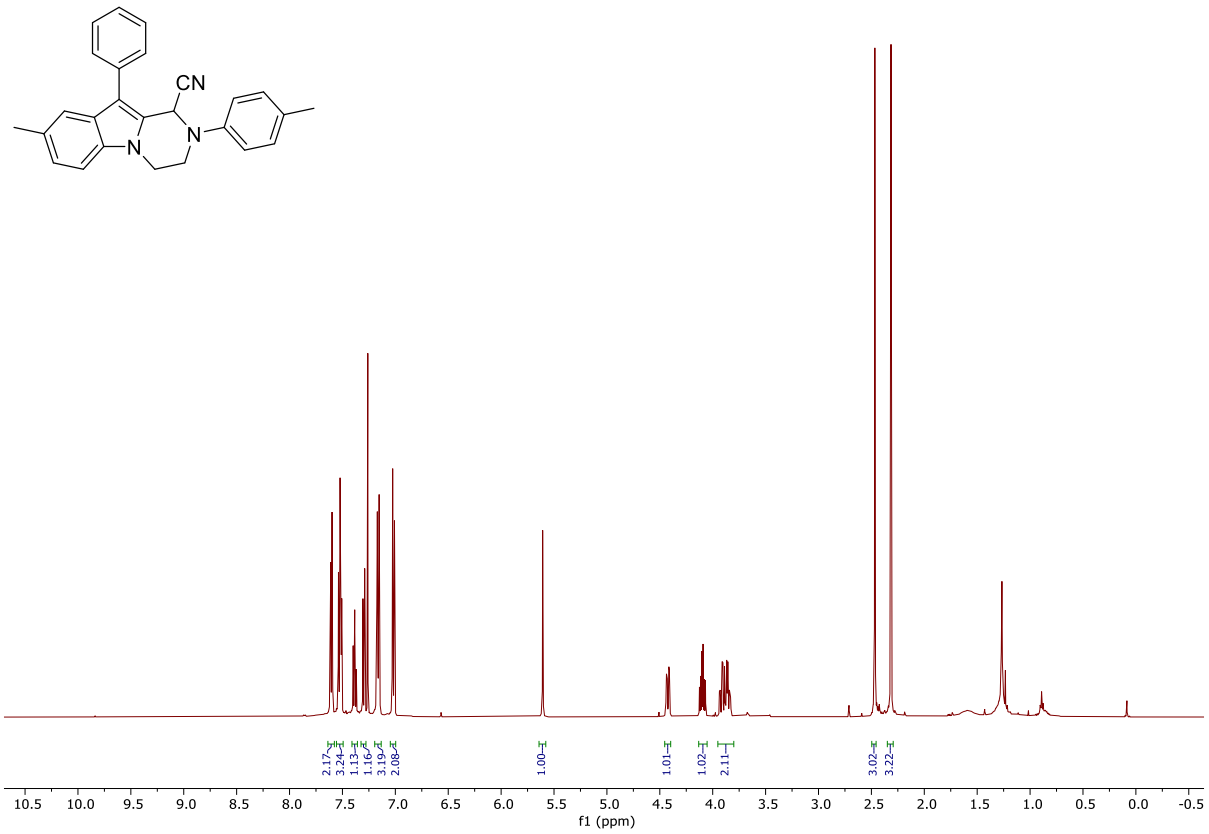
Compound 7 ^{1}H NMR ($CDCl_3$, 500 MHz)



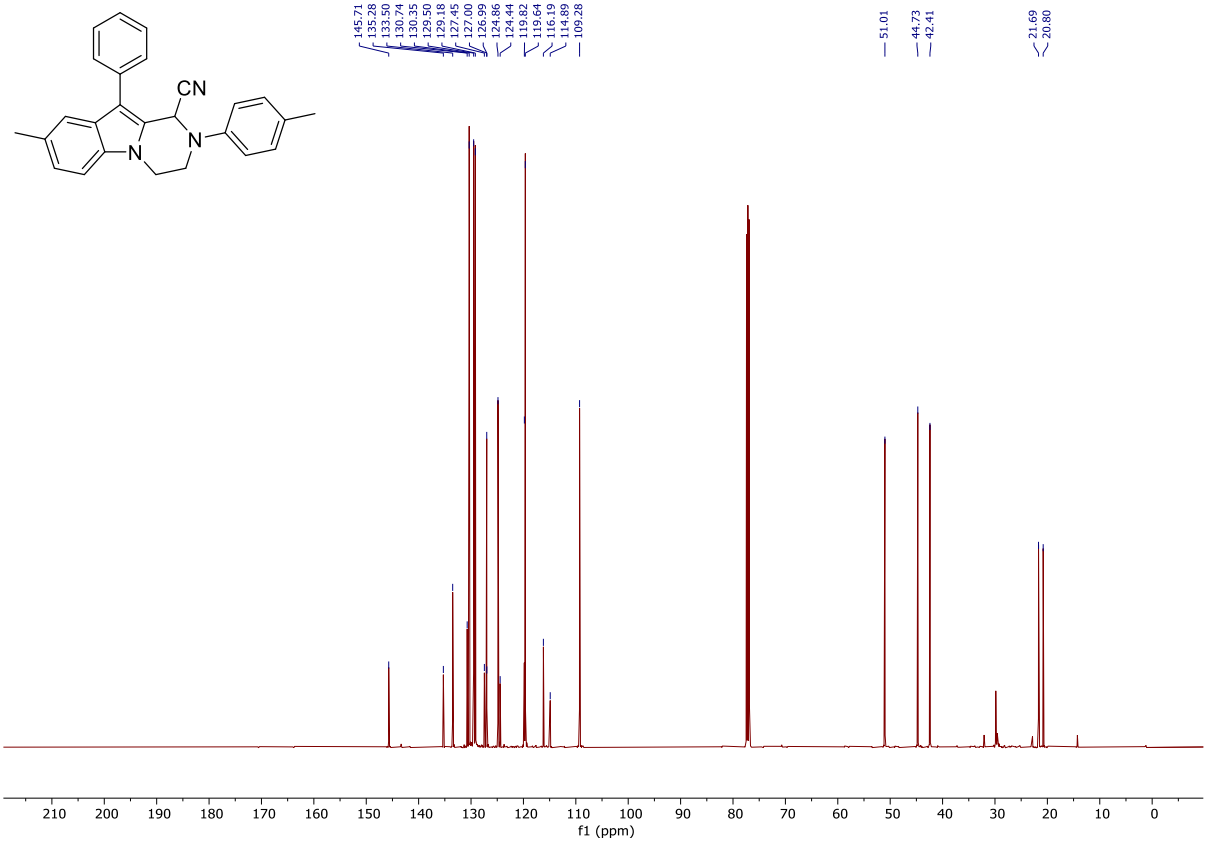
Compound 7 ^{13}C NMR ($CDCl_3$, 126 MHz)



Compound 8 ^{1}H NMR ($CDCl_3$, 500 MHz)



Compound 8 ^{13}C NMR ($CDCl_3$, 126 MHz)



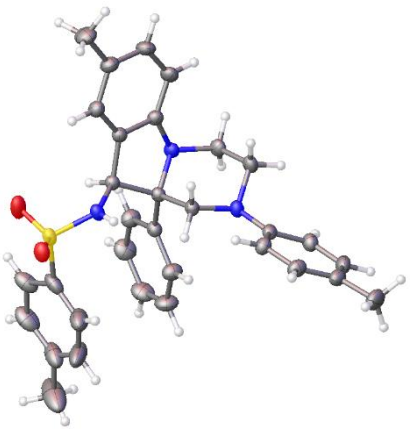
11. Crystallographic data

All data were collected on an Agilent supernova dual source diffractometer equipped with an Atlas detector, using Cu Kα radiation. Data reduction was carried out in the crysalis Pro Software.[4] Structure solution was made using direct methods (Shelxs[5] or sir2004[6]). Refinements were carried out in ShexlL[5] within the Olex2[7] software.

Details for the refinement for each structure are detailed below. For each structure, a representation of the asymmetric units shown as displacement ellipsoids, drawn as 50 percent probability is depicted (without showing disorder if present).

Compound 3aA''

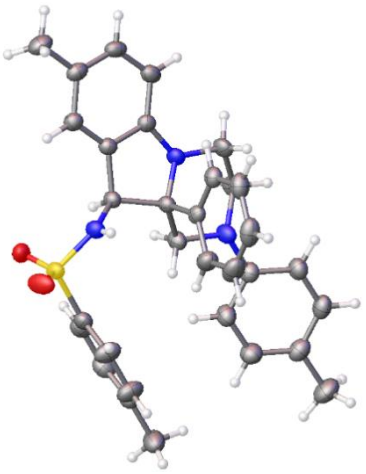
Empirical formula	$C_{32}H_{33}N_3O_2S$
CCDC	**2015201**
Formula weight	523.67
Temperature/K	180.00(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	18.90952(14)
b/Å	10.14583(6)
c/Å	28.4275(2)
α/°	90
β/°	93.3559(7)
γ/°	90
Volume/Å^3	5444.54(7)
Z	8
ρ_{calc}g/cm^3	1.278
μ/mm^{-1}	1.322
F(000)	2224.0
Crystal size/mm^3	0.332 × 0.169 × 0.104
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.228 to 147.27
Index ranges	-23 ≤ h ≤ 16, -12 ≤ k ≤ 12, -34 ≤ l ≤ 35
Reflections collected	23114
Independent reflections	5449 [R_{int} = 0.0202, R_{sigma} = 0.0136]
Data/restraints/parameters	5449/180/420
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0348, wR_2 = 0.0905
Final R indexes [all data]	R_1 = 0.0372, wR_2 = 0.0926
Largest diff. peak/hole / e Å^{-3}	0.22/-0.43



The methylphenyl group is disordered and was refined using two components. Restraints were applied on distances (same distances restraints), planarity of the ring and anisotropic displacement parameters.
The hydrogens bound to the carbon C9 are also disordered. 6 hydrogen atoms were used with half occupancies. Restraints were applied on the C-H distances.

Compound 3aA'

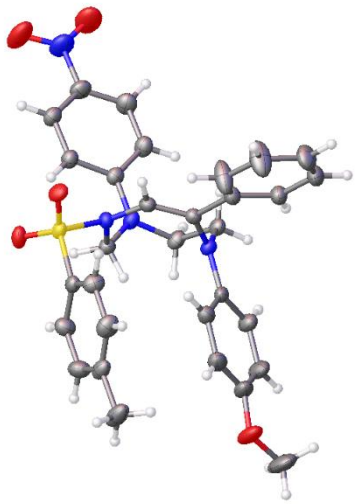
Empirical formula	$C_{32}H_{33}N_3O_2S$
CCDC	**2015202**
Formula weight	523.67
Temperature/K	180.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.9678(3)
b/Å	15.3212(4)
c/Å	17.9064(5)
α/°	111.225(3)
β/°	98.183(3)
γ/°	98.485(3)
Volume/Å^3	2710.90(15)
Z	4
ρ_{calc}g/cm^3	1.283
μ/mm^{-1}	1.327
F(000)	1112.0
Crystal size/mm^3	0.411 × 0.182 × 0.046
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.338 to 147.41
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -22 ≤ l ≤ 22
Reflections collected	42868
Independent reflections	10776 [R_{int} = 0.0370, R_{sigma} = 0.0292]
Data/restraints/parameters	10776/0/698
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.0989
Final R indexes [all data]	R_1 = 0.0480, wR_2 = 0.1064
Largest diff. peak/hole / e Å^{-3}	0.24/-0.42



There are two molecules per asymmetric unit. They can be overlaid. (root mean square deviations between the equivalent atoms in the two different molecules is 0.282A)

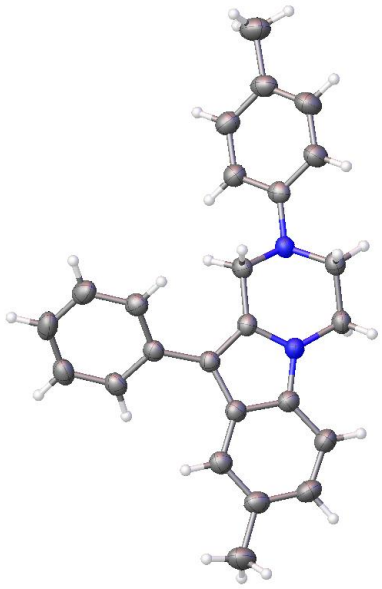
Compound 4aE

Empirical formula	$C_{31}H_{30}N_4O_5S$
CCDC	**2015200**
Formula weight	570.65
Temperature/K	180.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.14023(8)
b/Å	15.89219(10)
c/Å	18.23835(15)
α/°	90
β/°	105.5221(8)
γ/°	90
Volume/Å^3	2831.92(4)
Z	4
ρ_{calc}g/cm^3	1.338
μ/mm^{-1}	1.411
F(000)	1200.0
Crystal size/mm^3	0.426 × 0.303 × 0.19
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.5 to 147.26
Index ranges	-12 ≤ h ≤ 7, -19 ≤ k ≤ 19, -22 ≤ l ≤ 22
Reflections collected	19567
Independent reflections	5648 [R_{int} = 0.0234, R_{sigma} = 0.0189]
Data/restraints/parameters	5648/3/380
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0409, wR_2 = 0.1055
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.1083
Largest diff. peak/hole / e Å^{-3}	0.26/-0.53



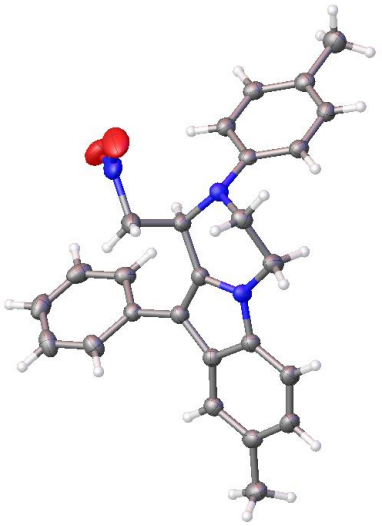
The O-methyl group is disordered and was refined using two components. Same distances restraints were applied, and anisotropic displacement parameters of identical atoms were constrained to be identical

Compound 5aA



Empirical formula	$C_{25}H_{24}N_2$
CCDC	**2015203**
Formula weight	352.46
Temperature/K	180.01(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	21.3021(10)
b/Å	7.7181(4)
c/Å	23.5444(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3871.0(3)
Z	8
ρ_{calc}g/cm^3	1.210
μ/mm^{-1}	0.539
F(000)	1504.0
Crystal size/mm^3	0.466 × 0.067 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.51 to 140.92
Index ranges	-17 ≤ h ≤ 25, -6 ≤ k ≤ 9, -28 ≤ l ≤ 19
Reflections collected	8929
Independent reflections	3621 [R_{int} = 0.0444, R_{sigma} = 0.0524]
Data/restraints/parameters	3621/0/247
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0549, wR_2 = 0.1293
Final R indexes [all data]	R_1 = 0.0881, wR_2 = 0.1547
Largest diff. peak/hole / e Å^{-3}	0.19/-0.21

Compound 6



CCDC	**2015204**
Empirical formula	$C_{26}H_{25}N_3O_2$
Formula weight	411.49
Temperature/K	149.99(10)
Crystal system	orthorhombic
Space group	Iba2
a/Å	18.50216(12)
b/Å	21.27952(14)
c/Å	10.92519(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4301.43(5)
Z	8
ρ_{calc}g/cm^3	1.271
μ/mm^{-1}	0.647
F(000)	1744.0
Crystal size/mm^3	0.652 × 0.112 × 0.049
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.33 to 149.794
Index ranges	$-23 \leq h \leq 23$, $-26 \leq k \leq 26$, $-13 \leq l \leq 12$
Reflections collected	89610
Independent reflections	4355 [R_{int} = 0.0318, R_{sigma} = 0.0090]
Data/restraints/parameters	4355/44/311
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0280, wR_2 = 0.0713
Final R indexes [all data]	R_1 = 0.0289, wR_2 = 0.0720
Largest diff. peak/hole / e Å^{-3}	0.11/-0.18
Flack parameter	-0.1(3)

The space group contains symmetry elements of the second kind.
The NO_2 group is disordered and was refined using two components with the same distance restraints on N-O distances and on C-N distances and rigid-bond restraints on displacement parameters.

12. Computational data

$Rh_2(Piv)_4$ with Me-Me imidazolidine – A to C

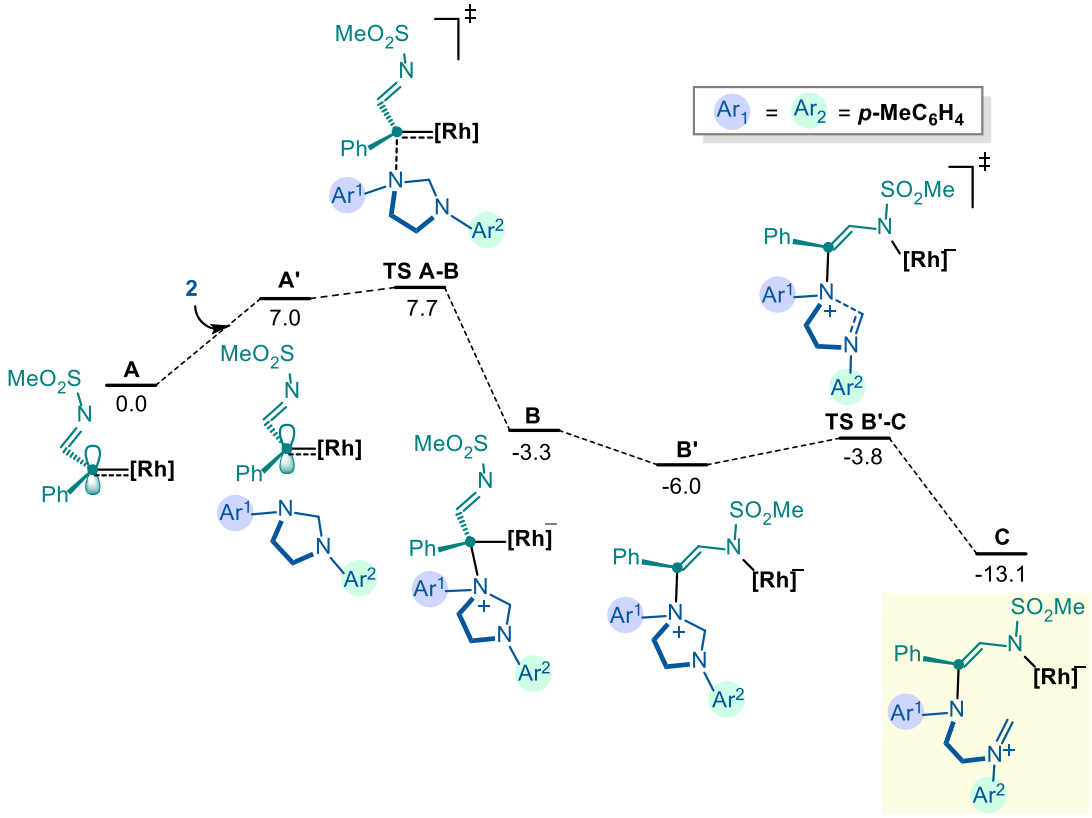


Fig. S1. Full Gibbs-energy profile for the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine ring opening by $Rh_2(Piv)_4$ system. Energies in kcal·mol^{-1}.

The full mechanism from **A** to **C** with the Me-Me (Ar^1, Ar^2 EDGs)imidazolidine and the $Rh_2(Piv)_4$ system is depicted in Fig. S1. The mechanism starts with the interaction of the imidazolidine **2** in **A'** found at 7.0 kcal·mol^{-1}. Then, **TS A-B** takes places with an overall barrier of 7.7 kcal·mol^{-1}, to form intermediate **B** placed at -3.3 kcal·mol^{-1} from the initial reactants. At this point, the next step would consist in the imidazolidine ring opening. Nevertheless, we were not able to find the transition state for this step while the Rh catalyst is attached to the C atom. Instead, the Rh catalyst switches from the C to the N atom in an exergonic step. At this point, the imidazolidine opening runs with a barrier of only 2.2 kcal·mol^{-1}, **TS B'-C**, to form intermediate **C** found at 13.1 kcal·mol^{-1} from the initial reactants.

$Rh_2(Piv)_4$ with Me-Me imidazolidine – C to 4

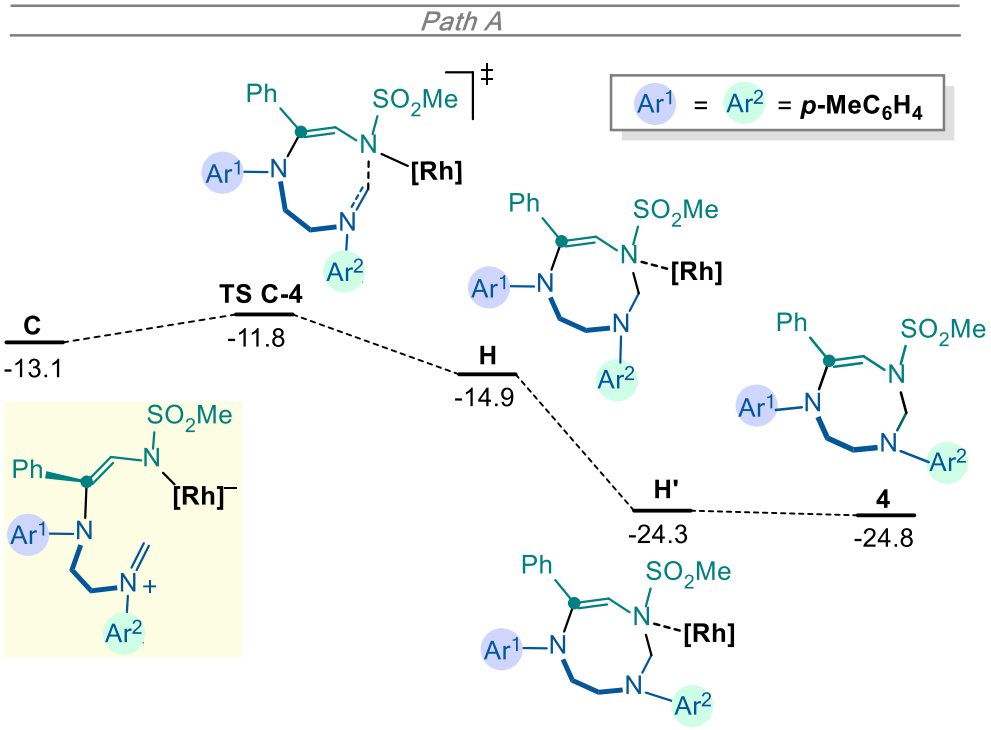


Fig. S2. Full Gibbs-energy profile for the formation of product **4** from intermediate **C** with the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine catalyzed by $Rh_2(Piv)_4$. Energies in kcal·mol^{-1}.

From intermediate **C**, product **4** is formed after a quasi-barrierless step, **TS C-4**, and subsequent rearrangement. The hexahydro-1,3,6-triazocines product **4** is found at 11.7 kcal·mol^{-1} below intermediate **C** and 24.8 kcal·mol^{-1} below **A** (Fig. S1).

$Rh_2(Piv)_4$ with Me-Me imidazolidine – C to 3 *via* Friedel-Crafts

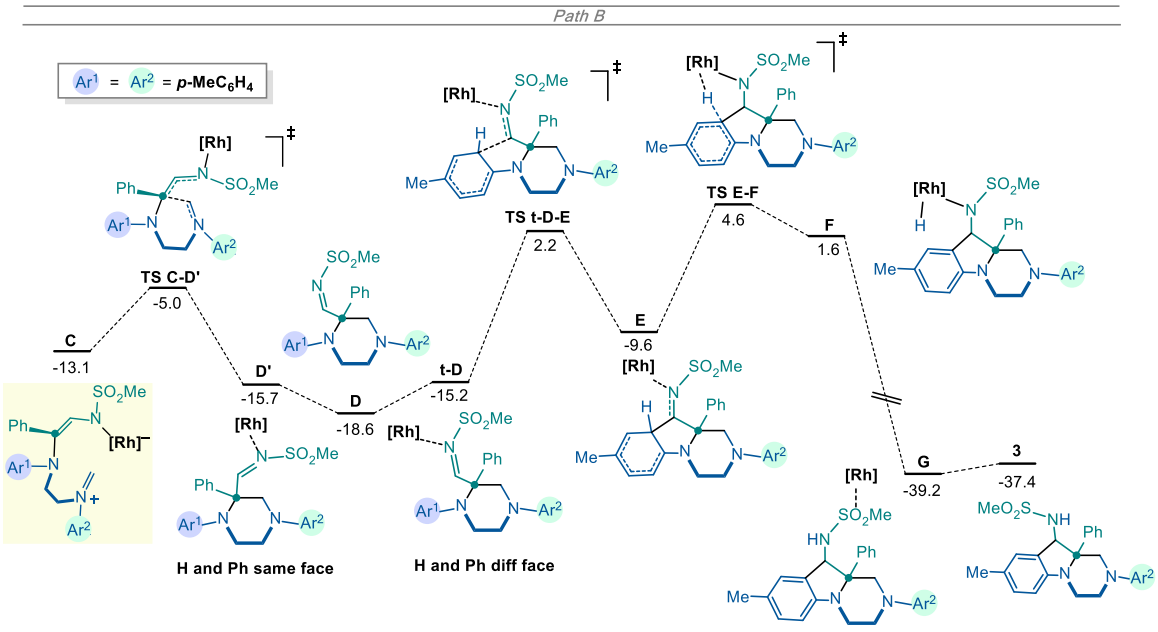


Fig. S3. Full Gibbs-energy profile for the formation of product **3** from intermediate **C** with the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine catalyzed by $Rh_2(Piv)_4$. Energies in kcal·mol^{-1}.

The full mechanism for the formation of the pyrazino-indoline **3** with the Me-Me imidazolidine catalyzed by $Rh_2(Piv)_4$ is depicted in Fig. S3. Starting from intermediate **C**, the first step consists in the C-C cyclization process with a related barrier of 8.1 kcal·mol^{-1}, to form intermediate **D'** found at 2.6 kcal·mol^{-1} below **C**. Intermediate **D'** presents the H (on the imine) and the Ph group on the same face. **D'** is able to rearrange to place the H and the Ph in opposite faces, in **t-D**. This process is almost isoenergetic and can take place upon the decoordination/coordination of the Rh catalyst. Intermediate **D** after the release of the Rh catalyst is found 5.5 kcal·mol^{-1} below intermediate **C**. From **t-D**, the reaction proceeds via a Friedel-Crafts process. The final product **3** is thus found at 37.4 kcal·mol^{-1} below the initial reactants **A** (Fig. S1). The highest point of this process is related with the catalyst assisted proton transfer (**TS E-F**), with a barrier of 23.2 kcal·mol^{-1} from intermediate **D**. We were not able to obtain the transition state connecting intermediate **F** and **G**. We assume that this step is barrierless considering the energy difference between the intermediates.

$Rh_2(Piv)_4$ with MeO-NO_2 imidazolidine – A to C

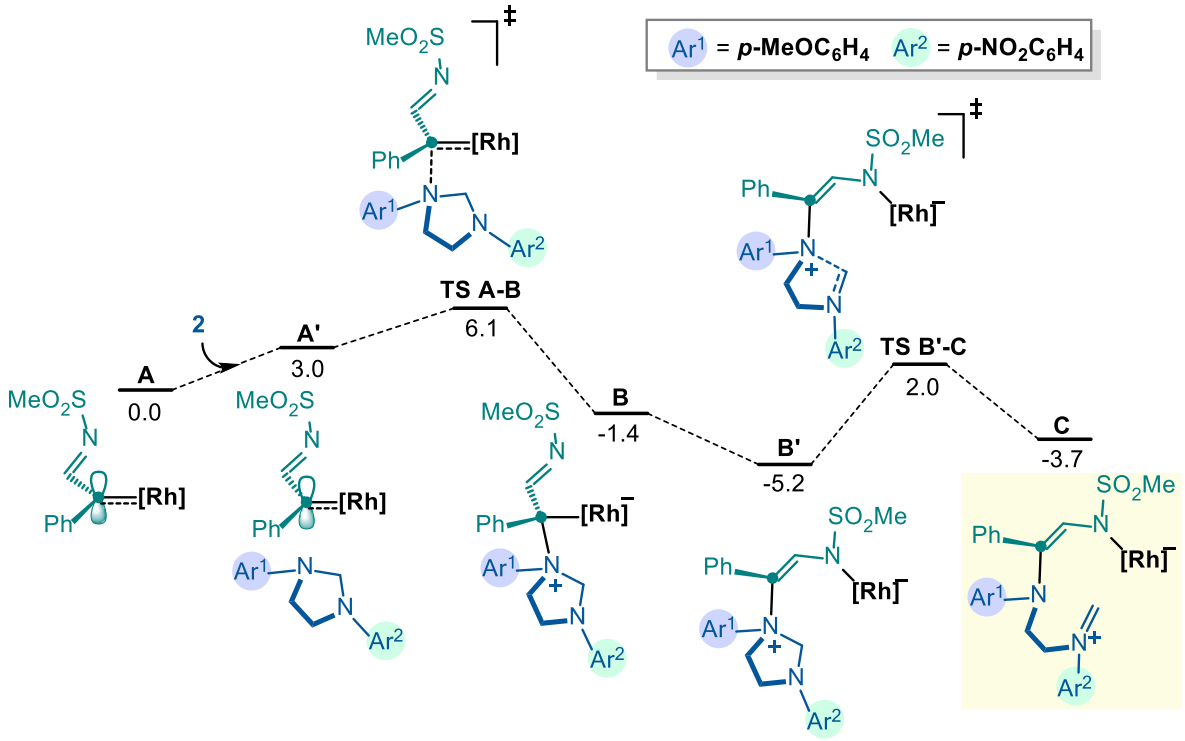


Fig. S4. Full Gibbs-energy profile for the MeO-NO_2 (Ar^1 EDG, Ar^2 EWG) imidazolidine ring opening by $Rh_2(Piv)_4$ system. Energies in kcal·mol^{-1}.

The results for the iminium intermediate **C** formation from **A** with the MeO-NO_2 imidazolidine, catalyzed by $Rh_2(Piv)_4$ is depicted in Fig. S4. The mechanism is the same as explained in Fig. S1. The main difference between the two systems is the relative energy of **C**.

$Rh_2(Piv)_4$ with MeO-NO_2 imidazolidine – C to 4 and C to E

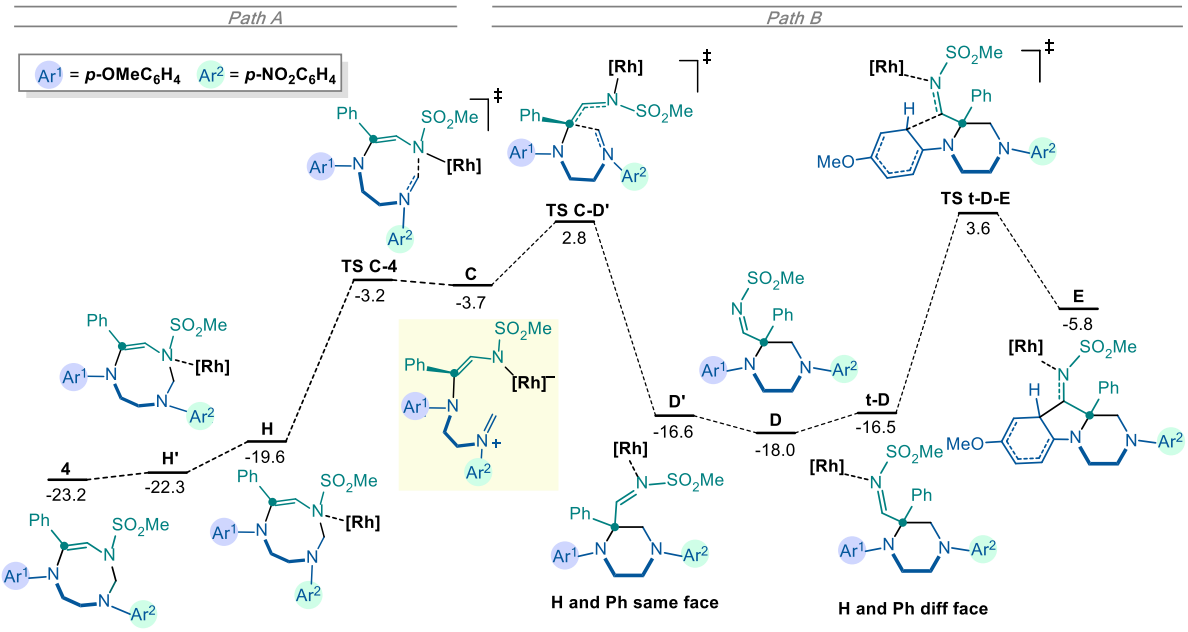


Fig. S5. Gibbs-energy profile for the 8-membered (left) or 6-membered (right) ring formation from the iminium intermediate **C**$_{(MeO\text{-}NO2)}$. Energies in kcal·mol^{-1}.

The formation of hexahydro-1,3,6-triazocines product **4** with the MeO-NO_2 runs almost barrierless (Fig. S5, Path A). The activation barrier is only 0.5 kcal·mol^{-1} to form the C—N bond. After rearrangement and catalyst liberation the final product **4** is found at 23.2 kcal·mol^{-1} below the initial reactants. The process to achieve product **3** (Fig. S5, Path B) would be exactly the same than the one explained in Fig. S3. Nevertheless, we did not calculate the full mechanism since experimentally product **3** while using the MeO-NO_2 imidazolidine is not observed. This can be rationalized due to the energy found for **TS C-D'** which will make the reaction irreversible once product **4** is formed.

$Rh_2(OAc)_4$ with Me-Me imidazolidine – A to C

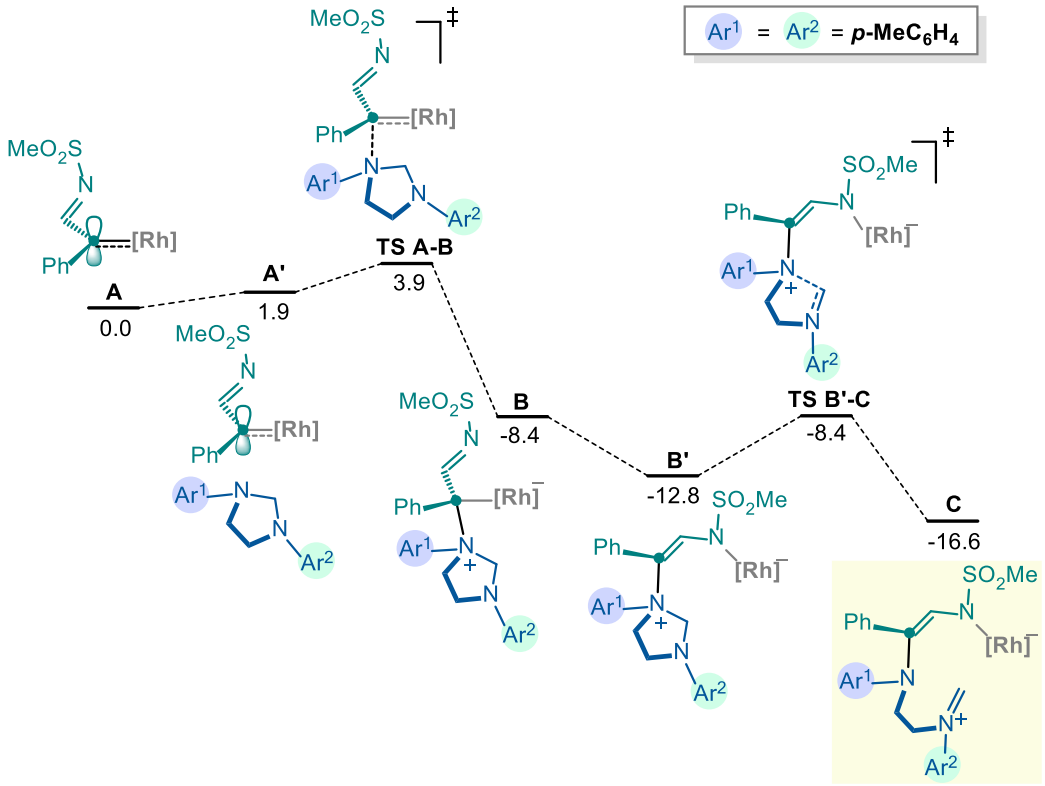


Fig. S6. Full Gibbs-energy profile for the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine ring opening by $Rh_2(OAc)_4$ system. Energies in kcal·mol^{-1}.

We have also calculated the formation of the iminium ion intermediate **C** with the Me-Me imidazolidine with the $Rh_2(OAc)_4$ catalyst (Fig. S6). The results are very similar to that obtained with the $Rh_2(Piv)_4$ catalyst and will not be further explained.

$Rh_2(OAc)_4$ with Me-Me imidazolidine – A to t-C

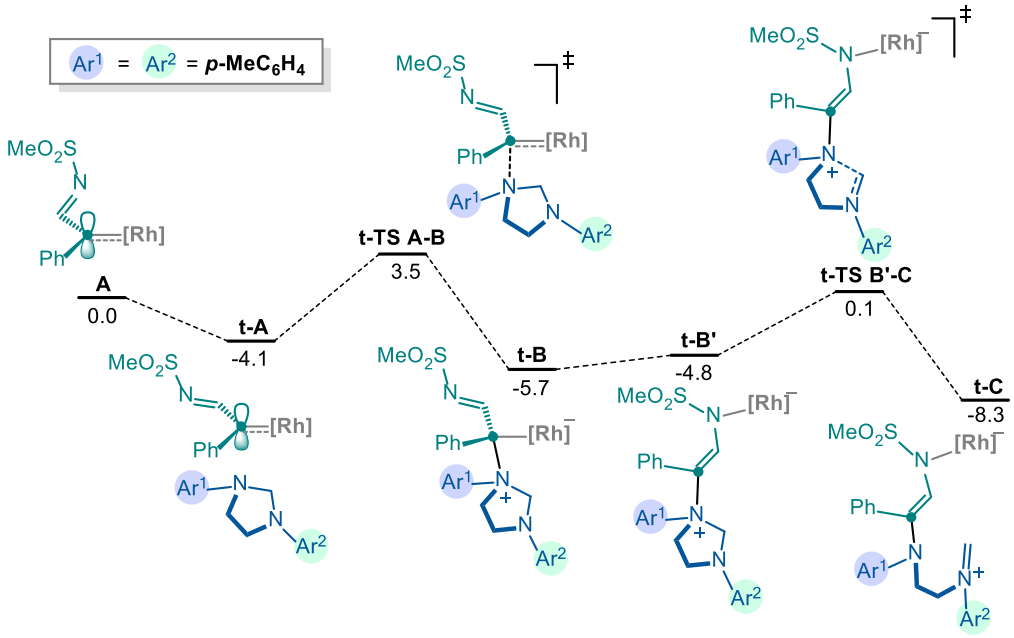


Fig. S7. Full Gibbs-energy profile for the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine ring opening by $Rh_2(OAc)_4$ system with a "*trans*" disposition of the carbene moiety. Energies in kcal·mol^{-1}.

We have also calculated the formation of the intermediate **t-C** with a *trans* disposition of the carbene moiety (Fig. S7); that is, with the N of the carbene and the N of the imidazolidine in a *trans* conformation. Although the adduct **t-A** is more stable than **A** in Fig. S6, the activation barrier for **t-TS A-B** is 3.7 kcal·mol^{-1} higher than that of **TS A-B**, favouring the mechanism with the *cis* conformation.

$Rh_2(OAc)_4$ with Me-Me imidazolidine – A to B'2

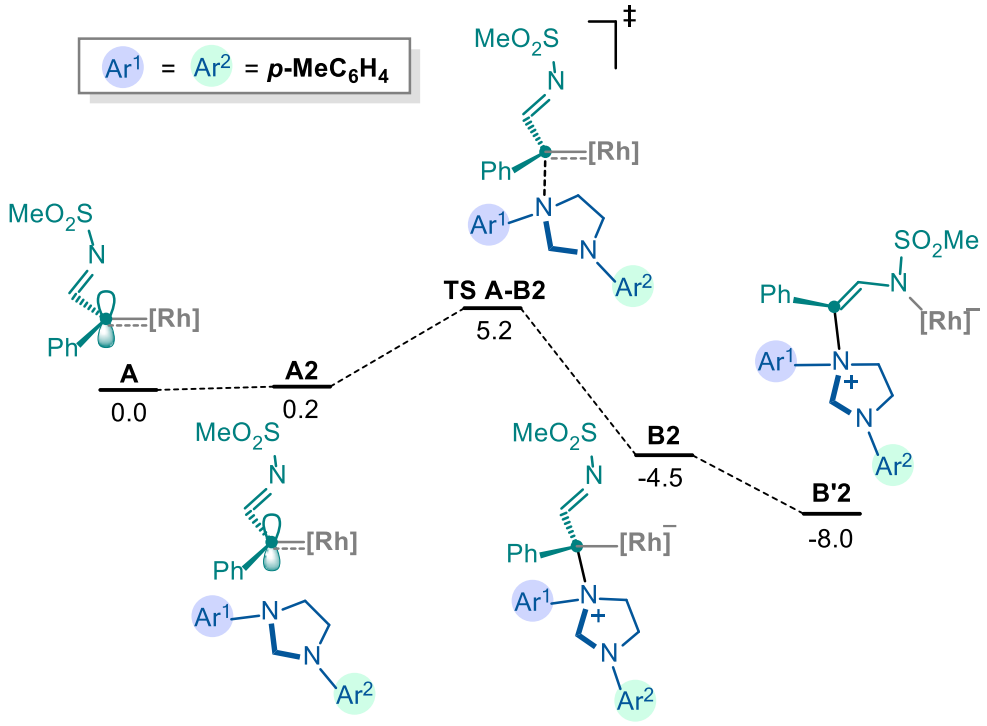


Fig. S8. Gibbs-energy profile for the Me-Me (Ar^1, Ar^2 EDGs) imidazolidine interaction with the $Rh_2(OAc)_4$ carbene complex. Energies in kcal·mol^{-1}.

We investigated the C—N formation step between the imidazolidine **2** and the carbene complex **A** with a different disposition of the imidazolidine. As shown in Fig. S8, the activation barrier for **TS A-B2** is only 5.2 kcal·mol^{-1}. Nevertheless, the one with the normal disposition is lower by 1.3 kcal·mol^{-1}, suggesting that the "normal" disposition will be the preferred one.

$Rh_2(OAc)_4$ with Me-Me imidazolidine – C to 4 and C to D'

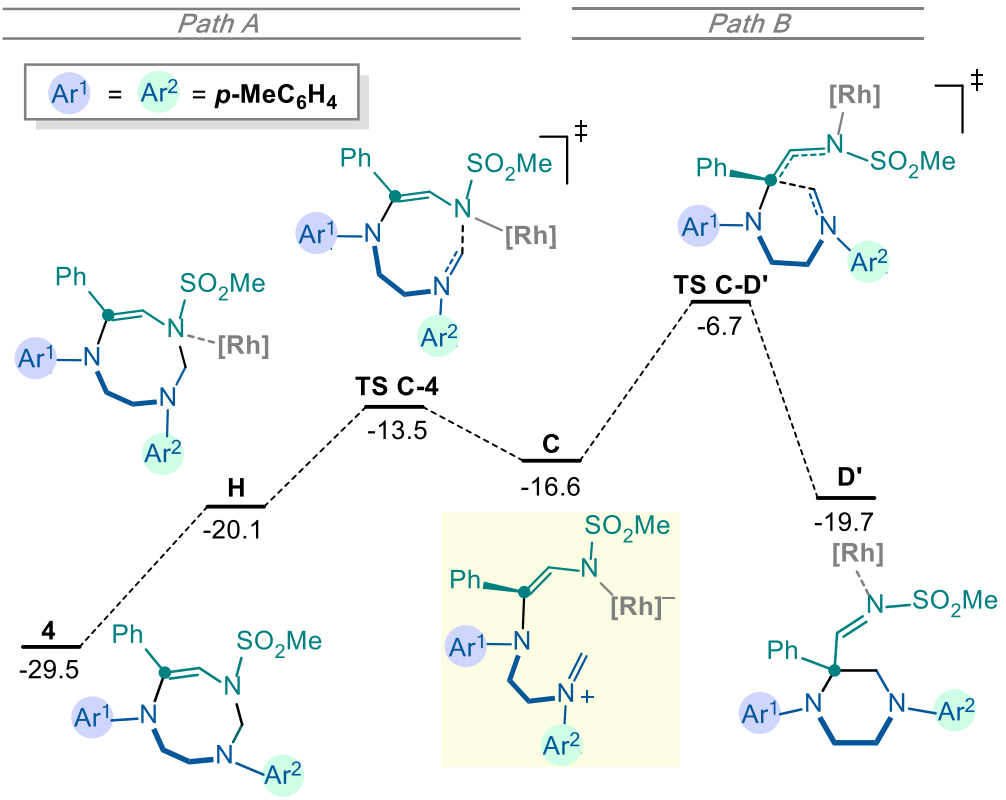


Fig. S9 Gibbs-energy profile for the 8-membered (left) or 6-membered (right) ring formation from the iminium intermediate **C** catalyzed by $Rh_2(OAc)_4$ with the Me-Me imidazolidine. Energies in kcal·mol^{-1}.

We have investigated the formation of product **4** and intermediate **D'** from intermediate **C** catalyzed with the $Rh_2(OAc)_4$ catalyst. The computed results show that product **4** can evolve backwards to form intermediate **D'** with a barrier of 22.8 kcal·mol^{-1}, thus permitted at the reactions conditions. From **D'**, the system would advance towards the formation of product **3** following the same mechanism shown in Fig. S3.

$Rh_2(OAc)_4$ with MeO-NO_2 imidazolidine – A to C

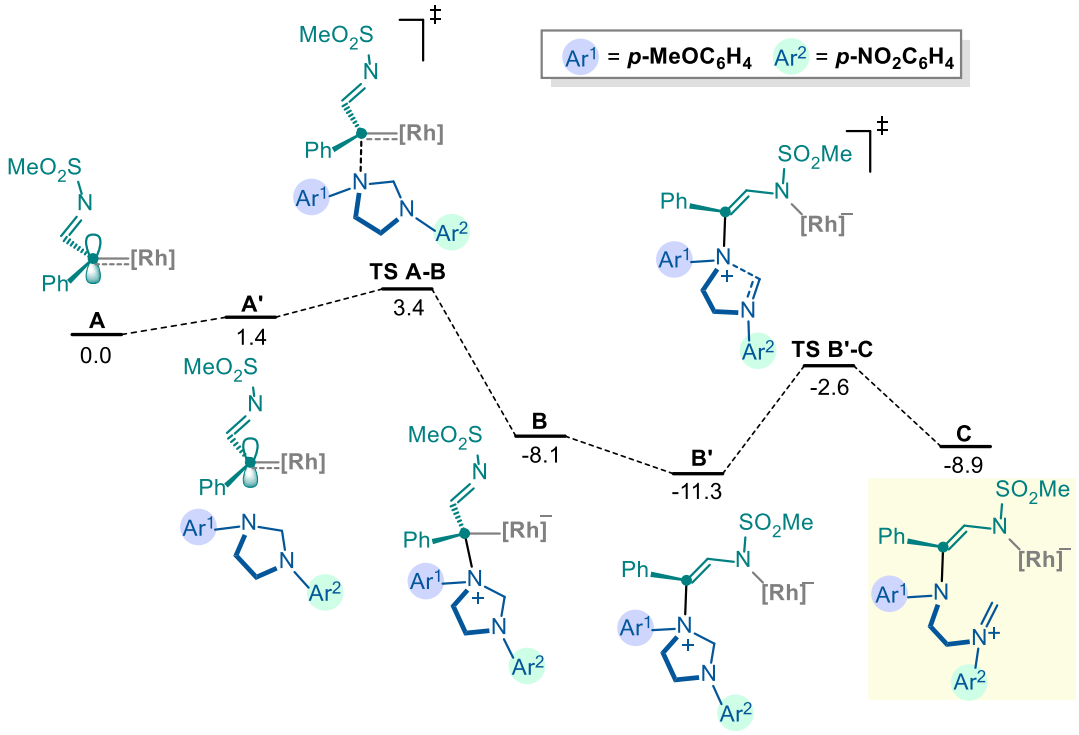


Fig. S10. Full Gibbs-energy profile for the MeO-NO_2 (Ar^1 EDG, Ar^2 EWG) imidazolidine ring opening by $Rh_2(OAc)_4$ system. Energies in kcal·mol^{-1}.

The computed results for the formation of the iminium ion intermediate **C** with the MeO-NO_2 imidazolidine with the $Rh_2(OAc)_4$ catalyst do not show any remarkable difference with that obtained with the $Rh_2(Piv)_4$ system. Interestingly, the energies of intermediate **C** with the different imidazolidines with the $Rh_2(OAc)_4$ (-16.6 and -8.9 kcal·mol^{-1} for the Me-Me and MeO-NO_2 imidazolidine, respectively) follow the same trends than that obtained with the real catalyst (-13.1 and -3.7 kcal·mol^{-1} for the Me-Me and MeO-NO_2 imidazolidine, respectively). This clearly suggests that the selectivity of the reactions is triggered by the nature of the substituents on the imidazolidine.

$Rh_2(OAc)_4$ with MeO-NO_2 imidazolidine – C to 4 and C to D'

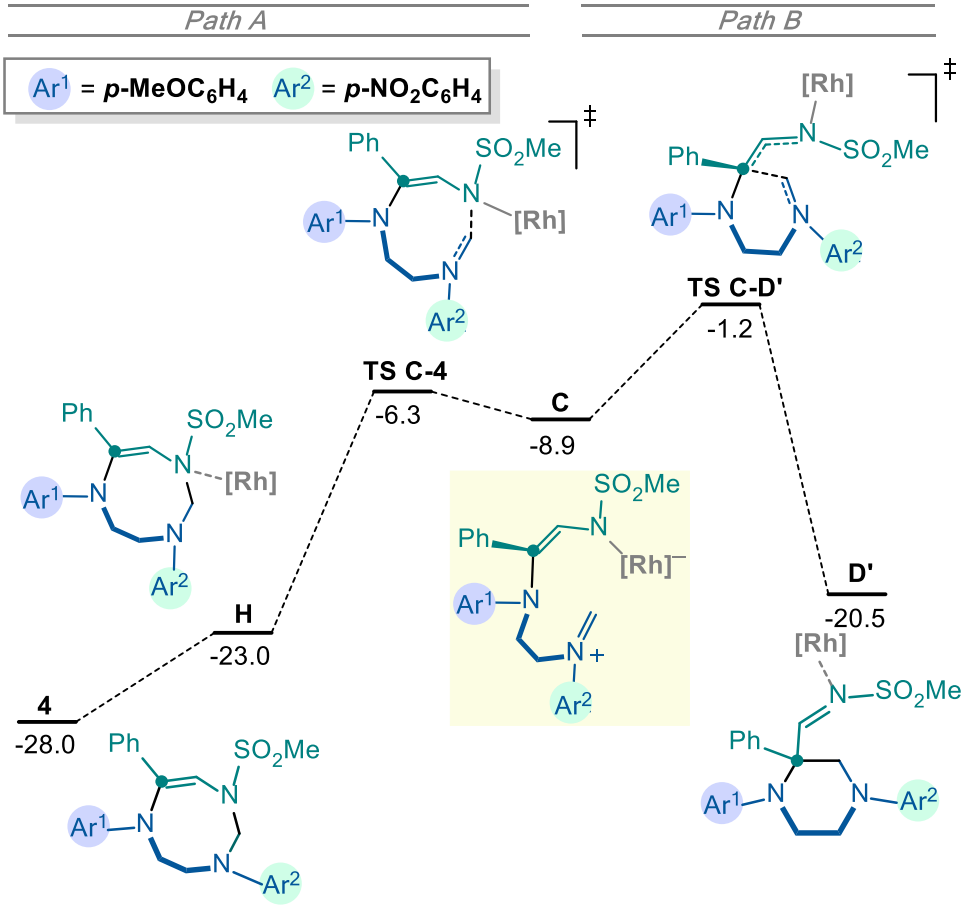


Fig. S11 Gibbs-energy profile for the 8-membered (left) or 6-membered (right) ring formation from the iminium intermediate **C** catalyzed by $Rh_2(OAc)_4$ with the MeO-NO_2 imidazolidine. Energies in kcal·mol^{-1}.

We have investigated the formation of product **4** and intermediate **D'** from intermediate **C** catalyzed with the $Rh_2(OAc)_4$ catalyst with the MeO-NO_2 imidazolidine. In this case, the computed results show that product 4 is formed preferentially and it cannot evolve backwards to form intermediate **D'**. The activation barrier to form **D'** is 26.8 kcal·mol^{-1} from product **4** to **TS C-D'**, thus not permitted at the reaction conditions.

$Rh_2(OAc)_4$ with MeO-NO_2 imidazolidine – A to t-B (N-selectivity)

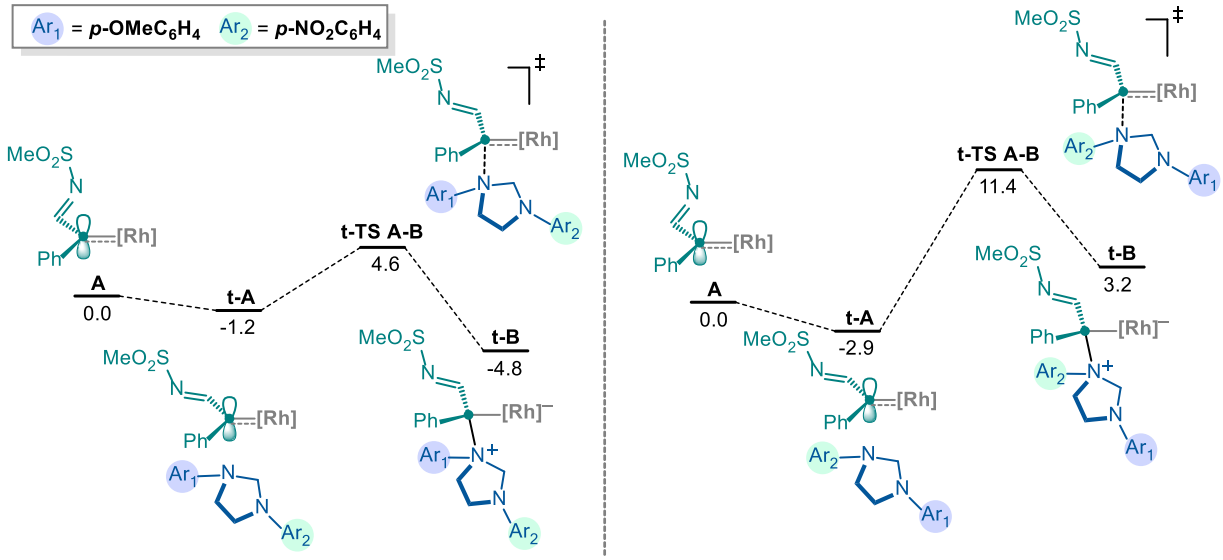


Fig. S12 Gibbs-energy profile for the formation of **t-B** from **A** with the MeO-NO_2 imidazolidine catalyzed by $Rh_2(OAc)_4$. Left: Carbene attack on the N bearing the *p*-$MeOC_6H_4$. Right: carbene attack on the N bearing the *p*-$NO_2C_6H_4$. Energies in kcal·mol^{-1}.

In order to check the N attack selectivity, we decided to compute the first step of the reaction with the MeO-NO_2 imidazolidine catalyzed by $Rh_2(OAc)_4$. The results are shown in Fig. S12. We can clearly see that while the attack on the N bearing the *p*-$MeOC_6H_4$ has a barrier of 5.8 kcal·mol^{-1} (Fig. S12, left), the attack on the N bearing the *p*-$NO_2C_6H_4$ has a barrier of 14.3 kcal·mol^{-1} (Fig. S12, right). This demonstrates the selectivity of the carbene attack towards the electron rich N of the imidazolidine.

$Rh_2(Piv)_4$ with Me-Me imidazolidine –diastereomeric product formation, *Major vs Minor*

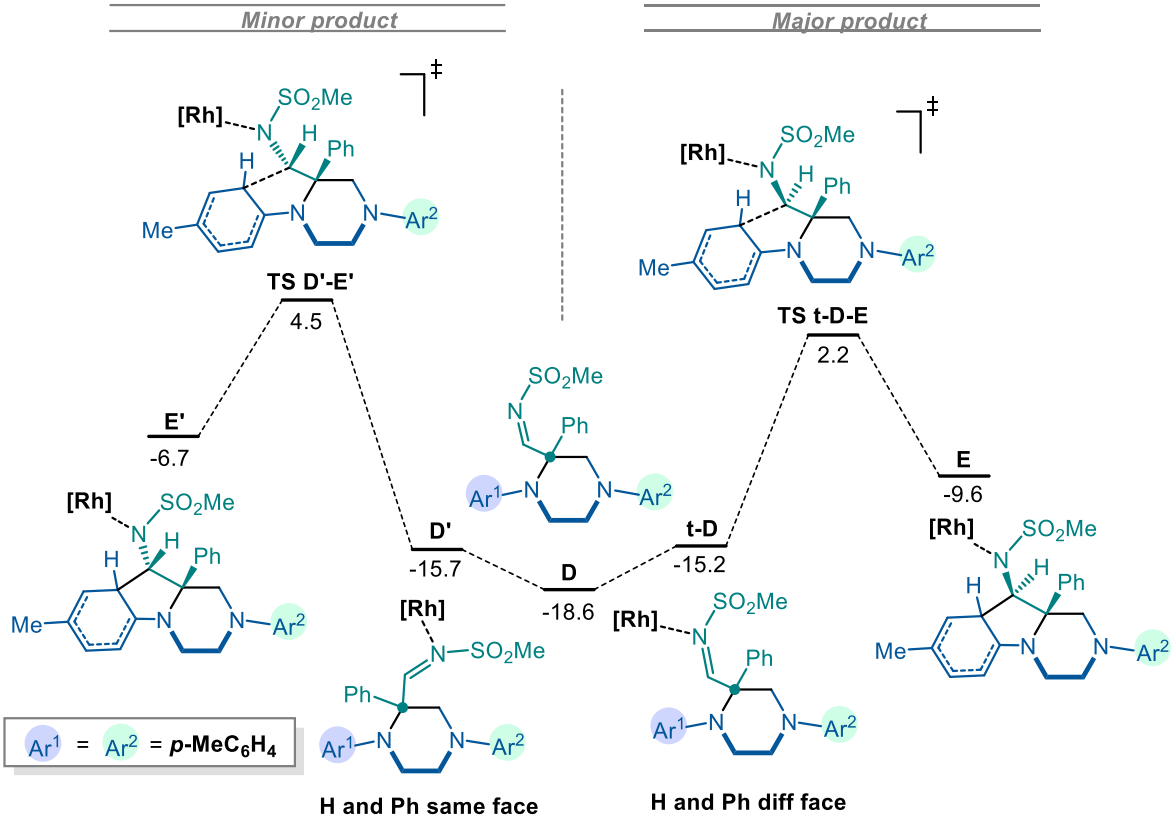


Fig. S13 Gibbs-energy profile for the formation of **E** and **E'** from **D** with the Me-Me imidazolidine catalyzed by $Rh_2(Piv)_4$. Left: formation pathway for the minor product. Right: formation pathway for the major product. Energies in kcal·mol^{-1}.

The final Friedel-Crafts reaction leads to the formation of a diastereomeric mixture of products with, somewhat surprisingly, a predominance for the *cis*-adduct over the *trans*. We investigated the initial step for the formation of (i, left) the minor product from intermediate **D'** to compare it to (ii, right) the formation of the major product. As shown in Fig. S13, **TS D'-E'** is 2.3 kcal·mol^{-1} higher that **TS t-D-E**, in agreement with the experimental results. However, the rational for the preferred *cis* selectivity is not trivial. We theorize that the steric clash between the organic moiety, that is, the skeleton of the imidazolidine; and the ligands in the $Rh_2(Piv)_4$ catalyst is larger in the **D'** disposition than in the **t-D** disposition.

13. Computational details

All calculations were carried out using Gaussian09 (Rev. D01) package[8] at the B3LYP-D3 level of theory.[9] Optimizations and frequency calculations were ran using the basis set 6-31G*[10] for light atoms and LANL2DZ[11] and its corresponding pseudopotential for the Rh atom; in dichloromethane solution (ε = 8.93), using the SMD model.[12] The potential energies for the $Rh_2(Piv)_4$ system were further refined with larger basis set: 6-311++G**[13] for light atoms and LANL2TZ(f) [14] for the Rh. All stationary points were assigned to a minima (zero imaginary frequencies) or transition state (one imaginary frequency) by frequency analysis. All the reports energies are Gibbs free energies in solution calculated at 298 K and 1 atm in $kcal \cdot mol^{-1}$.

14. XYZ Coordinates

A-OAc-Me-Me

Energy (POTENTIAL) = -2084.85010457 Eh

Atom	X	Y	Z
S	-7.6917	3.4652	0.2331
O	-9.1054	3.4975	0.6432
O	-7.1935	2.2799	-0.4932
N	-6.7487	3.7972	1.6288
C	-5.2842	2.8822	3.2539
C	-5.9180	2.8620	1.9556
H	-5.7776	1.9567	1.3515
C	-4.2749	3.8061	3.6202
C	-2.7127	5.5831	3.0152
H	-2.2754	6.2446	2.2738
C	-3.7014	4.6846	2.6514
H	-4.0440	4.6398	1.6230
C	-3.8120	3.8791	4.9673
H	-4.2476	3.2246	5.7091
C	-2.8298	4.7913	5.3201
H	-2.4865	4.8498	6.3484
C	-2.2781	5.6373	4.3483
H	-1.5033	6.3449	4.6306
C	-7.3310	4.9388	-0.7252
H	-7.5957	5.8152	-0.1298
H	-6.2677	4.9432	-0.9764
H	-7.9391	4.8927	-1.6328
Rh	-6.1091	1.3803	4.3459
Rh	-7.0846	-0.4742	5.6415
O	-8.0004	1.7176	3.5879
O	-8.9073	-0.0063	4.7534
O	-5.1894	-0.8100	6.4250
O	-4.2857	0.8801	5.2057
O	-5.7773	0.0048	2.8275
O	-6.6528	-1.7114	4.0281
O	-6.5315	2.6066	5.9607
O	-7.4525	0.9062	7.1505
C	-8.9713	0.9616	3.9357
C	-7.1063	2.1140	6.9939
C	-4.2232	-0.0831	6.0463
C	-6.1311	-1.2156	2.9860
C	-7.4048	3.0905	8.1045
C	-2.8541	-0.3663	6.6152
C	-5.9070	-2.1203	1.7997
C	-10.3110	1.2927	3.3265
H	-6.5091	3.6757	8.3349
H	-8.1797	3.7879	7.7654
H	-7.7530	2.5678	8.9973
H	-10.8825	1.8930	4.0453
H	-10.1770	1.8729	2.4108
H	-10.8724	0.3755	3.1290
H	-4.8715	-2.0322	1.4558
H	-6.5581	-1.7967	0.9794
H	-6.1306	-3.1577	2.0549
H	-2.4265	0.5561	7.0210
H	-2.1958	-0.7110	5.8097
H	-2.9066	-1.1295	7.3939

A_-OAc-Me-Me

Energy (POTENTIAL) = -2854.27317456 Eh

Atom	X	Y	Z
S	-5.5911	1.9112	-0.3511
O	-6.9455	1.6181	-0.8558
O	-4.6681	0.7823	-0.1142
N	-10.1559	4.0857	1.7969
N	-5.7918	2.8869	1.0350
C	-13.2926	1.2541	1.3968
C	-13.5418	2.5662	1.8216
H	-14.5634	2.8702	2.0427
C	-12.5197	3.5040	1.9632
H	-12.7662	4.5156	2.2702
C	-11.1777	3.1597	1.6831
C	-10.9209	1.8368	1.2517
H	-9.9092	1.5247	1.0190
C	-11.9607	0.9196	1.1133
H	-11.7253	-0.0871	0.7725
C	-10.2551	5.2608	2.6709
H	-10.9497	5.0914	3.5018
H	-10.5965	6.1417	2.1115
C	-8.8071	5.4362	3.1750
H	-8.5390	6.4789	3.3441
H	-8.6588	4.8705	4.0978

C	-5.6987	2.9719	3.4052
C	-5.3036	2.4100	2.1302
H	-4.7110	1.4876	2.1621
C	-8.7466	3.6572	1.7163
H	-8.4749	3.3050	0.7232
H	-8.5524	2.8468	2.4250
C	-5.2903	4.2493	3.8636
C	-5.4758	6.0713	5.4707
H	-5.9472	6.5189	6.3405
C	-5.8912	4.8294	5.0176
H	-6.6867	4.2939	5.5184
C	-7.4308	5.6875	1.1418
C	-7.6032	5.5238	-0.2440
H	-8.2413	4.7381	-0.6317
C	-6.9677	6.3792	-1.1462
H	-7.1291	6.2283	-2.2119
C	-6.1468	7.4314	-0.7179
C	-5.9914	7.5989	0.6654
C	-6.6112	6.7472	1.5768
H	-6.4436	6.8853	2.6397
C	-4.2607	4.9700	3.1925
H	-3.8085	4.5465	2.3022
C	-3.8260	6.1942	3.6794
H	-3.0296	6.7300	3.1723
C	-4.4347	6.7462	4.8138
H	-5.3599	8.4021	1.0406
N	-7.9847	4.8261	2.1148
H	-4.1004	7.7105	5.1866
C	-4.8060	3.0982	-1.4428
H	-5.4312	3.9926	-1.4889
H	-3.8165	3.3360	-1.0449
H	-4.7223	2.6293	-2.4270
C	-14.4041	0.2385	1.2690
H	-14.2230	-0.4525	0.4371
H	-14.5041	-0.3721	2.1777
H	-15.3724	0.7232	1.0982
C	-5.4348	8.3272	-1.7041
H	-5.9682	8.3747	-2.6603
H	-5.3360	9.3496	-1.3208
H	-4.4194	7.9640	-1.9177
Rh	-6.6627	1.4876	4.4252
Rh	-7.6812	-0.3952	5.6516
O	-8.4063	2.5391	4.8133
O	-9.4059	0.7536	5.7969
O	-5.8873	-1.4144	5.3984
O	-4.9977	0.2694	4.1650
O	-7.4812	0.6763	2.7054
O	-8.3283	-1.1167	3.8079
O	-5.8884	2.1238	6.2409
O	-6.9351	0.4703	7.3939
C	-9.4010	1.9410	5.3561
C	-6.1973	1.4971	7.3126
C	-4.9647	-0.8893	4.7093
C	-8.0874	-0.4486	2.7572
C	-5.5854	2.0281	8.5862
C	-3.6899	-1.6706	4.5073
C	-8.5581	-1.0161	1.4411
C	-10.6849	2.7274	5.4358
H	-5.5583	3.1210	8.5683
H	-6.1405	1.6743	9.4575
H	-4.5524	1.6652	8.6544
H	-10.4769	3.7864	5.6065
H	-11.2080	2.6330	4.4763
H	-11.3280	2.3330	6.2254
H	-8.2140	-0.3997	0.6083
H	-9.6522	-1.0634	1.4434
H	-8.1803	-2.0381	1.3326
H	-2.8734	-1.1663	5.0368
H	-3.4347	-1.6897	3.4431
H	-3.7950	-2.6888	4.8862

A-B-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.27217595 Eh

Atom	X	Y	Z
S	-5.3347	1.7176	-0.3162
O	-6.4929	1.0387	-0.9259
O	-4.2100	0.8900	0.1692
N	-10.1092	4.0565	1.8032
N	-5.9497	2.7514	0.8885
C	-13.3966	1.3778	1.5594
C	-13.5650	2.7077	1.9702
H	-14.5605	3.0631	2.2297

C	-12.4942	3.5968	2.0521
H	-12.6775	4.6234	2.3536
C	-11.1837	3.1819	1.7271
C	-11.0100	1.8455	1.2989
H	-10.0268	1.4786	1.0276
C	-12.0971	0.9766	1.2205
H	-11.9245	-0.0452	0.8871
C	-10.1003	5.2024	2.7209
H	-10.8061	5.0659	3.5474
H	-10.3564	6.1318	2.1964
C	-8.6492	5.2224	3.2341
H	-8.2954	6.2223	3.4766
H	-8.5525	4.5781	4.1053
C	-5.9502	3.1973	3.2782
C	-5.4401	2.6032	2.0624
H	-4.6232	1.8895	2.2465
C	-8.7430	3.5285	1.6713
H	-8.5145	3.2190	0.6557
H	-8.5934	2.6704	2.3252
C	-5.3700	4.3806	3.8311
C	-5.3425	6.1216	5.5357
H	-5.7559	6.5620	6.4385
C	-5.8876	4.9534	5.0231
H	-6.7176	4.4703	5.5197
C	-7.3386	5.5271	1.1744
C	-7.5051	5.3883	-0.2149
H	-8.1097	4.5888	-0.6241
C	-6.9094	6.2891	-1.0957
H	-7.0704	6.1596	-2.1639
C	-6.1235	7.3589	-0.6428
C	-5.9687	7.4977	0.7416
C	-6.5600	6.6056	1.6353
H	-6.4063	6.7478	2.6982
C	-4.2783	5.0256	3.1884
H	-3.8825	4.6121	2.2659
C	-3.7103	6.1714	3.7330
H	-2.8669	6.6463	3.2408
C	-4.2477	6.7258	4.8997
H	-5.3697	8.3155	1.1366
N	-7.8732	4.6128	2.1263
H	-3.8147	7.6311	5.3165
C	-4.7114	2.9373	-1.4759
H	-5.5198	3.6297	-1.7194
H	-3.8775	3.4694	-1.0121
H	-4.3773	2.4008	-2.3680
C	-14.5587	0.4141	1.5060
H	-14.4400	-0.3164	0.6970
H	-14.6562	-0.1559	2.4410
H	-15.5082	0.9389	1.3486
C	-5.4531	8.3051	-1.6095
H	-6.0168	8.3884	-2.5456
H	-5.3508	9.3097	-1.1835
H	-4.4427	7.9597	-1.8696
Rh	-6.8145	1.5844	4.3303
Rh	-7.6401	-0.4064	5.5334
O	-8.6780	2.4236	4.6880
O	-9.4571	0.5759	5.7475
O	-5.7816	-1.2767	5.2246
O	-5.0200	0.5532	4.1188
O	-7.5029	0.6823	2.5965
O	-8.2666	-1.1508	3.6932
O	-6.1442	2.2821	6.1691
O	-6.9434	0.4719	7.2838
C	-9.5870	1.7466	5.2815
C	-6.3466	1.5893	7.2231
C	-4.8980	-0.6320	4.5847
C	-8.0549	-0.4690	2.6442
C	-5.7799	2.1482	8.5062
C	-3.5651	-1.2960	4.3406
C	-8.5080	-1.0469	1.3262
C	-10.9369	2.4090	5.3972
H	-5.7772	3.2407	8.4819
H	-6.3474	1.7858	9.3663
H	-4.7426	1.8049	8.6057
H	-10.8204	3.4739	5.6160
H	-11.4535	2.3178	4.4346
H	-11.5376	1.9260	6.1707
H	-8.0561	-0.5033	0.4937
H	-9.6000	-0.9688	1.2651
H	-8.2455	-2.1078	1.2775
H	-2.7803	-0.7336	4.8590
H	-3.3384	-1.2724	3.2696

H	-3.5734	-2.3273	4.6978

B-OAc-Me-Me

Energy (POTENTIAL) = -2854.29465230 Eh

Atom	X	Y	Z
S	-5.1379	1.4538	0.0308
O	-5.9361	0.2674	-0.3410
O	-3.8282	1.2199	0.6819
N	-9.9360	4.0608	1.8298
N	-6.1162	2.5170	0.8733
C	-13.5211	1.9495	0.9861
C	-13.5312	3.3166	1.3049
H	-14.4783	3.8521	1.3282
C	-12.3596	4.0141	1.5864
H	-12.4082	5.0758	1.8090
C	-11.1122	3.3570	1.5643
C	-11.0904	1.9844	1.2457
H	-10.1549	1.4354	1.2238
C	-12.2778	1.3073	0.9606
H	-12.2287	0.2479	0.7176
C	-9.9152	5.1974	2.7607
H	-10.7297	5.1459	3.4914
H	-9.9858	6.1486	2.2223
C	-8.5743	5.0397	3.4717
H	-8.1287	5.9724	3.7998
H	-8.6527	4.3399	4.3004
C	-6.4129	3.6839	3.0015
C	-5.6942	2.8926	2.0550
H	-4.7211	2.5562	2.4151
C	-8.7057	3.3080	1.9616
H	-8.3733	2.8371	1.0448
H	-8.7473	2.5588	2.7465
C	-5.5861	4.6116	3.8450
C	-5.2176	5.9349	5.8617
H	-5.5602	6.2516	6.8436
C	-5.9919	5.0422	5.1215
H	-6.9022	4.6517	5.5549
C	-7.3444	5.3321	1.3353
C	-7.5796	5.0501	-0.0108
H	-8.0585	4.1347	-0.3241
C	-7.1988	5.9719	-0.9862
H	-7.3941	5.7371	-2.0293
C	-6.5814	7.1834	-0.6525
C	-6.3698	7.4522	0.7056
C	-6.7464	6.5438	1.6940
H	-6.5572	6.7930	2.7290
C	-4.3568	5.0968	3.3543
H	-4.0293	4.8157	2.3576
C	-3.5635	5.9635	4.1078
H	-2.6195	6.3172	3.7013
C	-3.9964	6.3965	5.3627
H	-5.9047	8.3880	1.0045
N	-7.7014	4.3461	2.4239
H	-3.3891	7.0831	5.9467
C	-4.8574	2.4108	-1.4666
H	-5.8230	2.6440	-1.9200
H	-4.3254	3.3286	-1.2055
H	-4.2560	1.7974	-2.1431
C	-14.8053	1.2052	0.7047
H	-14.6110	0.2356	0.2332
H	-15.3709	1.0143	1.6273
H	-15.4640	1.7772	0.0398
C	-6.1427	8.1578	-1.7173
H	-6.7317	8.0428	-2.6333
H	-6.2354	9.1941	-1.3744
H	-5.0890	7.9966	-1.9826
Rh	-6.8094	1.6074	4.3542
Rh	-7.2501	-0.4592	5.5918
O	-8.7258	2.2195	4.9083
O	-9.1552	0.2741	5.9891
O	-5.3403	-1.0911	5.0684
O	-4.9342	0.8396	3.9492
O	-7.5770	0.6344	2.6933
O	-7.9610	-1.2890	3.8282
O	-6.0457	2.3750	6.1249
O	-6.4979	0.4757	7.2845
C	-9.4855	1.4172	5.5519
C	-6.0446	1.6597	7.1788
C	-4.6183	-0.3274	4.3527
C	-7.9587	-0.5790	2.7736
C	-5.4082	2.2685	8.4052
C	-3.2505	-0.8136	3.9431

C	-8.4668	-1.2002	1.4970
C	-10.9052	1.8796	5.7688
H	-5.5365	3.3537	8.4047
H	-5.8288	1.8336	9.3148
H	-4.3330	2.0515	8.3812
H	-10.9166	2.9294	6.0765
H	-11.4427	1.8041	4.8155
H	-11.4090	1.2613	6.5141
H	-7.8416	-0.8696	0.6634
H	-9.4929	-0.8559	1.3183
H	-8.4706	-2.2899	1.5716
H	-2.4930	-0.2898	4.5386
H	-3.0819	-0.5646	2.8912
H	-3.1526	-1.8889	4.1050

B_-OAc-Me-Me

Energy (POTENTIAL) = -2854.30170042 Eh

Atom	X	Y	Z
S	-6.4765	2.7594	1.2415
O	-5.9937	3.9336	0.4664
O	-7.7225	2.1124	0.7935
N	-9.4756	5.7500	4.5940
N	-6.6767	3.2049	2.8169
C	-13.5651	4.6504	4.2265
C	-13.1196	5.4780	5.2624
H	-13.8348	5.8581	5.9886
C	-11.7751	5.8329	5.3972
H	-11.4814	6.4824	6.2151
C	-10.8158	5.3656	4.4799
C	-11.2548	4.5229	3.4359
H	-10.5517	4.1188	2.7164
C	-12.5994	4.1843	3.3205
H	-12.9033	3.5317	2.5045
C	-8.9482	6.3068	5.8376
H	-9.2480	5.7210	6.7183
H	-9.2958	7.3348	5.9759
C	-7.4266	6.2194	5.6505
H	-6.8727	7.1187	5.9046
H	-7.0116	5.3728	6.1912
C	-5.8689	5.1968	4.0016
C	-5.6901	4.0555	3.3031
H	-4.6440	3.7592	3.1944
C	-8.4401	4.9726	3.9602
H	-8.5972	4.8214	2.8995
H	-8.2443	4.0223	4.4509
C	-4.7303	5.8257	4.7165
C	-3.3057	7.7057	5.3142
H	-3.0657	8.7619	5.2251
C	-4.4014	7.1906	4.6206
H	-4.9890	7.8496	3.9922
C	-7.3233	7.0383	3.2282
C	-7.6736	8.3131	3.6610
H	-7.8674	8.5371	4.7019
C	-7.7678	9.3474	2.7253
H	-8.0371	10.3419	3.0710
C	-7.5277	9.1276	1.3648
C	-7.1832	7.8284	0.9610
C	-7.0774	6.7864	1.8773
H	-6.8008	5.7946	1.5340
C	-3.9257	4.9964	5.5228
H	-4.1928	3.9493	5.6242
C	-2.8203	5.5126	6.2009
H	-2.2128	4.8545	6.8166
C	-2.5098	6.8711	6.1047
H	-6.9879	7.6247	-0.0888
N	-7.2129	5.8656	4.1749
H	-1.6563	7.2776	6.6406
C	-5.1534	1.5342	1.1525
H	-4.2479	1.9554	1.5951
H	-5.4706	0.6445	1.6950
H	-4.9849	1.3120	0.0950
C	-15.0176	4.2628	4.0801
H	-15.4237	4.5860	3.1125
H	-15.1510	3.1743	4.1324
H	-15.6336	4.7124	4.8664
C	-7.6576	10.2389	0.3531
H	-7.6608	11.2228	0.8328
H	-6.8385	10.2125	-0.3748
H	-8.5939	10.1409	-0.2121
Rh	-6.9087	1.5821	4.4127
Rh	-7.0661	-0.1066	6.1661
O	-8.9603	1.8314	4.6047

O	-9.0746	0.3910	6.3562
O	-5.0378	-0.4672	5.8536
O	-4.8684	1.2313	4.3560
O	-7.2076	0.0525	3.0568
O	-7.5469	-1.4823	4.6915
O	-6.6285	2.9785	5.9531
O	-6.5819	1.3664	7.5464
C	-9.5791	1.2325	5.5461
C	-6.4995	2.5708	7.1566
C	-4.3875	0.2792	5.0570
C	-7.4909	-1.1178	3.4757
C	-6.2439	3.6274	8.2050
C	-2.9051	0.0345	4.9100
C	-7.8011	-2.1449	2.4145
C	-11.0360	1.5877	5.7205
H	-5.4899	4.3358	7.8504
H	-7.1731	4.1818	8.3846
H	-5.9204	3.1710	9.1425
H	-11.1048	2.5785	6.1854
H	-11.5270	1.6498	4.7464
H	-11.5405	0.8577	6.3567
H	-7.0047	-2.1506	1.6634
H	-8.7309	-1.8633	1.9071
H	-7.9103	-3.1392	2.8518
H	-2.3602	0.9494	5.1671
H	-2.6789	-0.2022	3.8646
H	-2.5767	-0.7842	5.5530

B-C-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.29327416 Eh

Atom	X	Y	Z
S	-6.0514	2.7217	1.2071
O	-5.5073	3.8878	0.4607
O	-7.2236	2.0377	0.6317
N	-9.5214	5.5193	4.3606
N	-6.4374	3.1866	2.7461
C	-12.5791	7.4929	2.1500
C	-12.6293	7.3891	3.5445
H	-13.4709	7.8151	4.0850
C	-11.6237	6.7369	4.2612
H	-11.7008	6.6485	5.3407
C	-10.5283	6.1869	3.5889
C	-10.4619	6.2772	2.1922
H	-9.6075	5.8867	1.6516
C	-11.4789	6.9195	1.4924
H	-11.4038	6.9936	0.4100
C	-8.9912	6.1156	5.5977
H	-9.2416	5.4952	6.4628
H	-9.4324	7.1020	5.7344
C	-7.4329	6.1799	5.4429
H	-7.0526	7.1582	5.7383
H	-6.9729	5.4289	6.0781
C	-5.7123	5.1628	4.0124
C	-5.4822	4.0147	3.3371
H	-4.4407	3.6871	3.3261
C	-8.6571	4.6280	3.8651
H	-8.7499	4.2873	2.8442
H	-8.2019	3.9455	4.5646
C	-4.6233	5.7791	4.8095
C	-3.3336	7.7034	5.5588
H	-3.1523	8.7749	5.5344
C	-4.3751	7.1646	4.8034
H	-4.9895	7.8194	4.1935
C	-7.2046	6.8724	3.0517
C	-7.7923	8.1010	3.3623
H	-8.0642	8.3584	4.3779
C	-8.0537	9.0293	2.3489
H	-8.5216	9.9745	2.6125
C	-7.7386	8.7616	1.0152
C	-7.1272	7.5293	0.7268
C	-6.8615	6.5945	1.7205
H	-6.4063	5.6480	1.4545
C	-3.8082	4.9556	5.6109
H	-4.0225	3.8918	5.6584
C	-2.7590	5.4968	6.3560
H	-2.1407	4.8436	6.9665
C	-2.5176	6.8729	6.3341
H	-6.8623	7.2901	-0.3007
N	-7.0233	5.8297	4.0543
H	-1.7064	7.2966	6.9203
C	-4.6912	1.5338	1.2796
H	-3.8454	1.9917	1.7980

H	-5.0305	0.6419	1.8035
H	-4.4136	1.3015	0.2477
C	-13.6613	8.1973	1.3680
H	-13.2474	9.0190	0.7701
H	-14.1569	7.5119	0.6687
H	-14.4276	8.6148	2.0293
C	-8.0559	9.7408	-0.0878
H	-8.4231	10.6920	0.3112
H	-7.1728	9.9478	-0.7046
H	-8.8270	9.3391	-0.7584
Rh	-6.8292	1.5232	4.2703
Rh	-7.2175	-0.1666	5.9924
O	-8.8916	1.7135	4.1282
O	-9.2535	0.1642	5.7481
O	-5.1496	-0.3672	6.1142
O	-4.7968	1.2259	4.5351
O	-6.8845	-0.0244	2.8975
O	-7.2687	-1.5928	4.4916
O	-6.7963	2.9241	5.8303
O	-7.1316	1.3385	7.4162
C	-9.6419	1.0169	4.8884
C	-6.9311	2.5328	7.0394
C	-4.4039	0.3591	5.3855
C	-7.0920	-1.2195	3.2895
C	-6.8484	3.5993	8.1057
C	-2.9090	0.2106	5.5363
C	-7.1557	-2.2736	2.2111
C	-11.1280	1.2285	4.7261
H	-5.9603	4.2172	7.9399
H	-7.7289	4.2492	8.0399
H	-6.8104	3.1509	9.1002
H	-11.3483	2.3005	4.7067
H	-11.4429	0.8075	3.7640
H	-11.6837	0.7431	5.5307
H	-6.3467	-2.1227	1.4905
H	-8.1051	-2.1691	1.6725
H	-7.0967	-3.2751	2.6417
H	-2.5043	1.1224	5.9909
H	-2.4475	0.0997	4.5501
H	-2.6618	-0.6471	6.1649

C-OAc-Me-Me

Energy (POTENTIAL) = -2854.30755981 Eh

Atom	X	Y	Z
S	-7.4398	2.9418	1.5555
O	-7.3493	4.1776	0.7344
O	-8.7034	2.1790	1.4765
N	-9.7806	5.2342	4.2182
N	-7.1916	3.2961	3.1508
C	-11.7072	7.4243	1.1313
C	-12.1852	7.4655	2.4499
H	-13.0550	8.0726	2.6869
C	-11.5625	6.7426	3.4660
H	-11.9449	6.7806	4.4816
C	-10.4485	5.9583	3.1593
C	-9.9583	5.8868	1.8558
H	-9.0690	5.3101	1.6301
C	-10.5937	6.6189	0.8545
H	-10.1972	6.5772	-0.1567
C	-9.3131	5.9973	5.4083
H	-9.7313	5.5332	6.3050
H	-9.7223	6.9995	5.3168
C	-7.7674	6.0104	5.5052
H	-7.4925	6.8344	6.1822
H	-7.4372	5.0805	5.9665
C	-5.9516	5.2346	4.0410
C	-6.0214	4.0310	3.4284
H	-5.0791	3.5149	3.2525
C	-9.4680	3.9848	4.1000
H	-9.8067	3.4114	3.2473
H	-8.9779	3.4917	4.9243
C	-4.6692	5.6997	4.6339
C	-3.1699	7.4866	5.3485
H	-2.9602	8.5498	5.4359
C	-4.3710	7.0691	4.7740
H	-5.0761	7.8129	4.4199
C	-7.2633	7.1898	3.3693
C	-7.8830	8.3765	3.8028
H	-8.1936	8.4933	4.8347
C	-8.0930	9.4374	2.9170
H	-8.5861	10.3350	3.2849
C	-7.6801	9.3772	1.5833

C	-7.0255	8.2044	1.1702
C	-6.8179	7.1344	2.0317
H	-6.3566	6.2264	1.6636
C	-3.7331	4.7668	5.1302
H	-3.9694	3.7080	5.0972
C	-2.5296	5.1873	5.6964
H	-1.8267	4.4476	6.0720
C	-2.2384	6.5501	5.8062
H	-6.6854	8.1190	0.1397
N	-7.1039	6.0757	4.2130
H	-1.3045	6.8785	6.2548
C	-6.0967	1.8835	0.9742
H	-5.1478	2.4058	1.1181
H	-6.1225	0.9461	1.5284
H	-6.2669	1.7129	-0.0925
C	-12.3442	8.2562	0.0460
H	-11.7981	9.2001	-0.0875
H	-12.3306	7.7346	-0.9174
H	-13.3823	8.5083	0.2873
C	-7.9460	10.5052	0.6146
H	-8.2453	11.4208	1.1370
H	-7.0604	10.7364	0.0095
H	-8.7528	10.2488	-0.0864
Rh	-7.0012	1.4426	4.5779
Rh	-6.6878	-0.2777	6.2841
O	-9.0482	1.2096	4.8591
O	-8.7539	-0.3805	6.4507
O	-4.6415	-0.0690	6.0139
O	-4.9303	1.4990	4.4033
O	-7.0371	-0.1013	3.1912
O	-6.7393	-1.6966	4.7773
O	-6.9691	2.8373	6.1146
O	-6.6351	1.2481	7.6975
C	-9.4732	0.3599	5.7097
C	-6.7787	2.4501	7.3174
C	-4.2108	0.7565	5.1497
C	-6.9003	-1.3091	3.5773
C	-6.7176	3.5389	8.3609
C	-2.7133	0.8840	5.0111
C	-6.9581	-2.3654	2.5010
C	-10.9713	0.2071	5.8112
H	-5.9220	4.2437	8.0967
H	-7.6630	4.0924	8.3690
H	-6.5300	3.1208	9.3514
H	-11.4594	1.1804	5.7100
H	-11.3132	-0.4280	4.9846
H	-11.2517	-0.2636	6.7558
H	-6.3088	-2.0834	1.6666
H	-7.9836	-2.4260	2.1179
H	-6.6620	-3.3395	2.8947
H	-2.3100	1.3322	5.9266
H	-2.4498	1.5089	4.1559
H	-2.2661	-0.1091	4.9035

C-4-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.30239020 Eh

Atom	X	Y	Z
S	-7.4314	3.1914	1.5245
O	-7.0885	4.4121	0.7626
O	-8.7353	2.5528	1.2689
N	-9.5782	5.2118	4.0251
N	-7.3654	3.5143	3.2016
C	-11.8301	7.1367	0.9707
C	-12.3526	6.9603	2.2613
H	-13.3507	7.3262	2.4908
C	-11.6183	6.3143	3.2542
H	-12.0404	6.1756	4.2458
C	-10.3326	5.8358	2.9732
C	-9.7954	6.0015	1.6963
H	-8.7897	5.6690	1.4784
C	-10.5474	6.6392	0.7081
H	-10.1140	6.7673	-0.2811
C	-9.3305	5.9890	5.2550
H	-9.8149	5.4987	6.1075
H	-9.8064	6.9574	5.1143
C	-7.8254	6.1510	5.5573
H	-7.6998	6.9885	6.2595
H	-7.4589	5.2519	6.0544
C	-5.9732	5.3600	4.1601
C	-6.1567	4.1652	3.5640
H	-5.2718	3.5531	3.4210
C	-9.1117	3.9579	3.9356

H	-9.6081	3.3044	3.2322
H	-8.8337	3.5281	4.8855
C	-4.6440	5.7046	4.7356
C	-2.9957	7.3670	5.4164
H	-2.7036	8.4105	5.5033
C	-4.2408	7.0460	4.8751
H	-4.8997	7.8426	4.5473
C	-7.1903	7.3814	3.4787
C	-7.9304	8.5238	3.8430
H	-8.3578	8.6097	4.8356
C	-8.1210	9.5683	2.9359
H	-8.7088	10.4294	3.2480
C	-7.5763	9.5393	1.6478
C	-6.8107	8.4134	1.3055
C	-6.6167	7.3573	2.1892
H	-6.0547	6.4877	1.8715
C	-3.7703	4.6991	5.2000
H	-4.0840	3.6610	5.1666
C	-2.5244	5.0232	5.7373
H	-1.8711	4.2292	6.0908
C	-2.1269	6.3589	5.8443
H	-6.3643	8.3528	0.3148
N	-7.0272	6.3024	4.3528
H	-1.1589	6.6119	6.2684
C	-6.1263	2.0034	1.1650
H	-5.1650	2.4064	1.4871
H	-6.3524	1.0590	1.6577
H	-6.1346	1.8896	0.0770
C	-12.6141	7.8735	-0.0887
H	-12.3189	7.5611	-1.0963
H	-13.6918	7.7068	0.0195
H	-12.4444	8.9569	-0.0209
C	-7.8241	10.6499	0.6544
H	-8.6262	10.3873	-0.0499
H	-8.1233	11.5779	1.1551
H	-6.9303	10.8631	0.0554
Rh	-7.0967	1.4479	4.6103
Rh	-6.6797	-0.2910	6.2501
O	-9.1180	1.2216	5.0158
O	-8.7250	-0.4005	6.5516
O	-4.6550	-0.0815	5.8741
O	-5.0445	1.5025	4.3022
O	-7.2622	-0.0630	3.2014
O	-6.8317	-1.6836	4.7276
O	-6.9282	2.8268	6.1446
O	-6.5280	1.2112	7.6822
C	-9.4912	0.3592	5.8789
C	-6.6595	2.4232	7.3263
C	-4.2765	0.7569	4.9965
C	-7.0937	-1.2793	3.5511
C	-6.4704	3.4984	8.3660
C	-2.7921	0.8926	4.7705
C	-7.2346	-2.3135	2.4634
C	-10.9778	0.2287	6.0948
H	-5.6217	4.1269	8.0735
H	-7.3596	4.1364	8.4012
H	-6.2867	3.0639	9.3502
H	-11.4264	1.2215	6.1963
H	-11.4218	-0.2492	5.2136
H	-11.1924	-0.3754	6.9783
H	-6.5993	-2.0435	1.6138
H	-8.2727	-2.3211	2.1122
H	-6.9664	-3.3056	2.8308
H	-2.3281	1.2857	5.6822
H	-2.5833	1.5646	3.9364
H	-2.3577	-0.0934	4.5770

H-OAc-Me-Me

Energy (POTENTIAL) = -2854.31360594 Eh

Atom	X	Y	Z
S	-7.7355	3.4953	1.6933
O	-7.5282	4.7891	1.0280
O	-8.9991	2.7732	1.5024
N	-9.3300	5.4445	3.8688
N	-7.5537	3.7005	3.4441
C	-12.0636	6.3813	0.7308
C	-12.1655	5.1726	1.4286
H	-12.9547	4.4702	1.1687
C	-11.2869	4.8503	2.4665
H	-11.4151	3.9097	2.9925
C	-10.2541	5.7277	2.8235
C	-10.1351	6.9364	2.1151

H	-9.3224	7.6125	2.3552
C	-11.0308	7.2581	1.1004
H	-10.9105	8.1998	0.5680
C	-9.2803	6.3532	5.0139
H	-9.9517	6.0243	5.8253
H	-9.6383	7.3273	4.6794
C	-7.8556	6.4872	5.5804
H	-7.8238	7.3390	6.2727
H	-7.5849	5.6049	6.1645
C	-5.9767	5.5174	4.3033
C	-6.3021	4.3187	3.7769
H	-5.4840	3.6229	3.6491
C	-8.8698	4.1164	4.0981
H	-9.5697	3.3562	3.7614
H	-8.6905	3.9541	5.1585
C	-4.5751	5.6928	4.7940
C	-2.6229	7.0904	5.2030
H	-2.1380	8.0607	5.1332
C	-3.9280	6.9407	4.7337
H	-4.4399	7.7952	4.3053
C	-6.9264	7.6615	3.5967
C	-7.5259	8.8911	3.9359
H	-7.9244	9.0483	4.9323
C	-7.6202	9.9206	2.9985
H	-8.1000	10.8522	3.2920
C	-7.1117	9.7872	1.7005
C	-6.4906	8.5702	1.3812
C	-6.3991	7.5258	2.2967
H	-5.9540	6.5858	1.9954
C	-3.8855	4.6138	5.3828
H	-4.3879	3.6595	5.4995
C	-2.5803	4.7674	5.8535
H	-2.0729	3.9207	6.3093
C	-1.9397	6.0051	5.7606
H	-6.0846	8.4252	0.3819
N	-6.8569	6.6145	4.5248
H	-0.9249	6.1274	6.1296
C	-6.3696	2.4143	1.2554
H	-5.4224	2.8798	1.5292
H	-6.5075	1.4476	1.7387
H	-6.4315	2.3158	0.1675
C	-13.0221	6.7408	-0.3799
H	-13.6256	7.6211	-0.1203
H	-12.4869	6.9848	-1.3066
H	-13.7116	5.9181	-0.5981
C	-7.2567	10.8861	0.6743
H	-7.4263	11.8594	1.1487
H	-6.3632	10.9692	0.0439
H	-8.1064	10.6976	0.0030
Rh	-7.2178	1.5341	4.7063
Rh	-6.7559	-0.2949	6.2201
O	-9.2104	1.3673	5.2320
O	-8.7846	-0.3716	6.6237
O	-4.7475	-0.1020	5.7455
O	-5.1915	1.5490	4.2607
O	-7.5087	0.1237	3.2214
O	-7.0287	-1.5896	4.6290
O	-6.8948	2.8282	6.2863
O	-6.4899	1.1205	7.7186
C	-9.5634	0.4563	6.0520
C	-6.5903	2.3542	7.4328
C	-4.4000	0.7634	4.8817
C	-7.3498	-1.1142	3.4939
C	-6.3294	3.3634	8.5214
C	-2.9326	0.8606	4.5513
C	-7.5888	-2.0841	2.3654
C	-11.0380	0.3323	6.3390
H	-5.5689	4.0731	8.1792
H	-7.2474	3.9283	8.7181
H	-5.9982	2.8731	9.4385
H	-11.5354	1.2972	6.2162
H	-11.4731	-0.3750	5.6220
H	-11.2002	-0.0565	7.3471
H	-7.0571	-1.7490	1.4697
H	-8.6599	-2.0957	2.1316
H	-7.2681	-3.0905	2.6406
H	-2.3446	0.8543	5.4737
H	-2.7221	1.7637	3.9757
H	-2.6419	-0.0185	3.9640

4

Energy (POTENTIAL) = -1721.12711114 Eh

Atom	X	Y	Z
S	-6.5330	1.5136	-0.5323
O	-7.4602	1.0268	-1.5648
O	-5.7975	0.5481	0.2948
N	-9.7164	3.2414	0.9636
N	-7.4071	2.5400	0.4941
C	-11.0165	-0.3088	2.9335
C	-11.2507	0.9581	3.4828
H	-11.7690	1.0408	4.4362
C	-10.8260	2.1267	2.8515
H	-11.0162	3.0759	3.3386
C	-10.1499	2.0772	1.6155
C	-9.9174	0.8035	1.0539
H	-9.4069	0.7024	0.1034
C	-10.3446	-0.3524	1.7051
H	-10.1463	-1.3148	1.2374
C	-10.0784	4.5767	1.4371
H	-11.1034	4.5595	1.8181
H	-10.0851	5.2363	0.5647
C	-9.1292	5.1485	2.5108
H	-9.3241	6.2175	2.6499
H	-9.3139	4.6628	3.4721
C	-7.1975	3.6754	2.6518
C	-6.9893	2.6246	1.8271
H	-6.4797	1.7430	2.1963
C	-8.6772	3.1644	-0.0238
H	-8.4636	4.1736	-0.3748
H	-8.9675	2.5516	-0.8781
C	-6.9176	3.5739	4.1021
C	-6.2593	4.6445	6.1889
H	-5.9681	5.5419	6.7290
C	-6.5469	4.7222	4.8267
H	-6.4763	5.6738	4.3082
C	-7.0219	5.7073	1.2689
C	-7.6272	6.7968	0.6072
H	-8.6676	7.0436	0.7838
C	-6.8988	7.5866	-0.2842
H	-7.4037	8.4187	-0.7712
C	-5.5520	7.3368	-0.5713
C	-4.9535	6.2573	0.0953
C	-5.6592	5.4605	0.9923
H	-5.1522	4.6439	1.4935
C	-7.0265	2.3524	4.7940
H	-7.3792	1.4688	4.2699
C	-6.7269	2.2752	6.1544
H	-6.8185	1.3226	6.6701
C	-6.3409	3.4194	6.8588
H	-3.9040	6.0328	-0.0861
N	-7.7228	4.9169	2.1867
H	-6.1196	3.3601	7.9212
C	-5.3410	2.6058	-1.3136
H	-5.8792	3.3828	-1.8607
H	-4.7141	3.0464	-0.5363
H	-4.7389	2.0003	-1.9973
C	-11.4328	-1.5696	3.6537
H	-11.6071	-2.3942	2.9530
H	-10.6591	-1.9031	4.3597
H	-12.3517	-1.4173	4.2320
C	-4.7868	8.1701	-1.5722
H	-4.8794	7.7669	-2.5908
H	-5.1546	9.2024	-1.6007
H	-3.7171	8.1998	-1.3345

C-D-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.29278710 Eh

Atom	X	Y	Z
S	-8.3054	4.6399	2.0177
O	-8.6895	6.0611	2.1123
O	-9.3872	3.6737	1.7806
N	-9.1898	6.6188	5.1385
N	-7.4508	4.0818	3.3473
C	-12.8029	4.5444	4.2718
C	-12.7544	5.9424	4.3018
H	-13.6580	6.5168	4.1136
C	-11.5643	6.6217	4.5713
H	-11.5643	7.7058	4.6031
C	-10.3934	5.8986	4.8161
C	-10.4182	4.4998	4.7838
H	-9.5132	3.9182	4.9067
C	-11.6131	3.8430	4.5192
H	-11.5992	2.7603	4.4637
C	-8.9466	7.9384	4.4852

H	-9.4456	8.7243	5.0635
H	-9.3979	7.8697	3.4978
C	-7.4493	8.2511	4.3511
H	-7.3702	9.1742	3.7739
H	-7.0201	8.4808	5.3355
C	-6.3076	6.0753	4.5070
C	-6.6524	4.7592	4.1938
H	-6.1464	4.0525	4.8388
C	-8.2737	6.1328	5.9399
H	-8.4057	5.1445	6.3628
H	-7.5725	6.7980	6.4194
C	-5.2768	6.2802	5.5655
C	-3.4635	7.6189	6.5086
H	-2.8173	8.4905	6.4407
C	-4.4303	7.4049	5.5240
H	-4.5171	8.1053	4.6997
C	-6.0470	7.4089	2.4634
C	-6.6153	8.2536	1.4891
H	-7.5706	8.7314	1.6767
C	-5.9885	8.4469	0.2611
H	-6.4596	9.1012	-0.4702
C	-4.7854	7.8035	-0.0681
C	-4.2307	6.9574	0.8996
C	-4.8381	6.7622	2.1414
H	-4.3680	6.1073	2.8673
C	-5.1428	5.4030	6.6652
H	-5.8131	4.5531	6.7648
C	-4.1702	5.6131	7.6409
H	-4.0876	4.9147	8.4701
C	-3.3202	6.7218	7.5694
H	-3.2960	6.4419	0.6879
N	-6.6594	7.2057	3.7100
H	-2.5668	6.8875	8.3346
C	-7.1175	4.4355	0.6812
H	-6.2488	5.0695	0.8609
H	-6.8394	3.3794	0.6594
H	-7.6182	4.7261	-0.2469
C	-14.0789	3.7998	3.9634
H	-14.9175	4.4849	3.8021
H	-13.9667	3.1857	3.0607
H	-14.3496	3.1191	4.7806
C	-4.1406	7.9971	-1.4203
H	-4.1284	9.0542	-1.7138
H	-3.1066	7.6347	-1.4262
H	-4.6829	7.4541	-2.2070
Rh	-7.3971	1.8821	3.8212
Rh	-7.0863	-0.4227	4.5561
O	-9.4345	1.4578	3.7400
O	-9.1219	-0.6989	4.3777
O	-5.0477	-0.0195	4.7011
O	-5.3432	2.1140	3.9943
O	-7.1243	1.2174	1.8809
O	-6.8461	-0.9327	2.5597
O	-7.6230	2.4176	5.8184
O	-7.3463	0.2725	6.5040
C	-9.8441	0.2869	4.0174
C	-7.5354	1.5102	6.7130
C	-4.6266	1.1404	4.4031
C	-6.9165	-0.0236	1.6727
C	-7.6249	1.9627	8.1506
C	-3.1467	1.4134	4.5245
C	-6.7636	-0.4394	0.2295
C	-11.3340	0.0442	3.9400
H	-6.6076	2.1289	8.5269
H	-8.1821	2.8989	8.2302
H	-8.0918	1.1896	8.7657
H	-11.7827	0.2788	4.9131
H	-11.7885	0.6898	3.1850
H	-11.5378	-1.0054	3.7142
H	-6.0717	0.2375	-0.2810
H	-7.7376	-0.3572	-0.2674
H	-6.4068	-1.4684	0.1550
H	-2.9904	2.3428	5.0814
H	-2.7248	1.5515	3.5221
H	-2.6355	0.5866	5.0214

D_-OAc-Me-Me

Energy (POTENTIAL) = -2854.31634308 Eh

Atom	X	Y	Z
S	-8.4893	4.9018	1.9348

O	-8.7808	6.3369	1.9646
O	-9.6121	3.9685	1.8345
N	-9.2240	6.7998	4.9746
N	-7.5367	4.3006	3.2850
C	-12.6702	4.3097	4.7807
C	-12.7073	5.6522	4.3856
H	-13.6390	6.0735	4.0121
C	-11.5838	6.4770	4.4601
H	-11.6743	7.5147	4.1580
C	-10.3503	5.9780	4.9288
C	-10.3109	4.6267	5.3362
H	-9.3847	4.1650	5.6571
C	-11.4466	3.8264	5.2649
H	-11.3624	2.7847	5.5665
C	-9.1770	8.0862	4.2839
H	-9.7038	8.8727	4.8485
H	-9.6557	7.9785	3.3104
C	-7.7075	8.5114	4.0931
H	-7.6550	9.2727	3.3175
H	-7.3295	8.9824	5.0110
C	-6.7723	6.3360	4.7452
C	-6.8765	4.9191	4.1990
H	-6.3243	4.2202	4.8201
C	-8.0369	6.4828	5.7029
H	-8.1498	5.5733	6.2890
H	-7.7875	7.2786	6.4158
C	-5.5436	6.4314	5.6842
C	-3.6395	7.6850	6.5305
H	-2.9938	8.5568	6.4665
C	-4.7014	7.5487	5.6331
H	-4.8693	8.3111	4.8803
C	-6.0457	7.3439	2.5965
C	-6.3581	8.1128	1.4531
H	-7.2431	8.7376	1.4438
C	-5.5791	8.0406	0.3040
H	-5.8641	8.6424	-0.5570
C	-4.4593	7.1974	0.2133
C	-4.1548	6.4319	1.3419
C	-4.9200	6.4989	2.5099
H	-4.6139	5.8925	3.3537
C	-5.3140	5.4641	6.6775
H	-5.9662	4.5999	6.7716
C	-4.2510	5.5986	7.5728
H	-4.0903	4.8354	8.3296
C	-3.4066	6.7089	7.5015
H	-3.2962	5.7639	1.3227
N	-6.8423	7.3858	3.7466
H	-2.5793	6.8135	8.1981
C	-7.3086	4.5574	0.6300
H	-6.4133	5.1592	0.7882
H	-7.0853	3.4890	0.6481
H	-7.8022	4.8404	-0.3045
C	-13.8758	3.4088	4.6502
H	-14.8124	3.9709	4.7457
H	-13.8996	2.9069	3.6724
H	-13.8747	2.6230	5.4149
C	-3.6455	7.1130	-1.0560
H	-3.2955	8.1020	-1.3788
H	-2.7660	6.4734	-0.9241
H	-4.2356	6.6986	-1.8847
Rh	-7.4122	2.0208	3.6212
Rh	-7.0498	-0.2981	4.2381
O	-9.4234	1.5622	3.4910
O	-9.0891	-0.5956	4.1060
O	-5.0182	0.1493	4.3644
O	-5.3740	2.3232	3.8302
O	-7.1277	1.4709	1.6481
O	-6.8357	-0.7060	2.2141
O	-7.6477	2.4284	5.6424
O	-7.2865	0.2667	6.2230
C	-9.8262	0.3928	3.7788
C	-7.5227	1.4848	6.4946
C	-4.6282	1.3403	4.1596
C	-6.9147	0.2424	1.3723
C	-7.6299	1.8644	7.9504
C	-3.1552	1.6383	4.2913
C	-6.7661	-0.0976	-0.0895
C	-11.3146	0.1444	3.7354
H	-6.6185	2.0222	8.3453
H	-8.2006	2.7881	8.0688
H	-8.0933	1.0555	8.5208
H	-11.6592	-0.1574	4.7308

H	-11.8489	1.0413	3.4181
H	-11.5276	-0.6806	3.0474
H	-6.0736	0.6039	-0.5648
H	-7.7411	0.0121	-0.5791
H	-6.4112	-1.1219	-0.2177
H	-3.0156	2.5724	4.8439
H	-2.7301	1.7750	3.2898
H	-2.6348	0.8201	4.7928

Rh-OAc

Energy (POTENTIAL) = -1133.17573809 Eh

Atom	X	Y	Z
Rh	-11.4398	0.6512	-9.3564
Rh	-9.9388	1.3889	-11.0788
O	-9.8450	-0.3342	-8.4832
O	-8.4294	0.3543	-10.1142
O	-11.5330	2.3782	-11.9501
O	-12.9486	1.6857	-10.3208
O	-11.8382	-1.0107	-10.5203
O	-10.4189	-0.3159	-12.1465
O	-10.9611	2.3575	-8.2892
O	-9.5390	3.0503	-9.9137
C	-8.6991	-0.2714	-9.0373
C	-10.1170	3.1743	-8.7845
C	-12.6754	2.3267	-11.3880
C	-11.2617	-1.1335	-11.6503
C	-9.7403	4.3740	-7.9538
C	-13.7944	3.1187	-12.0146
C	-11.6390	-2.3327	-12.4814
C	-7.5585	-0.9661	-8.3389
H	-10.5412	4.6278	-7.2562
H	-8.8392	4.1297	-7.3776
H	-9.5111	5.2254	-8.5995
H	-6.7843	-1.2479	-9.0561
H	-7.1216	-0.2707	-7.6114
H	-7.9195	-1.8451	-7.7998
H	-11.8697	-3.1838	-11.8361
H	-10.8376	-2.5874	-13.1782
H	-12.5391	-2.0871	-13.0587
H	-13.5953	3.2992	-13.0731
H	-13.8653	4.0855	-11.5007
H	-14.7460	2.5964	-11.8877

2_Me-Me

Energy (POTENTIAL) = -769.399133853 Eh

Atom	X	Y	Z
N	-10.1346	3.9657	2.0620
C	-13.2012	2.8871	-0.6696
C	-13.4306	3.8103	0.3587
H	-14.4168	4.2587	0.4626
C	-12.4291	4.1846	1.2544
H	-12.6581	4.9120	2.0259
C	-11.1343	3.6328	1.1570
C	-10.8941	2.7056	0.1182
H	-9.9138	2.2537	0.0051
C	-11.9096	2.3493	-0.7666
H	-11.6876	1.6333	-1.5558
C	-10.2696	5.0853	2.9884
H	-11.1026	4.9286	3.6799
H	-10.4324	6.0373	2.4580
C	-8.9260	5.0769	3.7106
H	-8.6452	6.0762	4.0562
H	-8.9428	4.4009	4.5806
C	-8.7316	3.7628	1.7206
H	-8.5129	4.0687	0.6842
H	-8.4534	2.7004	1.8177
C	-6.6616	4.4086	2.9098
C	-6.0409	4.9054	4.0748
H	-6.6246	5.4255	4.8268
C	-4.6705	4.7389	4.2767
H	-4.2254	5.1372	5.1864
C	-3.8587	4.0731	3.3503
C	-4.4830	3.5770	2.1960
C	-5.8483	3.7341	1.9707
H	-6.2796	3.3452	1.0538
H	-3.8867	3.0546	1.4499
N	-8.0159	4.6023	2.6732
C	-14.2995	2.4677	-1.6188
H	-13.9178	2.3204	-2.6363
H	-14.7612	1.5195	-1.3091
H	-15.0980	3.2171	-1.6642
C	-2.3793	3.8755	3.5840

H	-2.0213	4.4855	4.4208
H	-2.1432	2.8278	3.8165
H	-1.7910	4.1444	2.6975

t-A-OAc-Me-Me

Energy (POTENTIAL) = -2854.28472268 Eh

Atom	X	Y	Z
S	-3.0664	2.3140	0.7262
O	-2.1885	3.3908	0.2369
O	-4.0115	1.6888	-0.2224
N	-10.4782	4.4696	2.2909
N	-3.8591	2.9313	2.1152
C	-13.2396	1.3439	3.0521
C	-13.6110	2.6882	3.1866
H	-14.6208	2.9314	3.5115
C	-12.7255	3.7340	2.9160
H	-13.0613	4.7582	3.0408
C	-11.4082	3.4616	2.4983
C	-11.0337	2.1093	2.3451
H	-10.0201	1.8697	2.0563
C	-11.9287	1.0829	2.6235
H	-11.5876	0.0549	2.5219
C	-10.8480	5.8790	2.2328
H	-11.2719	6.2155	3.1838
H	-11.5820	6.0774	1.4355
C	-9.5121	6.5540	1.9320
H	-9.6460	7.4925	1.3868
H	-8.9510	6.7641	2.8568
C	-5.9001	3.1181	3.3052
C	-5.1481	2.8209	2.1062
H	-5.6958	2.3686	1.2752
C	-9.2974	4.2196	1.4735
H	-9.5404	3.6303	0.5738
H	-8.5373	3.6592	2.0407
C	-5.9415	4.4102	3.8864
C	-6.5610	5.8828	5.7298
H	-7.0103	6.0349	6.7065
C	-6.5378	4.6174	5.1667
H	-6.9583	3.7737	5.6944
C	-7.5778	5.7440	0.5735
C	-6.8630	4.6663	0.0045
H	-7.2957	3.6715	-0.0127
C	-5.5952	4.8597	-0.5416
H	-5.0729	4.0018	-0.9585
C	-4.9769	6.1187	-0.5508
C	-5.6951	7.1845	0.0092
C	-6.9645	7.0141	0.5606
H	-7.4679	7.8683	1.0003
C	-5.3830	5.5328	3.2028
H	-4.9469	5.4000	2.2201
C	-5.4122	6.7917	3.7795
H	-4.9920	7.6401	3.2491
C	-6.0002	6.9681	5.0397
H	-5.2480	8.1766	0.0265
N	-8.8425	5.5538	1.1080
H	-6.0234	7.9582	5.4869
C	-2.0700	1.0328	1.4855
H	-1.4130	1.4949	2.2250
H	-2.7434	0.3161	1.9581
H	-1.4866	0.5577	0.6920
C	-14.1988	0.2150	3.3482
H	-14.4301	-0.3668	2.4456
H	-13.7786	-0.4882	4.0792
H	-15.1463	0.5892	3.7516
C	-3.6044	6.3097	-1.1519
H	-3.6458	6.3466	-2.2498
H	-3.1476	7.2461	-0.8118
H	-2.9375	5.4840	-0.8798
Rh	-6.8017	1.4029	3.9170
Rh	-7.9878	-0.6415	4.6250
O	-8.4900	2.4423	4.5117
O	-9.5610	0.5718	5.2222
O	-6.3124	-1.7043	4.0134
O	-5.1981	0.1753	3.3952
O	-7.5898	1.0754	2.0206
O	-8.7172	-0.7818	2.6789
O	-6.0832	1.5402	5.8516
O	-7.1455	-0.3598	6.5023
C	-9.4589	1.8267	5.0785
C	-6.4029	0.6456	6.7104
C	-5.3117	-1.0922	3.5360
C	-8.3293	0.0504	1.8074

C	-5.8008	0.7970	8.0854
C	-4.1344	-1.9174	3.0753
C	-8.7476	-0.1742	0.3755
C	-10.5566	2.6834	5.6567
H	-5.5917	1.8470	8.3029
H	-6.4687	0.3749	8.8401
H	-4.8545	0.2425	8.1136
H	-10.4506	3.7200	5.3351
H	-11.5294	2.2931	5.3476
H	-10.4982	2.6320	6.7507
H	-8.8801	0.7792	-0.1415
H	-9.6658	-0.7634	0.3302
H	-7.9493	-0.7290	-0.1332
H	-3.2172	-1.5483	3.5450
H	-4.0239	-1.8109	1.9903
H	-4.2808	-2.9703	3.3229

t-A-B-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.27387087 Eh

Atom	X	Y	Z
S	-3.8305	2.0775	0.3436
O	-2.8518	2.9748	-0.2933
O	-5.0087	1.6533	-0.4432
N	-10.1512	4.0908	1.8424
N	-4.2671	2.8242	1.8210
C	-13.7862	1.8972	1.6852
C	-13.7707	3.2742	1.9470
H	-14.7112	3.7969	2.1099
C	-12.5831	4.0021	1.9974
H	-12.6219	5.0716	2.1797
C	-11.3396	3.3680	1.7929
C	-11.3478	1.9819	1.5176
H	-10.4197	1.4465	1.3479
C	-12.5493	1.2758	1.4653
H	-12.5183	0.2089	1.2521
C	-10.0103	5.2900	2.6816
H	-10.7645	5.3239	3.4745
H	-10.0898	6.2059	2.0837
C	-8.6101	5.1137	3.2757
H	-8.1223	6.0390	3.5620
H	-8.6510	4.4534	4.1398
C	-6.1122	3.3527	3.2753
C	-5.5436	2.8999	2.0242
H	-6.2450	2.4825	1.3031
C	-8.8793	3.3621	1.8267
H	-8.6728	2.9292	0.8514
H	-8.8604	2.5705	2.5713
C	-5.6499	4.5285	3.9804
C	-5.7514	5.9741	5.9432
H	-6.1557	6.1946	6.9271
C	-6.1612	4.8317	5.2669
H	-6.8811	4.1611	5.7162
C	-7.2930	5.1568	1.1572
C	-7.0244	4.5873	-0.1039
H	-7.3103	3.5695	-0.3347
C	-6.3591	5.3126	-1.0856
H	-6.1607	4.8349	-2.0419
C	-5.9328	6.6313	-0.8675
C	-6.2022	7.1917	0.3838
C	-6.8610	6.4738	1.3841
H	-7.0201	6.9595	2.3370
C	-4.7218	5.4283	3.3967
H	-4.3279	5.2257	2.4092
C	-4.2985	6.5587	4.0907
H	-3.5778	7.2315	3.6348
C	-4.8137	6.8364	5.3602
H	-5.8847	8.2095	0.5965
N	-7.8700	4.3691	2.2187
H	-4.4880	7.7244	5.8955
C	-2.9973	0.6100	0.9464
H	-2.1892	0.9135	1.6142
H	-3.7313	0.0020	1.4757
H	-2.6009	0.0779	0.0770
C	-15.0750	1.1094	1.6625
H	-15.0653	0.3451	0.8762
H	-15.2455	0.5869	2.6144
H	-15.9398	1.7599	1.4897
C	-5.2174	7.4013	-1.9497
H	-5.8743	7.5757	-2.8119
H	-4.8720	8.3755	-1.5886
H	-4.3457	6.8470	-2.3189
Rh	-6.7478	1.5248	4.2090

Rh	-7.4513	-0.5991	5.2618
O	-8.6095	2.2664	4.7829
O	-9.3113	0.2695	5.5989
O	-5.5463	-1.3136	4.8682
O	-4.9305	0.5950	3.7997
O	-7.5180	0.7620	2.4293
O	-8.0972	-1.2146	3.3778
O	-5.9723	2.0413	6.0644
O	-6.7498	0.1544	7.0611
C	-9.4896	1.4831	5.2849
C	-6.1468	1.2707	7.0673
C	-4.7119	-0.5776	4.2586
C	-7.9961	-0.4222	2.3944
C	-5.5388	1.7335	8.3698
C	-3.3328	-1.1527	4.0347
C	-8.4924	-0.9145	1.0559
C	-10.8692	2.0657	5.4672
H	-5.6386	2.8176	8.4714
H	-6.0053	1.2257	9.2167
H	-4.4686	1.4928	8.3598
H	-10.8091	3.1264	5.7238
H	-11.4062	1.9768	4.5142
H	-11.4220	1.5192	6.2343
H	-8.2769	-0.1928	0.2660
H	-9.5729	-1.0874	1.1136
H	-8.0170	-1.8727	0.8221
H	-2.6142	-0.3658	3.8002
H	-3.3709	-1.8619	3.1991
H	-3.0152	-1.7022	4.9252

t-B-OAc-Me-Me

Energy (POTENTIAL) = -2854.29263340 Eh

Atom	X	Y	Z
S	-4.5215	0.9585	0.2847
O	-3.3990	1.3661	-0.5836
O	-5.7836	0.5625	-0.3872
N	-9.9326	4.1059	2.1608
N	-4.7251	2.1665	1.4231
C	-13.7184	2.3913	1.2936
C	-13.5967	3.5387	2.0890
H	-14.4928	4.0057	2.4924
C	-12.3575	4.1079	2.3771
H	-12.3139	5.0077	2.9822
C	-11.1720	3.5353	1.8742
C	-11.2835	2.3827	1.0688
H	-10.4000	1.9064	0.6567
C	-12.5352	1.8350	0.7888
H	-12.5872	0.9458	0.1640
C	-9.7266	4.9404	3.3467
H	-10.3706	4.6355	4.1792
H	-9.9251	5.9939	3.1224
C	-8.2714	4.6779	3.7085
H	-7.7361	5.5157	4.1420
H	-8.1870	3.8253	4.3740
C	-6.3073	3.4499	2.7032
C	-5.9571	2.5520	1.6496
H	-6.7637	2.1189	1.0586
C	-8.7278	3.3858	1.8110
H	-8.6054	3.3067	0.7326
H	-8.6695	2.3987	2.2707
C	-5.2525	4.3759	3.2573
C	-4.2438	5.6199	5.0957
H	-4.2218	5.8626	6.1554
C	-5.1982	4.7177	4.6175
H	-5.8882	4.2563	5.3104
C	-7.3318	5.4006	1.4715
C	-6.9138	5.1119	0.1675
H	-6.8266	4.0923	-0.1879
C	-6.5706	6.1454	-0.6970
H	-6.2441	5.9004	-1.7043
C	-6.6241	7.4877	-0.2902
C	-7.0471	7.7524	1.0142
C	-7.3968	6.7245	1.8957
H	-7.7060	6.9954	2.8957
C	-4.3139	4.9699	2.3905
H	-4.3346	4.7308	1.3343
C	-3.3589	5.8669	2.8669
H	-2.6481	6.3106	2.1744
C	-3.3200	6.1987	4.2242
H	-7.1025	8.7794	1.3647
N	-7.6176	4.2414	2.4022
H	-2.5758	6.8979	4.5967

C	-3.9645	-0.4133	1.3023
H	-3.0395	-0.1190	1.8003
H	-4.7401	-0.6384	2.0324
H	-3.7902	-1.2656	0.6396
C	-15.0631	1.7633	1.0125
H	-15.1090	1.3495	-0.0018
H	-15.2749	0.9378	1.7065
H	-15.8750	2.4919	1.1170
C	-6.2172	8.5923	-1.2325
H	-6.7432	8.5096	-2.1911
H	-6.4281	9.5798	-0.8103
H	-5.1426	8.5422	-1.4508
Rh	-6.8586	1.4428	4.1928
Rh	-7.1808	-0.5530	5.5757
O	-8.9378	1.6699	4.2629
O	-9.2223	-0.1722	5.5538
O	-5.1260	-0.8242	5.4840
O	-4.8363	1.0705	4.2686
O	-7.0905	0.1874	2.5550
O	-7.4012	-1.6564	3.8357
O	-6.7754	2.5094	5.9805
O	-6.9519	0.6417	7.2534
C	-9.6551	0.8242	4.8976
C	-6.8117	1.8938	7.0980
C	-4.4106	0.0352	4.8760
C	-7.3238	-1.0562	2.7186
C	-6.6380	2.7411	8.3343
C	-2.9207	-0.2049	4.8615
C	-7.5358	-1.8666	1.4643
C	-11.1463	1.0472	4.8398
H	-7.1786	3.6853	8.2243
H	-6.9810	2.2088	9.2238
H	-5.5724	2.9752	8.4486
H	-11.3837	2.0432	5.2280
H	-11.4722	1.0185	3.7946
H	-11.6783	0.2885	5.4166
H	-7.0585	-1.3720	0.6154
H	-8.6138	-1.9383	1.2719
H	-7.1470	-2.8797	1.5958
H	-2.3965	0.6244	4.3838
H	-2.7128	-1.1333	4.3179
H	-2.5606	-0.3339	5.8873

t-B_-OAc-Me-Me

Energy (POTENTIAL) = -2854.28923420 Eh

Atom	X	Y	Z
S	-6.4544	2.7273	1.1136
O	-7.6852	2.3775	0.3585
O	-5.3370	1.7688	1.0972
N	-11.2641	5.5668	4.6310
N	-6.7494	3.1717	2.6811
C	-15.2138	4.0776	5.1021
C	-14.7249	5.1255	5.8919
H	-15.3710	5.5753	6.6426
C	-13.4255	5.6132	5.7484
H	-13.0935	6.4301	6.3806
C	-12.5570	5.0598	4.7894
C	-13.0359	3.9981	3.9950
H	-12.3972	3.5238	3.2582
C	-14.3378	3.5282	4.1550
H	-14.6747	2.7043	3.5292
C	-10.5970	6.3082	5.7024
H	-10.7402	5.8394	6.6848
H	-10.9772	7.3323	5.7538
C	-9.1197	6.2451	5.3078
H	-8.5547	7.1616	5.4494
H	-8.6076	5.4291	5.8125
C	-7.7981	5.1663	3.5074
C	-7.8479	4.0155	2.8054
H	-8.7854	3.6816	2.3622
C	-10.2875	4.8532	3.8541
H	-10.6222	4.6621	2.8370
H	-9.9187	3.9294	4.3164
C	-6.5742	5.8148	4.0388
C	-5.1092	7.7511	4.2342
H	-4.8988	8.7913	3.9996
C	-6.2782	7.1605	3.7511
H	-6.9517	7.7465	3.1356
C	-9.4197	6.9625	2.8754
C	-9.6847	8.2572	3.3114
H	-9.6877	8.5241	4.3598
C	-9.9416	9.2554	2.3672

H	-10.1435	10.2645	2.7162
C	-9.9438	8.9841	0.9951
C	-9.6853	7.6665	0.5866
C	-9.4202	6.6616	1.5118
H	-9.2088	5.6563	1.1660
C	-5.6585	5.0732	4.8075
H	-5.8705	4.0383	5.0363
C	-4.4852	5.6657	5.2763
H	-3.7888	5.0743	5.8657
C	-4.2069	7.0064	4.9978
H	-9.6834	7.4216	-0.4722
N	-9.1132	5.8372	3.8322
H	-3.2941	7.4655	5.3682
C	-5.8413	4.2675	0.3839
H	-6.6175	5.0344	0.4441
H	-4.9508	4.5860	0.9297
H	-5.5974	4.0606	-0.6620
C	-16.6265	3.5633	5.2464
H	-16.6535	2.4671	5.2761
H	-17.0980	3.9371	6.1619
H	-17.2551	3.8753	4.4011
C	-10.1816	10.0744	-0.0192
H	-9.2275	10.4572	-0.4056
H	-10.7530	9.7034	-0.8771
H	-10.7233	10.9190	0.4186
Rh	-7.3314	1.5224	4.1896
Rh	-7.8850	-0.1822	5.8537
O	-9.3189	1.4586	3.5776
O	-9.8218	-0.1518	5.0965
O	-5.9114	-0.0786	6.4881
O	-5.4050	1.5097	4.9472
O	-6.8853	-0.0325	2.9128
O	-7.3700	-1.6207	4.4594
O	-7.8890	2.9435	5.6464
O	-8.3621	1.3367	7.1771
C	-10.1165	0.6457	4.1517
C	-8.2507	2.5443	6.8037
C	-5.1157	0.7291	5.9116
C	-6.9987	-1.2366	3.3032
C	-8.6034	3.6099	7.8151
C	-3.6832	0.7603	6.3890
C	-6.6856	-2.3132	2.2921
C	-11.5535	0.6521	3.6867
H	-7.8663	4.4174	7.7833
H	-9.5851	4.0301	7.5657
H	-8.6499	3.1866	8.8203
H	-11.9507	-0.3665	3.6830
H	-12.1510	1.2467	4.3877
H	-11.6375	1.0934	2.6913
H	-7.6282	-2.7286	1.9154
H	-6.1270	-3.1242	2.7682
H	-6.1196	-1.9019	1.4541
H	-3.3347	1.7952	6.4546
H	-3.0554	0.2430	5.6536
H	-3.5826	0.2640	7.3564

t-B-C-ts-OAc-Me-Me

Energy (POTENTIAL) = -2854.28176223 Eh

Atom	X	Y	Z
S	-6.5709	2.6143	1.1397
O	-7.8661	2.2517	0.5066
O	-5.4444	1.6783	0.9853
N	-11.3598	4.6987	5.0338
N	-6.7123	3.0293	2.7361
C	-15.2146	5.9733	3.7556
C	-14.9131	5.7836	5.1097
H	-15.6807	5.9566	5.8598
C	-13.6469	5.3614	5.5189
H	-13.4414	5.1991	6.5730
C	-12.6458	5.1385	4.5696
C	-12.9246	5.3279	3.2106
H	-12.1495	5.2006	2.4627
C	-14.1965	5.7363	2.8184
H	-14.3944	5.8939	1.7609
C	-10.6535	5.4211	6.1023
H	-10.5275	4.7846	6.9822
H	-11.2396	6.2952	6.3839
C	-9.2382	5.8000	5.5400
H	-9.0001	6.8417	5.7555
H	-8.4846	5.1750	6.0116
C	-7.8224	4.9584	3.7119
C	-7.8325	3.8172	2.9831

H	-8.7844	3.4562	2.5963
C	-10.5003	4.0033	4.2858
H	-10.8311	3.6439	3.3184
H	-9.7400	3.4138	4.7883
C	-6.6290	5.6948	4.1843
C	-5.5198	7.8160	4.6730
H	-5.5592	8.9017	4.7122
C	-6.6437	7.1031	4.2552
H	-7.5351	7.6508	3.9667
C	-9.7237	6.4850	3.1795
C	-10.4674	7.5692	3.6542
H	-10.5703	7.7644	4.7140
C	-11.1074	8.4292	2.7574
H	-11.6844	9.2615	3.1522
C	-11.0298	8.2361	1.3759
C	-10.2645	7.1521	0.9146
C	-9.6208	6.2879	1.7932
H	-9.0469	5.4575	1.4004
C	-5.4438	5.0254	4.5534
H	-5.4091	3.9465	4.5251
C	-4.3216	5.7451	4.9658
H	-3.4207	5.2047	5.2471
C	-4.3496	7.1409	5.0298
H	-10.1736	6.9771	-0.1547
N	-9.1412	5.5059	4.0825
H	-3.4728	7.6952	5.3545
C	-6.0648	4.1801	0.3849
H	-6.8444	4.9294	0.5440
H	-5.1301	4.5045	0.8470
H	-5.9241	4.0038	-0.6852
C	-16.5904	6.4023	3.3071
H	-17.1382	5.5626	2.8590
H	-17.1873	6.7777	4.1447
H	-16.5347	7.1902	2.5465
C	-11.7594	9.1359	0.4092
H	-11.1257	9.4063	-0.4435
H	-12.6479	8.6333	0.0036
H	-12.0938	10.0588	0.8940
Rh	-6.9540	1.3717	4.2969
Rh	-7.1695	-0.2947	6.0729
O	-9.0043	1.1929	3.9969
O	-9.2242	-0.2709	5.7179
O	-5.1086	-0.1672	6.3092
O	-4.9344	1.4637	4.7382
O	-6.6351	-0.2084	3.0041
O	-6.9331	-1.7616	4.6329
O	-7.3373	2.8094	5.7841
O	-7.3835	1.2542	7.4350
C	-9.6853	0.4514	4.7806
C	-7.4200	2.4481	7.0041
C	-4.4552	0.6818	5.6227
C	-6.7005	-1.4031	3.4330
C	-7.6080	3.5434	8.0286
C	-2.9639	0.7619	5.8470
C	-6.4346	-2.4980	2.4276
C	-11.1843	0.4801	4.5918
H	-7.0105	4.4190	7.7609
H	-8.6644	3.8385	8.0477
H	-7.3308	3.1888	9.0237
H	-11.6491	-0.4064	5.0284
H	-11.5841	1.3697	5.0958
H	-11.4319	0.5539	3.5296
H	-6.9656	-3.4117	2.7059
H	-5.3584	-2.7118	2.4225
H	-6.7251	-2.1764	1.4248
H	-2.6411	1.8070	5.8435
H	-2.4552	0.2517	5.0202
H	-2.6843	0.2816	6.7870

t-C-OAc-Me-Me

Energy (POTENTIAL) = -2854.29577078 Eh

Atom	X	Y	Z
S	-8.3932	2.5567	1.3883
O	-9.8009	2.0732	1.4495
O	-7.3899	1.6394	0.8208
N	-11.8383	4.5659	4.7474
N	-7.8293	3.1381	2.8368
C	-12.9067	6.0890	0.9140
C	-13.2178	6.7980	2.0829
H	-13.7170	7.7603	2.0115
C	-12.8849	6.3062	3.3417
H	-13.1500	6.8856	4.2167

C	-12.2354	5.0713	3.4491
C	-11.9453	4.3277	2.2979
H	-11.4169	3.3812	2.3426
C	-12.2796	4.8420	1.0485
H	-12.0214	4.2666	0.1639
C	-11.3941	5.5259	5.8069
H	-11.7073	5.1163	6.7682
H	-11.9211	6.4606	5.6489
C	-9.8677	5.7216	5.8032
H	-9.6504	6.4582	6.5924
H	-9.3910	4.7843	6.0963
C	-8.2151	5.2657	4.0337
C	-8.6098	4.1898	3.3028
H	-9.6739	4.1594	3.0885
C	-11.7739	3.3054	5.0031
H	-12.0922	2.5744	4.2724
H	-11.3992	2.9889	5.9672
C	-6.8530	5.6514	4.4400
C	-5.3714	7.1622	5.6699
H	-5.2517	8.0378	6.3037
C	-6.6510	6.7811	5.2617
H	-7.5023	7.3722	5.5822
C	-9.5960	7.3090	3.9000
C	-10.2765	8.3477	4.5659
H	-10.5420	8.2531	5.6135
C	-10.6041	9.5301	3.8971
H	-11.1318	10.3093	4.4437
C	-10.2684	9.7396	2.5556
C	-9.5656	8.7111	1.9065
C	-9.2339	7.5256	2.5526
H	-8.6950	6.7511	2.0177
C	-5.7112	4.9212	4.0417
H	-5.8378	4.0340	3.4378
C	-4.4366	5.3068	4.4518
H	-3.5786	4.7187	4.1339
C	-4.2531	6.4267	5.2704
H	-9.2749	8.8386	0.8653
N	-9.3018	6.0870	4.5160
H	-3.2566	6.7194	5.5914
C	-8.4299	4.0251	0.3259
H	-9.1703	4.7357	0.6995
H	-7.4364	4.4786	0.3123
H	-8.7083	3.6867	-0.6761
C	-13.1983	6.6746	-0.4431
H	-12.4198	7.3984	-0.7200
H	-13.2227	5.9020	-1.2182
H	-14.1547	7.2092	-0.4522
C	-10.6625	11.0006	1.8232
H	-10.8876	11.8169	2.5189
H	-9.8655	11.3414	1.1513
H	-11.5572	10.8441	1.2040
Rh	-7.5879	1.5835	4.5151
Rh	-7.1344	0.0158	6.3385
O	-9.6313	1.2713	4.8820
O	-9.1854	-0.2674	6.4942
O	-5.1153	0.3742	6.0562
O	-5.5377	1.7538	4.3038
O	-7.5862	-0.0534	3.2495
O	-7.0734	-1.4963	4.9244
O	-7.5823	3.0769	5.9648
O	-7.1996	1.6186	7.6603
C	-9.9689	0.3825	5.7338
C	-7.3813	2.7854	7.1870
C	-4.7619	1.1602	5.1189
C	-7.3227	-1.2082	3.7094
C	-7.3963	3.9382	8.1645
C	-3.2867	1.4518	4.9801
C	-7.3189	-2.3381	2.7067
C	-11.4458	0.0855	5.8775
H	-7.0510	4.8522	7.6753
H	-8.4246	4.0984	8.5119
H	-6.7732	3.7121	9.0332
H	-11.8757	0.7374	6.6483
H	-11.9709	0.2630	4.9359
H	-11.5905	-0.9495	6.1958
H	-6.6585	-2.0843	1.8715
H	-8.3298	-2.4615	2.3018
H	-6.9947	-3.2724	3.1694
H	-3.0496	2.3329	5.5892
H	-3.0373	1.6769	3.9405
H	-2.6910	0.6103	5.3420

A2-OAc-Me-Me

Energy (POTENTIAL) = -2854.27559853 Eh

Atom	X	Y	Z
S	-3.9616	1.6164	0.5168
O	-4.6664	0.4389	-0.0200
O	-2.7217	1.3988	1.2911
N	-9.9681	4.5127	2.1759
N	-5.1143	2.5327	1.3916
C	-13.3769	4.7418	4.6947
C	-13.1224	3.6099	3.9059
H	-13.8138	2.7698	3.9400
C	-12.0011	3.5180	3.0857
H	-11.8421	2.6131	2.5095
C	-11.0708	4.5791	3.0144
C	-11.3180	5.7194	3.8086
H	-10.6312	6.5594	3.7883
C	-12.4477	5.7871	4.6253
H	-12.6050	6.6811	5.2257
C	-9.5436	3.2534	1.5719
H	-10.3148	2.8591	0.9035
H	-9.3144	2.5028	2.3357
C	-8.2974	3.6602	0.7958
H	-7.5776	2.8450	0.7247
H	-8.5628	4.0063	-0.2146
C	-5.7751	3.1418	3.6467
C	-4.8529	2.6460	2.6486
H	-3.9274	2.2376	3.0803
C	-8.8035	5.3509	2.4237
H	-8.5094	5.3438	3.4866
H	-9.0066	6.3924	2.1367
C	-5.6571	4.4379	4.2073
C	-6.3406	6.0968	5.8609
H	-7.0019	6.4129	6.6621
C	-6.5195	4.8589	5.2629
H	-7.3125	4.1974	5.5845
C	-6.7686	5.6010	1.0648
C	-6.4401	6.8234	1.6857
H	-6.9373	7.1206	2.6023
C	-5.4500	7.6519	1.1542
H	-5.2239	8.5866	1.6631
C	-4.7363	7.3036	0.0030
C	-5.0560	6.0761	-0.6008
C	-6.0455	5.2407	-0.0931
H	-6.2482	4.2992	-0.5866
C	-4.6342	5.3305	3.7703
H	-3.9906	5.0399	2.9462
C	-4.4432	6.5508	4.4020
H	-3.6494	7.2137	4.0723
C	-5.2940	6.9344	5.4455
H	-4.5180	5.7665	-1.4947
N	-7.7491	4.7664	1.5946
H	-5.1467	7.8936	5.9345
C	-3.6021	2.7396	-0.8327
H	-4.5209	2.9260	-1.3903
H	-3.1965	3.6670	-0.4241
H	-2.8636	2.2427	-1.4679
C	-14.6063	4.8252	5.5688
H	-14.5295	5.6463	6.2904
H	-15.5154	4.9942	4.9751
H	-14.7623	3.8971	6.1327
C	-3.6779	8.2076	-0.5829
H	-3.3684	8.9783	0.1315
H	-2.7844	7.6434	-0.8780
H	-4.0410	8.7223	-1.4833
Rh	-6.7979	1.5146	4.3682
Rh	-7.9210	-0.4953	5.2554
O	-8.5433	2.5547	4.8209
O	-9.5014	0.7390	5.7888
O	-6.2462	-1.5862	4.6886
O	-5.1431	0.2922	4.0589
O	-7.5038	0.9365	2.5140
O	-8.6890	-0.8106	3.3509
O	-6.1659	1.8953	6.3089
O	-7.0454	-0.0497	7.0897
C	-9.4372	1.9793	5.5362
C	-6.3934	1.0292	7.2236
C	-5.2469	-0.9741	4.2082
C	-8.2852	-0.0688	2.4047
C	-5.7998	1.3347	8.5776
C	-4.0564	-1.7812	3.7537
C	-8.7810	-0.3580	1.0092
C	-10.4709	2.8697	6.1766

H	-5.9647	2.3863	8.8298
H	-6.2320	0.6895	9.3450
H	-4.7169	1.1667	8.5346
H	-10.5700	3.8125	5.6392
H	-11.4342	2.3590	6.2315
H	-10.1366	3.0790	7.2014
H	-7.9578	-0.2583	0.2961
H	-9.5467	0.3813	0.7461
H	-9.2153	-1.3581	0.9512
H	-3.1501	-1.4061	4.2402
H	-3.9303	-1.6456	2.6737
H	-4.1923	-2.8399	3.9814

B_2-OAc-Me-Me

Energy (POTENTIAL) = -2854.29653367 Eh

Atom	X	Y	Z
S	-7.7137	2.0595	4.5955
O	-6.9687	1.5220	5.7567
O	-6.8739	2.3214	3.3877
N	-10.4387	6.1684	3.1923
N	-8.6424	3.3812	4.8997
C	-13.9856	8.0337	4.5631
C	-13.8252	6.6379	4.5843
H	-14.6204	6.0150	4.9899
C	-12.6699	6.0238	4.1155
H	-12.5661	4.9482	4.1845
C	-11.6039	6.7963	3.6084
C	-11.7614	8.1941	3.5597
H	-10.9812	8.8256	3.1460
C	-12.9319	8.7893	4.0392
H	-13.0214	9.8727	3.9948
C	-10.3831	4.7621	2.7909
H	-11.1080	4.5344	1.9969
H	-10.5594	4.1080	3.6428
C	-8.9584	4.6147	2.2611
H	-8.4651	3.6837	2.5112
H	-8.9061	4.7908	1.1858
C	-7.7573	5.6473	4.3260
C	-7.9155	4.5632	5.1091
H	-7.4737	4.6914	6.1003
C	-9.2801	6.8666	2.7434
H	-9.0341	7.7300	3.3590
H	-9.3019	7.1478	1.6827
C	-7.1615	6.8833	4.9211
C	-7.4383	8.7619	6.4452
H	-8.0575	9.3173	7.1448
C	-7.9447	7.6157	5.8298
H	-8.9441	7.2594	6.0544
C	-6.9666	6.0817	2.0573
C	-6.7185	7.3465	1.5327
H	-7.4015	8.1738	1.6791
C	-5.5317	7.5666	0.8276
H	-5.3387	8.5569	0.4243
C	-4.5873	6.5499	0.6516
C	-4.8638	5.2895	1.2068
C	-6.0398	5.0475	1.9107
H	-6.2185	4.0779	2.3653
C	-5.8476	7.3075	4.6622
H	-5.2144	6.7344	3.9940
C	-5.3426	8.4532	5.2798
H	-4.3222	8.7660	5.0750
C	-6.1372	9.1872	6.1654
H	-4.1412	4.4848	1.0970
N	-8.1892	5.7967	2.8748
H	-5.7389	10.0785	6.6430
C	-8.9572	0.8651	4.0976
H	-9.6234	0.6661	4.9354
H	-9.5035	1.2660	3.2418
H	-8.4162	-0.0410	3.8112
C	-15.2403	8.6783	5.1032
H	-15.3382	8.5182	6.1855
H	-15.2433	9.7595	4.9268
H	-16.1422	8.2603	4.6376
C	-3.3039	6.7885	-0.1041
H	-3.1671	7.8480	-0.3423
H	-2.4367	6.4534	0.4773
H	-3.2935	6.2272	-1.0474
Rh	-10.1461	3.2776	6.6100
Rh	-11.8311	3.2551	8.3787
O	-10.5175	5.3234	6.4293
O	-12.1343	5.2680	8.0215
O	-11.4270	1.2427	8.6731

O	-9.8947	1.2511	7.0007
O	-11.6682	2.8060	5.2719
O	-13.2297	2.7527	6.9188
O	-8.7425	3.7454	8.0559
O	-10.3076	3.7598	9.7011
C	-11.3761	5.8705	7.1960
C	-9.1196	3.8887	9.2651
C	-10.5687	0.6834	7.9220
C	-12.8568	2.6531	5.7085
C	-8.0441	4.2095	10.2749
C	-10.3135	-0.7920	8.1169
C	-13.9272	2.3585	4.6842
C	-11.4716	7.3762	7.1733
H	-7.2370	4.7789	9.8076
H	-8.4631	4.7624	11.1190
H	-7.6257	3.2677	10.6514
H	-10.7265	7.7739	7.8742
H	-11.2613	7.7698	6.1788
H	-12.4604	7.6998	7.5043
H	-13.4854	2.0212	3.7444
H	-14.4973	3.2769	4.4980
H	-14.6222	1.6066	5.0688
H	-9.2415	-0.9622	8.2600
H	-10.6166	-1.3314	7.2122
H	-10.8702	-1.1757	8.9741

B2-OAc-Me-Me

Energy (POTENTIAL) = -2854.29089146 Eh

Atom	X	Y	Z
S	-3.8165	1.8107	1.0341
O	-4.2469	0.5303	0.4285
O	-2.7816	1.7615	2.0943
N	-9.3469	4.4097	3.1755
N	-5.1520	2.7081	1.4412
C	-12.7089	5.2126	5.6394
C	-12.6911	4.1348	4.7464
H	-13.5542	3.4746	4.6890
C	-11.5935	3.8729	3.9269
H	-11.6232	3.0135	3.2667
C	-10.4513	4.6963	3.9713
C	-10.4604	5.7863	4.8676
H	-9.6028	6.4459	4.9457
C	-11.5663	6.0251	5.6805
H	-11.5373	6.8707	6.3647
C	-9.3679	3.3523	2.1751
H	-10.2230	3.4443	1.4900
H	-9.4078	2.3794	2.6616
C	-8.0670	3.5594	1.3910
H	-7.4938	2.6540	1.2251
H	-8.2739	4.0564	0.4448
C	-6.3367	3.8070	3.2674
C	-5.2735	3.0709	2.7067
H	-4.5070	2.7802	3.4266
C	-8.3605	5.3798	2.8264
H	-7.9964	5.9476	3.6757
H	-8.6659	6.0658	2.0238
C	-6.0883	4.5469	4.5425
C	-6.8147	5.3565	6.7240
H	-7.5988	5.4445	7.4721
C	-7.0773	4.6779	5.5350
H	-8.0402	4.2092	5.3803
C	-6.3657	5.4587	1.4079
C	-5.8753	6.6169	2.0162
H	-6.1208	6.8569	3.0424
C	-5.0364	7.4715	1.3020
H	-4.6607	8.3670	1.7898
C	-4.6714	7.1958	-0.0219
C	-5.1767	6.0283	-0.6085
C	-6.0128	5.1585	0.0925
H	-6.3471	4.2496	-0.3854
C	-4.8209	5.1054	4.7961
H	-4.0467	5.0390	4.0372
C	-4.5479	5.7592	5.9997
H	-3.5586	6.1754	6.1720
C	-5.5469	5.8953	6.9664
H	-4.9045	5.7809	-1.6314
N	-7.2357	4.5426	2.2258
H	-5.3400	6.4144	7.8988
C	-3.1497	2.8143	-0.3045
H	-3.9087	2.9258	-1.0814
H	-2.8590	3.7897	0.0918
H	-2.2768	2.2879	-0.7011

C	-13.9146	5.5117	6.4988
H	-13.6211	5.9037	7.4798
H	-14.5643	6.2657	6.0325
H	-14.5232	4.6152	6.6618
C	-3.7819	8.1322	-0.8012
H	-3.1748	8.7556	-0.1366
H	-3.1083	7.5802	-1.4662
H	-4.3788	8.8057	-1.4310
Rh	-6.9531	1.3475	4.2233
Rh	-7.4912	-0.7888	5.2685
O	-8.7215	2.0676	5.0633
O	-9.1793	0.0914	6.0755
O	-5.7625	-1.5783	4.4534
O	-5.2312	0.4273	3.5453
O	-7.9390	0.6505	2.5323
O	-8.5078	-1.3030	3.5324
O	-5.9569	1.8466	5.9623
O	-6.4349	-0.1482	6.9317
C	-9.3929	1.3268	5.8516
C	-5.9029	1.0082	6.9190
C	-5.0133	-0.8056	3.7714
C	-8.4896	-0.4992	2.5485
C	-5.1088	1.4250	8.1324
C	-3.7662	-1.3823	3.1546
C	-9.1539	-0.9431	1.2682
C	-10.5548	1.9558	6.5817
H	-5.1995	2.5025	8.2905
H	-5.4391	0.8781	9.0184
H	-4.0511	1.1949	7.9532
H	-10.4957	3.0441	6.5468
H	-11.4914	1.6405	6.1098
H	-10.5651	1.6056	7.6181
H	-8.3764	-1.2620	0.5636
H	-9.6949	-0.1080	0.8141
H	-9.8311	-1.7799	1.4510
H	-2.9187	-0.7261	3.3703
H	-3.8915	-1.3822	2.0668
H	-3.5798	-2.3945	3.5188

A-B-ts2-OAc-Me-Me
Energy (POTENTIAL) = -2854.27226276 Eh

Atom	X	Y	Z
S	-3.8643	1.6657	0.6714
O	-4.3020	0.3009	0.3210
O	-2.6790	1.8178	1.5413
N	-9.8318	4.4401	2.2944
N	-5.2209	2.5067	1.2610
C	-13.3265	4.9524	4.6434
C	-13.1829	3.8665	3.7686
H	-13.9875	3.1382	3.6874
C	-12.0321	3.6788	3.0057
H	-11.9644	2.8133	2.3556
C	-10.9614	4.5956	3.0816
C	-11.0966	5.6908	3.9636
H	-10.3000	6.4218	4.0579
C	-12.2552	5.8527	4.7226
H	-12.3234	6.7053	5.3958
C	-9.5099	3.1830	1.6364
H	-10.2718	2.9177	0.8964
H	-9.4129	2.3683	2.3564
C	-8.1956	3.5016	0.9439
H	-7.5545	2.6348	0.8251
H	-8.3898	3.9684	-0.0280
C	-6.1724	3.4135	3.3418
C	-5.1258	2.9010	2.4872
H	-4.2000	2.7221	3.0502
C	-8.6238	5.1839	2.5906
H	-8.3828	5.1824	3.6581
H	-8.7249	6.2248	2.2657
C	-5.8797	4.5449	4.1992
C	-6.4460	5.9583	6.1062
H	-7.1091	6.1981	6.9326
C	-6.7282	4.8700	5.2870
H	-7.5926	4.2478	5.4817
C	-6.6261	5.4177	1.1867
C	-6.2970	6.6424	1.7922
H	-6.7374	6.9263	2.7403
C	-5.3818	7.5078	1.1912
H	-5.1449	8.4453	1.6883
C	-4.7597	7.1887	-0.0200
C	-5.0922	5.9613	-0.6143
C	-6.0038	5.0872	-0.0295

H	-6.2130	4.1440	-0.5137
C	-4.7340	5.3507	3.9820
H	-4.0734	5.1279	3.1504
C	-4.4366	6.4159	4.8266
H	-3.5456	7.0119	4.6510
C	-5.2979	6.7285	5.8830
H	-4.6275	5.6797	-1.5564
N	-7.5331	4.5137	1.8289
H	-5.0723	7.5679	6.5354
C	-3.5738	2.5705	-0.8495
H	-4.4769	2.5299	-1.4616
H	-3.3169	3.6026	-0.6039
H	-2.7435	2.0777	-1.3626
C	-14.5909	5.1613	5.4431
H	-14.3795	5.6107	6.4206
H	-15.2900	5.8331	4.9249
H	-15.1182	4.2156	5.6131
C	-3.7867	8.1330	-0.6825
H	-3.3778	8.8551	0.0323
H	-2.9498	7.5905	-1.1372
H	-4.2741	8.7039	-1.4847
Rh	-6.9742	1.5930	4.1861
Rh	-7.7550	-0.4922	5.2506
O	-8.7829	2.4514	4.7566
O	-9.4623	0.5580	5.8111
O	-6.0010	-1.3999	4.6097
O	-5.2170	0.5584	3.7789
O	-7.7464	0.8201	2.4211
O	-8.6135	-1.0162	3.4344
O	-6.1945	2.1181	6.0384
O	-6.8351	0.1618	6.9953
C	-9.5788	1.7836	5.5030
C	-6.2753	1.3000	7.0146
C	-5.1365	-0.6954	4.0041
C	-8.3950	-0.2789	2.4254
C	-5.6098	1.7347	8.2987
C	-3.8957	-1.3716	3.4774
C	-8.9769	-0.7026	1.0984
C	-10.7508	2.5269	6.0947
H	-5.7187	2.8140	8.4345
H	-6.0293	1.1982	9.1527
H	-4.5384	1.5082	8.2332
H	-10.8127	3.5429	5.7062
H	-11.6786	1.9890	5.8804
H	-10.6268	2.5538	7.1838
H	-8.2420	-0.5486	0.3029
H	-9.8478	-0.0738	0.8773
H	-9.2903	-1.7481	1.1259
H	-3.0072	-0.8512	3.8494
H	-3.8927	-1.2816	2.3854
H	-3.8658	-2.4225	3.7713

A_-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.67101473 Eh

Atom	X	Y	Z
S	-5.6817	1.7613	-0.3396
O	-7.0690	1.5209	-0.7798
O	-4.7972	0.5973	-0.1311
N	-10.0883	3.9732	1.9129
N	-5.7800	2.7574	1.0439
C	-13.2281	1.3267	1.2027
C	-13.5013	2.6156	1.6853
H	-14.5278	2.9118	1.8658
C	-12.4660	3.4992	1.9209
H	-12.6932	4.4975	2.2766
C	-11.1138	3.1187	1.6827
C	-10.8649	1.8044	1.1885
H	-9.8501	1.4784	0.9981
C	-11.9056	0.9280	0.9547
H	-11.7074	-0.0703	0.5833
C	-10.1904	5.2296	2.6588
H	-10.9074	5.1471	3.4814
H	-10.5001	6.0516	2.0009
C	-8.7470	5.4184	3.1645
H	-8.4769	6.4670	3.2869
H	-8.6088	4.8941	4.1132
C	-5.6395	2.8536	3.4048
C	-5.2999	2.2541	2.1315
H	-4.7662	1.2966	2.1572
C	-8.6686	3.5821	1.7617
H	-8.4403	3.2434	0.7533
H	-8.4457	2.7674	2.4533

C	-5.1767	4.1266	3.8211
C	-5.2880	6.0063	5.3670
H	-5.7406	6.5005	6.2213
C	-5.7524	4.7678	4.9551
H	-6.5696	4.2820	5.4714
C	-7.3559	5.5995	1.1351
C	-7.5793	5.4461	-0.2455
H	-8.2584	4.6868	-0.6166
C	-6.9372	6.2676	-1.1682
H	-7.1171	6.1445	-2.2325
C	-6.0616	7.2787	-0.7459
C	-5.8417	7.4533	0.6258
C	-6.4775	6.6149	1.5439
H	-6.2703	6.7385	2.6017
C	-4.1212	4.7831	3.1248
H	-3.6882	4.3120	2.2486
C	-3.6372	6.0044	3.5717
H	-2.8205	6.4915	3.0481
C	-4.2214	6.6166	4.6881
H	-5.1670	8.2181	0.9934
N	-7.9204	4.7649	2.1345
H	-3.8485	7.5783	5.0298
C	-4.8997	2.9065	-1.4761
H	-5.4967	3.8205	-1.5124
H	-3.8884	3.1165	-1.1198
H	-4.8688	2.4215	-2.4554
Rh	-6.6407	1.4370	4.4824
Rh	-7.6951	-0.3696	5.7902
O	-8.3496	2.5537	4.8524
O	-9.3817	0.8383	5.9229
O	-5.9381	-1.4501	5.5331
O	-5.0196	0.1633	4.2299
O	-7.5164	0.5893	2.8053
O	-8.3982	-1.1347	3.9883
O	-5.8267	2.1112	6.2663
O	-6.9042	0.5310	7.4918
C	-9.3540	2.0029	5.4269
C	-6.1590	1.5477	7.3663
C	-5.0140	-0.9795	4.8082
C	-8.1559	-0.5142	2.9093
C	-5.6145	2.1889	8.6196
C	-3.7717	-1.8103	4.6035
C	-8.6705	-1.1153	1.6249
C	-10.6224	2.8177	5.4735
H	-4.5387	2.3594	8.5137
H	-6.0942	3.1654	8.7548
H	-5.8120	1.5642	9.4926
H	-10.3939	3.8825	5.5583
H	-11.1700	2.6576	4.5365
H	-11.2544	2.4962	6.3041
H	-8.3042	-0.5577	0.7608
H	-9.7660	-1.1022	1.6385
H	-8.3508	-2.1603	1.5605
H	-2.9294	-1.3241	5.1092
H	-3.5347	-1.8621	3.5363
H	-3.9069	-2.8154	5.0074
N	-14.3100	0.4124	0.9552
O	-15.4702	0.7869	1.1909
O	-14.0447	-0.7174	0.5143
O	-5.4841	8.0258	-1.7346
C	-4.5889	9.0640	-1.3502
H	-4.2545	9.5322	-2.2788
H	-5.0864	9.8185	-0.7261
H	-3.7166	8.6685	-0.8125

A-B-ts-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.67007103 Eh

Atom	X	Y	Z
S	-5.4347	1.5099	-0.2951
O	-6.6427	0.8800	-0.8593
O	-4.3389	0.6364	0.1751
N	-10.0518	3.9575	1.9018
N	-5.9634	2.5935	0.9063
C	-13.3847	1.5076	1.3825
C	-13.5507	2.8138	1.8664
H	-14.5446	3.1737	2.1039
C	-12.4508	3.6331	2.0327
H	-12.5939	4.6460	2.3909
C	-11.1413	3.1676	1.7234
C	-11.0027	1.8421	1.2182
H	-10.0240	1.4498	0.9709
C	-12.1073	1.0286	1.0566

H	-11.9933	0.0173	0.6847
C	-10.0193	5.1738	2.7168
H	-10.7218	5.1132	3.5530
H	-10.2590	6.0591	2.1148
C	-8.5615	5.1927	3.2036
H	-8.2001	6.1968	3.4127
H	-8.4577	4.5715	4.0908
C	-5.8936	3.0878	3.2802
C	-5.4328	2.4415	2.0708
H	-4.6469	1.6931	2.2508
C	-8.6838	3.4610	1.6694
H	-8.5233	3.1823	0.6326
H	-8.4969	2.5856	2.2885
C	-5.2827	4.2807	3.7719
C	-5.1826	6.0837	5.4091
H	-5.5648	6.5638	6.3052
C	-5.7608	4.9082	4.9538
H	-6.5863	4.4596	5.4885
C	-7.2515	5.4342	1.1291
C	-7.3850	5.2576	-0.2625
H	-7.9770	4.4475	-0.6691
C	-6.7652	6.1219	-1.1555
H	-6.8831	5.9815	-2.2260
C	-5.9836	7.1950	-0.6982
C	-5.8415	7.3854	0.6797
C	-6.4663	6.5114	1.5728
H	-6.3232	6.6759	2.6338
C	-4.1991	4.8850	3.0761
H	-3.8356	4.4311	2.1596
C	-3.5988	6.0405	3.5630
H	-2.7624	6.4838	3.0310
C	-4.0944	6.6448	4.7232
H	-5.2432	8.1972	1.0769
N	-7.8110	4.5508	2.0977
H	-3.6352	7.5563	5.0961
C	-4.7851	2.6765	-1.4941
H	-5.5632	3.4063	-1.7265
H	-3.9104	3.1719	-1.0665
H	-4.5063	2.1081	-2.3856
Rh	-6.8039	1.5433	4.3901
Rh	-7.6802	-0.3735	5.6725
O	-8.6516	2.4384	4.7078
O	-9.4714	0.6602	5.8531
O	-5.8430	-1.2993	5.3989
O	-5.0371	0.4608	4.2143
O	-7.5362	0.5989	2.6946
O	-8.3389	-1.1697	3.8665
O	-6.1064	2.2903	6.1974
O	-6.9535	0.5510	7.3867
C	-9.5740	1.8111	5.3346
C	-6.3232	1.6462	7.2792
C	-4.9431	-0.7046	4.7342
C	-8.1247	-0.5320	2.7912
C	-5.7354	2.2351	8.5389
C	-3.6236	-1.4073	4.5302
C	-8.6233	-1.1375	1.5024
C	-10.9069	2.5118	5.4262
H	-5.5844	3.3115	8.4311
H	-6.3812	2.0225	9.3946
H	-4.7619	1.7629	8.7209
H	-10.7630	3.5780	5.6210
H	-11.4233	2.4103	4.4645
H	-11.5239	2.0644	6.2079
H	-8.1530	-0.6532	0.6440
H	-9.7103	-1.0017	1.4483
H	-8.4201	-2.2123	1.4944
H	-2.8369	-0.8569	5.0588
H	-3.3710	-1.4080	3.4651
H	-3.6674	-2.4314	4.9054
N	-14.5329	0.6558	1.2152
O	-15.6513	1.1010	1.5176
O	-14.3615	-0.4918	0.7752
O	-5.4188	7.9780	-1.6611
C	-4.6135	9.0772	-1.2434
H	-4.2725	9.5644	-2.1595
H	-5.1897	9.7957	-0.6457
H	-3.7416	8.7416	-0.6665

B-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.69045527 Eh

Atom	X	Y	Z
S	-5.2379	1.4326	0.0496

O	-6.0562	0.2518	-0.2938
O	-3.9114	1.1939	0.6629
N	-9.9883	3.9602	2.0243
N	-6.1859	2.5016	0.9230
C	-13.4711	2.1745	0.5927
C	-13.5244	3.4655	1.1350
H	-14.4695	3.9936	1.1720
C	-12.3702	4.0572	1.6140
H	-12.4171	5.0619	2.0184
C	-11.1306	3.3692	1.5616
C	-11.1021	2.0594	1.0125
H	-10.1761	1.4969	0.9782
C	-12.2598	1.4740	0.5322
H	-12.2372	0.4725	0.1199
C	-9.9588	5.1104	2.9311
H	-10.7563	5.0608	3.6794
H	-10.0477	6.0502	2.3760
C	-8.5988	4.9616	3.6047
H	-8.1636	5.8992	3.9315
H	-8.6467	4.2513	4.4271
C	-6.4255	3.6504	3.0667
C	-5.7288	2.8710	2.0922
H	-4.7439	2.5373	2.4211
C	-8.7319	3.2411	2.0726
H	-8.4287	2.8134	1.1261
H	-8.7277	2.4636	2.8294
C	-5.5821	4.5990	3.8697
C	-5.1618	5.9501	5.8571
H	-5.4740	6.2729	6.8472
C	-5.9493	5.0389	5.1544
H	-6.8389	4.6418	5.6230
C	-7.4373	5.3011	1.4373
C	-7.6942	5.0277	0.0889
H	-8.1514	4.1028	-0.2290
C	-7.3600	5.9596	-0.8847
H	-7.5593	5.7526	-1.9312
C	-6.7611	7.1802	-0.5363
C	-6.5156	7.4579	0.8145
C	-6.8579	6.5207	1.7904
H	-6.6484	6.7639	2.8231
C	-4.3788	5.0963	3.3292
H	-4.0831	4.8080	2.3247
C	-3.5719	5.9826	4.0445
H	-2.6483	6.3452	3.6009
C	-3.9659	6.4230	5.3097
H	-6.0613	8.3911	1.1247
N	-7.7420	4.2967	2.5252
H	-3.3479	7.1238	5.8647
C	-4.9979	2.3879	-1.4554
H	-5.9753	2.6317	-1.8769
H	-4.4477	3.2997	-1.2114
H	-4.4255	1.7691	-2.1518
Rh	-6.7547	1.5888	4.4355
Rh	-7.1071	-0.4867	5.6876
O	-8.6869	2.1331	5.0025
O	-9.0227	0.1960	6.1319
O	-5.1985	-1.0660	5.1139
O	-4.8609	0.8840	4.0077
O	-7.5286	0.5875	2.7949
O	-7.8541	-1.3356	3.9487
O	-5.9970	2.3883	6.1941
O	-6.3340	0.4684	7.3589
C	-9.4022	1.3179	5.6814
C	-5.9376	1.6718	7.2456
C	-4.5099	-0.2803	4.3898
C	-7.9059	-0.6263	2.8955
C	-5.2999	2.3060	8.4582
C	-3.1448	-0.7345	3.9380
C	-8.4842	-1.2408	1.6463
C	-10.8276	1.7456	5.9313
H	-5.4508	3.3881	8.4497
H	-5.7010	1.8705	9.3765
H	-4.2209	2.1095	8.4246
H	-10.8467	2.7714	6.3127
H	-11.3687	1.7350	4.9773
H	-11.3217	1.0739	6.6355
H	-7.8802	-0.9386	0.7866
H	-9.5020	-0.8557	1.5052
H	-8.5263	-2.3290	1.7295
H	-2.3802	-0.1728	4.4878
H	-3.0279	-0.5068	2.8741
H	-3.0072	-1.8022	4.1198

N	-14.6807	1.5558	0.1008
O	-14.6080	0.4163	-0.3800
O	-15.7422	2.1900	0.1807
O	-6.4701	8.0136	-1.5651
C	-5.8415	9.2629	-1.2722
H	-5.6969	9.7550	-2.2360
H	-6.4769	9.8916	-0.6357
H	-4.8675	9.1166	-0.7887

B_-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.69798022 Eh

Atom	X	Y	Z
S	-5.9849	2.8164	1.0881
O	-5.3459	3.9555	0.3771
O	-7.1590	2.1918	0.4547
N	-9.2312	6.0877	4.0283
N	-6.4283	3.3121	2.6012
C	-13.2325	5.7563	2.8919
C	-12.8676	6.6427	3.9122
H	-13.6261	7.2428	4.4000
C	-11.5412	6.7440	4.2922
H	-11.2727	7.4332	5.0841
C	-10.5434	5.9635	3.6537
C	-10.9400	5.0618	2.6315
H	-10.2147	4.4193	2.1473
C	-12.2679	4.9659	2.2549
H	-12.5662	4.2737	1.4770
C	-8.7989	6.7815	5.2398
H	-9.3045	6.3974	6.1343
H	-9.0018	7.8531	5.1620
C	-7.3033	6.4641	5.3027
H	-6.6726	7.2833	5.6344
H	-7.1086	5.5865	5.9131
C	-5.6383	5.2300	3.9211
C	-5.4614	4.0735	3.2501
H	-4.4453	3.6788	3.3156
C	-8.1812	5.2308	3.5297
H	-8.2262	5.0712	2.4594
H	-8.1272	4.2802	4.0535
C	-4.5697	5.7509	4.8100
C	-3.0187	7.4604	5.5742
H	-2.6158	8.4657	5.4840
C	-4.0386	7.0497	4.7147
H	-4.4064	7.7332	3.9578
C	-6.7746	7.1700	2.9069
C	-6.9414	8.4996	3.2752
H	-7.1797	8.7922	4.2894
C	-6.7857	9.5138	2.3245
H	-6.9182	10.5426	2.6360
C	-6.4644	9.1894	1.0007
C	-6.2928	7.8396	0.6449
C	-6.4415	6.8365	1.5887
H	-6.2809	5.8045	1.2940
C	-4.0454	4.8760	5.7815
H	-4.4666	3.8792	5.8667
C	-3.0142	5.2861	6.6283
H	-2.6204	4.5955	7.3695
C	-2.5024	6.5824	6.5322
H	-6.0331	7.5946	-0.3800
N	-6.9227	6.0292	3.8858
H	-1.7053	6.9066	7.1958
C	-4.7005	1.5580	1.2499
H	-3.8526	1.9801	1.7947
H	-5.1161	0.7035	1.7820
H	-4.3913	1.2787	0.2388
Rh	-7.0180	1.7212	4.1486
Rh	-7.5575	0.0692	5.8605
O	-9.0573	2.0462	3.9382
O	-9.5614	0.4944	5.5185
O	-5.5070	-0.2232	6.0853
O	-5.0174	1.3166	4.4903
O	-7.1062	0.1746	2.7779
O	-7.5998	-1.3660	4.3685
O	-6.9782	3.1334	5.7002
O	-7.4665	1.5783	7.2773
C	-9.8726	1.3709	4.6503
C	-7.1894	2.7582	6.9039
C	-4.6993	0.4497	5.3719
C	-7.3730	-1.0091	3.1699
C	-7.1070	3.8260	7.9684
C	-3.2211	0.2051	5.5558
C	-7.4513	-2.0677	2.0976

C	-11.3411	1.6227	4.4083
H	-6.1936	4.4134	7.8321
H	-7.9640	4.5025	7.8702
H	-7.1201	3.3811	8.9650
H	-11.5158	2.6834	4.2105
H	-11.6490	1.0623	3.5168
H	-11.9386	1.2868	5.2584
H	-6.6521	-1.9244	1.3652
H	-8.4086	-1.9639	1.5725
H	-7.3923	-3.0670	2.5338
H	-2.6996	1.1611	5.6655
H	-2.8280	-0.2863	4.6581
H	-3.0340	-0.4276	6.4254
O	-6.2944	10.0885	0.0020
C	-6.4491	11.4777	0.2991
H	-6.2773	12.0029	-0.6424
H	-7.4621	11.6987	0.6582
H	-5.7143	11.8119	1.0421
N	-14.6199	5.6480	2.5010
O	-14.9184	4.8531	1.5995
O	-15.4537	6.3556	3.0834

B-C-ts-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.68186316 Eh

Atom	X	Y	Z
S	-6.1123	2.7059	1.2495
O	-5.5666	3.8616	0.4883
O	-7.3198	2.0527	0.7118
N	-9.4327	5.5747	4.3509
N	-6.4370	3.1704	2.8025
C	-12.0602	7.8902	2.0386
C	-12.2057	7.8600	3.4254
H	-12.9818	8.4424	3.9059
C	-11.3401	7.0739	4.1757
H	-11.4543	7.0359	5.2533
C	-10.3323	6.3329	3.5400
C	-10.2257	6.3440	2.1412
H	-9.4380	5.7997	1.6366
C	-11.0851	7.1309	1.3883
H	-10.9836	7.1784	0.3114
C	-8.8883	6.1302	5.6062
H	-9.1866	5.5002	6.4476
H	-9.2879	7.1303	5.7568
C	-7.3226	6.1366	5.4875
H	-6.9324	7.0960	5.8344
H	-6.9112	5.3561	6.1201
C	-5.6034	5.0984	4.0719
C	-5.4323	3.9466	3.3835
H	-4.4098	3.5658	3.3576
C	-8.6871	4.5788	3.8954
H	-8.8015	4.2076	2.8883
H	-8.2142	3.9354	4.6185
C	-4.4887	5.6539	4.8759
C	-3.1633	7.5233	5.7007
H	-2.9708	8.5928	5.7291
C	-4.2255	7.0356	4.9395
H	-4.8449	7.7279	4.3779
C	-7.0496	6.8586	3.1261
C	-7.6350	8.0887	3.4395
H	-7.8728	8.3563	4.4610
C	-7.9514	9.0150	2.4385
H	-8.4242	9.9481	2.7210
C	-7.6755	8.7170	1.1019
C	-7.0392	7.5008	0.7908
C	-6.7320	6.5851	1.7831
H	-6.2772	5.6415	1.5067
C	-3.6689	4.7815	5.6198
H	-3.8963	3.7191	5.6215
C	-2.5996	5.2723	6.3707
H	-1.9787	4.5816	6.9356
C	-2.3415	6.6451	6.4148
H	-6.8138	7.2797	-0.2482
N	-6.8750	5.8184	4.1161
H	-1.5143	7.0285	7.0061
C	-4.7767	1.4890	1.2686
H	-3.9050	1.9242	1.7633
H	-5.1188	0.5988	1.7934
H	-4.5361	1.2621	0.2262
Rh	-6.8483	1.4952	4.3171
Rh	-7.2392	-0.2002	6.0338
O	-8.9122	1.6928	4.1802
O	-9.2747	0.1278	5.7848

O	-5.1724	-0.4011	6.1592
O	-4.8164	1.1896	4.5787
O	-6.9079	-0.0511	2.9423
O	-7.2871	-1.6246	4.5321
O	-6.8241	2.8938	5.8781
O	-7.1583	1.3028	7.4591
C	-9.6631	0.9859	4.9313
C	-6.9609	2.4985	7.0864
C	-4.4251	0.3155	5.4225
C	-7.1136	-1.2478	3.3307
C	-6.8791	3.5604	8.1571
C	-2.9339	0.1007	5.5180
C	-7.1781	-2.2984	2.2492
C	-11.1496	1.1891	4.7636
H	-5.9569	4.1368	8.0310
H	-7.7240	4.2508	8.0542
H	-6.9028	3.1106	9.1512
H	-11.3773	2.2595	4.7405
H	-11.4587	0.7627	3.8019
H	-11.7050	0.7024	5.5676
H	-6.3653	-2.1494	1.5325
H	-8.1246	-2.1876	1.7068
H	-7.1257	-3.3014	2.6772
H	-2.4065	1.0540	5.4247
H	-2.6196	-0.5407	4.6853
H	-2.6707	-0.3895	6.4576
N	-12.9360	8.7527	1.2489
O	-12.7244	8.8409	0.0364
O	-13.8393	9.3568	1.8338
O	-7.9730	9.5192	0.0449
C	-8.7120	10.7141	0.2924
H	-8.8688	11.1758	-0.6847
H	-9.6859	10.4936	0.7489
H	-8.1547	11.4088	0.9340

C-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.69245375 Eh

Atom	X	Y	Z
S	-7.4238	2.9661	1.5735
O	-7.3414	4.2122	0.7677
O	-8.6781	2.1906	1.4751
N	-9.7542	5.2269	4.2102
N	-7.2002	3.3119	3.1803
C	-11.3886	7.7039	1.2543
C	-11.9228	7.7491	2.5433
H	-12.7171	8.4449	2.7820
C	-11.4069	6.8951	3.5100
H	-11.8083	6.9144	4.5174
C	-10.3618	6.0254	3.1737
C	-9.8636	5.9578	1.8719
H	-9.0288	5.3131	1.6249
C	-10.3811	6.8088	0.9010
H	-9.9735	6.8100	-0.1015
C	-9.3143	5.9077	5.4589
H	-9.7129	5.3508	6.3099
H	-9.7645	6.8958	5.4593
C	-7.7659	5.9774	5.5644
H	-7.5277	6.8081	6.2467
H	-7.4102	5.0570	6.0248
C	-5.9429	5.2302	4.0974
C	-6.0242	4.0350	3.4715
H	-5.0884	3.5098	3.2904
C	-9.4504	3.9768	4.0305
H	-9.7845	3.4523	3.1450
H	-9.0289	3.4291	4.8578
C	-4.6555	5.6867	4.6834
C	-3.1548	7.4710	5.3986
H	-2.9469	8.5338	5.4948
C	-4.3616	7.0556	4.8348
H	-5.0750	7.7994	4.4963
C	-7.2912	7.1668	3.4244
C	-8.0142	8.3031	3.8228
H	-8.3401	8.4191	4.8499
C	-8.3542	9.3104	2.9104
H	-8.9465	10.1493	3.2581
C	-7.9426	9.2190	1.5792
C	-7.1371	8.1338	1.1956
C	-6.8166	7.1288	2.0945
H	-6.2546	6.2689	1.7528
C	-3.7117	4.7509	5.1577
H	-3.9448	3.6916	5.1149
C	-2.5032	5.1696	5.7145

H	-1.7934	4.4286	6.0742
C	-2.2154	6.5322	5.8353
H	-6.8010	8.0748	0.1642
N	-7.0891	6.0710	4.2836
H	-1.2772	6.8588	6.2760
C	-6.0599	1.9300	1.0053
H	-5.1206	2.4680	1.1525
H	-6.0751	0.9927	1.5603
H	-6.2235	1.7557	-0.0618
Rh	-7.0026	1.4308	4.5871
Rh	-6.6832	-0.3096	6.2687
O	-9.0486	1.1982	4.8720
O	-8.7487	-0.4092	6.4447
O	-4.6384	-0.1030	5.9909
O	-4.9329	1.4871	4.4034
O	-7.0426	-0.0944	3.1811
O	-6.7467	-1.7103	4.7465
O	-6.9662	2.8087	6.1377
O	-6.6190	1.2010	7.6985
C	-9.4711	0.3397	5.7160
C	-6.7657	2.4076	7.3342
C	-4.2104	0.7326	5.1350
C	-6.9094	-1.3076	3.5516
C	-6.6954	3.4835	8.3904
C	-2.7138	0.8575	4.9880
C	-6.9756	-2.3501	2.4626
C	-10.9684	0.1868	5.8228
H	-5.8984	4.1882	8.1306
H	-7.6386	4.0403	8.4101
H	-6.5040	3.0527	9.3747
H	-11.4575	1.1600	5.7250
H	-11.3130	-0.4477	4.9969
H	-11.2450	-0.2856	6.7678
H	-6.3345	-2.0565	1.6259
H	-8.0046	-2.4069	2.0886
H	-6.6750	-3.3288	2.8412
H	-2.3040	1.2995	5.9037
H	-2.4544	1.4871	4.1350
H	-2.2695	-0.1359	4.8718
N	-11.8606	8.6668	0.2569
O	-12.6431	9.5469	0.6278
O	-11.4425	8.5616	-0.8969
O	-8.2649	10.1082	0.5904
C	-9.1735	11.1566	0.9047
H	-8.7519	11.8525	1.6433
H	-9.3500	11.6930	-0.0303
H	-10.1300	10.7707	1.2828

C-4-ts-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.69038246 Eh

Atom	X	Y	Z
S	-7.3804	3.1102	1.5310
O	-7.1125	4.3399	0.7510
O	-8.6559	2.4086	1.2938
N	-9.5935	5.2010	4.0758
N	-7.3261	3.4627	3.1992
C	-11.3675	7.6390	1.1596
C	-11.9150	7.6025	2.4443
H	-12.7645	8.2262	2.6927
C	-11.3494	6.7592	3.3902
H	-11.7741	6.7153	4.3872
C	-10.2300	5.9765	3.0579
C	-9.7280	5.9887	1.7530
H	-8.8446	5.4226	1.4944
C	-10.2944	6.8255	0.7988
H	-9.8756	6.8837	-0.1977
C	-9.3130	5.8422	5.3800
H	-9.7252	5.2175	6.1782
H	-9.8404	6.7918	5.3954
C	-7.7954	6.0510	5.6225
H	-7.6762	6.8897	6.3243
H	-7.3910	5.1605	6.1027
C	-5.9612	5.3171	4.1767
C	-6.1271	4.1309	3.5581
H	-5.2303	3.5406	3.3961
C	-9.1758	3.9450	3.8745
H	-9.6286	3.3970	3.0600
H	-8.9557	3.4009	4.7784
C	-4.6320	5.6860	4.7345
C	-3.0076	7.3819	5.3873
H	-2.7332	8.4308	5.4665
C	-4.2535	7.0356	4.8641

H	-4.9324	7.8174	4.5402
C	-7.2722	7.2906	3.5159
C	-8.0968	8.3725	3.8687
H	-8.4920	8.4571	4.8746
C	-8.4584	9.3502	2.9343
H	-9.1299	10.1432	3.2442
C	-7.9724	9.2858	1.6262
C	-7.0709	8.2627	1.2925
C	-6.7264	7.2841	2.2129
H	-6.0846	6.4685	1.9038
C	-3.7339	4.6982	5.1886
H	-4.0289	3.6542	5.1603
C	-2.4876	5.0477	5.7089
H	-1.8142	4.2677	6.0559
C	-2.1148	6.3911	5.8070
H	-6.6783	8.2247	0.2803
N	-7.0346	6.2293	4.3998
H	-1.1461	6.6639	6.2174
C	-6.0225	1.9853	1.1686
H	-5.0759	2.4522	1.4445
H	-6.1810	1.0462	1.6963
H	-6.0579	1.8354	0.0855
Rh	-7.0722	1.4270	4.6131
Rh	-6.6816	-0.3136	6.2594
O	-9.1024	1.1845	4.9691
O	-8.7330	-0.4312	6.5171
O	-4.6504	-0.0952	5.9231
O	-5.0144	1.4962	4.3521
O	-7.1764	-0.0825	3.1956
O	-6.7890	-1.7044	4.7322
O	-6.9711	2.8015	6.1571
O	-6.5803	1.1859	7.6975
C	-9.4893	0.3204	5.8251
C	-6.7361	2.3959	7.3455
C	-4.2581	0.7463	5.0549
C	-7.0123	-1.2985	3.5483
C	-6.6311	3.4655	8.4034
C	-2.7702	0.8813	4.8519
C	-7.1119	-2.3321	2.4553
C	-10.9788	0.1627	5.9984
H	-5.8144	4.1467	8.1411
H	-7.5574	4.0494	8.4270
H	-6.4463	3.0270	9.3856
H	-11.4786	1.1288	5.8894
H	-11.3523	-0.5033	5.2108
H	-11.2105	-0.2800	6.9695
H	-6.4760	-2.0425	1.6130
H	-8.1460	-2.3675	2.0936
H	-6.8217	-3.3179	2.8231
H	-2.3223	1.2875	5.7660
H	-2.5481	1.5429	4.0129
H	-2.3313	-0.1064	4.6791
N	-11.8923	8.5940	0.1891
O	-12.7683	9.3817	0.5635
O	-11.4249	8.5851	-0.9524
O	-8.3111	10.1444	0.6149
C	-9.3252	11.1085	0.8689
H	-9.0009	11.8538	1.6083
H	-9.5121	11.6085	-0.0842
H	-10.2565	10.6439	1.2191

D-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.71966556 Eh

Atom	X	Y	Z
S	-6.9084	3.7190	0.8674
O	-5.6359	4.3535	0.5029
O	-8.0850	3.8512	-0.0052
N	-9.3873	4.9605	3.6455
N	-7.3444	4.3446	2.3828
C	-11.6202	7.9491	1.7358
C	-11.7465	7.7575	3.1164
H	-12.4035	8.3981	3.6921
C	-11.0164	6.7604	3.7363
H	-11.1154	6.6330	4.8071
C	-10.1454	5.9222	2.9952
C	-10.0682	6.1122	1.5931
H	-9.3924	5.5204	0.9906
C	-10.7878	7.1194	0.9753
H	-10.6842	7.2891	-0.0894
C	-9.0015	5.1407	5.0506
H	-8.4320	4.2578	5.3397
H	-9.8829	5.1770	5.7004

C	-8.1313	6.4018	5.2799
H	-8.7564	7.2890	5.3493
H	-7.6284	6.2936	6.2491
C	-6.1653	5.5378	4.1676
C	-6.2557	4.5201	3.2843
H	-5.4486	3.7985	3.2126
C	-8.6882	3.9471	2.9028
H	-9.2838	3.6458	2.0424
H	-8.5718	3.0786	3.5578
C	-5.0592	5.6188	5.1566
C	-3.7164	6.9648	6.6818
H	-3.5058	7.9285	7.1384
C	-4.7643	6.8512	5.7670
H	-5.3591	7.7221	5.5116
C	-7.3003	7.4958	3.1616
C	-8.1899	8.5810	3.2480
H	-8.7746	8.7513	4.1430
C	-8.3825	9.4653	2.1824
H	-9.1041	10.2659	2.2992
C	-7.6655	9.3071	0.9938
C	-6.7332	8.2650	0.9145
C	-6.5500	7.3817	1.9719
H	-5.8322	6.5814	1.8520
C	-4.2811	4.4994	5.5085
H	-4.5202	3.5298	5.0950
C	-3.2278	4.6166	6.4136
H	-2.6425	3.7364	6.6687
C	-2.9402	5.8500	7.0088
H	-6.1632	8.1398	-0.0018
N	-7.1331	6.5827	4.2300
H	-2.1259	5.9380	7.7230
C	-6.6129	1.9661	1.1392
H	-5.7950	1.8444	1.8520
H	-7.5270	1.5052	1.5191
H	-6.3429	1.5267	0.1745
Rh	-7.0725	1.3166	4.7949
Rh	-6.2615	-0.2916	6.3823
O	-8.9806	0.9761	5.5073
O	-8.2290	-0.6044	6.9463
O	-4.3398	0.1022	5.7171
O	-5.1153	1.5253	4.1359
O	-7.3197	-0.2295	3.4447
O	-6.4569	-1.7330	4.9062
O	-6.8166	2.7717	6.2387
O	-6.1160	1.2481	7.7619
C	-9.1521	0.0846	6.4030
C	-6.4139	2.4333	7.4007
C	-4.1797	0.8867	4.7303
C	-6.9594	-1.4061	3.7822
C	-6.2426	3.5339	8.4133
C	-2.7858	1.0843	4.1975
C	-7.1834	-2.5062	2.7780
C	-10.5673	-0.2050	6.8300
H	-5.2232	3.9276	8.3249
H	-6.9402	4.3499	8.2111
H	-6.3832	3.1488	9.4258
H	-11.2223	0.6369	6.5963
H	-10.9200	-1.0888	6.2840
H	-10.6011	-0.4305	7.8988
H	-7.1009	-2.1172	1.7604
H	-8.1985	-2.8993	2.9156
H	-6.4729	-3.3206	2.9358
H	-2.0432	0.6853	4.8907
H	-2.6036	2.1473	4.0142
H	-2.7009	0.5604	3.2378
N	-12.3163	9.0432	1.1021
O	-13.0756	9.7407	1.7892
O	-12.1200	9.2498	-0.1058
O	-7.7929	10.0986	-0.1169
C	-8.8652	11.0345	-0.1458
H	-8.7607	11.8033	0.6323
H	-8.8171	11.5163	-1.1254
H	-9.8383	10.5363	-0.0361

4-MeO-NO2

Energy (POTENTIAL) = -1961.52129144 Eh

Atom	X	Y	Z
S	-6.3626	1.6660	-0.4658
O	-7.2444	1.1597	-1.5275
O	-5.5814	0.7242	0.3442
N	-9.6564	3.2056	1.0076
N	-7.3275	2.5840	0.5868

C	-11.0266	-0.3768	2.7006
C	-11.3646	0.8444	3.2939
H	-11.9695	0.8569	4.1924
C	-10.9099	2.0279	2.7400
H	-11.1640	2.9562	3.2349
C	-10.1070	2.0279	1.5694
C	-9.7743	0.7725	0.9936
H	-9.1665	0.7169	0.1000
C	-10.2299	-0.4091	1.5503
H	-9.9753	-1.3599	1.0977
C	-10.0886	4.5239	1.4851
H	-11.1278	4.4714	1.8174
H	-10.0733	5.1941	0.6221
C	-9.1955	5.0867	2.6074
H	-9.4442	6.1384	2.7856
H	-9.3893	4.5489	3.5392
C	-7.1890	3.7099	2.7617
C	-6.9192	2.6839	1.9235
H	-6.3638	1.8258	2.2822
C	-8.5765	3.1970	0.0457
H	-8.3852	4.2272	-0.2524
H	-8.8344	2.6188	-0.8425
C	-6.8991	3.6050	4.2106
C	-6.2818	4.6861	6.3039
H	-6.0338	5.5916	6.8520
C	-6.5844	4.7637	4.9449
H	-6.5678	5.7232	4.4368
C	-7.0868	5.7938	1.4436
C	-7.7301	6.8833	0.8151
H	-8.7835	7.0769	0.9798
C	-7.0299	7.7431	-0.0264
H	-7.5403	8.5757	-0.5022
C	-5.6668	7.5535	-0.2837
C	-5.0134	6.4816	0.3359
C	-5.7141	5.6224	1.1848
H	-5.1785	4.8073	1.6576
C	-6.9362	2.3717	4.8886
H	-7.2400	1.4750	4.3562
C	-6.6233	2.2956	6.2460
H	-6.6588	1.3338	6.7512
C	-6.2935	3.4512	6.9602
H	-3.9563	6.3019	0.1742
N	-7.7739	4.9299	2.3127
H	-6.0608	3.3919	8.0202
C	-5.2400	2.8711	-1.1807
H	-5.8265	3.6370	-1.6929
H	-4.6503	3.3115	-0.3748
H	-4.5952	2.3420	-1.8881
N	-11.4890	-1.6126	3.2896
O	-11.1610	-2.6808	2.7547
O	-12.1946	-1.5541	4.3066
O	-5.0800	8.4497	-1.1364
C	-3.6999	8.2769	-1.4372
H	-3.5085	7.3089	-1.9206
H	-3.4395	9.0807	-2.1298
H	-3.0743	8.3606	-0.5383

2_MeO-NO2

Energy (POTENTIAL) = -1009.79516639 Eh

Atom	X	Y	Z
N	-10.1116	3.6662	2.2621
C	-13.1056	2.4386	-0.4759
C	-13.4080	3.3470	0.5438
H	-14.4094	3.7466	0.6571
C	-12.4148	3.7653	1.4353
H	-12.6863	4.4757	2.2085
C	-11.0979	3.2830	1.3436
C	-10.8076	2.3668	0.3083
H	-9.8072	1.9619	0.1968
C	-11.7937	1.9552	-0.5806
H	-11.5583	1.2515	-1.3740
C	-10.2949	4.8522	3.0963
H	-11.1303	4.7217	3.7887
H	-10.4820	5.7540	2.4906
C	-8.9630	4.9517	3.8378
H	-8.6990	5.9896	4.0608
H	-8.9768	4.3838	4.7776
C	-8.7136	3.5866	1.8620
H	-8.5356	4.0157	0.8599
H	-8.3646	2.5457	1.8497
C	-6.6712	4.3639	3.0284
C	-6.0529	4.9997	4.1411

H	-6.6595	5.4759	4.9021
C	-4.6779	5.0100	4.2753
H	-4.2131	5.4919	5.1271
C	-3.8752	4.3868	3.3090
C	-4.4590	3.7519	2.2035
C	-5.8334	3.7381	2.0624
H	-6.2667	3.2522	1.1959
H	-3.8269	3.2770	1.4629
N	-8.0227	4.3590	2.8873
N	-2.4418	4.3999	3.4524
O	-1.7540	3.8393	2.5854
O	-1.9495	4.9719	4.4372
O	-13.9957	1.9719	-1.4051
C	-15.3352	2.4493	-1.3428
H	-15.3837	3.5392	-1.4716
H	-15.8654	1.9675	-2.1676
H	-15.8199	2.1748	-0.3959

D_-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.71504116 Eh

Atom	X	Y	Z
S	-8.6067	4.9495	2.0324
O	-8.9118	6.3802	2.1171
O	-9.7236	4.0075	1.9583
N	-9.2106	6.8049	5.1228
N	-7.5955	4.3281	3.3321
C	-12.5178	4.2508	4.8409
C	-12.6194	5.5829	4.4183
H	-13.5579	5.9486	4.0195
C	-11.5287	6.4260	4.5222
H	-11.6355	7.4561	4.2063
C	-10.2909	5.9616	5.0447
C	-10.2205	4.6064	5.4700
H	-9.2936	4.1736	5.8203
C	-11.3114	3.7683	5.3664
H	-11.2246	2.7315	5.6642
C	-9.1791	8.1139	4.4568
H	-9.6889	8.8762	5.0633
H	-9.6846	8.0283	3.4967
C	-7.7137	8.5340	4.2273
H	-7.6866	9.3102	3.4650
H	-7.3007	8.9862	5.1395
C	-6.7721	6.3423	4.7991
C	-6.9018	4.9297	4.2308
H	-6.3252	4.2200	4.8166
C	-7.9878	6.4789	5.8062
H	-8.0807	5.5716	6.3970
H	-7.7310	7.2780	6.5093
C	-5.5049	6.4121	5.6917
C	-3.5535	7.6332	6.4726
H	-2.9021	8.4995	6.3946
C	-4.6561	7.5232	5.6219
H	-4.8497	8.2996	4.8899
C	-6.1298	7.3829	2.6338
C	-6.5012	8.1508	1.5154
H	-7.3958	8.7607	1.5488
C	-5.7756	8.1150	0.3239
H	-6.1123	8.7245	-0.5071
C	-4.6549	7.2835	0.2010
C	-4.2814	6.4994	1.2986
C	-4.9969	6.5518	2.4924
H	-4.6497	5.9395	3.3158
C	-5.2417	5.4256	6.6572
H	-5.8973	4.5655	6.7654
C	-4.1381	5.5341	7.5056
H	-3.9509	4.7561	8.2408
C	-3.2868	6.6377	7.4147
H	-3.4142	5.8514	1.2106
N	-6.8777	7.4076	3.8235
H	-2.4273	6.7219	8.0740
C	-7.4770	4.6438	0.6752
H	-6.5798	5.2486	0.8075
H	-7.2457	3.5767	0.6663
H	-8.0096	4.9388	-0.2336
Rh	-7.4687	2.0404	3.6402
Rh	-7.0659	-0.2823	4.2146
O	-9.4799	1.5547	3.5336
O	-9.0914	-0.6254	4.0277
O	-5.0470	0.2031	4.3881
O	-5.4297	2.3626	3.8194
O	-7.2126	1.5312	1.6546
O	-6.8203	-0.6387	2.1832

O	-7.6709	2.4201	5.6703
O	-7.3382	0.2427	6.2055
C	-9.8506	0.3530	3.7237
C	-7.5609	1.4567	6.5029
C	-4.6727	1.3972	4.1748
C	-6.9482	0.3177	1.3570
C	-7.6686	1.8063	7.9659
C	-3.2085	1.7241	4.3308
C	-6.7952	0.0087	-0.1111
C	-11.3196	0.0645	3.5415
H	-6.6570	1.9505	8.3654
H	-8.2343	2.7307	8.1031
H	-8.1377	0.9885	8.5185
H	-11.9226	0.8391	4.0236
H	-11.5478	0.0843	2.4688
H	-11.5755	-0.9187	3.9421
H	-6.1116	0.7290	-0.5711
H	-7.7709	0.1156	-0.5996
H	-6.4256	-1.0076	-0.2595
H	-3.0975	2.6545	4.8965
H	-2.7722	1.8827	3.3374
H	-2.6780	0.9115	4.8306
O	-3.8806	7.1667	-0.9205
C	-4.2436	7.9346	-2.0628
H	-4.2064	9.0127	-1.8559
H	-3.5089	7.6926	-2.8341
H	-5.2461	7.6714	-2.4263
N	-13.6552	3.3775	4.7356
O	-13.5496	2.2096	5.1494
O	-14.7037	3.8197	4.2429

C-D-ts-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.68077324 Eh

Atom	X	Y	Z
S	-8.3697	4.7232	2.1024
O	-8.7611	6.1396	2.2286
O	-9.4562	3.7572	1.8914
N	-9.1785	6.6517	5.2093
N	-7.4750	4.1451	3.4051
C	-12.6488	4.4991	4.2426
C	-12.6594	5.8917	4.1629
H	-13.5600	6.4144	3.8658
C	-11.5026	6.5936	4.4776
H	-11.5168	7.6758	4.4348
C	-10.3434	5.9019	4.8639
C	-10.3518	4.5009	4.9393
H	-9.4567	3.9389	5.1722
C	-11.5047	3.7997	4.6279
H	-11.4950	2.7205	4.6452
C	-8.9422	7.9821	4.5699
H	-9.4334	8.7589	5.1670
H	-9.4005	7.9315	3.5857
C	-7.4435	8.2946	4.4195
H	-7.3730	9.2114	3.8302
H	-7.0063	8.5344	5.3977
C	-6.3068	6.1185	4.5727
C	-6.6678	4.8005	4.2528
H	-6.1627	4.0825	4.8869
C	-8.2573	6.1795	6.0265
H	-8.3752	5.1936	6.4560
H	-7.5882	6.8675	6.5210
C	-5.2685	6.3117	5.6260
C	-3.4485	7.6436	6.5636
H	-2.8032	8.5159	6.4977
C	-4.4225	7.4363	5.5846
H	-4.5173	8.1426	4.7661
C	-6.0749	7.4262	2.5099
C	-6.6965	8.1925	1.5123
H	-7.6672	8.6372	1.6999
C	-6.1185	8.3519	0.2506
H	-6.6413	8.9449	-0.4913
C	-4.9031	7.7260	-0.0534
C	-4.2736	6.9559	0.9343
C	-4.8437	6.8150	2.1957
H	-4.3317	6.2176	2.9426
C	-5.1260	5.4248	6.7164
H	-5.7964	4.5750	6.8164
C	-4.1464	5.6285	7.6861
H	-4.0568	4.9243	8.5094
C	-3.2976	6.7385	7.6162
H	-3.3281	6.4748	0.7004
N	-6.6600	7.2458	3.7790

H	-2.5390	6.8989	8.3773
C	-7.2141	4.5416	0.7368
H	-6.3408	5.1712	0.9074
H	-6.9383	3.4858	0.6914
H	-7.7363	4.8487	-0.1739
Rh	-7.4174	1.9288	3.8143
Rh	-7.0939	-0.3957	4.4673
O	-9.4543	1.5032	3.7445
O	-9.1259	-0.6799	4.2710
O	-5.0580	0.0167	4.6332
O	-5.3632	2.1642	3.9749
O	-7.1640	1.3343	1.8486
O	-6.8408	-0.8302	2.4549
O	-7.6250	2.3918	5.8308
O	-7.3677	0.2201	6.4406
C	-9.8573	0.3174	3.9646
C	-7.5522	1.4504	6.6928
C	-4.6419	1.1851	4.3625
C	-6.9316	0.1054	1.5982
C	-7.6547	1.8520	8.1443
C	-3.1635	1.4616	4.4911
C	-6.7723	-0.2587	0.1421
C	-11.3453	0.0677	3.8874
H	-6.6414	2.0129	8.5334
H	-8.2192	2.7812	8.2514
H	-8.1207	1.0552	8.7291
H	-11.7714	0.1524	4.8947
H	-11.8327	0.8028	3.2447
H	-11.5390	-0.9450	3.5241
H	-6.0841	0.4412	-0.3420
H	-7.7455	-0.1666	-0.3546
H	-6.4068	-1.2815	0.0328
H	-3.0111	2.3881	5.0538
H	-2.7386	1.6059	3.4909
H	-2.6519	0.6329	4.9844
O	-4.2618	7.8011	-1.2600
C	-4.9073	8.5044	-2.3157
H	-5.0383	9.5686	-2.0764
H	-4.2508	8.4123	-3.1840
H	-5.8853	8.0658	-2.5558
N	-13.8564	3.7549	3.9005
O	-13.8290	2.5235	3.9939
O	-14.8507	4.3904	3.5374

t-A-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.67467382 Eh

Atom	X	Y	Z
S	-3.5749	2.3482	0.5323
O	-2.6798	3.3905	0.0037
O	-4.6514	1.8230	-0.3304
N	-10.1769	4.3278	2.4014
N	-4.1728	2.9399	2.0291
C	-13.4281	1.8670	3.2845
C	-13.4852	3.2324	3.5954
H	-14.3694	3.6366	4.0733
C	-12.4172	4.0552	3.2883
H	-12.4802	5.1088	3.5320
C	-11.2537	3.5339	2.6604
C	-11.2352	2.1510	2.3320
H	-10.3663	1.7221	1.8536
C	-12.2982	1.3294	2.6510
H	-12.2625	0.2720	2.4180
C	-10.1315	5.7566	2.6903
H	-10.4075	5.9494	3.7302
H	-10.8165	6.3166	2.0369
C	-8.6698	6.1235	2.4099
H	-8.6032	7.0979	1.9162
H	-8.0819	6.1665	3.3342
C	-6.0965	3.2794	3.3920
C	-5.4606	2.9871	2.1287
H	-6.1210	2.6743	1.3133
C	-9.1685	3.9840	1.4090
H	-9.6087	3.9625	0.3959
H	-8.7221	3.0107	1.6205
C	-6.0032	4.5398	4.0356
C	-6.5476	6.0070	5.9096
H	-7.0574	6.1817	6.8524
C	-6.6661	4.7792	5.2760
H	-7.2679	3.9937	5.7103
C	-7.2487	5.2802	0.5370
C	-7.0441	4.3417	-0.5017
H	-7.6175	3.4221	-0.5351

C	-6.0894	4.5612	-1.4854
H	-5.9303	3.8247	-2.2660
C	-5.2938	5.7153	-1.4749
C	-5.4722	6.6466	-0.4457
C	-6.4347	6.4302	0.5442
H	-6.5352	7.1651	1.3342
C	-5.2327	5.5974	3.4631
H	-4.7288	5.4400	2.5181
C	-5.1116	6.8149	4.1162
H	-4.5141	7.6079	3.6766
C	-5.7661	7.0215	5.3378
H	-4.8694	7.5463	-0.3958
N	-8.1838	5.0503	1.5414
H	-5.6706	7.9779	5.8445
C	-2.5984	0.9658	1.1206
H	-1.8721	1.3272	1.8513
H	-3.2796	0.2450	1.5725
H	-2.0923	0.5331	0.2531
Rh	-6.9330	1.5367	4.0658
Rh	-7.9557	-0.5532	4.8956
O	-8.6643	2.4895	4.6896
O	-9.6160	0.5683	5.4372
O	-6.2024	-1.5213	4.3619
O	-5.2603	0.3899	3.5746
O	-7.7506	1.0687	2.2098
O	-8.6880	-0.8531	2.9717
O	-6.1698	1.8063	5.9690
O	-7.1234	-0.1043	6.7472
C	-9.5782	1.8264	5.2915
C	-6.4308	0.9478	6.8831
C	-5.2533	-0.8613	3.8430
C	-8.4045	-0.0235	2.0596
C	-5.8319	1.2370	8.2378
C	-3.9988	-1.6205	3.4815
C	-8.8489	-0.3489	0.6545
C	-10.6955	2.6210	5.9189
H	-6.0572	2.2680	8.5282
H	-6.2150	0.5424	8.9876
H	-4.7419	1.1405	8.1742
H	-10.6359	3.6741	5.6442
H	-11.6597	2.2088	5.6118
H	-10.6182	2.5216	7.0081
H	-8.9179	0.5540	0.0442
H	-9.8070	-0.8742	0.6716
H	-8.1024	-1.0142	0.2030
H	-3.1160	-0.9936	3.6288
H	-4.0483	-1.9058	2.4236
H	-3.9217	-2.5304	4.0809
N	-14.5377	1.0093	3.6190
O	-14.4654	-0.1933	3.3257
O	-15.5209	1.5074	4.1879
O	-4.3928	5.8348	-2.4954
C	-3.5325	6.9680	-2.4951
H	-2.8976	6.8632	-3.3778
H	-4.0979	7.9071	-2.5686
H	-2.9001	6.9950	-1.5974

t-A-B-ts-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.67098145 Eh

Atom	X	Y	Z
S	-4.2023	1.6442	0.2083
O	-3.0221	2.2046	-0.4685
O	-5.4677	1.5433	-0.5542
N	-10.1617	3.9968	2.1040
N	-4.3919	2.5385	1.6590
C	-13.6381	1.7651	1.5426
C	-13.7136	3.0337	2.1362
H	-14.6756	3.4226	2.4476
C	-12.5656	3.7809	2.3154
H	-12.6409	4.7667	2.7595
C	-11.2980	3.2765	1.9121
C	-11.2500	1.9903	1.3019
H	-10.3043	1.5695	0.9806
C	-12.4035	1.2497	1.1242
H	-12.3594	0.2680	0.6679
C	-10.0368	5.1773	2.9593
H	-10.7099	5.1201	3.8192
H	-10.2468	6.0976	2.4005
C	-8.5746	5.0849	3.3957
H	-8.1426	6.0324	3.6973
H	-8.4797	4.3766	4.2153
C	-6.0370	3.3336	3.2295

C	-5.6260	2.8053	1.9471
H	-6.4230	2.4820	1.2810
C	-8.8403	3.4709	1.7425
H	-8.7631	3.3241	0.6659
H	-8.6534	2.5258	2.2498
C	-5.4674	4.5254	3.7996
C	-5.3085	6.1117	5.6460
H	-5.5921	6.4179	6.6490
C	-5.8261	4.9411	5.1079
H	-6.5037	4.3266	5.6838
C	-7.3201	5.3691	1.2436
C	-6.9297	4.8729	-0.0209
H	-7.0979	3.8395	-0.2970
C	-6.2874	5.6836	-0.9432
H	-5.9886	5.2846	-1.9075
C	-6.0006	7.0257	-0.6449
C	-6.3684	7.5298	0.6060
C	-7.0079	6.7055	1.5360
H	-7.2528	7.1423	2.4947
C	-4.5848	5.3497	3.0510
H	-4.3144	5.0672	2.0412
C	-4.0520	6.5085	3.6072
H	-3.3702	7.1211	3.0246
C	-4.4140	6.8932	4.9013
H	-6.1583	8.5565	0.8817
N	-7.8833	4.4865	2.2244
H	-4.0039	7.8035	5.3307
C	-3.8101	0.0191	0.8616
H	-2.9184	0.0998	1.4841
H	-4.6646	-0.3282	1.4445
H	-3.6264	-0.6375	0.0064
Rh	-6.7511	1.5637	4.2392
Rh	-7.4322	-0.5581	5.3144
O	-8.6873	2.2275	4.6298
O	-9.3344	0.2480	5.5291
O	-5.4872	-1.2193	5.0297
O	-4.8828	0.7016	3.9803
O	-7.3986	0.7077	2.4525
O	-7.9420	-1.2670	3.4222
O	-6.1504	2.1812	6.1291
O	-6.8836	0.2792	7.1288
C	-9.5483	1.4376	5.1503
C	-6.3604	1.4340	7.1439
C	-4.6519	-0.4664	4.4423
C	-7.8255	-0.4976	2.4241
C	-5.9332	2.0025	8.4758
C	-3.2572	-1.0100	4.2423
C	-8.2493	-1.0163	1.0719
C	-10.9524	1.9744	5.2828
H	-6.4432	2.9570	8.6452
H	-6.1633	1.3107	9.2881
H	-4.8564	2.2028	8.4546
H	-10.9382	3.0530	5.4574
H	-11.4857	1.7880	4.3435
H	-11.4827	1.4656	6.0909
H	-7.7034	-0.4998	0.2787
H	-9.3216	-0.8230	0.9422
H	-8.0880	-2.0952	1.0095
H	-2.5597	-0.2106	3.9863
H	-3.2755	-1.7448	3.4287
H	-2.9273	-1.5240	5.1496
N	-14.8372	0.9865	1.3626
O	-14.7435	-0.1330	0.8369
O	-15.9168	1.4658	1.7411
O	-5.3712	7.7326	-1.6198
C	-5.0097	9.0855	-1.3459
H	-4.5048	9.4470	-2.2439
H	-5.8933	9.7072	-1.1520
H	-4.3231	9.1509	-0.4921

t-B-OAc-MeO-NO2

Energy (POTENTIAL) = -3094.68807736 Eh

Atom	X	Y	Z
S	-4.5209	0.9676	0.2423
O	-3.4012	1.3869	-0.6232
O	-5.7822	0.5700	-0.4298
N	-9.9552	4.0352	2.2394
N	-4.7310	2.1688	1.3901
C	-13.7240	2.6042	1.1723
C	-13.6159	3.7040	2.0331
H	-14.5120	4.1774	2.4152
C	-12.3667	4.1805	2.3861

H	-12.2969	5.0407	3.0415
C	-11.1894	3.5649	1.8865
C	-11.3255	2.4509	1.0162
H	-10.4502	1.9469	0.6235
C	-12.5783	1.9809	0.6637
H	-12.6780	1.1284	0.0029
C	-9.7130	4.9661	3.3415
H	-10.3581	4.7522	4.1990
H	-9.8757	6.0016	3.0238
C	-8.2662	4.6757	3.7010
H	-7.7184	5.5056	4.1322
H	-8.1969	3.8222	4.3677
C	-6.3144	3.4299	2.6870
C	-5.9629	2.5480	1.6166
H	-6.7667	2.1192	1.0179
C	-8.7410	3.3668	1.8133
H	-8.6647	3.3282	0.7298
H	-8.6530	2.3679	2.2377
C	-5.2589	4.3614	3.2309
C	-4.2309	5.6019	5.0605
H	-4.1915	5.8358	6.1216
C	-5.1830	4.6917	4.5926
H	-5.8562	4.2176	5.2936
C	-7.3478	5.3844	1.4552
C	-7.0225	5.1010	0.1212
H	-7.0288	4.0884	-0.2632
C	-6.6602	6.1220	-0.7427
H	-6.4043	5.9046	-1.7745
C	-6.6030	7.4522	-0.2922
C	-6.9277	7.7340	1.0393
C	-7.2931	6.6996	1.9055
H	-7.5193	6.9640	2.9290
C	-4.3451	4.9753	2.3513
H	-4.3848	4.7475	1.2928
C	-3.3928	5.8805	2.8171
H	-2.7017	6.3398	2.1149
C	-3.3317	6.2002	4.1765
H	-6.8954	8.7458	1.4238
N	-7.6296	4.2286	2.3895
H	-2.5893	6.9055	4.5411
C	-3.9583	-0.4037	1.2569
H	-3.0346	-0.1062	1.7557
H	-4.7333	-0.6327	1.9865
H	-3.7807	-1.2540	0.5927
Rh	-6.8592	1.4392	4.1640
Rh	-7.1828	-0.5592	5.5450
O	-8.9404	1.6617	4.2259
O	-9.2251	-0.1773	5.5213
O	-5.1281	-0.8284	5.4543
O	-4.8372	1.0702	4.2450
O	-7.0815	0.1852	2.5236
O	-7.3986	-1.6592	3.8018
O	-6.7893	2.5039	5.9541
O	-6.9583	0.6338	7.2244
C	-9.6575	0.8174	4.8637
C	-6.8242	1.8865	7.0711
C	-4.4122	0.0320	4.8487
C	-7.3144	-1.0593	2.6855
C	-6.6562	2.7329	8.3088
C	-2.9227	-0.2096	4.8316
C	-7.5162	-1.8705	1.4302
C	-11.1486	1.0442	4.8091
H	-7.1933	3.6787	8.1960
H	-7.0063	2.2009	9.1957
H	-5.5906	2.9633	8.4304
H	-11.3835	2.0337	5.2155
H	-11.4761	1.0326	3.7640
H	-11.6825	0.2776	5.3734
H	-7.0508	-1.3667	0.5802
H	-8.5932	-1.9640	1.2419
H	-7.1077	-2.8763	1.5590
H	-2.3976	0.6231	4.3609
H	-2.7164	-1.1333	4.2794
H	-2.5622	-0.3484	5.8560
N	-15.0311	2.1097	0.8041
O	-15.1004	1.1297	0.0495
O	-16.0291	2.6870	1.2574
O	-6.2263	8.3715	-1.2121
C	-6.1014	9.7352	-0.8022
H	-5.7693	10.2807	-1.6874
H	-7.0631	10.1411	-0.4646
H	-5.3550	9.8450	-0.0057

t-A-OAc-NO2-MeO

Energy (POTENTIAL) = -3094.67870688 Eh

Atom	X	Y	Z
S	-3.0855	2.5475	0.8818
O	-2.3357	3.7234	0.4149
O	-3.9721	1.8424	-0.0676
N	-10.1832	4.5255	2.4089
N	-3.9313	3.0551	2.2904
C	-13.1542	1.5687	3.0052
C	-13.4482	2.9246	3.2115
H	-14.4461	3.1958	3.5444
C	-12.4871	3.9087	2.9982
H	-12.7522	4.9459	3.1742
C	-11.1885	3.5644	2.5716
C	-10.9119	2.2046	2.3512
H	-9.9183	1.9036	2.0510
C	-11.8725	1.2158	2.5666
H	-11.5947	0.1806	2.4068
C	-10.5143	5.9426	2.2723
H	-10.9426	6.3372	3.1975
H	-11.2304	6.1187	1.4533
C	-9.1586	6.5761	1.9601
H	-9.2629	7.4632	1.3298
H	-8.6160	6.8523	2.8738
C	-6.0056	3.0689	3.4488
C	-5.2056	2.8399	2.2645
H	-5.7008	2.3529	1.4201
C	-9.0768	4.2077	1.5180
H	-9.4188	3.7386	0.5782
H	-8.3685	3.5210	1.9999
C	-6.1570	4.3499	4.0381
C	-6.9735	5.7609	5.8533
H	-7.4640	5.8705	6.8157
C	-6.8056	4.5016	5.3000
H	-7.1522	3.6217	5.8223
C	-7.3293	5.6378	0.5194
C	-6.7391	4.5108	-0.1168
H	-7.1971	3.5325	-0.0307
C	-5.5707	4.6378	-0.8463
H	-5.1158	3.7703	-1.3067
C	-4.9516	5.8885	-0.9560
C	-5.5127	7.0170	-0.3402
C	-6.6869	6.8991	0.3794
H	-7.1044	7.7771	0.8577
C	-5.6796	5.5193	3.3725
H	-5.1838	5.4246	2.4148
C	-5.8601	6.7726	3.9335
H	-5.5036	7.6561	3.4138
C	-6.5099	6.8947	5.1705
H	-5.0193	7.9772	-0.4322
N	-8.4655	5.5012	1.2526
H	-6.6513	7.8797	5.6072
C	-1.9576	1.3557	1.6039
H	-1.3555	1.8580	2.3639
H	-2.5470	0.5482	2.0430
H	-1.3238	0.9795	0.7960
Rh	-6.8413	1.3023	3.9945
Rh	-7.9493	-0.8206	4.5906
O	-8.5805	2.2435	4.5965
O	-9.5778	0.3058	5.2257
O	-6.2217	-1.7787	3.9374
O	-5.1718	0.1797	3.4703
O	-7.5742	1.0099	2.0668
O	-8.6650	-0.8976	2.6366
O	-6.1822	1.3999	5.9509
O	-7.1319	-0.5930	6.4868
C	-9.5225	1.5691	5.1388
C	-6.4599	0.4454	6.7595
C	-5.2353	-1.0975	3.5282
C	-8.2872	-0.0230	1.8037
C	-5.9156	0.5970	8.1583
C	-4.0107	-1.8374	3.0473
C	-8.6815	-0.2016	0.3585
C	-10.6500	2.3569	5.7557
H	-6.2347	1.5592	8.5720
H	-6.2592	-0.2171	8.7991
H	-4.8204	0.5989	8.1209
H	-10.5402	3.4221	5.5507
H	-11.6051	1.9987	5.3624
H	-10.6427	2.1859	6.8386
H	-8.8389	0.7665	-0.1228

H	-9.5790	-0.8183	0.2775
H	-7.8598	-0.7097	-0.1616
H	-3.1209	-1.4448	3.5493
H	-3.8911	-1.6679	1.9712
H	-4.1042	-2.9081	3.2383
N	-3.7291	6.0159	-1.7111
O	-3.3308	5.0419	-2.3617
O	-3.1318	7.1036	-1.6852
O	-14.1684	0.6845	3.2542
C	-13.8801	-0.7047	3.1316
H	-14.7985	-1.2285	3.4070
H	-13.6078	-0.9740	2.1021
H	-13.0721	-1.0107	3.8104

t-A-B-OAc-NO2-MeO

Energy (POTENTIAL) = -3094.66074667 Eh

Atom	X	Y	Z
S	-4.2511	1.5774	0.1886
O	-3.0751	2.1311	-0.5017
O	-5.5065	1.4212	-0.5805
N	-10.1169	4.1098	1.8536
N	-4.4657	2.5258	1.5993
C	-13.4941	1.5484	1.8857
C	-13.6127	2.9036	2.2295
H	-14.5891	3.2853	2.5139
C	-12.5085	3.7460	2.2043
H	-12.6402	4.7928	2.4594
C	-11.2307	3.2603	1.8502
C	-11.1273	1.9061	1.4831
H	-10.1729	1.4803	1.1938
C	-12.2420	1.0598	1.4996
H	-12.1098	0.0215	1.2166
C	-10.0162	5.2245	2.8096
H	-10.7397	5.1271	3.6248
H	-10.1769	6.1884	2.3123
C	-8.5919	5.0860	3.3464
H	-8.1555	6.0089	3.7115
H	-8.5642	4.3415	4.1372
C	-6.1339	3.4092	3.1024
C	-5.7001	2.8289	1.8470
H	-6.4846	2.4995	1.1690
C	-8.8004	3.4957	1.6851
H	-8.6109	3.2386	0.6451
H	-8.6912	2.6008	2.2942
C	-5.4607	4.5351	3.7210
C	-5.2437	6.0779	5.5974
H	-5.5601	6.4071	6.5832
C	-5.8540	4.9777	5.0068
H	-6.6340	4.4415	5.5285
C	-7.2605	5.4100	1.2513
C	-6.9697	4.9977	-0.0674
H	-7.2274	4.0097	-0.4229
C	-6.3169	5.8430	-0.9525
H	-6.0982	5.5154	-1.9612
C	-5.9388	7.1171	-0.5285
C	-6.1950	7.5475	0.7704
C	-6.8434	6.6939	1.6547
H	-7.0040	7.0467	2.6632
C	-4.4386	5.2516	3.0482
H	-4.1345	4.9477	2.0543
C	-3.8101	6.3338	3.6582
H	-3.0195	6.8628	3.1339
C	-4.2142	6.7527	4.9290
H	-5.8814	8.5330	1.0913
N	-7.8362	4.5013	2.1971
H	-3.7309	7.6056	5.3981
C	-3.8310	-0.0102	0.9097
H	-2.9513	0.1176	1.5412
H	-4.6846	-0.3570	1.4940
H	-3.6181	-0.6943	0.0835
Rh	-6.8513	1.6111	4.1655
Rh	-7.4919	-0.5114	5.2529
O	-8.8113	2.2283	4.5493
O	-9.4294	0.2171	5.3935
O	-5.5174	-1.1091	5.0582
O	-4.9556	0.7954	3.9579
O	-7.4374	0.7149	2.3783
O	-7.8986	-1.2754	3.3578
O	-6.2974	2.2699	6.0560
O	-7.0444	0.3807	7.0698
C	-9.6628	1.4137	5.0465
C	-6.5299	1.5406	7.0778

C	-4.6935	-0.3449	4.4682
C	-7.7917	-0.5126	2.3522
C	-6.1180	2.1149	8.4118
C	-3.2745	-0.8426	4.3296
C	-8.1354	-1.0719	0.9933
C	-11.0745	1.9230	5.2004
H	-6.3064	3.1914	8.4374
H	-6.6469	1.6157	9.2265
H	-5.0404	1.9567	8.5431
H	-11.0788	3.0031	5.3636
H	-11.6251	1.7136	4.2761
H	-11.5739	1.4121	6.0270
H	-7.5709	-0.5510	0.2160
H	-9.2059	-0.9163	0.8097
H	-7.9362	-2.1458	0.9601
H	-2.5983	-0.0271	4.0673
H	-3.2419	-1.6035	3.5408
H	-2.9550	-1.3142	5.2632
N	-5.2517	8.0094	-1.4586
O	-5.0460	7.6058	-2.6060
O	-4.9107	9.1234	-1.0511
O	-14.6434	0.8088	1.9505
C	-14.5638	-0.5745	1.6244
H	-15.5739	-0.9716	1.7485
H	-14.2422	-0.7287	0.5855
H	-13.8808	-1.1105	2.2974

t-B-OAc-NO2-MeO

Energy (POTENTIAL) = -3094.67491032 Eh

Atom	X	Y	Z
S	-4.4781	1.0311	0.2940
O	-3.3614	1.4577	-0.5716
O	-5.7368	0.6236	-0.3772
N	-9.9487	4.0805	2.1652
N	-4.6984	2.2355	1.4373
C	-13.6803	2.2222	1.4205
C	-13.6033	3.4275	2.1346
H	-14.5227	3.8801	2.4941
C	-12.3788	4.0366	2.3770
H	-12.3558	4.9760	2.9200
C	-11.1789	3.4552	1.9165
C	-11.2636	2.2494	1.2004
H	-10.3699	1.7589	0.8296
C	-12.4985	1.6398	0.9509
H	-12.5148	0.7087	0.3962
C	-9.7576	4.9235	3.3516
H	-10.4052	4.6197	4.1815
H	-9.9605	5.9745	3.1194
C	-8.3037	4.6742	3.7264
H	-7.7781	5.5144	4.1665
H	-8.2143	3.8197	4.3890
C	-6.3044	3.4842	2.7211
C	-5.9369	2.5940	1.6661
H	-6.7355	2.1426	1.0777
C	-8.7391	3.3511	1.8559
H	-8.6138	3.2214	0.7837
H	-8.6685	2.3870	2.3598
C	-5.2745	4.4404	3.2677
C	-4.2984	5.7207	5.0976
H	-4.2794	5.9680	6.1562
C	-5.2259	4.7873	4.6269
H	-5.8986	4.3060	5.3235
C	-7.3857	5.3878	1.4784
C	-7.0663	5.0956	0.1467
H	-7.0460	4.0799	-0.2262
C	-6.7459	6.1202	-0.7346
H	-6.4944	5.9016	-1.7646
C	-6.7422	7.4337	-0.2682
C	-7.0543	7.7412	1.0512
C	-7.3763	6.7085	1.9291
H	-7.6055	6.9677	2.9522
C	-4.3575	5.0587	2.3947
H	-4.3748	4.8139	1.3391
C	-3.4290	5.9867	2.8641
H	-2.7343	6.4494	2.1678
C	-3.3965	6.3246	4.2200
H	-7.0412	8.7681	1.3933
N	-7.6406	4.2384	2.4215
H	-2.6733	7.0482	4.5872
C	-3.9072	-0.3376	1.3069
H	-2.9872	-0.0350	1.8091
H	-4.6829	-0.5753	2.0330

H	-3.7215	-1.1843	0.6402
Rh	-6.8130	1.4626	4.2273
Rh	-7.0920	-0.5427	5.6025
O	-8.8939	1.6673	4.3350
O	-9.1386	-0.1878	5.6137
O	-5.0362	-0.7851	5.4810
O	-4.7871	1.1156	4.2668
O	-7.0556	0.2180	2.5839
O	-7.3185	-1.6381	3.8575
O	-6.7080	2.5213	6.0162
O	-6.8579	0.6463	7.2823
C	-9.5933	0.8086	4.9729
C	-6.7345	1.9007	7.1316
C	-4.3392	0.0858	4.8681
C	-7.2629	-1.0312	2.7428
C	-6.6026	2.7542	8.3687
C	-2.8463	-0.1310	4.8412
C	-7.4704	-1.8381	1.4857
C	-11.0877	1.0133	4.9366
H	-7.3998	3.5055	8.3777
H	-6.6581	2.1460	9.2733
H	-5.6460	3.2870	8.3384
H	-11.3309	2.0157	5.3035
H	-11.4313	0.9543	3.8979
H	-11.6004	0.2622	5.5401
H	-7.0001	-1.3348	0.6379
H	-8.5480	-1.9194	1.2950
H	-7.0709	-2.8478	1.6110
H	-2.3402	0.6979	4.3438
H	-2.6285	-1.0662	4.3136
H	-2.4743	-0.2345	5.8659
N	-6.3940	8.5196	-1.1928
O	-6.1215	8.2212	-2.3563
O	-6.3927	9.6715	-0.7560
O	-14.9354	1.7120	1.2389
C	-15.0620	0.4856	0.5263
H	-16.1314	0.2651	0.4961
H	-14.6826	0.5719	-0.5007
H	-14.5394	-0.3347	1.0369

Rh-Piv

Energy (POTENTIAL) = -1605.4405554 Eh

Atom	X	Y	Z
Rh	-6.0781	1.3057	4.2986
Rh	-7.0566	-0.4604	5.5957
O	-7.9469	1.6750	3.5055
O	-8.8768	0.0290	4.7465
O	-5.1825	-0.8386	6.3754
O	-4.2649	0.8417	5.1713
O	-5.7252	-0.0837	2.8134
O	-6.6646	-1.7456	4.0256
O	-6.5064	2.5967	5.8542
O	-7.4014	0.9259	7.0873
C	-8.9401	0.9871	3.9075
C	-7.0734	2.1419	6.9021
C	-4.1994	-0.1161	6.0103
C	-6.1056	-1.2895	2.9765
C	-7.4092	3.1573	7.9994
C	-2.8283	-0.3871	6.6379
C	-5.8908	-2.2379	1.7925
C	-10.3326	1.3647	3.3928
C	-6.8208	-1.7523	0.6574
H	-6.5825	-0.7241	0.3670
H	-6.7027	-2.3976	-0.2208
H	-7.8723	-1.7878	0.9680
C	-4.4181	-2.1418	1.3462
H	-3.7409	-2.4500	2.1522
H	-4.2480	-2.8022	0.4880
H	-4.1595	-1.1198	1.0543
C	-6.2356	-3.6841	2.1749
H	-5.6082	-4.0382	2.9999
H	-7.2821	-3.7784	2.4809
H	-6.0687	-4.3395	1.3121
C	-1.7841	-0.4992	5.5089
H	-1.7375	0.4203	4.9183
H	-0.7934	-0.6866	5.9388
H	-2.0245	-1.3294	4.8334
C	-2.8500	-1.6796	7.4663
H	-1.8615	-1.8461	7.9098
H	-3.5856	-1.6248	8.2746
H	-3.0956	-2.5464	6.8431

C	-2.5025	0.8202	7.5461
H	-3.2470	0.9239	8.3451
H	-1.5208	0.6790	8.0132
H	-2.4822	1.7518	6.9713
C	-8.5094	4.0820	7.4315
H	-8.7771	4.8394	8.1772
H	-8.1651	4.5922	6.5263
H	-9.4131	3.5119	7.1836
C	-6.1426	3.9762	8.3193
H	-6.3704	4.7221	9.0895
H	-5.3417	3.3298	8.6986
H	-5.7718	4.4961	7.4313
C	-7.9157	2.4514	9.2655
H	-8.8203	1.8691	9.0649
H	-7.1590	1.7718	9.6724
H	-8.1508	3.1994	10.0318
C	-11.1034	0.0829	3.0248
H	-11.1969	-0.5847	3.8858
H	-12.1093	0.3432	2.6758
H	-10.5953	-0.4636	2.2208
C	-11.0403	2.0977	4.5565
H	-10.4896	3.0017	4.8435
H	-12.0487	2.3967	4.2473
H	-11.1251	1.4517	5.4367
C	-10.2325	2.2923	2.1724
H	-9.7023	1.8056	1.3463
H	-11.2400	2.5522	1.8272
H	-9.7032	3.2183	2.4156

Rh-OH-Piv

Energy (POTENTIAL) = -1605.8402179 Eh

Atom	X	Y	Z
Rh	-6.2995	1.4809	4.3567
Rh	-7.4538	-0.3094	5.5696
O	-8.0886	1.8711	3.3995
O	-9.0940	0.1139	4.4130
O	-5.6414	-0.6132	6.6089
O	-4.5674	0.9141	5.3334
O	-5.8983	0.0658	2.9545
O	-6.8038	-1.5755	4.1955
O	-6.6264	3.1186	5.6320
O	-6.2735	2.2629	7.6974
C	-9.0782	1.0944	3.5887
C	-6.5294	3.2582	6.8625
C	-4.5771	-0.0341	6.1862
C	-6.1882	-1.1497	3.1503
C	-6.7081	4.6066	7.5334
C	-3.2249	-0.4559	6.7560
C	-5.8524	-2.1777	2.0761
C	-10.3481	1.3002	2.7626
C	-7.0754	-2.2062	1.1260
H	-7.2447	-1.2240	0.6717
H	-6.8883	-2.9285	0.3237
H	-7.9831	-2.5097	1.6585
C	-4.5923	-1.7329	1.3134
H	-3.7306	-1.6536	1.9859
H	-4.3600	-2.4763	0.5434
H	-4.7381	-0.7651	0.8255
C	-5.6369	-3.5629	2.7102
H	-4.8090	-3.5450	3.4281
H	-6.5339	-3.9137	3.2282
H	-5.3901	-4.2821	1.9222
C	-2.3658	-0.9617	5.5749
H	-2.2279	-0.1803	4.8214
H	-1.3802	-1.2641	5.9458
H	-2.8291	-1.8309	5.0924
C	-3.3913	-1.5618	7.8066
H	-2.4059	-1.8446	8.1929
H	-4.0045	-1.2238	8.6483
H	-3.8603	-2.4532	7.3781
C	-2.5731	0.7931	7.3894
H	-3.1938	1.1930	8.2003
H	-1.5975	0.5222	7.8075
H	-2.4246	1.5825	6.6467
C	-7.8760	4.4872	8.5404
H	-8.0317	5.4609	9.0163
H	-8.8062	4.2016	8.0353
H	-7.6611	3.7521	9.3215
C	-7.0186	5.6770	6.4781
H	-7.1416	6.6442	6.9760
H	-6.2069	5.7659	5.7491
H	-7.9424	5.4492	5.9362

C	-5.3954	4.9453	8.2773
H	-5.1598	4.1960	9.0386
H	-4.5530	5.0145	7.5797
H	-5.5114	5.9159	8.7708
C	-10.4421	0.0976	1.7944
H	-10.5050	-0.8469	2.3441
H	-11.3406	0.1990	1.1756
H	-9.5717	0.0564	1.1290
C	-11.5637	1.3081	3.7119
H	-11.5005	2.1345	4.4302
H	-12.4814	1.4360	3.1272
H	-11.6384	0.3702	4.2697
C	-10.2795	2.6144	1.9725
H	-9.4350	2.6205	1.2767
H	-11.2022	2.7362	1.3942
H	-10.1775	3.4760	2.6410
H	-6.1662	1.4071	7.2324

A-Piv

Energy (POTENTIAL) = -2557.3111108 Eh

Atom	X	Y	Z
S	-7.4735	3.4680	0.1071
O	-8.9195	3.5832	0.3569
O	-6.9588	2.2202	-0.4950
N	-6.6746	3.8375	1.5814
C	-5.3492	2.9435	3.3476
C	-5.8909	2.9023	2.0108
H	-5.7150	1.9790	1.4451
C	-4.3505	3.8596	3.7636
C	-2.7195	5.5983	3.2334
H	-2.2246	6.2401	2.5110
C	-3.7013	4.7126	2.8210
H	-3.9793	4.6590	1.7738
C	-3.9685	3.9432	5.1352
H	-4.4585	3.3061	5.8571
C	-2.9928	4.8427	5.5364
H	-2.7133	4.9084	6.5835
C	-2.3661	5.6645	4.5896
H	-1.5966	6.3617	4.9093
C	-6.9411	4.8625	-0.8884
H	-7.2227	5.7838	-0.3742
H	-5.8591	4.8066	-1.0282
H	-7.4573	4.7861	-1.8494
Rh	-6.1749	1.4174	4.3956
Rh	-7.0734	-0.5087	5.6391
O	-8.0745	1.7023	3.6382
O	-8.9218	-0.0372	4.8161
O	-5.1526	-0.8356	6.3604
O	-4.3412	0.9610	5.2440
O	-5.7932	0.0970	2.8463
O	-6.6703	-1.6672	3.9590
O	-6.6466	2.5772	6.0387
O	-7.4158	0.8007	7.2139
C	-9.0258	0.9262	3.9978
C	-7.1387	2.0291	7.0863
C	-4.2197	-0.0509	6.0180
C	-6.1608	-1.1259	2.9346
C	-7.4138	2.9775	8.2597
C	-2.8027	-0.3072	6.5477
C	-5.9780	-1.9609	1.6617
C	-10.3838	1.1838	3.3340
C	-6.9652	-1.4019	0.6115
H	-6.7796	-0.3427	0.4072
H	-6.8607	-1.9601	-0.3264
H	-8.0015	-1.5053	0.9547
C	-4.5280	-1.7959	1.1636
H	-3.8098	-2.1429	1.9170
H	-4.3802	-2.3895	0.2539
H	-4.3044	-0.7500	0.9341
C	-6.2785	-3.4417	1.9327
H	-5.6030	-3.8542	2.6901
H	-7.3055	-3.5830	2.2832
H	-6.1478	-4.0161	1.0081
C	-1.9024	-0.6124	5.3310
H	-1.8918	0.2278	4.6298
H	-0.8754	-0.8003	5.6656
H	-2.2538	-1.5031	4.7955
C	-2.7905	-1.4920	7.5239
H	-1.7693	-1.6565	7.8875
H	-3.4366	-1.3044	8.3879
H	-3.1345	-2.4109	7.0386
C	-2.3144	0.9736	7.2559

H	-2.9695	1.2329	8.0970
H	-1.3032	0.8185	7.6498
H	-2.2907	1.8221	6.5657
C	-8.4961	3.9794	7.8015
H	-8.7203	4.6815	8.6131
H	-8.1602	4.5503	6.9301
H	-9.4247	3.4605	7.5344
C	-6.1065	3.7270	8.5920
H	-6.2696	4.3992	9.4423
H	-5.3082	3.0247	8.8631
H	-5.7652	4.3231	7.7406
C	-7.9019	2.1965	9.4876
H	-8.8282	1.6541	9.2736
H	-7.1539	1.4689	9.8200
H	-8.0934	2.8931	10.3123
C	-11.5016	0.4602	4.0992
H	-11.5695	0.8169	5.1332
H	-12.4633	0.6496	3.6081
H	-11.3347	-0.6207	4.1245
C	-10.6537	2.7004	3.2980
H	-9.8966	3.2204	2.7067
H	-11.6346	2.8879	2.8447
H	-10.6620	3.1225	4.3108
C	-10.2830	0.6340	1.8923
H	-10.0669	-0.4413	1.8957
H	-11.2370	0.7868	1.3732
H	-9.5016	1.1502	1.3279

A_-tBu

Energy (POTENTIAL) = -3326.9401418 Eh

Atom	X	Y	Z
S	-5.4876	2.0119	-0.3085
O	-6.7948	1.9180	-0.9833
O	-4.7365	0.7654	-0.0469
N	-10.1729	4.0507	1.5451
N	-5.7406	2.9296	1.1083
C	-13.4627	1.7847	0.1212
C	-13.6494	2.9861	0.8175
H	-14.6609	3.3456	0.9984
C	-12.5773	3.7430	1.2894
H	-12.7742	4.6732	1.8120
C	-11.2458	3.3155	1.0849
C	-11.0515	2.1114	0.3682
H	-10.0490	1.7481	0.1733
C	-12.1390	1.3756	-0.0959
H	-11.9482	0.4514	-0.6384
C	-10.2946	5.1677	2.4825
H	-11.0612	4.9890	3.2462
H	-10.5470	6.0982	1.9555
C	-8.8848	5.2287	3.1054
H	-8.5824	6.2391	3.3770
H	-8.8298	4.5895	3.9892
C	-5.8441	2.9224	3.4896
C	-5.4297	2.3532	2.2202
H	-4.9545	1.3676	2.2564
C	-8.7954	3.5304	1.5718
H	-8.4515	3.1924	0.5969
H	-8.7059	2.6866	2.2699
C	-5.4130	4.1996	3.9438
C	-5.6256	6.0557	5.5091
H	-6.1294	6.5311	6.3453
C	-6.0554	4.8196	5.0523
H	-6.8935	4.3183	5.5184
C	-7.4159	5.5472	1.1552
C	-7.4940	5.4118	-0.2412
H	-8.0743	4.6153	-0.6908
C	-6.8181	6.2991	-1.0814
H	-6.9038	6.1667	-2.1582
C	-6.0489	7.3565	-0.5785
C	-5.9850	7.4936	0.8156
C	-6.6456	6.6105	1.6657
H	-6.5458	6.7294	2.7391
C	-4.3257	4.8739	3.3212
H	-3.8358	4.4205	2.4665
C	-3.8778	6.0932	3.8126
H	-3.0359	6.5920	3.3424
C	-4.5277	6.6856	4.9018
H	-5.3944	8.2986	1.2491
N	-8.0093	4.6452	2.0726
H	-4.1821	7.6446	5.2779
C	-4.4477	3.1579	-1.2159
H	-4.9683	4.1168	-1.2713
H	-3.4933	3.2582	-0.6936

H	-4.2977	2.7385	-2.2146
C	-14.6294	0.9470	-0.3477
H	-14.4358	0.4995	-1.3302
H	-14.8371	0.1188	0.3451
H	-15.5463	1.5426	-0.4248
C	-5.2973	8.2953	-1.4922
H	-5.6700	8.2378	-2.5209
H	-5.3841	9.3367	-1.1591
H	-4.2247	8.0571	-1.5187
Rh	-6.6830	1.4587	4.6305
Rh	-7.3718	-0.4415	6.0445
O	-8.4746	2.3762	5.1320
O	-9.1369	0.5940	6.3657
O	-5.5782	-1.3788	5.5793
O	-4.9772	0.3426	4.2402
O	-7.5947	0.5085	3.0380
O	-8.1690	-1.2732	4.3129
O	-5.8103	2.2394	6.3398
O	-6.5084	0.5345	7.6598
C	-9.3257	1.7306	5.8418
C	-5.9281	1.6442	7.4652
C	-4.8169	-0.8283	4.7320
C	-8.0984	-0.6552	3.2077
C	-5.3166	2.3796	8.6654
C	-3.6179	-1.6109	4.1847
C	-8.7086	-1.3342	1.9767
C	-10.7002	2.3870	6.0178
C	-11.3921	2.3234	4.6372
H	-12.3627	2.8307	4.6791
H	-10.7816	2.8024	3.8695
H	-11.5646	1.2845	4.3315
C	-11.5365	1.6298	7.0598
H	-11.0504	1.6358	8.0416
H	-12.5168	2.1103	7.1601
H	-11.6930	0.5878	6.7657
C	-10.5144	3.8509	6.4612
H	-11.4941	4.3220	6.6014
H	-9.9710	3.9070	7.4128
H	-9.9600	4.4293	5.7188
C	-8.1546	-0.7107	0.6870
H	-7.0681	-0.8318	0.6212
H	-8.6083	-1.1995	-0.1836
H	-8.3643	0.3582	0.6304
C	-8.3916	-2.8398	2.0154
H	-8.7916	-3.3092	2.9184
H	-8.8345	-3.3323	1.1418
H	-7.3087	-3.0133	1.9904
C	-10.2353	-1.1100	2.0732
H	-10.4799	-0.0428	2.0717
H	-10.7334	-1.5720	1.2126
H	-10.6406	-1.5581	2.9873
C	-3.8392	2.6875	8.3461
H	-3.7509	3.3084	7.4497
H	-3.3808	3.2223	9.1863
H	-3.2715	1.7633	8.1816
C	-6.1005	3.6983	8.8455
H	-7.1640	3.5029	9.0311
H	-5.7024	4.2522	9.7037
H	-6.0148	4.3295	7.9560
C	-5.4178	1.5263	9.9373
H	-4.9738	2.0694	10.7799
H	-6.4597	1.3001	10.1847
H	-4.8847	0.5766	9.8221
C	-2.3592	-0.7247	4.2517
H	-1.5006	-1.2693	3.8419
H	-2.4917	0.1958	3.6762
H	-2.1253	-0.4513	5.2880
C	-3.9520	-1.9461	2.7119
H	-3.1344	-2.5284	2.2711
H	-4.8700	-2.5432	2.6433
H	-4.0905	-1.0390	2.1145
C	-3.3999	-2.9036	4.9838
H	-3.1946	-2.6889	6.0382
H	-4.2769	-3.5564	4.9364
H	-2.5424	-3.4483	4.5717

A-B-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9405468 Eh

Atom	X	Y	Z
S	-5.1699	1.8113	-0.2279
O	-6.2992	1.3225	-1.0361
O	-4.1617	0.8360	0.2427

N	-10.1434	3.9838	1.6436
N	-5.8411	2.7203	1.0501
C	-13.5658	2.0519	0.0557
C	-13.6672	3.2559	0.7666
H	-14.6469	3.7074	0.9128
C	-12.5499	3.8993	1.2962
H	-12.6788	4.8364	1.8280
C	-11.2564	3.3526	1.1313
C	-11.1466	2.1447	0.4045
H	-10.1762	1.6885	0.2452
C	-12.2792	1.5219	-0.1158
H	-12.1536	0.5917	-0.6669
C	-10.1952	5.1009	2.5838
H	-10.9603	4.9582	3.3569
H	-10.4039	6.0463	2.0646
C	-8.7776	5.0806	3.1872
H	-8.4239	6.0666	3.4814
H	-8.7407	4.4134	4.0481
C	-5.9321	3.0113	3.4502
C	-5.4017	2.4405	2.2285
H	-4.6381	1.6677	2.3919
C	-8.7974	3.3975	1.6364
H	-8.4963	3.0505	0.6519
H	-8.7187	2.5525	2.3301
C	-5.4605	4.2612	3.9527
C	-5.6085	6.0728	5.5756
H	-6.0915	6.5326	6.4327
C	-6.0720	4.8602	5.0875
H	-6.9121	4.3629	5.5535
C	-7.3884	5.3892	1.1828
C	-7.4965	5.2362	-0.2100
H	-8.0755	4.4270	-0.6378
C	-6.8631	6.1279	-1.0762
H	-6.9753	5.9831	-2.1487
C	-6.1002	7.2045	-0.6034
C	-6.0076	7.3605	0.7857
C	-6.6338	6.4772	1.6626
H	-6.5220	6.6274	2.7299
C	-4.3654	4.9294	3.3401
H	-3.8985	4.4957	2.4617
C	-3.8782	6.1204	3.8650
H	-3.0289	6.6115	3.3996
C	-4.5030	6.6964	4.9764
H	-5.4269	8.1841	1.1962
N	-7.9448	4.4784	2.1229
H	-4.1318	7.6357	5.3772
C	-4.3391	3.1258	-1.1261
H	-5.0592	3.9260	-1.3116
H	-3.5028	3.4900	-0.5249
H	-3.9799	2.6992	-2.0667
C	-14.7891	1.3395	-0.4723
H	-14.5658	0.7821	-1.3898
H	-15.1828	0.6152	0.2554
H	-15.5997	2.0434	-0.6949
C	-5.3883	8.1453	-1.5458
H	-5.7926	8.0783	-2.5617
H	-5.4739	9.1872	-1.2144
H	-4.3153	7.9154	-1.6043
Rh	-6.7084	1.4783	4.6004
Rh	-7.3461	-0.4382	6.0192
O	-8.5309	2.3352	5.1007
O	-9.1307	0.5583	6.3709
O	-5.5431	-1.3351	5.5235
O	-4.9611	0.4230	4.2250
O	-7.5945	0.4882	3.0110
O	-8.1716	-1.2766	4.3101
O	-5.8518	2.2792	6.3100
O	-6.4648	0.5372	7.6233
C	-9.3587	1.6767	5.8244
C	-5.9153	1.6624	7.4276
C	-4.7798	-0.7508	4.7000
C	-8.1215	-0.6615	3.2015
C	-5.2747	2.3875	8.6192
C	-3.5547	-1.4992	4.1631
C	-8.7996	-1.3300	1.9992
C	-10.7556	2.2891	5.9841
C	-11.4376	2.1728	4.6017
H	-12.4297	2.6377	4.6303
H	-10.8447	2.6660	3.8289
H	-11.5624	1.1221	4.3140
C	-11.5696	1.5244	7.0380
H	-11.0913	1.5722	8.0226

H	-12.5685	1.9684	7.1210
H	-11.6835	0.4705	6.7677
C	-10.6247	3.7677	6.3962
H	-11.6216	4.2049	6.5258
H	-10.0853	3.8646	7.3466
H	-10.0925	4.3505	5.6411
C	-8.2823	-0.7331	0.6830
H	-7.2089	-0.9102	0.5617
H	-8.8029	-1.1963	-0.1637
H	-8.4393	0.3456	0.6387
C	-8.5282	-2.8448	2.0340
H	-8.9050	-3.2966	2.9559
H	-9.0231	-3.3278	1.1832
H	-7.4537	-3.0538	1.9648
C	-10.3147	-1.0629	2.1572
H	-10.5329	0.0100	2.1573
H	-10.8600	-1.5187	1.3224
H	-10.6922	-1.4942	3.0910
C	-3.8150	2.7272	8.2538
H	-3.7679	3.3644	7.3658
H	-3.3364	3.2555	9.0868
H	-3.2378	1.8158	8.0537
C	-6.0743	3.6876	8.8546
H	-7.1265	3.4688	9.0752
H	-5.6546	4.2319	9.7088
H	-6.0338	4.3384	7.9761
C	-5.3146	1.5092	9.8773
H	-4.8510	2.0453	10.7139
H	-6.3428	1.2591	10.1571
H	-4.7687	0.5722	9.7255
C	-2.3270	-0.5694	4.2057
H	-1.4510	-1.0947	3.8077
H	-2.4911	0.3307	3.6065
H	-2.1011	-0.2622	5.2343
C	-3.8844	-1.8717	2.6982
H	-3.0503	-2.4362	2.2648
H	-4.7827	-2.4996	2.6459
H	-4.0529	-0.9801	2.0859
C	-3.2876	-2.7685	4.9848
H	-3.0867	-2.5278	6.0346
H	-4.1403	-3.4535	4.9523
H	-2.4120	-3.2890	4.5794

B-Piv-Me-Me

Energy (POTENTIAL) = -3326.964343 Eh

Atom	X	Y	Z
S	-5.2869	1.4925	0.2009
O	-5.7182	0.0801	0.1233
O	-3.8779	1.7501	0.5796
N	-10.2854	3.6128	2.1811
N	-6.3775	2.3701	1.1132
C	-12.9381	3.4168	-1.1359
C	-13.1243	4.3328	-0.0942
H	-13.9711	5.0152	-0.1273
C	-12.2559	4.3991	0.9958
H	-12.4548	5.1189	1.7822
C	-11.1411	3.5419	1.0805
C	-10.9558	2.6036	0.0429
H	-10.1292	1.9032	0.0714
C	-11.8337	2.5583	-1.0374
H	-11.6542	1.8263	-1.8223
C	-10.3211	4.7397	3.1134
H	-11.1173	4.6465	3.8603
H	-10.4571	5.6839	2.5728
C	-8.9511	4.6849	3.7824
H	-8.5982	5.6529	4.1190
H	-8.9259	3.9668	4.5978
C	-6.6782	3.5883	3.2118
C	-5.9296	2.8578	2.2455
H	-4.8913	2.6915	2.5331
C	-8.9998	2.9725	2.2531
H	-8.6548	2.5208	1.3347
H	-8.9382	2.2369	3.0489
C	-5.9160	4.6360	3.9739
C	-5.6366	6.1113	5.8953
H	-5.9633	6.4277	6.8821
C	-6.3009	5.0643	5.2565
H	-7.1069	4.5578	5.7710
C	-7.8418	5.1270	1.6030
C	-8.0153	4.8036	0.2567
H	-8.3328	3.8213	-0.0563
C	-7.7808	5.7677	-0.7244

H	-7.9312	5.4971	-1.7663
C	-7.3613	7.0621	-0.3972
C	-7.1982	7.3677	0.9601
C	-7.4358	6.4193	1.9532
H	-7.2880	6.7032	2.9863
C	-4.8023	5.2655	3.3817
H	-4.4942	4.9806	2.3800
C	-4.1075	6.2820	4.0390
H	-3.2522	6.7467	3.5555
C	-4.5340	6.7237	5.2929
H	-6.8804	8.3648	1.2539
N	-8.0508	4.1044	2.6932
H	-4.0102	7.5301	5.7992
C	-5.5763	2.2373	-1.4093
H	-6.6298	2.1145	-1.6697
H	-5.3121	3.2960	-1.3635
H	-4.9421	1.7136	-2.1297
C	-13.8974	3.3294	-2.2992
H	-13.3676	3.1709	-3.2463
H	-14.5998	2.4925	-2.1812
H	-14.4938	4.2436	-2.3959
C	-7.0719	8.0865	-1.4656
H	-7.6121	7.8637	-2.3918
H	-7.3489	9.0948	-1.1387
H	-6.0003	8.1060	-1.7060
Rh	-6.7416	1.5209	4.6417
Rh	-6.8655	-0.5235	5.9877
O	-8.6411	1.9762	5.3507
O	-8.8059	0.0319	6.4929
O	-4.9510	-0.9659	5.3507
O	-4.8646	0.8790	4.0460
O	-7.6398	0.4228	3.1295
O	-7.6390	-1.4915	4.3336
O	-5.8071	2.4028	6.2841
O	-6.0473	0.5423	7.5534
C	-9.2837	1.1163	6.0459
C	-5.5881	1.7072	7.3287
C	-4.3915	-0.2179	4.4878
C	-7.9048	-0.8115	3.2919
C	-4.6101	2.2776	8.3640
C	-3.0787	-0.7080	3.8672
C	-8.5848	-1.5565	2.1363
C	-10.7617	1.4336	6.3065
C	-11.4824	1.3575	4.9404
H	-12.5524	1.5558	5.0739
H	-11.0824	2.0909	4.2335
H	-11.3760	0.3610	4.4935
C	-10.8787	2.8578	6.8840
H	-11.9316	3.0929	7.0791
H	-10.3300	2.9465	7.8296
H	-10.4849	3.6044	6.1882
C	-11.3741	0.4178	7.2810
H	-10.8586	0.4345	8.2473
H	-12.4297	0.6604	7.4505
H	-11.3145	-0.6005	6.8844
C	-3.2125	1.8093	7.8889
H	-2.9873	2.2021	6.8909
H	-2.4437	2.1690	8.5831
H	-3.1579	0.7154	7.8502
C	-4.6651	3.8114	8.3882
H	-5.6641	4.1659	8.6694
H	-3.9493	4.1964	9.1245
H	-4.4187	4.2332	7.4121
C	-4.9054	1.7113	9.7624
H	-4.1750	2.1033	10.4801
H	-5.9060	2.0023	10.1040
H	-4.8482	0.6195	9.7724
C	-2.3042	-1.5783	4.8700
H	-1.3808	-1.9424	4.4044
H	-2.0300	-1.0053	5.7639
H	-2.8932	-2.4429	5.1889
C	-3.4923	-1.5535	2.6374
H	-4.0480	-0.9516	1.9110
H	-2.5951	-1.9472	2.1444
H	-4.1195	-2.4016	2.9363
C	-2.2184	0.4832	3.4128
H	-1.9674	1.1354	4.2583
H	-1.2807	0.1131	2.9807
H	-2.7356	1.0763	2.6550
C	-9.0953	-0.5661	1.0801
H	-8.2724	0.0220	0.6668
H	-9.5812	-1.1149	0.2643

H	-9.8323	0.1185	1.5131
C	-9.7612	-2.3753	2.7029
H	-10.2603	-2.9183	1.8916
H	-9.4192	-3.1005	3.4470
H	-10.5031	-1.7213	3.1791
C	-7.5272	-2.4966	1.5172
H	-7.1448	-3.2013	2.2634
H	-7.9785	-3.0714	0.6993
H	-6.6894	-1.9200	1.1127

B_-Piv-Me-Me

Energy (POTENTIAL) = -3326.9675724 Eh

Atom	X	Y	Z
S	-6.5263	2.6673	1.3604
O	-6.1058	3.8381	0.5433
O	-7.7638	1.9758	0.9567
N	-9.4587	5.8062	4.5949
N	-6.6998	3.1440	2.9340
C	-13.6221	5.3161	3.9270
C	-13.1339	6.1111	4.9692
H	-13.8350	6.6137	5.6322
C	-11.7657	6.2733	5.1957
H	-11.4395	6.8894	6.0265
C	-10.8226	5.6380	4.3661
C	-11.3051	4.8352	3.3105
H	-10.6188	4.3077	2.6575
C	-12.6734	4.6873	3.1058
H	-13.0107	4.0524	2.2891
C	-8.9273	6.4741	5.7746
H	-9.2414	5.9931	6.7111
H	-9.2499	7.5187	5.8027
C	-7.4083	6.3340	5.5934
H	-6.8317	7.2333	5.7897
H	-7.0125	5.5133	6.1867
C	-5.8685	5.1998	3.9990
C	-5.7081	4.0150	3.3672
H	-4.6659	3.7098	3.2496
C	-8.4468	4.9646	4.0259
H	-8.6173	4.7105	2.9879
H	-8.2335	4.0641	4.6035
C	-4.6945	5.8827	4.5981
C	-3.2674	7.8125	5.0129
H	-3.0774	8.8757	4.8913
C	-4.4221	7.2574	4.4605
H	-5.0977	7.8963	3.9049
C	-7.3492	6.9823	3.1219
C	-7.6844	8.2859	3.4753
H	-7.8398	8.5839	4.5035
C	-7.8120	9.2522	2.4734
H	-8.0706	10.2686	2.7580
C	-7.6175	8.9379	1.1244
C	-7.2831	7.6136	0.8022
C	-7.1463	6.6378	1.7852
H	-6.8792	5.6256	1.5004
C	-3.7696	5.0910	5.3082
H	-3.9900	4.0414	5.4666
C	-2.6055	5.6453	5.8401
H	-1.9101	5.0092	6.3815
C	-2.3506	7.0113	5.6995
H	-7.1215	7.3356	-0.2363
N	-7.2082	5.8779	4.1453
H	-1.4508	7.4488	6.1234
C	-5.1532	1.5000	1.2453
H	-4.2413	2.0117	1.5586
H	-5.3583	0.6440	1.8834
H	-5.0697	1.2012	0.1970
C	-15.1020	5.1305	3.6882
H	-15.4105	5.5466	2.7198
H	-15.3765	4.0678	3.6792
H	-15.6973	5.6225	4.4652
C	-7.7745	9.9780	0.0431
H	-7.8489	10.9866	0.4620
H	-6.9290	9.9566	-0.6546
H	-8.6814	9.7930	-0.5473
Rh	-6.8472	1.5136	4.5521
Rh	-6.9386	-0.3073	6.1706
O	-8.8917	1.7354	4.8176
O	-8.9695	0.0743	6.3576
O	-4.8920	-0.5346	5.8781
O	-4.8052	1.2061	4.4318
O	-7.1765	0.0702	3.1248
O	-7.3459	-1.6180	4.6178

O	-6.5535	2.8250	6.2006
O	-6.5596	1.0776	7.6406
C	-9.4990	0.9999	5.6654
C	-6.4852	2.3159	7.3700
C	-4.2708	0.2758	5.1232
C	-7.4006	-1.1424	3.4413
C	-6.3442	3.2680	8.5704
C	-2.7435	0.1588	5.0236
C	-7.8419	-2.0693	2.3029
C	-10.9904	1.2959	5.8699
C	-5.2501	4.3101	8.2858
H	-5.4740	4.9050	7.4004
H	-5.1518	4.9891	9.1411
H	-4.2803	3.8255	8.1244
C	-7.7135	3.9573	8.7595
H	-8.4950	3.2212	8.9835
H	-7.6637	4.6668	9.5939
H	-8.0124	4.5050	7.8621
C	-5.9852	2.4848	9.8439
H	-5.0347	1.9527	9.7271
H	-5.8857	3.1815	10.6848
H	-6.7552	1.7496	10.0944
C	-2.1415	1.4967	5.5056
H	-1.0468	1.4479	5.4669
H	-2.4732	2.3264	4.8751
H	-2.4341	1.7116	6.5412
C	-2.2247	-0.9961	5.8916
H	-2.6458	-1.9551	5.5723
H	-1.1330	-1.0557	5.8100
H	-2.4827	-0.8489	6.9453
C	-2.3723	-0.0782	3.5453
H	-1.2835	-0.1561	3.4423
H	-2.8164	-1.0089	3.1710
H	-2.7210	0.7446	2.9150
C	-7.1674	-1.6489	0.9852
H	-7.5142	-2.2973	0.1717
H	-7.4037	-0.6110	0.7362
H	-6.0767	-1.7453	1.0521
C	-7.5092	-3.5312	2.6384
H	-8.0054	-3.8523	3.5589
H	-7.8406	-4.1835	1.8218
H	-6.4296	-3.6714	2.7687
C	-9.3740	-1.8847	2.1869
H	-9.7654	-2.5235	1.3862
H	-9.8759	-2.1609	3.1218
H	-9.6243	-0.8445	1.9520
C	-11.6378	0.2575	6.7961
H	-11.1649	0.2511	7.7833
H	-12.7008	0.4938	6.9250
H	-11.5594	-0.7520	6.3784
C	-11.0857	2.7019	6.5012
H	-10.6160	3.4492	5.8588
H	-12.1365	2.9812	6.6395
H	-10.5912	2.7261	7.4805
C	-11.6838	1.2845	4.4929
H	-11.6099	0.2946	4.0259
H	-12.7462	1.5294	4.6088
H	-11.2331	2.0175	3.8200

B-C-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9611575 Eh

Atom	X	Y	Z
S	-5.9009	2.6981	1.3899
O	-5.2980	3.8309	0.6363
O	-7.0582	2.0250	0.7717
N	-9.4879	5.5612	4.2885
N	-6.3489	3.2161	2.8997
C	-12.5888	7.0523	1.7859
C	-12.6778	7.1082	3.1824
H	-13.5640	7.5329	3.6478
C	-11.6557	6.6163	3.9952
H	-11.7594	6.6465	5.0756
C	-10.5033	6.0729	3.4184
C	-10.3923	6.0132	2.0240
H	-9.4914	5.6323	1.5566
C	-11.4282	6.4951	1.2275
H	-11.3205	6.4537	0.1463
C	-9.0218	6.3282	5.4533
H	-9.3000	5.8275	6.3837
H	-9.4859	7.3133	5.4385
C	-7.4607	6.4019	5.3470
H	-7.1008	7.4069	5.5680
H	-7.0144	5.7150	6.0621
C	-5.6781	5.2967	4.0396
C	-5.4257	4.0957	3.4651
H	-4.3761	3.7945	3.4777
C	-8.5675	4.6608	3.9218
H	-8.6135	4.1987	2.9476
H	-8.1118	4.0748	4.7065
C	-4.5829	6.0365	4.7155
C	-3.4030	8.1009	5.2582
H	-3.3309	9.1826	5.1784
C	-4.4620	7.4377	4.6377
H	-5.1875	8.0121	4.0719
C	-7.2015	6.8775	2.9073
C	-7.8357	8.1091	3.0935
H	-8.1320	8.4537	4.0754
C	-8.1021	8.9338	1.9963
H	-8.6034	9.8836	2.1650
C	-7.7447	8.5607	0.6983
C	-7.0859	7.3310	0.5358
C	-6.8152	6.4973	1.6153
H	-6.3151	5.5527	1.4433
C	-3.6074	5.3302	5.4485
H	-3.7062	4.2563	5.5685
C	-2.5416	5.9941	6.0554
H	-1.8060	5.4224	6.6156
C	-2.4340	7.3844	5.9665
H	-6.7825	7.0119	-0.4588
N	-7.0058	5.9347	4.0055
H	-1.6103	7.9038	6.4487
C	-4.5587	1.5018	1.5623
H	-3.7270	1.9949	2.0692
H	-4.9088	0.6475	2.1354
H	-4.2569	1.2080	0.5532
C	-13.7100	7.5504	0.9064
H	-13.3244	8.0202	-0.0056
H	-14.3621	6.7238	0.5927
H	-14.3364	8.2815	1.4288
C	-8.0761	9.4256	-0.4926
H	-8.2964	10.4561	-0.1943
H	-7.2517	9.4453	-1.2148
H	-8.9582	9.0390	-1.0207
Rh	-6.8178	1.5638	4.4371
Rh	-7.2856	-0.2177	6.0401
O	-8.8676	1.8348	4.2893
O	-9.2986	0.2548	5.8519
O	-5.2298	-0.5359	6.1172
O	-4.8077	1.1813	4.7007
O	-6.9256	0.0996	2.9947
O	-7.4719	-1.5375	4.4561
O	-6.7479	2.8870	6.0944
O	-7.0704	1.1745	7.5374
C	-9.6505	1.1746	5.0471
C	-6.8188	2.3886	7.2691
C	-4.4491	0.2200	5.4595
C	-7.2770	-1.0905	3.2836
C	-6.6161	3.3270	8.4708
C	-2.9382	-0.0370	5.5417
C	-7.4865	-2.0261	2.0865
C	-11.1289	1.5859	5.0321

C	-5.4330	4.2700	8.1965
H	-5.5847	4.8592	7.2918
H	-5.2990	4.9578	9.0398
H	-4.5030	3.7031	8.0713
C	-7.9204	4.1327	8.6489
H	-8.7738	3.4669	8.8243
H	-7.8295	4.8054	9.5098
H	-8.1362	4.7393	7.7660
C	-6.3392	2.5124	9.7455
H	-7.1759	1.8526	9.9917
H	-5.4423	1.8937	9.6311
H	-6.1785	3.1959	10.5878
C	-11.2614	2.7180	6.0792
H	-10.6267	3.5712	5.8156
H	-12.3003	3.0656	6.1216
H	-10.9753	2.3667	7.0774
C	-12.0207	0.3979	5.4255
H	-13.0720	0.7090	5.4301
H	-11.9128	-0.4281	4.7126
H	-11.7671	0.0220	6.4206
C	-11.5256	2.1124	3.6418
H	-11.3867	1.3429	2.8732
H	-12.5824	2.4044	3.6448
H	-10.9317	2.9848	3.3573
C	-8.5780	-1.3916	1.1965
H	-8.2762	-0.3913	0.8722
H	-8.7476	-2.0175	0.3121
H	-9.5277	-1.3077	1.7402
C	-7.9164	-3.4245	2.5502
H	-8.0695	-4.0695	1.6767
H	-7.1551	-3.8864	3.1879
H	-8.8527	-3.3862	3.1164
C	-6.1617	-2.1091	1.3003
H	-5.3478	-2.4873	1.9316
H	-6.2778	-2.7930	0.4512
H	-5.8735	-1.1274	0.9149
C	-2.2302	1.2951	5.8641
H	-1.1466	1.1379	5.9197
H	-2.4317	2.0458	5.0946
H	-2.5647	1.6949	6.8295
C	-2.6180	-1.0823	6.6193
H	-3.1073	-2.0375	6.4052
H	-1.5355	-1.2517	6.6585
H	-2.9492	-0.7485	7.6086
C	-2.4867	-0.5509	4.1565
H	-1.4099	-0.7570	4.1687
H	-3.0068	-1.4800	3.8918
H	-2.6886	0.1882	3.3755

C-Piv-Me-Me

Energy (POTENTIAL) = -3326.9776979 Eh

Atom	X	Y	Z
S	-7.1784	2.9005	1.5877
O	-7.0947	4.1271	0.7511
O	-8.3825	2.0606	1.4175
N	-9.8075	5.1223	3.9925
N	-7.0856	3.3031	3.1929
C	-11.5564	7.2762	0.7785
C	-12.1296	7.3024	2.0589
H	-13.0255	7.8923	2.2342
C	-11.5670	6.5887	3.1157
H	-12.0215	6.6171	4.1016
C	-10.4172	5.8292	2.8886
C	-9.8355	5.7686	1.6227
H	-8.9214	5.2088	1.4609
C	-10.4123	6.4905	0.5797
H	-9.9440	6.4605	-0.4008
C	-9.4543	5.8914	5.2158
H	-9.9052	5.3971	6.0803
H	-9.9021	6.8753	5.1099
C	-7.9231	5.9661	5.4162
H	-7.7303	6.7709	6.1431
H	-7.5874	5.0314	5.8634
C	-5.9694	5.3172	4.0853
C	-5.9625	4.0886	3.5231
H	-4.9960	3.5994	3.4201
C	-9.4450	3.8837	3.8982
H	-9.7022	3.3013	3.0236
H	-9.0149	3.3983	4.7582
C	-4.7300	5.8583	4.7054
C	-3.3328	7.7269	5.4182
H	-3.1760	8.8004	5.4883

C	-4.4985	7.2422	4.8228
H	-5.2273	7.9456	4.4367
C	-7.3350	7.2066	3.3301
C	-8.0552	8.3514	3.7165
H	-8.4448	8.4451	4.7241
C	-8.2737	9.3950	2.8116
H	-8.8506	10.2578	3.1384
C	-7.7671	9.3603	1.5098
C	-7.0120	8.2314	1.1471
C	-6.7970	7.1772	2.0254
H	-6.2573	6.2976	1.6952
C	-3.7659	4.9819	5.2490
H	-3.9577	3.9140	5.2489
C	-2.5964	5.4683	5.8318
H	-1.8719	4.7683	6.2405
C	-2.3701	6.8452	5.9174
H	-6.5991	8.1673	0.1421
N	-7.1672	6.1035	4.1825
H	-1.4637	7.2263	6.3803
C	-5.7181	1.9293	1.1518
H	-4.8311	2.5436	1.3205
H	-5.6968	1.0266	1.7588
H	-5.8034	1.6870	0.0892
C	-12.1238	8.1068	-0.3459
H	-11.5695	9.0503	-0.4442
H	-12.0486	7.5854	-1.3065
H	-13.1749	8.3595	-0.1710
C	-8.0206	10.4745	0.5222
H	-8.6108	11.2814	0.9706
H	-7.0826	10.9116	0.1548
H	-8.5676	10.1114	-0.3582
Rh	-6.8869	1.4743	4.6529
Rh	-6.5692	-0.3259	6.2706
O	-8.9302	1.2368	4.9551
O	-8.6292	-0.3852	6.5034
O	-4.5309	-0.1480	5.9417
O	-4.8236	1.5256	4.4479
O	-6.9745	-0.0002	3.2150
O	-6.7383	-1.6800	4.7119
O	-6.8354	2.8114	6.2603
O	-6.4572	1.1364	7.7336
C	-9.3559	0.3891	5.8085
C	-6.6407	2.3567	7.4383
C	-4.1001	0.7148	5.1138
C	-6.9485	-1.2308	3.5410
C	-6.6613	3.3743	8.5885
C	-2.5788	0.8076	4.9358
C	-7.2821	-2.2427	2.4383
C	-10.8788	0.3258	5.9860
C	-5.6714	4.5123	8.2733
H	-5.9115	5.0126	7.3338
H	-5.6957	5.2564	9.0782
H	-4.6468	4.1306	8.1967
C	-8.1020	3.9235	8.6887
H	-8.8134	3.1172	8.9069
H	-8.1634	4.6585	9.4998
H	-8.4130	4.4115	7.7608
C	-6.2740	2.7046	9.9156
H	-6.9666	1.8981	10.1752
H	-5.2652	2.2814	9.8668
H	-6.2949	3.4496	10.7199
C	-11.3679	1.7315	6.3950
H	-11.1617	2.4662	5.6106
H	-12.4498	1.7127	6.5701
H	-10.8793	2.0667	7.3185
C	-11.2632	-0.6982	7.0628
H	-12.3535	-0.7225	7.1749
H	-10.9229	-1.7036	6.7949
H	-10.8242	-0.4403	8.0323
C	-11.4968	-0.0716	4.6287
H	-11.1599	-1.0682	4.3194
H	-12.5903	-0.0914	4.7079
H	-11.2176	0.6408	3.8465
C	-2.2175	1.6647	3.7128
H	-2.5737	2.6930	3.8186
H	-1.1279	1.6911	3.5934
H	-2.6511	1.2490	2.7964
C	-2.0204	1.4544	6.2240
H	-2.2467	0.8398	7.1017
H	-0.9318	1.5601	6.1465
H	-2.4485	2.4511	6.3839
C	-2.0083	-0.6141	4.7693

H	-2.4138	-1.0981	3.8723
H	-0.9179	-0.5677	4.6659
H	-2.2485	-1.2404	5.6330
C	-6.9800	-1.6524	1.0514
H	-7.2657	-2.3718	0.2749
H	-7.5314	-0.7227	0.8882
H	-5.9108	-1.4382	0.9369
C	-6.4943	-3.5454	2.6518
H	-6.7157	-3.9895	3.6263
H	-6.7588	-4.2699	1.8727
H	-5.4137	-3.3665	2.5970
C	-8.8006	-2.5110	2.5735
H	-9.1195	-3.2348	1.8140
H	-9.0407	-2.9196	3.5615
H	-9.3747	-1.5883	2.4310

C-4-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9742159 Eh

Atom	X	Y	Z
S	-7.6293	3.4016	1.8329
O	-7.5475	4.6961	1.1275
O	-8.8835	2.6340	1.7264
N	-9.5948	5.3355	4.1797
N	-7.3264	3.5985	3.4843
C	-12.2852	5.8857	0.9340
C	-12.5430	4.9387	1.9336
H	-13.4439	4.3326	1.8801
C	-11.6674	4.7660	3.0066
H	-11.8843	4.0379	3.7829
C	-10.5050	5.5356	3.0830
C	-10.2237	6.4823	2.0931
H	-9.3076	7.0591	2.1401
C	-11.1129	6.6521	1.0349
H	-10.8841	7.3827	0.2626
C	-9.2615	6.4832	5.0492
H	-9.8180	6.3893	5.9898
H	-9.6214	7.3777	4.5437
C	-7.7629	6.5939	5.3568
H	-7.5980	7.5178	5.9310
H	-7.4513	5.7715	6.0021
C	-5.8976	5.5459	4.1521
C	-6.1046	4.2693	3.7664
H	-5.2424	3.6119	3.7500
C	-9.0856	4.1332	4.4107
H	-9.5584	3.2931	3.9291
H	-8.6195	3.9614	5.3709
C	-4.5646	5.9504	4.6905
C	-2.9226	7.6698	5.2476
H	-2.6434	8.7203	5.2619
C	-4.1679	7.3006	4.7358
H	-4.8295	8.0730	4.3629
C	-6.9315	7.5673	3.2209
C	-7.5608	8.8036	3.4661
H	-8.0699	8.9927	4.4038
C	-7.5325	9.8219	2.5080
H	-8.0339	10.7613	2.7330
C	-6.8753	9.6685	1.2845
C	-6.2445	8.4345	1.0505
C	-6.2718	7.4053	1.9829
H	-5.8056	6.4556	1.7539
C	-3.6755	4.9910	5.2233
H	-3.9753	3.9505	5.2812
C	-2.4292	5.3611	5.7256
H	-1.7689	4.5977	6.1289
C	-2.0403	6.7037	5.7354
H	-5.7276	8.2710	0.1066
N	-6.9429	6.5233	4.1566
H	-1.0712	6.9933	6.1330
C	-6.2717	2.3905	1.2130
H	-5.3334	2.9286	1.3617
H	-6.2745	1.4367	1.7375
H	-6.4562	2.2493	0.1443
C	-13.2386	6.0917	-0.2185
H	-12.7074	6.0863	-1.1778
H	-14.0057	5.3111	-0.2496
H	-13.7507	7.0600	-0.1406
C	-6.8216	10.7772	0.2603
H	-7.1329	10.4264	-0.7320
H	-7.4733	11.6126	0.5391
H	-5.8033	11.1752	0.1511
Rh	-7.0780	1.5653	4.7131
Rh	-6.7063	-0.3079	6.2199

O	-9.0906	1.3875	5.1619
O	-8.7476	-0.3517	6.5662
O	-4.6848	-0.1499	5.7942
O	-5.0340	1.5519	4.3484
O	-7.3114	0.1700	3.2047
O	-6.9576	-1.5751	4.6027
O	-6.8491	2.8266	6.3406
O	-6.4946	1.0897	7.7447
C	-9.4903	0.4991	5.9806
C	-6.6262	2.3264	7.4948
C	-4.2870	0.7111	4.9483
C	-7.2134	-1.0755	3.4625
C	-6.5277	3.3248	8.6545
C	-2.7821	0.7545	4.6569
C	-7.4162	-2.0245	2.2742
C	-10.9904	0.4478	6.2951
C	-11.7449	1.5552	5.5433
H	-12.8130	1.5034	5.7852
H	-11.3774	2.5475	5.8264
H	-11.6325	1.4498	4.4596
C	-11.1586	0.6318	7.8180
H	-12.2217	0.5938	8.0831
H	-10.6347	-0.1542	8.3702
H	-10.7624	1.6020	8.1437
C	-11.5152	-0.9385	5.8667
H	-11.3779	-1.0942	4.7895
H	-10.9918	-1.7391	6.3983
H	-12.5861	-1.0169	6.0877
C	-2.4776	1.6520	3.4479
H	-2.7888	2.6857	3.6234
H	-1.3985	1.6493	3.2534
H	-2.9875	1.2917	2.5477
C	-2.2904	-0.6809	4.3858
H	-1.2110	-0.6736	4.1947
H	-2.4882	-1.3346	5.2399
H	-2.7886	-1.1071	3.5062
C	-2.0981	1.3179	5.9224
H	-1.0142	1.3702	5.7673
H	-2.4589	2.3280	6.1484
H	-2.2936	0.6812	6.7914
C	-6.2454	-1.7982	1.2925
H	-6.3479	-2.4719	0.4336
H	-6.2329	-0.7689	0.9208
H	-5.2807	-2.0043	1.7724
C	-8.7506	-1.6637	1.5892
H	-8.9080	-2.3120	0.7193
H	-9.5952	-1.8045	2.2750
H	-8.7525	-0.6224	1.2551
C	-7.4371	-3.4875	2.7390
H	-6.4939	-3.7693	3.2178
H	-8.2460	-3.6652	3.4557
H	-7.5942	-4.1441	1.8752
C	-7.8969	4.0277	8.7802
H	-7.8670	4.7580	9.5974
H	-8.1567	4.5562	7.8578
H	-8.6938	3.3058	8.9984
C	-5.4345	4.3565	8.3093
H	-5.3471	5.0911	9.1185
H	-4.4597	3.8700	8.1863
H	-5.6657	4.8866	7.3820
C	-6.1827	2.6072	9.9668
H	-6.9474	1.8703	10.2321
H	-5.2228	2.0855	9.8924
H	-6.1135	3.3402	10.7790

H-Piv-Me-Me

Energy (POTENTIAL) = -3326.9816596 Eh

Atom	X	Y	Z
S	-7.6416	3.5246	1.8337
O	-7.5414	4.8136	1.1365
O	-8.8552	2.7136	1.6844
N	-9.2717	5.4770	3.9450
N	-7.4449	3.7656	3.5790
C	-12.2136	6.0513	0.9110
C	-12.2448	4.9157	1.7281
H	-13.0307	4.1766	1.5877
C	-11.2967	4.7137	2.7345
H	-11.3699	3.8271	3.3571
C	-10.2666	5.6413	2.9394
C	-10.2220	6.7787	2.1149
H	-9.4150	7.4923	2.2452
C	-11.1853	6.9824	1.1315

H	-11.1248	7.8706	0.5054
C	-9.2239	6.4645	5.0219
H	-9.8664	6.1761	5.8717
H	-9.6197	7.4004	4.6266
C	-7.7914	6.6741	5.5440
H	-7.7591	7.5850	6.1568
H	-7.5011	5.8523	6.2012
C	-5.8943	5.6311	4.3565
C	-6.1973	4.3958	3.9045
H	-5.3793	3.6928	3.8280
C	-8.7583	4.1824	4.2420
H	-9.4429	3.3863	3.9652
H	-8.5429	4.0833	5.3042
C	-4.5045	5.8904	4.8420
C	-2.6951	7.4497	5.3338
H	-2.3226	8.4707	5.3480
C	-3.9926	7.2006	4.8860
H	-4.6084	8.0316	4.5634
C	-6.8635	7.7004	3.4740
C	-7.5343	8.9212	3.6888
H	-8.0226	9.1218	4.6358
C	-7.5833	9.8936	2.6876
H	-8.1191	10.8197	2.8868
C	-6.9582	9.7130	1.4488
C	-6.2725	8.5040	1.2520
C	-6.2234	7.5168	2.2303
H	-5.7137	6.5838	2.0244
C	-3.6818	4.8451	5.3117
H	-4.0710	3.8342	5.3684
C	-2.3835	5.0966	5.7547
H	-1.7722	4.2729	6.1130
C	-1.8792	6.3997	5.7621
H	-5.7730	8.3225	0.3022
N	-6.8123	6.7146	4.4661
H	-0.8696	6.5959	6.1129
C	-6.1959	2.5528	1.3899
H	-5.2960	3.1409	1.5728
H	-6.1971	1.6180	1.9459
H	-6.3052	2.3686	0.3172
C	-13.2362	6.2734	-0.1784
H	-13.7488	7.2367	-0.0586
H	-12.7663	6.2848	-1.1707
H	-13.9980	5.4865	-0.1802
C	-7.0409	10.7515	0.3552
H	-7.3786	11.7186	0.7445
H	-6.0690	10.9048	-0.1301
H	-7.7463	10.4507	-0.4320
Rh	-7.1478	1.5930	4.7803
Rh	-6.7450	-0.3193	6.2042
O	-9.1410	1.4347	5.2838
O	-8.7752	-0.3665	6.6018
O	-4.7379	-0.1678	5.7043
O	-5.1265	1.5751	4.3206
O	-7.4586	0.2694	3.2284
O	-7.0527	-1.5229	4.5476
O	-6.8317	2.8010	6.4242
O	-6.4830	1.0174	7.7691
C	-9.5314	0.4976	6.0550
C	-6.5990	2.2647	7.5593
C	-4.3685	0.6940	4.8462
C	-7.3542	-0.9851	3.4361
C	-6.4777	3.2263	8.7460
C	-2.8954	0.6680	4.4248
C	-7.6597	-1.8914	2.2391
C	-11.0430	0.3929	6.2822
C	-11.6376	1.8050	6.4398
H	-11.4664	2.4097	5.5448
H	-12.7185	1.7353	6.6078
H	-11.1932	2.3275	7.2958
C	-11.6217	-0.2846	5.0175
H	-11.2041	-1.2894	4.8836
H	-12.7101	-0.3770	5.1114
H	-11.3999	0.3035	4.1205
C	-11.3497	-0.4558	7.5252
H	-10.9152	-0.0096	8.4271
H	-12.4349	-0.5217	7.6663
H	-10.9532	-1.4704	7.4249
C	-2.6233	1.6805	3.3020
H	-1.5683	1.6255	3.0096
H	-3.2347	1.4662	2.4188
H	-2.8346	2.7052	3.6208
C	-2.5639	-0.7580	3.9373

H	-1.5096	-0.8125	3.6425
H	-2.7440	-1.4963	4.7240
H	-3.1745	-1.0280	3.0666
C	-2.0531	1.0107	5.6723
H	-0.9885	1.0162	5.4121
H	-2.3138	2.0016	6.0625
H	-2.2122	0.2767	6.4685
C	-6.8660	-1.3851	1.0179
H	-7.0732	-2.0233	0.1511
H	-7.1437	-0.3580	0.7646
H	-5.7859	-1.4130	1.2092
C	-9.1765	-1.7680	1.9671
H	-9.4538	-2.4011	1.1161
H	-9.7609	-2.0911	2.8370
H	-9.4490	-0.7336	1.7352
C	-7.2918	-3.3494	2.5470
H	-7.5218	-3.9774	1.6783
H	-6.2241	-3.4514	2.7701
H	-7.8544	-3.7303	3.4049
C	-7.8543	3.9048	8.9235
H	-7.8130	4.6175	9.7554
H	-8.1448	4.4475	8.0185
H	-8.6339	3.1658	9.1461
C	-5.4098	4.2855	8.4064
H	-5.3135	4.9938	9.2376
H	-4.4309	3.8200	8.2422
H	-5.6737	4.8429	7.5040
C	-6.0896	2.4727	10.0255
H	-6.8396	1.7205	10.2897
H	-5.1269	1.9635	9.9093
H	-6.0044	3.1815	10.8572

H_-Piv-Me-Me

Energy (POTENTIAL) = -3326.9964355 Eh

Atom	X	Y	Z
S	-6.9764	3.1738	1.3266
O	-7.1341	2.0554	0.3476
O	-5.8642	3.1330	2.2815
N	-10.8706	3.3403	2.1742
N	-8.3956	3.3662	2.1751
C	-12.3880	0.1964	4.6304
C	-11.1697	0.0726	3.9459
H	-10.6019	-0.8519	4.0176
C	-10.6516	1.1084	3.1743
H	-9.6904	0.9597	2.7072
C	-11.3584	2.3181	3.0133
C	-12.5764	2.4529	3.7052
H	-13.1558	3.3660	3.6332
C	-13.0691	1.4109	4.4945
H	-14.0139	1.5552	5.0143
C	-11.3685	4.7113	2.2889
H	-12.4619	4.7258	2.2182
H	-10.9913	5.2544	1.4204
C	-10.9345	5.4297	3.5834
H	-11.2884	6.4659	3.5652
H	-11.4036	4.9434	4.4440
C	-8.9923	4.1798	4.3552
C	-8.3610	3.2664	3.5863
H	-7.8692	2.4012	4.0107
C	-9.7011	3.1263	1.3973
H	-9.6927	3.8272	0.5607
H	-9.6777	2.1101	1.0087
C	-9.2436	3.9522	5.7947
C	-9.7340	2.4624	7.6546
H	-9.9536	1.4625	8.0199
C	-9.5235	2.6664	6.2904
H	-9.6139	1.8372	5.5970
C	-8.6222	6.2878	3.1564
C	-9.0638	7.2061	2.1866
H	-10.1007	7.2278	1.8728
C	-8.1732	8.1151	1.6057
H	-8.5525	8.8068	0.8562
C	-6.8198	8.1527	1.9513
C	-6.3865	7.2361	2.9257
C	-7.2563	6.3285	3.5172
H	-6.8804	5.6373	4.2631
C	-9.2250	5.0351	6.6920
H	-9.0312	6.0340	6.3120
C	-9.4389	4.8292	8.0543
H	-9.4107	5.6735	8.7382
C	-9.6887	3.5414	8.5417
H	-5.3416	7.2338	3.2300

N	-9.4917	5.3978	3.8058
H	-9.8606	3.3838	9.6032
C	-6.8559	4.6490	0.3133
H	-7.7744	4.7629	-0.2661
H	-6.7015	5.5014	0.9752
H	-6.0030	4.5098	-0.3564
C	-12.9122	-0.9267	5.4930
H	-13.9472	-0.7458	5.8030
H	-12.8817	-1.8865	4.9623
H	-12.3102	-1.0464	6.4043
C	-5.8563	9.1272	1.3168
H	-5.4195	9.8054	2.0620
H	-5.0200	8.6079	0.8307
H	-6.3520	9.7428	0.5582
Rh	-7.4281	-0.2361	0.8344
Rh	-7.8579	-2.5890	1.1585
O	-9.4585	-0.0202	0.4697
O	-9.8761	-2.1979	0.8990
O	-5.8092	-2.8370	1.3465
O	-5.4189	-0.6237	1.0884
O	-7.2446	-0.6145	-1.1815
O	-7.7043	-2.8105	-0.8921
O	-7.5003	-0.0206	2.9183
O	-7.9161	-2.2235	3.1985
C	-10.2228	-1.0388	0.5020
C	-7.5630	-1.0772	3.6281
C	-5.0395	-1.8263	1.2721
C	-7.4152	-1.8006	-1.6123
C	-7.1366	-1.0182	5.1041
C	-3.5270	-2.0641	1.3540
C	-7.1981	-2.0543	-3.1086
C	-11.6440	-0.8958	-0.0558
C	-2.8787	-0.9587	2.2079
H	-1.7949	-1.1159	2.2560
H	-3.0672	0.0317	1.7844
H	-3.2700	-0.9700	3.2325
C	-2.9993	-1.9887	-0.0978
H	-1.9171	-2.1647	-0.1088
H	-3.4757	-2.7477	-0.7298
H	-3.1937	-1.0033	-0.5346
C	-3.2238	-3.4454	1.9539
H	-2.1390	-3.5974	1.9974
H	-3.6220	-3.5322	2.9712
H	-3.6594	-4.2478	1.3512
C	-5.7977	-2.6989	-3.2352
H	-5.5817	-2.9146	-4.2883
H	-5.0189	-2.0259	-2.8573
H	-5.7463	-3.6373	-2.6727
C	-8.2741	-3.0253	-3.6285
H	-9.2773	-2.5957	-3.5219
H	-8.1037	-3.2306	-4.6918
H	-8.2505	-3.9733	-3.0840
C	-7.2468	-0.7379	-3.8988
H	-7.0868	-0.9425	-4.9639
H	-8.2195	-0.2451	-3.7874
H	-6.4745	-0.0399	-3.5627
C	-11.6323	-1.6370	-1.4146
H	-11.3826	-2.6947	-1.2843
H	-12.6213	-1.5666	-1.8825
H	-10.8995	-1.1914	-2.0988
C	-12.0168	0.5775	-0.2727
H	-13.0226	0.6388	-0.7048
H	-12.0174	1.1298	0.6708
H	-11.3190	1.0691	-0.9575
C	-12.6479	-1.5646	0.9009
H	-12.6616	-1.0560	1.8710
H	-13.6561	-1.5121	0.4734
H	-12.3969	-2.6164	1.0664
C	-6.0106	-2.0640	5.2790
H	-5.6616	-2.0580	6.3180
H	-6.3619	-3.0700	5.0335
H	-5.1554	-1.8323	4.6320
C	-6.6051	0.3685	5.4879
H	-7.3936	1.1227	5.4613
H	-6.2140	0.3385	6.5118
H	-5.8005	0.6897	4.8192
C	-8.3409	-1.3937	5.9904
H	-8.0325	-1.4171	7.0422
H	-9.1476	-0.6596	5.8897
H	-8.7350	-2.3793	5.7232

C-D-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9633245 Eh

Atom	X	Y	Z
S	-8.5112	4.5939	2.1534
O	-8.8576	6.0271	2.2263
O	-9.6235	3.6515	1.9526
N	-9.3020	6.8956	5.1077
N	-7.6718	4.0450	3.4947
C	-13.0504	5.0558	4.2989
C	-12.8962	6.4457	4.2469
H	-13.7511	7.0737	4.0095
C	-11.6622	7.0490	4.4992
H	-11.5778	8.1302	4.4699
C	-10.5549	6.2544	4.8044
C	-10.6820	4.8614	4.8489
H	-9.8155	4.2300	5.0097
C	-11.9205	4.2812	4.6051
H	-12.0029	3.1995	4.6187
C	-8.9158	8.1206	4.3447
H	-9.3429	8.9972	4.8445
H	-9.3611	8.0093	3.3591
C	-7.3930	8.2789	4.2171
H	-7.2241	9.1385	3.5650
H	-6.9582	8.5552	5.1871
C	-6.4427	6.0328	4.5744
C	-6.8749	4.7286	4.3445
H	-6.4489	4.0331	5.0569
C	-8.4730	6.4024	5.9871
H	-8.7279	5.4844	6.5021
H	-7.6906	7.0164	6.4036
C	-5.4344	6.2482	5.6501
C	-3.5257	7.4946	6.5296
H	-2.7994	8.2942	6.4068
C	-4.4870	7.2850	5.5389
H	-4.4910	7.9155	4.6557
C	-6.0390	7.1643	2.4397
C	-6.5352	7.9400	1.3751
H	-7.4614	8.4910	1.4947
C	-5.8814	7.9605	0.1443
H	-6.3009	8.5609	-0.6608
C	-4.7208	7.2096	-0.0924
C	-4.2385	6.4295	0.9678
C	-4.8728	6.4065	2.2093
H	-4.4679	5.7885	3.0032
C	-5.4036	5.4632	6.8233
H	-6.1438	4.6831	6.9682
C	-4.4386	5.6674	7.8074
H	-4.4393	5.0359	8.6924
C	-3.4878	6.6837	7.6665
H	-3.3434	5.8270	0.8263
N	-6.6862	7.1203	3.6840
H	-2.7382	6.8469	8.4359
C	-7.3621	4.3418	0.7934
H	-6.4830	4.9689	0.9330
H	-7.0964	3.2842	0.7931
H	-7.8877	4.6162	-0.1258
C	-14.3772	4.3924	4.0223
H	-14.7518	3.8701	4.9123
H	-15.1356	5.1196	3.7150
H	-14.2844	3.6419	3.2276
C	-4.0104	7.2527	-1.4249
H	-3.5004	6.3061	-1.6381
H	-4.7080	7.4532	-2.2464
H	-3.2467	8.0431	-1.4498
Rh	-7.4317	1.8295	3.8146
Rh	-6.9110	-0.4837	4.3746
O	-9.4284	1.2833	3.8072
O	-8.9368	-0.8880	4.2263
O	-4.9107	0.0859	4.5133
O	-5.3992	2.2107	3.9108
O	-7.2108	1.3087	1.8243
O	-6.6702	-0.8275	2.3413
O	-7.5932	2.1976	5.8483
O	-7.1711	0.0366	6.3708
C	-9.7475	0.0719	4.0222
C	-7.4311	1.2420	6.6764
C	-4.5927	1.2913	4.2700
C	-6.8521	0.1238	1.5197
C	-7.4949	1.5958	8.1685
C	-3.1277	1.7212	4.4255
C	-6.5962	-0.1378	0.0295
C	-11.2510	-0.2308	4.0982

C	-3.0807	2.8042	5.5258
H	-2.0476	3.1388	5.6779
H	-3.6875	3.6715	5.2522
H	-3.4549	2.4138	6.4802
C	-2.6585	2.3198	3.0826
H	-1.6185	2.6570	3.1662
H	-2.7103	1.5738	2.2799
H	-3.2778	3.1750	2.7949
C	-2.2423	0.5303	4.8158
H	-1.2027	0.8626	4.9217
H	-2.5613	0.0933	5.7676
H	-2.2750	-0.2567	4.0550
C	-5.3545	0.6920	-0.3682
H	-5.1267	0.5364	-1.4294
H	-5.5230	1.7609	-0.2037
H	-4.4767	0.3893	0.2162
C	-7.8256	0.3329	-0.7736
H	-7.6545	0.1689	-1.8442
H	-8.7224	-0.2279	-0.4829
H	-8.0232	1.3965	-0.6116
C	-6.3343	-1.6282	-0.2285
H	-5.4610	-1.9817	0.3286
H	-7.1935	-2.2400	0.0671
H	-6.1497	-1.7902	-1.2972
C	-11.7162	0.2703	5.4853
H	-12.7938	0.1048	5.6029
H	-11.1992	-0.2669	6.2899
H	-11.5141	1.3391	5.6069
C	-11.9851	0.5327	2.9804
H	-11.6677	0.1771	1.9923
H	-13.0669	0.3743	3.0666
H	-11.7793	1.6043	3.0296
C	-11.5180	-1.7382	3.9734
H	-12.5965	-1.9275	4.0342
H	-11.1581	-2.1264	3.0139
H	-11.0242	-2.3004	4.7715
C	-6.0360	1.8613	8.6098
H	-6.0113	2.1343	9.6715
H	-5.4163	0.9687	8.4695
H	-5.5913	2.6811	8.0343
C	-8.3513	2.8538	8.3921
H	-9.3675	2.7161	8.0046
H	-8.4199	3.0671	9.4654
H	-7.9176	3.7285	7.8995
C	-8.0776	0.4154	8.9636
H	-8.0915	0.6587	10.0325
H	-9.1059	0.1986	8.6503
H	-7.4821	-0.4904	8.8224

D_-Piv-Me-Me

Energy (POTENTIAL) = -3326.9855089 Eh

Atom	X	Y	Z
S	-8.6173	4.8909	2.0338
O	-8.8573	6.3360	2.0365
O	-9.7731	3.9926	2.0041
N	-9.2115	6.9720	4.9799
N	-7.6514	4.2886	3.3737
C	-12.7742	4.6505	4.7866
C	-12.7357	5.9827	4.3563
H	-13.6399	6.4433	3.9622
C	-11.5724	6.7486	4.4262
H	-11.6059	7.7836	4.1038
C	-10.3705	6.1992	4.9217
C	-10.4034	4.8554	5.3523
H	-9.5082	4.3538	5.7000
C	-11.5816	4.1166	5.2925
H	-11.5601	3.0846	5.6331
C	-9.0772	8.2275	4.2437
H	-9.5454	9.0676	4.7813
H	-9.5659	8.1198	3.2756
C	-7.5816	8.5401	4.0341
H	-7.4770	9.2692	3.2329
H	-7.1652	9.0125	4.9346
C	-6.7958	6.3349	4.7683
C	-6.9754	4.9042	4.2775
H	-6.4605	4.2027	4.9274
C	-8.0475	6.5980	5.7169
H	-8.2239	5.7165	6.3299
H	-7.7466	7.3965	6.4059
C	-5.5595	6.3954	5.6995
C	-3.5282	7.5054	6.4412
H	-2.7973	8.2988	6.3097

C	-4.6109	7.4158	5.5628
H	-4.7092	8.1349	4.7573
C	-6.0294	7.1964	2.5684
C	-6.3112	7.9291	1.3942
H	-7.1579	8.6046	1.3655
C	-5.5518	7.7584	0.2420
H	-5.8113	8.3366	-0.6429
C	-4.4834	6.8486	0.1799
C	-4.2111	6.1166	1.3392
C	-4.9560	6.2831	2.5096
H	-4.6763	5.6991	3.3781
C	-5.4154	5.4857	6.7597
H	-6.1466	4.6974	6.9119
C	-4.3344	5.5737	7.6382
H	-4.2418	4.8519	8.4453
C	-3.3808	6.5818	7.4783
H	-3.3930	5.3996	1.3442
N	-6.8041	7.3424	3.7246
H	-2.5360	6.6498	8.1582
C	-7.5018	4.4785	0.6935
H	-6.5910	5.0692	0.7889
H	-7.2944	3.4092	0.7443
H	-8.0332	4.7360	-0.2274
C	-14.0283	3.8168	4.6707
H	-14.9278	4.4091	4.8789
H	-14.1426	3.4019	3.6597
H	-14.0134	2.9706	5.3671
C	-3.6886	6.6628	-1.0905
H	-3.3058	7.6186	-1.4705
H	-2.8324	5.9981	-0.9319
H	-4.3034	6.2257	-1.8891
Rh	-7.4657	2.0050	3.6649
Rh	-6.9545	-0.3024	4.2062
O	-9.4557	1.4520	3.5635
O	-8.9735	-0.7064	4.0450
O	-4.9504	0.2543	4.3345
O	-5.4445	2.4006	3.8268
O	-7.1889	1.5125	1.6806
O	-6.7044	-0.6400	2.1720
O	-7.7075	2.3564	5.6934
O	-7.2329	0.2030	6.1960
C	-9.7815	0.2436	3.7809
C	-7.5499	1.3918	6.5141
C	-4.6288	1.4629	4.1177
C	-6.8577	0.3220	1.3589
C	-7.7012	1.6965	8.0097
C	-3.1523	1.8700	4.1949
C	-6.6180	0.0751	-0.1348
C	-11.2764	-0.1013	3.7814
C	-3.0258	2.9977	5.2414
H	-1.9799	3.3161	5.3213
H	-3.6301	3.8656	4.9642
H	-3.3527	2.6561	6.2308
C	-2.7422	2.3990	2.8030
H	-1.6957	2.7256	2.8222
H	-2.8400	1.6182	2.0385
H	-3.3653	3.2483	2.5060
C	-2.2718	0.6772	4.5905
H	-1.2233	0.9940	4.6366
H	-2.5543	0.2825	5.5721
H	-2.3526	-0.1366	3.8626
C	-8.5215	2.9771	8.2320
H	-8.6371	3.1549	9.3076
H	-8.0337	3.8536	7.7964
H	-9.5207	2.8917	7.7914
C	-6.2680	1.8801	8.5612
H	-6.3069	2.1049	9.6335
H	-5.6739	0.9709	8.4200
H	-5.7543	2.7072	8.0572
C	-8.3874	0.5073	8.7068
H	-8.4876	0.7142	9.7784
H	-9.3904	0.3378	8.2967
H	-7.8098	-0.4128	8.5835
C	-5.4329	0.9675	-0.5655
H	-5.2247	0.8192	-1.6315
H	-5.6529	2.0267	-0.4001
H	-4.5254	0.7147	-0.0031
C	-7.8935	0.4841	-0.9015
H	-7.7473	0.3241	-1.9762
H	-8.7538	-0.1168	-0.5821
H	-8.1345	1.5388	-0.7375
C	-6.2900	-1.4007	-0.4006

H	-6.1207	-1.5520	-1.4732
H	-5.3879	-1.7111	0.1363
H	-7.1111	-2.0540	-0.0876
C	-12.0823	0.9770	3.0410
H	-13.1494	0.7279	3.0782
H	-11.9362	1.9633	3.4861
H	-11.7817	1.0384	1.9889
C	-11.7049	-0.1649	5.2659
H	-12.7731	-0.4023	5.3349
H	-11.1438	-0.9363	5.8049
H	-11.5370	0.7947	5.7687
C	-11.4918	-1.4729	3.1167
H	-12.5591	-1.7238	3.1254
H	-11.1540	-1.4610	2.0733
H	-10.9470	-2.2618	3.6429

t-D-Piv-Me-Me

Energy (POTENTIAL) = -3326.9823836 Eh

Atom	X	Y	Z
S	-7.2475	3.3124	-1.5119
O	-8.0310	4.1049	-2.4813
O	-7.1658	1.8557	-1.7003
N	-12.2022	4.4997	1.6803
N	-7.8481	3.5324	0.1060
C	-13.4013	2.2258	5.0907
C	-13.0722	1.6168	3.8691
H	-13.1329	0.5341	3.7782
C	-12.6794	2.3616	2.7630
H	-12.4589	1.8474	1.8326
C	-12.5757	3.7674	2.8301
C	-12.9187	4.3822	4.0471
H	-12.8504	5.4577	4.1616
C	-13.3273	3.6204	5.1452
H	-13.5759	4.1337	6.0719
C	-12.2882	5.9568	1.6580
H	-13.1589	6.2956	2.2236
H	-12.4354	6.2567	0.6125
C	-11.0176	6.6149	2.1912
H	-11.0754	7.6879	2.0049
H	-10.9593	6.4765	3.2785
C	-9.6796	4.6238	1.4003
C	-8.7957	4.3881	0.1919
H	-9.1049	4.9831	-0.6739
C	-11.0823	4.0707	0.8679
H	-11.2366	4.4594	-0.1446
H	-11.0255	2.9863	0.8075
C	-9.3187	3.8572	2.6816
C	-9.0723	1.7353	3.8490
H	-9.0164	0.6516	3.8117
C	-9.2184	2.4561	2.6647
H	-9.2734	1.9184	1.7242
C	-8.6401	6.8904	1.5570
C	-8.7149	8.2405	1.1629
H	-9.6589	8.6498	0.8165
C	-7.5899	9.0618	1.1919
H	-7.6900	10.1014	0.8869
C	-6.3352	8.5785	1.5899
C	-6.2570	7.2273	1.9515
C	-7.3795	6.3977	1.9452
H	-7.2604	5.3774	2.2839
C	-9.2141	4.5116	3.9153
H	-9.2423	5.5925	3.9603
C	-9.0747	3.7914	5.1035
H	-9.0149	4.3252	6.0478
C	-9.0222	2.3982	5.0778
H	-5.3100	6.7979	2.2655
N	-9.8119	6.0861	1.5225
H	-8.9389	1.8353	6.0032
C	-5.6085	4.0148	-1.4038
H	-5.6960	5.0405	-1.0446
H	-5.0111	3.4097	-0.7259
H	-5.1988	3.9919	-2.4176
C	-13.7863	1.4007	6.2954
H	-14.2804	2.0113	7.0594
H	-14.4657	0.5830	6.0250
H	-12.9042	0.9414	6.7633
C	-5.1171	9.4712	1.6163
H	-4.4121	9.2146	0.8153
H	-5.3916	10.5243	1.4907
H	-4.5725	9.3769	2.5636
Rh	-5.0003	3.0510	2.2454
Rh	-2.8449	2.6731	3.2583

O	-5.6699	1.3845	3.2701
O	-3.6455	1.0295	4.2094
O	-2.1348	4.3034	2.2204
O	-4.1439	4.6690	1.2538
O	-4.3912	1.8286	0.7003
O	-2.3624	1.4822	1.6314
O	-5.4617	4.2756	3.8405
O	-3.4461	3.9097	4.7961
C	-4.8586	0.7129	3.9862
C	-4.6087	4.4312	4.7728
C	-2.9131	4.9376	1.4367
C	-3.2070	1.3555	0.6883
C	-5.0371	5.2482	5.9955
C	-2.3030	6.1324	0.6947
C	-2.7539	0.6582	-0.5968
C	-5.3977	-0.5541	4.6596
C	-3.8178	5.9418	6.6259
H	-4.1346	6.5173	7.5034
H	-3.0645	5.2153	6.9432
H	-3.3478	6.6337	5.9169
C	-6.0967	6.2903	5.6021
H	-6.9710	5.8184	5.1488
H	-6.4190	6.8389	6.4951
H	-5.6955	7.0140	4.8840
C	-5.6413	4.2262	6.9882
H	-4.8979	3.4749	7.2783
H	-5.9783	4.7451	7.8934
H	-6.4997	3.7101	6.5450
C	-4.2414	-1.4719	5.0869
H	-3.5768	-0.9745	5.7990
H	-4.6459	-2.3725	5.5635
H	-3.6421	-1.7823	4.2235
C	-6.3250	-1.2971	3.6797
H	-6.7240	-2.1981	4.1600
H	-7.1629	-0.6681	3.3690
H	-5.7795	-1.6048	2.7791
C	-6.1919	-0.0907	5.9010
H	-7.0045	0.5823	5.6156
H	-6.6217	-0.9601	6.4128
H	-5.5424	0.4370	6.6096
C	-0.9715	5.6919	0.0547
H	-0.5177	6.5389	-0.4729
H	-0.2658	5.3361	0.8108
H	-1.1303	4.8852	-0.6715
C	-3.2549	6.6566	-0.3897
H	-4.2243	6.9426	0.0258
H	-2.8103	7.5349	-0.8718
H	-3.4270	5.8990	-1.1616
C	-2.0395	7.2247	1.7557
H	-1.6081	8.1114	1.2770
H	-2.9676	7.5261	2.2537
H	-1.3397	6.8676	2.5181
C	-1.6438	-0.3609	-0.2958
H	-1.3241	-0.8419	-1.2276
H	-0.7730	0.1182	0.1609
H	-1.9999	-1.1419	0.3861
C	-3.9473	-0.0322	-1.2795
H	-4.7521	0.6740	-1.5007
H	-3.6159	-0.4917	-2.2180
H	-4.3595	-0.8230	-0.6413
C	-2.2042	1.7866	-1.5043
H	-1.3609	2.2997	-1.0276
H	-1.8559	1.3611	-2.4526
H	-2.9791	2.5287	-1.7271

t-D-E-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9571731 Eh

Atom	X	Y	Z
N	-6.3891	0.4471	-7.4225
N	-3.4353	-1.2705	-6.1497
N	-2.1813	1.2129	-5.7623
C	-5.2975	-0.2976	-7.1946
H	-4.6973	-0.5256	-8.0765
C	-5.5545	-2.2126	-6.5897
C	-6.3259	-3.1613	-7.3232
H	-7.3970	-2.9961	-7.3702
C	-5.7497	-4.2715	-7.9071
C	-4.3547	-4.4728	-7.7012
C	-3.5521	-3.5747	-7.0230
H	-2.4892	-3.7663	-6.9306
C	-4.1278	-2.3824	-6.5217
C	-2.0129	-1.2312	-5.8117

H	-1.8887	-1.3557	-4.7289
H	-1.5035	-2.0572	-6.3106
C	-1.3733	0.0847	-6.2386
H	-1.2785	0.1193	-7.3384
H	-0.3697	0.1327	-5.8126
C	-1.5140	2.4620	-5.6558
C	-0.4333	2.5764	-4.7590
H	-0.1406	1.7124	-4.1683
C	0.2383	3.7832	-4.6013
H	1.0651	3.8414	-3.8960
C	-0.1417	4.9329	-5.3155
C	0.5844	6.2421	-5.1147
H	1.6573	6.1432	-5.3254
H	0.1864	7.0257	-5.7683
H	0.4946	6.5942	-4.0786
C	-1.2199	4.8155	-6.1971
H	-1.5401	5.6839	-6.7690
C	-1.8939	3.6026	-6.3788
H	-2.7097	3.5584	-7.0929
C	-3.4738	1.1950	-6.4286
H	-4.0568	2.0694	-6.1420
H	-3.3623	1.2099	-7.5261
C	-4.2787	-0.0724	-6.0153
C	-4.8286	0.0965	-4.5970
C	-4.4376	-0.7628	-3.5609
H	-3.8046	-1.6170	-3.7705
C	-4.8630	-0.5464	-2.2482
H	-4.5413	-1.2241	-1.4618
C	-5.7039	0.5276	-1.9531
H	-6.0391	0.7002	-0.9338
C	-6.1159	1.3746	-2.9840
H	-6.7900	2.1971	-2.7741
C	-5.6711	1.1709	-4.2892
H	-6.0089	1.8375	-5.0714
S	-6.4732	0.9599	-9.0569
O	-6.9215	2.3613	-9.0348
O	-5.1951	0.6690	-9.7514
H	-3.8934	-5.3667	-8.1158
C	-6.5462	-5.2754	-8.7047
H	-7.6217	-5.1346	-8.5632
H	-6.3376	-5.1852	-9.7795
H	-6.2973	-6.3038	-8.4157
C	-7.7089	-0.0674	-9.8603
H	-7.3881	-1.1064	-9.7730
H	-8.6743	0.0857	-9.3887
H	-7.7264	0.2406	-10.9093
H	-6.0755	-1.7548	-5.7514
Rh	-10.7750	0.2555	-5.3220
Rh	-8.5677	0.3450	-6.3315
O	-9.9999	-0.9966	-3.8855
O	-7.9538	-1.0081	-4.8450
O	-9.4352	1.5082	-7.8045
O	-11.4791	1.4682	-6.8445
O	-11.1593	-1.4061	-6.4984
O	-9.0963	-1.3458	-7.4221
O	-10.3071	1.9563	-4.2542
O	-8.2975	2.1193	-5.2776
C	-8.8222	-1.4606	-4.0311
C	-9.2273	2.5724	-4.5389
C	-10.6705	1.8117	-7.7632
C	-10.2709	-1.8292	-7.3021
C	-9.0804	3.9912	-3.9691
C	-11.1987	2.7041	-8.8940
C	-10.6280	-3.0469	-8.1663
C	-8.4739	-2.6673	-3.1459
C	-9.2649	3.9373	-2.4392
H	-9.1953	4.9489	-2.0224
H	-10.2424	3.5215	-2.1767
H	-8.4938	3.3217	-1.9619
C	-10.2087	4.8415	-4.5961
H	-10.1726	5.8601	-4.1920
H	-10.0938	4.9036	-5.6838
H	-11.1922	4.4146	-4.3771
C	-7.7192	4.6036	-4.3314
H	-6.8872	4.0366	-3.9047
H	-7.5778	4.6393	-5.4162
H	-7.6651	5.6277	-3.9434
C	-7.1334	-3.2933	-3.5494
H	-6.3190	-2.5706	-3.4784
H	-6.9075	-4.1345	-2.8830
H	-7.1648	-3.6728	-4.5759
C	-9.5991	-3.7112	-3.3116

H	-9.3753	-4.5943	-2.7014
H	-10.5660	-3.3078	-2.9985
H	-9.6853	-4.0323	-4.3566
C	-8.4215	-2.1814	-1.6819
H	-8.2175	-3.0300	-1.0179
H	-7.6278	-1.4400	-1.5435
H	-9.3732	-1.7299	-1.3831
C	-12.1254	-3.0112	-8.5202
H	-12.3800	-3.8814	-9.1363
H	-12.7488	-3.0292	-7.6221
H	-12.3741	-2.1069	-9.0885
C	-9.7894	-3.0572	-9.4552
H	-8.7190	-3.0975	-9.2437
H	-10.0531	-3.9337	-10.0583
H	-9.9799	-2.1603	-10.0561
C	-10.3210	-4.3004	-7.3145
H	-10.9441	-4.3239	-6.4139
H	-10.5288	-5.2049	-7.8983
H	-9.2706	-4.3281	-7.0044
C	-10.9501	4.1641	-8.4508
H	-11.2913	4.8518	-9.2337
H	-11.4979	4.3951	-7.5307
H	-9.8836	4.3449	-8.2762
C	-12.7025	2.4643	-9.1023
H	-13.0705	3.1093	-9.9088
H	-12.9014	1.4227	-9.3817
H	-13.2729	2.6857	-8.1957
C	-10.4269	2.4164	-10.1937
H	-10.5747	1.3787	-10.5169
H	-10.7935	3.0735	-10.9911
H	-9.3549	2.5841	-10.0628

E-Piv-Me-Me

Energy (POTENTIAL) = -3326.9773384 Eh

Atom	X	Y	Z
N	-6.6346	0.5135	-7.1734
N	-3.7539	-1.1729	-5.5980
N	-2.0992	1.0826	-5.7621
C	-5.4494	-0.3084	-7.0629
H	-4.8952	-0.3253	-8.0078
C	-5.6911	-1.7949	-6.6921
C	-6.1900	-2.7205	-7.7406
H	-7.0207	-2.3674	-8.3389
C	-5.7027	-3.9813	-7.8570
C	-4.6517	-4.4063	-6.9467
C	-4.0183	-3.5806	-6.0591
H	-3.1858	-3.9330	-5.4615
C	-4.4124	-2.2115	-6.0598
C	-2.5047	-1.1567	-4.8331
H	-2.7388	-0.7929	-3.8280
H	-2.1053	-2.1683	-4.7603
C	-1.4925	-0.2253	-5.5044
H	-1.1446	-0.6845	-6.4465
H	-0.6326	-0.1258	-4.8411
C	-1.2295	2.1868	-5.9277
C	-0.2888	2.4813	-4.9190
H	-0.2438	1.8576	-4.0307
C	0.5572	3.5789	-5.0279
H	1.2668	3.7800	-4.2275
C	0.5001	4.4452	-6.1329
C	1.4134	5.6447	-6.2238
H	2.4702	5.3485	-6.1933
H	1.2498	6.2042	-7.1512
H	1.2516	6.3349	-5.3853
C	-0.4403	4.1547	-7.1251
H	-0.5139	4.8008	-7.9972
C	-1.2854	3.0431	-7.0394
H	-1.9795	2.8520	-7.8509
C	-3.2396	0.9492	-6.6567
H	-3.6366	1.9179	-6.9455
H	-2.9610	0.4342	-7.5898
C	-4.3659	0.1378	-5.9792
C	-4.9115	0.8264	-4.7290
C	-5.4042	0.0709	-3.6564
H	-5.4538	-1.0080	-3.7335
C	-5.8165	0.6816	-2.4711
H	-6.1837	0.0693	-1.6519
C	-5.7338	2.0677	-2.3324
H	-6.0295	2.5465	-1.4032
C	-5.2685	2.8341	-3.4031
H	-5.2059	3.9151	-3.3151
C	-4.8719	2.2209	-4.5919

H	-4.5119	2.8464	-5.3997
S	-6.5641	1.5845	-8.4067
O	-7.2912	2.8218	-8.0590
O	-5.1626	1.7622	-8.8882
H	-4.3224	-5.4413	-7.0123
C	-6.1970	-4.9736	-8.8795
H	-6.6557	-5.8463	-8.3975
H	-6.9385	-4.5252	-9.5455
H	-5.3668	-5.3453	-9.4937
C	-7.4358	0.8183	-9.7953
H	-6.8954	-0.0899	-10.0755
H	-8.4522	0.5824	-9.4854
H	-7.4372	1.5226	-10.6318
H	-6.4481	-1.8123	-5.8854
Rh	-10.9924	-0.3869	-5.4490
Rh	-8.7507	0.0604	-6.3329
O	-10.1473	-1.8089	-4.2109
O	-8.0553	-1.3183	-4.9064
O	-9.6934	1.2823	-7.7067
O	-11.7304	1.0298	-6.7594
O	-11.1870	-1.8511	-6.8996
O	-9.0673	-1.5405	-7.6341
O	-10.6827	1.1328	-4.0927
O	-8.6873	1.6712	-5.0191
C	-8.8961	-2.0156	-4.2468
C	-9.6789	1.9014	-4.2579
C	-10.9329	1.5408	-7.6096
C	-10.1972	-2.1336	-7.6420
C	-9.6915	3.2047	-3.4444
C	-11.5088	2.5972	-8.5616
C	-10.3446	-3.3349	-8.5866
C	-8.3670	-3.1770	-3.3897
C	-12.8664	2.1122	-9.1017
H	-13.5747	1.9255	-8.2894
H	-13.2946	2.8694	-9.7691
H	-12.7504	1.1826	-9.6729
C	-10.5394	2.8714	-9.7213
H	-10.9450	3.6656	-10.3598
H	-9.5565	3.1764	-9.3522
H	-10.4047	1.9764	-10.3396
C	-11.6979	3.8795	-7.7191
H	-10.7392	4.2273	-7.3169
H	-12.1160	4.6779	-8.3439
H	-12.3812	3.7022	-6.8819
C	-9.6445	-3.0435	-9.9256
H	-8.5805	-2.8376	-9.7919
H	-9.7457	-3.9063	-10.5944
H	-10.0952	-2.1753	-10.4217
C	-9.6662	-4.5227	-7.8650
H	-10.1858	-4.7550	-6.9276
H	-9.6941	-5.4160	-8.5001
H	-8.6226	-4.2950	-7.6297
C	-11.8269	-3.6540	-8.8358
H	-12.3363	-2.8131	-9.3202
H	-11.9098	-4.5277	-9.4932
H	-12.3517	-3.8747	-7.9021
C	-8.6255	4.1795	-3.9614
H	-8.6372	5.0960	-3.3586
H	-7.6277	3.7417	-3.9099
H	-8.8162	4.4527	-5.0049
C	-11.0879	3.8473	-3.5658
H	-11.8674	3.1822	-3.1836
H	-11.1161	4.7819	-2.9927
H	-11.3225	4.0827	-4.6108
C	-9.4152	2.8282	-1.9728
H	-8.4397	2.3417	-1.8702
H	-9.4156	3.7303	-1.3490
H	-10.1828	2.1456	-1.5924
C	-8.2828	-2.6571	-1.9377
H	-7.8984	-3.4455	-1.2797
H	-7.6115	-1.7934	-1.8674
H	-9.2695	-2.3526	-1.5723
C	-9.3542	-4.3567	-3.4731
H	-9.4424	-4.7217	-4.5040
H	-8.9966	-5.1837	-2.8486
H	-10.3504	-4.0673	-3.1288
C	-6.9827	-3.6354	-3.8705
H	-6.6492	-4.4910	-3.2720
H	-7.0088	-3.9451	-4.9209
H	-6.2370	-2.8437	-3.7696

E-F-ts-Piv-Me-Me

Energy (POTENTIAL) = -3326.9517473 Eh

Atom	X	Y	Z
N	-6.6462	0.5266	-7.0522
N	-3.8008	-1.0589	-5.3309
N	-2.0284	1.0673	-5.7217
C	-5.4505	-0.2989	-6.9295
H	-4.9241	-0.3369	-7.8915
C	-5.6368	-1.7779	-6.5156
C	-6.2768	-2.7949	-7.2912
H	-7.0844	-2.4966	-7.9487
C	-5.9515	-4.1307	-7.1330
C	-4.8670	-4.4541	-6.2716
C	-4.1291	-3.5034	-5.5921
H	-3.2784	-3.7958	-4.9864
C	-4.4752	-2.1426	-5.7593
C	-2.5644	-1.0266	-4.5632
H	-2.7498	-0.5459	-3.5961
H	-2.2223	-2.0463	-4.3793
C	-1.4954	-0.2409	-5.3214
H	-1.1779	-0.8150	-6.2104
H	-0.6263	-0.1141	-4.6737
C	-1.0700	2.0519	-6.0704
C	-0.0881	2.4218	-5.1278
H	-0.0862	1.9527	-4.1480
C	0.8555	3.3995	-5.4214
H	1.5952	3.6636	-4.6678
C	0.8611	4.0680	-6.6578
C	1.8890	5.1336	-6.9574
H	2.9076	4.7231	-6.9528
H	1.7194	5.5899	-7.9386
H	1.8662	5.9346	-6.2072
C	-0.1201	3.7066	-7.5848
H	-0.1478	4.2012	-8.5536
C	-1.0654	2.7123	-7.3100
H	-1.7908	2.4571	-8.0746
C	-3.1808	0.9120	-6.6040
H	-3.5139	1.8801	-6.9619
H	-2.9246	0.3100	-7.4928
C	-4.3477	0.2069	-5.8724
C	-4.9180	1.0783	-4.7549
C	-5.2218	0.5418	-3.4977
H	-5.0800	-0.5182	-3.3182
C	-5.6783	1.3543	-2.4564
H	-5.8915	0.9133	-1.4862
C	-5.8489	2.7242	-2.6595
H	-6.1985	3.3606	-1.8512
C	-5.5851	3.2647	-3.9208
H	-5.7348	4.3257	-4.1021
C	-5.1319	2.4500	-4.9580
H	-4.9469	2.8939	-5.9288
S	-6.5658	1.6976	-8.1837
O	-7.3477	2.8739	-7.7512
O	-5.1537	1.9524	-8.5862
H	-4.5945	-5.5014	-6.1557
C	-6.6999	-5.2321	-7.8453
H	-7.2696	-5.8519	-7.1398
H	-7.4078	-4.8243	-8.5727
H	-6.0155	-5.9024	-8.3805
C	-7.3612	1.0492	-9.6743
H	-6.7901	0.1802	-10.0106
H	-8.3836	0.7647	-9.4352
H	-7.3422	1.8316	-10.4384
H	-6.7669	-1.7630	-5.5279
Rh	-10.9030	-0.9119	-5.7243
Rh	-8.7146	-0.0578	-6.4177
O	-9.8525	-2.1570	-4.4061
O	-7.8390	-1.4752	-5.0940
O	-9.7580	1.2610	-7.5731
O	-11.7813	0.4001	-7.0323
O	-10.7927	-2.2759	-7.2870
O	-8.8810	-1.3392	-8.0540
O	-10.9334	0.5629	-4.2915
O	-8.8396	1.2577	-4.8063
C	-8.6157	-2.1720	-4.2760
C	-9.9361	1.3450	-4.1636
C	-11.0284	1.2206	-7.6488
C	-9.9071	-2.0867	-8.1797
C	-10.0602	2.4629	-3.1176
C	-11.6937	2.3059	-8.5016
C	-10.1418	-2.7536	-9.5408
C	-8.0132	-2.8726	-3.0674
C	-12.9986	1.7734	-9.1161
H	-13.7035	1.4555	-8.3425
H	-13.4724	2.5616	-9.7126
H	-12.8055	0.9176	-9.7735
C	-10.7335	2.7830	-9.6046
H	-11.2050	3.5911	-10.1760
H	-9.7945	3.1491	-9.1812
H	-10.4965	1.9696	-10.3008
C	-12.0000	3.4709	-7.5305
H	-11.0806	3.8499	-7.0698
H	-12.4741	4.2934	-8.0787
H	-12.6814	3.1503	-6.7343

C	-8.8967	-2.6683	-10.4355
H	-8.0457	-3.1980	-9.9952
H	-9.1128	-3.1268	-11.4074
H	-8.5967	-1.6301	-10.6036
C	-10.5586	-4.2211	-9.3334
H	-11.4606	-4.2927	-8.7187
H	-10.7622	-4.6893	-10.3034
H	-9.7623	-4.7924	-8.8416
C	-11.3018	-1.9606	-10.1908
H	-11.0281	-0.9072	-10.3272
H	-11.5326	-2.3824	-11.1760
H	-12.2038	-2.0052	-9.5724
C	-9.3382	3.7227	-3.6254
H	-9.3926	4.5116	-2.8657
H	-8.2890	3.5180	-3.8423
H	-9.8065	4.0992	-4.5429
C	-11.5406	2.7815	-2.8492
H	-12.0759	1.9106	-2.4604
H	-11.6117	3.5888	-2.1107
H	-12.0468	3.1111	-3.7636
C	-9.3946	1.9452	-1.8231
H	-8.3462	1.6894	-1.9954
H	-9.4368	2.7225	-1.0505
H	-9.9132	1.0574	-1.4421
C	-8.0246	-1.7942	-1.9518
H	-7.5788	-2.2157	-1.0438
H	-7.4448	-0.9141	-2.2468
H	-9.0470	-1.4762	-1.7227
C	-8.9010	-4.0628	-2.6660
H	-8.9246	-4.8191	-3.4592
H	-8.4917	-4.5276	-1.7627
H	-9.9270	-3.7480	-2.4589
C	-6.5821	-3.3479	-3.3261
H	-6.2168	-3.8909	-2.4480
H	-6.5371	-4.0206	-4.1864
H	-5.9029	-2.5123	-3.5026

F-Piv-Me-Me

Energy (POTENTIAL) = -3326.9625413 Eh

Atom	X	Y	Z
N	-6.5958	0.4789	-7.1270
N	-3.6449	-1.0963	-5.5748
N	-1.9662	1.1070	-5.8560
C	-5.3599	-0.3123	-7.0804
H	-4.8641	-0.2662	-8.0592
C	-5.4747	-1.7995	-6.7629
C	-6.3066	-2.7647	-7.3146
H	-7.1194	-2.4527	-7.9584
C	-6.1184	-4.1325	-7.0275
C	-5.0318	-4.4918	-6.2209
C	-4.1543	-3.5440	-5.6799
H	-3.3229	-3.8609	-5.0584
C	-4.3781	-2.1887	-5.9567
C	-2.3995	-1.0818	-4.8352
H	-2.5564	-0.6944	-3.8187
H	-2.0141	-2.1012	-4.7543
C	-1.3746	-0.2018	-5.5527
H	-1.0548	-0.6986	-6.4865
H	-0.4959	-0.0821	-4.9168
C	-1.0723	2.1761	-6.0926
C	-0.1067	2.4994	-5.1151
H	-0.0686	1.9260	-4.1930
C	0.7717	3.5612	-5.2968
H	1.4986	3.7841	-4.5178
C	0.7257	4.3663	-6.4480
C	1.6756	5.5277	-6.6207
H	2.7229	5.1983	-6.5976
H	1.5098	6.0433	-7.5730
H	1.5580	6.2670	-5.8172
C	-0.2381	4.0502	-7.4095
H	-0.3038	4.6480	-8.3164
C	-1.1167	2.9734	-7.2492
H	-1.8283	2.7589	-8.0390
C	-3.1228	0.9697	-6.7373
H	-3.4925	1.9471	-7.0266
H	-2.8563	0.4361	-7.6656
C	-4.2441	0.1727	-6.0313
C	-4.8194	0.9616	-4.8511
C	-5.0809	0.3360	-3.6252
H	-4.9118	-0.7314	-3.5231
C	-5.5126	1.0703	-2.5164
H	-5.6839	0.5645	-1.5696
C	-5.7061	2.4485	-2.6201
H	-6.0308	3.0249	-1.7581
C	-5.4953	3.0761	-3.8507
H	-5.6642	4.1446	-3.9542
C	-5.0658	2.3394	-4.9542
H	-4.9211	2.8496	-5.8991
S	-6.5597	1.6991	-8.2122
O	-7.3677	2.8368	-7.7266
O	-5.1632	2.0152	-8.6238
H	-4.8665	-5.5429	-5.9924
C	-7.0821	-5.1635	-7.5685
H	-8.1092	-4.9634	-7.2344

H	-7.1011	-5.1724	-8.6660
H	-6.8166	-6.1729	-7.2354
C	-7.3468	1.0736	-9.7183
H	-6.7526	0.2286	-10.0761
H	-8.3605	0.7544	-9.4862
H	-7.3497	1.8735	-10.4640
H	-7.0199	-1.9294	-5.1479
Rh	-10.9242	-0.8779	-5.7530
Rh	-8.7008	-0.1090	-6.4712
O	-9.9752	-2.0830	-4.2896
O	-7.9721	-1.6657	-5.1229
O	-9.6951	1.2476	-7.5931
O	-11.7359	0.3829	-7.1326
O	-10.8086	-2.3262	-7.2415
O	-8.9463	-1.3725	-8.1046
O	-10.9370	0.6682	-4.4001
O	-8.7703	1.1768	-4.8277
C	-8.7588	-2.2252	-4.1801
C	-9.8799	1.3595	-4.2277
C	-10.9636	1.2125	-7.7115
C	-9.9553	-2.1508	-8.1693
C	-9.9403	2.4786	-3.1800
C	-11.5994	2.3158	-8.5608
C	-10.2088	-2.8648	-9.5019
C	-8.1228	-2.8994	-2.9820
C	-12.8906	1.7996	-9.2172
H	-13.6185	1.4755	-8.4679
H	-13.3420	2.6003	-9.8142
H	-12.6849	0.9527	-9.8821
C	-10.6107	2.8125	-9.6290
H	-11.0627	3.6425	-10.1842
H	-9.6763	3.1546	-9.1765
H	-10.3713	2.0177	-10.3451
C	-11.9249	3.4606	-7.5710
H	-11.0150	3.8280	-7.0830
H	-12.3851	4.2943	-8.1137
H	-12.6245	3.1249	-6.7974
C	-8.9458	-2.8852	-10.3759
H	-8.1345	-3.4398	-9.8934
H	-9.1699	-3.3752	-11.3304
H	-8.5870	-1.8732	-10.5841
C	-10.7097	-4.2973	-9.2479
H	-11.6171	-4.2997	-8.6374
H	-10.9346	-4.7837	-10.2041
H	-9.9484	-4.8959	-8.7349
C	-11.3136	-2.0333	-10.1999
H	-10.9803	-1.0027	-10.3710
H	-11.5526	-2.4800	-11.1720
H	-12.2267	-2.0056	-9.5963
C	-9.1742	3.7052	-3.7059
H	-9.1715	4.4941	-2.9445
H	-8.1421	3.4516	-3.9521
H	-9.6495	4.1051	-4.6099
C	-11.3983	2.8600	-2.8785
H	-11.9630	2.0123	-2.4794
H	-11.4154	3.6662	-2.1357
H	-11.9102	3.2155	-3.7795
C	-9.2689	1.9291	-1.9016
H	-8.2358	1.6316	-2.0967
H	-9.2647	2.7044	-1.1261
H	-9.8171	1.0624	-1.5133
C	-7.9730	-1.7662	-1.9323
H	-7.4833	-2.1763	-1.0425
H	-7.3595	-0.9478	-2.3194
H	-8.9491	-1.3653	-1.6419
C	-9.0682	-3.9954	-2.4629
H	-9.1973	-4.7885	-3.2077
H	-8.6366	-4.4383	-1.5596
H	-10.0522	-3.5896	-2.2135
C	-6.7477	-3.4908	-3.3230
H	-6.3609	-4.0183	-2.4458
H	-6.8073	-4.2046	-4.1500
H	-6.0117	-2.7213	-3.5791

G-Piv-Me-Me

Energy (POTENTIAL) = -3327.0229342 Eh

Atom	X	Y	Z
N	-5.4675	-0.7232	-5.9425
N	-2.5735	-2.7713	-5.0664
N	-0.8282	-0.6246	-4.7569
C	-4.3074	-1.5736	-6.0946
H	-3.8763	-1.3953	-7.0890
C	-4.6539	-3.0374	-5.9644
C	-5.8011	-3.7104	-6.3320
H	-6.6456	-3.1573	-6.7352
C	-5.8819	-5.1052	-6.1364
C	-4.7762	-5.7574	-5.5746
C	-3.6095	-5.0777	-5.1837
H	-2.7874	-5.6135	-4.7185
C	-3.5589	-3.6959	-5.3772
C	-1.3012	-3.0221	-4.4220
H	-1.3759	-2.9729	-3.3256
H	-0.9583	-4.0245	-4.6957
C	-0.2865	-1.9845	-4.9075

H	-0.0452	-2.1791	-5.9676
H	0.6328	-2.0842	-4.3289
C	0.1097	0.4352	-4.7349
C	1.1466	0.4211	-3.7781
H	1.2080	-0.4008	-3.0704
C	2.0676	1.4597	-3.7033
H	2.8502	1.4180	-2.9479
C	1.9983	2.5687	-4.5642
C	2.9924	3.7006	-4.4537
H	4.0261	3.3366	-4.5168
H	2.8483	4.4392	-5.2497
H	2.8983	4.2255	-3.4935
C	0.9650	2.5837	-5.5049
H	0.8803	3.4229	-6.1924
C	0.0419	1.5370	-5.6040
H	-0.7236	1.5891	-6.3706
C	-2.0382	-0.4447	-5.5539
H	-2.3846	0.5838	-5.4738
H	-1.8528	-0.6514	-6.6226
C	-3.1325	-1.4044	-5.0524
C	-3.6588	-0.9865	-3.6681
C	-3.8050	-1.9127	-2.6272
H	-3.5480	-2.9534	-2.7877
C	-4.2958	-1.5227	-1.3777
H	-4.3944	-2.2626	-0.5876
C	-4.6689	-0.1978	-1.1501
H	-5.0538	0.1066	-0.1805
C	-4.5506	0.7324	-2.1868
H	-4.8477	1.7662	-2.0307
C	-4.0509	0.3419	-3.4300
H	-3.9801	1.0808	-4.2204
S	-5.6748	0.6598	-6.7912
O	-6.9693	1.2170	-6.3057
O	-4.4762	1.5054	-6.7025
H	-4.8290	-6.8315	-5.4085
C	-7.1386	-5.8556	-6.5146
H	-8.0329	-5.2474	-6.3309
H	-7.1486	-6.1285	-7.5791
H	-7.2394	-6.7841	-5.9412
C	-5.8890	0.1886	-8.5094
H	-5.0007	-0.3512	-8.8463
H	-6.7821	-0.4338	-8.5740
H	-6.0074	1.1117	-9.0833
H	-6.2347	-1.0004	-5.3279
Rh	-10.9981	-1.2856	-5.8281
Rh	-8.9160	-0.1178	-6.1437
O	-10.0694	-2.3801	-4.3399
O	-8.0967	-1.3247	-4.6561
O	-9.8427	1.0126	-7.5917
O	-11.7994	-0.0862	-7.3112
O	-10.4129	-2.6137	-7.3029
O	-8.4567	-1.5251	-7.6175
O	-11.4827	0.1367	-4.4051
O	-9.5144	1.2108	-4.6982
C	-8.8654	-2.1311	-4.0232
C	-10.6504	1.0614	-4.1388
C	-11.0697	0.7976	-7.8638
C	-9.3403	-2.3871	-7.9474
C	-11.0286	2.1047	-3.0821
C	-11.7227	1.7259	-8.8938
C	-9.1530	-3.1228	-9.2795
C	-8.3094	-2.7814	-2.7527
C	-12.9904	1.0824	-9.4775
H	-13.7245	0.8630	-8.6970
H	-13.4492	1.7666	-10.2007
H	-12.7572	0.1452	-9.9962
C	-10.7227	2.0447	-10.0195
H	-11.1852	2.7260	-10.7431
H	-9.8191	2.5193	-9.6271
H	-10.4259	1.1332	-10.5524
C	-12.0892	3.0188	-8.1270
H	-11.1962	3.4931	-7.7057
H	-12.5700	3.7305	-8.8081
H	-12.7855	2.8053	-7.3073
C	-7.6672	-3.3381	-9.6083
H	-7.1800	-3.9747	-8.8631
H	-7.5801	-3.8332	-10.5825
H	-7.1212	-2.3925	-9.6591
C	-9.8919	-4.4704	-9.2662
H	-10.9591	-4.3389	-9.0685
H	-9.7780	-4.9604	-10.2402
H	-9.4823	-5.1388	-8.5003
C	-9.7904	-2.1800	-10.3323
H	-9.2770	-1.2121	-10.3526
H	-9.7137	-2.6317	-11.3280
H	-10.8500	-2.0044	-10.1141
C	-11.1963	3.4538	-3.8160
H	-11.4622	4.2369	-3.0962
H	-10.2689	3.7454	-4.3190
H	-11.9925	3.3977	-4.5685
C	-12.3365	1.7206	-2.3752
H	-12.2433	0.7571	-1.8627
H	-12.5865	2.4833	-1.6284
H	-13.1676	1.6473	-3.0834

C	-9.8784	2.1990	-2.0587
H	-8.9411	2.4893	-2.5421
H	-10.1225	2.9461	-1.2945
H	-9.7191	1.2373	-1.5561
C	-8.1050	-1.6297	-1.7408
H	-7.7175	-2.0315	-0.7976
H	-7.3930	-0.8926	-2.1217
H	-9.0543	-1.1212	-1.5315
C	-9.3007	-3.8088	-2.1873
H	-9.4938	-4.6127	-2.9059
H	-8.8811	-4.2564	-1.2787
H	-10.2586	-3.3454	-1.9315
C	-6.9655	-3.4625	-3.0603
H	-6.5439	-3.8746	-2.1365
H	-7.0909	-4.2844	-3.7721
H	-6.2444	-2.7585	-3.4773

2_Me-Me

Energy (POTENTIAL) = -769.6116649 Eh

Atom	X	Y	Z
N	-10.1346	3.9657	2.0620
C	-13.2012	2.8871	-0.6696
C	-13.4306	3.8103	0.3587
H	-14.4168	4.2587	0.4626
C	-12.4291	4.1846	1.2544
H	-12.6581	4.9120	2.0259
C	-11.1343	3.6328	1.1570
C	-10.8941	2.7056	0.1182
H	-9.9138	2.2537	0.0051
C	-11.9096	2.3493	-0.7666
H	-11.6876	1.6333	-1.5558
C	-10.2696	5.0853	2.9884
H	-11.1026	4.9286	3.6799
H	-10.4324	6.0373	2.4580
C	-8.9260	5.0769	3.7106
H	-8.6452	6.0762	4.0562
H	-8.9428	4.4009	4.5806
C	-8.7316	3.7628	1.7206
H	-8.5129	4.0687	0.6842
H	-8.4534	2.7004	1.8177
C	-6.6616	4.4086	2.9098
C	-6.0409	4.9054	4.0748
H	-6.6246	5.4255	4.8268
C	-4.6705	4.7389	4.2767
H	-4.2254	5.1372	5.1864
C	-3.8587	4.0731	3.3503
C	-4.4830	3.5770	2.1960
C	-5.8483	3.7341	1.9707
H	-6.2796	3.3452	1.0538
H	-3.8867	3.0546	1.4499
N	-8.0159	4.6023	2.6732
C	-14.2995	2.4677	-1.6188
H	-13.9178	2.3204	-2.6363
H	-14.7612	1.5195	-1.3092
H	-15.0980	3.2171	-1.6642
C	-2.3793	3.8755	3.5840
H	-2.0213	4.4855	4.4208
H	-2.1432	2.8278	3.8165
H	-1.7910	4.1444	2.6975

TS D'-E'-Piv-Me-Me

Energy (POTENTIAL) = -3326.95505059 Eh

N	-5.45145	0.89282	-8.2365
N	-4.1077	-0.5849	-5.18833
N	-1.9491	1.20811	-5.43261
C	-5.3202	0.22418	-7.07826
H	-6.22799	-0.02512	-6.53242
C	-4.64599	-1.62208	-7.23958
C	-5.39287	-2.63312	-7.91894
H	-5.56985	-2.4956	-8.98169
C	-5.80827	-3.7738	-7.26539
C	-5.42531	-3.9332	-5.89937
C	-4.74481	-2.96379	-5.18231
H	-4.53895	-3.10171	-4.12551
C	-4.42405	-1.75099	-5.82876
C	-3.16602	-0.4673	-4.07619
H	-3.55061	0.26457	-3.36042
H	-3.06973	-1.43232	-3.5748
C	-1.80565	-0.01186	-4.61756
H	-1.36509	-0.82856	-5.21656
H	-1.13955	0.18242	-3.77512
C	-0.73135	1.8732	-5.73548
C	0.08552	2.3338	-4.68274
H	-0.23636	2.1896	-3.6551
C	1.2811	2.99604	-4.94006
H	1.88356	3.34459	-4.1033
C	1.7179	3.24106	-6.25305
C	3.02153	3.95625	-6.51697
H	3.88267	3.34871	-6.20741
H	3.14398	4.18598	-7.58091
H	3.08057	4.89995	-5.95993
C	0.89934	2.79315	-7.29355
H	1.20651	2.95488	-8.32415
C	-0.30237	2.11939	-7.05048
H	-0.8915	1.7869	-7.89683
C	-2.86305	1.0021	-6.5643
H	-2.92204	1.90582	-7.16612

H	-2.50574	0.20571	-7.22203
C	-4.24597	0.62869	-6.02176
C	-4.9039	1.76209	-5.21544
C	-5.87559	1.44759	-4.25258
H	-6.08891	0.40481	-4.03515
C	-6.56358	2.45335	-3.57119
H	-7.3055	2.18649	-2.82311
C	-6.30241	3.79569	-3.85659
H	-6.83969	4.58203	-3.33331
C	-5.34739	4.11874	-4.8237
H	-5.13829	5.1589	-5.05871
C	-4.65396	3.112	-5.49851
H	-3.92265	3.39449	-6.24638
S	-7.02998	1.22468	-8.75642
O	-7.12348	2.68714	-8.92439
O	-7.39788	0.36606	-9.89639
H	-5.71687	-4.84745	-5.38644
C	-6.59425	-4.85963	-7.95786
H	-7.5701	-5.01263	-7.47877
H	-6.77142	-4.61078	-9.00923
H	-6.06485	-5.82036	-7.92154
C	-8.18462	0.8078	-7.41901
H	-8.20778	-0.26917	-7.23959
H	-7.94631	1.36429	-6.51024
H	-9.15235	1.13417	-7.80915
H	-3.83846	-1.19665	-7.82937
Rh	-3.91843	0.84643	-10.04916
Rh	-2.46626	0.90166	-12.00393
O	-2.49991	-0.46766	-9.21945
O	-1.1102	-0.28296	-10.98421
O	-3.92069	2.00108	-12.97766
O	-5.1862	2.0585	-11.10598
O	-4.77285	-0.86647	-10.84099
O	-3.39712	-0.83283	-12.63805
O	-2.97957	2.57437	-9.40609
O	-1.68851	2.68419	-11.26037
C	-1.45189	-0.78937	-9.87309
C	-2.19784	3.1846	-10.2065
C	-4.9739	2.31077	-12.33296
C	-4.32251	-1.34575	-11.92952
C	-1.93538	4.67062	-9.93435
C	-6.12656	2.98304	-13.08438
C	-4.91211	-2.68515	-12.39296
C	-0.53099	-1.84957	-9.24984
C	-7.18974	1.8761	-13.28426
H	-7.51923	1.47858	-12.31914
H	-8.05694	2.28519	-13.81659
H	-6.785	1.04695	-13.87844
C	-5.65915	3.5268	-14.4412
H	-6.50333	3.99586	-14.96053
H	-4.87321	4.28099	-14.31833
H	-5.26449	2.7291	-15.07809
C	-6.7093	4.11562	-12.21846
H	-5.96797	4.90926	-12.06219
H	-7.57585	4.55911	-12.724
H	-7.0208	3.74023	-11.23989
C	-4.69208	-2.87797	-13.90198
H	-3.62836	-2.87478	-14.15641
H	-5.11991	-3.83702	-14.21726
H	-5.18019	-2.08172	-14.47578
C	-4.16205	-3.78523	-11.6057
H	-4.29685	-3.66247	-10.52614
H	-4.54405	-4.77307	-11.89006
H	-3.08792	-3.76081	-11.82392
C	-6.41658	-2.73562	-12.07259
H	-6.95579	-1.93556	-12.59321
H	-6.83076	-3.69668	-12.40016
H	-6.60525	-2.62272	-11.00226
C	-0.49416	5.04697	-10.31412
H	-0.34446	6.12401	-10.17451
H	0.22991	4.52204	-9.6815
H	-0.28113	4.80042	-11.35809
C	-2.93598	5.41769	-10.85225
H	-3.96894	5.15092	-10.60157
H	-2.82043	6.50031	-10.7227
H	-2.76139	5.17378	-11.90589
C	-2.21592	5.02706	-8.46584
H	-1.55825	4.47156	-7.78957
H	-2.0404	6.09799	-8.3092
H	-3.25209	4.805	-8.19453
C	0.30303	-1.15788	-8.151
H	0.98151	-1.8854	-7.68963
H	0.90657	-0.34139	-8.56256
H	-0.33708	-0.74254	-7.3677
C	-1.3869	-2.97002	-8.62871
H	-2.04913	-3.42453	-9.37462
H	-0.73234	-3.75425	-8.2307
H	-2.00678	-2.59734	-7.80971
C	0.40151	-2.43799	-10.32116
H	1.04678	-3.19931	-9.86766
H	-0.16978	-2.91	-11.1283
H	1.0382	-1.6671	-10.7647

E'-Piv-Me-Me

Energy (POTENTIAL) = -3326.97485742 Eh

N	-5.12212	1.25162	-8.2875
N	-3.93117	-0.93701	-5.60383
N	-1.92006	0.96214	-5.33432
C	-5.23684	0.2769	-7.2187
H	-6.23238	0.28582	-6.76281
C	-5.00605	-1.1997	-7.63208
C	-6.14471	-1.93972	-8.23354

H	-6.75696	-1.40217	-8.94938
C	-6.34486	-3.24862	-7.94074
C	-5.42982	-3.9013	-7.01716
C	-4.47435	-3.25332	-6.2789
H	-3.8885	-3.77652	-5.53212
C	-4.41712	-1.83877	-6.42638
C	-2.96911	-1.11939	-4.51701
H	-3.38469	-0.66531	-3.61431
H	-2.80209	-2.18261	-4.34106
C	-1.66458	-0.4233	-4.92456
H	-1.19641	-0.99705	-5.74047
H	-0.9849	-0.44142	-4.07156
C	-0.81536	1.84665	-5.3225
C	-0.08785	2.03052	-4.12862
H	-0.38211	1.48903	-3.2339
C	0.98177	2.91704	-4.07342
H	1.52038	3.0382	-3.13549
C	1.3639	3.67799	-5.19142
C	2.52446	4.6412	-5.11294
H	3.46969	4.11608	-4.9206
H	2.64157	5.20358	-6.04544
H	2.39228	5.36577	-4.29898
C	0.63169	3.5009	-6.36879
H	0.8998	4.07103	-7.25495
C	-0.43426	2.59863	-6.44588
H	-0.95196	2.47731	-7.39046
C	-2.86666	1.06344	-6.44925
H	-3.01495	2.10599	-6.72724
H	-2.52219	0.53757	-7.34453
C	-4.21525	0.47324	-6.01666
C	-4.86248	1.21306	-4.84447
C	-5.92099	0.59966	-4.15471
H	-6.22442	-0.40948	-4.42123
C	-6.59788	1.26753	-3.13378
H	-7.416	0.77296	-2.61694
C	-6.22657	2.56827	-2.78313
H	-6.75423	3.09432	-1.99216
C	-5.16953	3.18419	-3.45571
H	-4.868	4.1938	-3.18983
C	-4.48864	2.51102	-4.47337
H	-3.67054	3.01489	-4.97391
S	-6.50046	2.11467	-8.49964
O	-6.22974	3.25213	-9.40137
O	-7.6669	1.24177	-8.81943
H	-5.55528	-4.97151	-6.86598
C	-7.45152	-4.07456	-8.54526
H	-8.06296	-4.54362	-7.76399
H	-8.10702	-3.46224	-9.17044
H	-7.04523	-4.88331	-9.16571
C	-6.92159	2.89877	-6.9143
H	-7.15715	2.16418	-6.14395
H	-6.08862	3.52783	-6.59885
H	-7.80265	3.51403	-7.11726
H	-4.18952	-1.21571	-8.37757
Rh	-3.9481	0.83731	-10.28911
Rh	-2.62408	0.64238	-12.33798
O	-2.36314	-0.13361	-9.31856
O	-1.16951	-0.33634	-11.22776
O	-4.161	1.57486	-13.35603
O	-5.43175	1.60524	-11.48402
O	-4.70065	-1.06287	-10.73204
O	-3.51773	-1.19172	-12.66026
O	-3.06566	2.69038	-10.03397
O	-1.83876	2.51066	-11.92851
C	-1.37622	-0.57241	-9.99924
C	-2.26607	3.14575	-10.91198
C	-5.23265	1.83101	-12.71631
C	-4.32817	-1.65482	-11.79917
C	-1.80937	4.5982	-10.71583
C	-6.39156	2.50314	-13.46292
C	-4.893	-3.06173	-12.04189
C	-0.3611	-1.44215	-9.24376
C	-7.68731	1.72466	-13.15837
H	-7.89813	1.71999	-12.08567
H	-8.53226	2.19009	-13.67993
H	-7.61126	0.68375	-13.49773
C	-6.13197	2.53191	-14.97512
H	-6.9674	3.02783	-15.48392
H	-5.21324	3.07717	-15.21278
H	-6.03701	1.51891	-15.38242
C	-6.50206	3.93923	-12.90364
H	-5.59553	4.51681	-13.12539
H	-7.35337	4.4554	-13.36446
H	-6.63909	3.91735	-11.81823
C	-4.48527	-3.58713	-13.42573
H	-3.39724	-3.64997	-13.52582
H	-4.90309	-4.59018	-13.57489
H	-4.86093	-2.93794	-14.22373
C	-4.31189	-3.97783	-10.94238
H	-4.58672	-3.61914	-9.94772
H	-4.69557	-4.99799	-11.06343
H	-3.21722	-4.01903	-11.00719
C	-6.42872	-2.99735	-11.93611
H	-6.84571	-2.34504	-12.71341
H	-6.85758	-3.99785	-12.06686
H	-6.73913	-2.60773	-10.96525
C	-0.82247	5.0201	-11.81343
H	-0.52068	6.06268	-11.65661
H	0.07889	4.39775	-11.80185
H	-1.27374	4.93961	-12.80753
C	-3.07493	5.48113	-10.76733
H	-3.79475	5.17564	-10.00216

H	-2.80688	6.53185	-10.60337
H	-3.56711	5.40231	-11.74465
C	-1.14168	4.71138	-9.33138
H	-0.27253	4.04648	-9.26324
H	-0.79671	5.73839	-9.16171
H	-1.84031	4.44613	-8.53336
C	0.42497	-0.51546	-8.29194
H	1.15614	-1.09916	-7.71975
H	0.96861	0.2561	-8.85022
H	-0.24004	-0.01368	-7.58569
C	-1.13454	-2.50126	-8.4326
H	-1.7303	-3.14634	-9.09007
H	-0.4318	-3.13495	-7.87881
H	-1.81345	-2.03152	-7.71714
C	0.6004	-2.13138	-10.2225
H	1.31062	-2.75333	-9.6647
H	0.0576	-2.7752	-10.9234
H	1.1681	-1.4007	-10.8065

4-Me-Me

Energy (POTENTIAL) = -1721.5273898 Eh

Atom	X	Y	Z
S	-6.5330	1.5136	-0.5323
O	-7.4602	1.0268	-1.5648
O	-5.7975	0.5481	0.2948
N	-9.7164	3.2414	0.9636
N	-7.4071	2.5400	0.4941
C	-11.0165	-0.3088	2.9335
C	-11.2507	0.9581	3.4828
H	-11.7690	1.0408	4.4362
C	-10.8260	2.1267	2.8515
H	-11.0162	3.0759	3.3386
C	-10.1499	2.0772	1.6155
C	-9.9174	0.8035	1.0539
H	-9.4069	0.7024	0.1034
C	-10.3446	-0.3524	1.7051
H	-10.1463	-1.3148	1.2374
C	-10.0784	4.5767	1.4371
H	-11.1034	4.5595	1.8180
H	-10.0851	5.2363	0.5647
C	-9.1292	5.1485	2.5108
H	-9.3241	6.2175	2.6499
H	-9.3139	4.6628	3.4721
C	-7.1975	3.6754	2.6518
C	-6.9893	2.6246	1.8271
H	-6.4797	1.7430	2.1963
C	-8.6772	3.1644	-0.0238
H	-8.4636	4.1736	-0.3748
H	-8.9675	2.5516	-0.8781
C	-6.9176	3.5739	4.1021
C	-6.2593	4.6445	6.1889
H	-5.9681	5.5419	6.7290
C	-6.5469	4.7222	4.8267
H	-6.4763	5.6738	4.3082
C	-7.0219	5.7073	1.2689
C	-7.6272	6.7968	0.6072
H	-8.6676	7.0436	0.7838
C	-6.8988	7.5866	-0.2842
H	-7.4037	8.4187	-0.7712
C	-5.5520	7.3368	-0.5713
C	-4.9535	6.2573	0.0953
C	-5.6592	5.4605	0.9923
H	-5.1522	4.6439	1.4935
C	-7.0265	2.3524	4.7940
H	-7.3792	1.4688	4.2699
C	-6.7269	2.2752	6.1544
H	-6.8185	1.3226	6.6701
C	-6.3409	3.4194	6.8588
H	-3.9040	6.0328	-0.0861
N	-7.7228	4.9169	2.1867
H	-6.1196	3.3601	7.9212
C	-5.3410	2.6058	-1.3136
H	-5.8792	3.3828	-1.8607
H	-4.7141	3.0464	-0.5363
H	-4.7388	2.0003	-1.9973
C	-11.4328	-1.5696	3.6537
H	-11.6071	-2.3942	2.9530
H	-10.6591	-1.9031	4.3597
H	-12.3517	-1.4173	4.2320
C	-4.7868	8.1701	-1.5722
H	-4.8794	7.7669	-2.5908
H	-5.1546	9.2024	-1.6007
H	-3.7171	8.1998	-1.3345

D-noRh

Energy (POTENTIAL) = -1721.5153267 Eh

Atom	X	Y	Z
N	-6.7843	5.6561	-4.4588
N	-3.4551	4.3846	-4.1895
N	-2.4283	7.0370	-3.7746
C	-5.5836	5.3907	-4.8014
H	-5.3038	5.1725	-5.8354
C	-3.6132	2.2533	-2.9133
C	-4.1124	0.9586	-2.7847
H	-3.8436	0.3719	-1.9086

C	-4.9699	0.4059	-3.7476
C	-5.2870	1.1928	-4.8613
C	-4.7699	2.4812	-5.0121
H	-4.9980	3.0397	-5.9134
C	-3.9427	3.0430	-4.0286
C	-2.1168	4.6223	-3.6336
H	-2.1163	4.6619	-2.5330
H	-1.4749	3.7930	-3.9438
C	-1.5527	5.9285	-4.1691
H	-1.4667	5.8746	-5.2686
H	-0.5541	6.0804	-3.7572
C	-1.8961	8.3470	-3.8633
C	-0.6791	8.6422	-3.2123
H	-0.1642	7.8631	-2.6579
C	-0.1414	9.9231	-3.2471
H	0.7975	10.1155	-2.7315
C	-0.7911	10.9775	-3.9120
C	-0.1991	12.3669	-3.9241
H	0.8238	12.3639	-4.3219
H	-0.7952	13.0510	-4.5376
H	-0.1448	12.7887	-2.9115
C	-2.0010	10.6841	-4.5458
H	-2.5326	11.4726	-5.0745
C	-2.5473	9.3956	-4.5341
H	-3.4775	9.2222	-5.0635
C	-3.7807	6.8422	-4.2730
H	-4.4300	7.6334	-3.8916
H	-3.8007	6.8908	-5.3759
C	-4.4133	5.4790	-3.8350
C	-4.8354	5.4352	-2.3589
C	-4.2613	6.2787	-1.3958
H	-3.5261	7.0157	-1.6949
C	-4.6101	6.1699	-0.0461
H	-4.1518	6.8381	0.6787
C	-5.5354	5.2117	0.3692
H	-5.8063	5.1270	1.4185
C	-6.1111	4.3619	-0.5791
H	-6.8345	3.6106	-0.2732
C	-5.7650	4.4720	-1.9259
H	-6.2292	3.8054	-2.6429
S	-7.9555	5.5448	-5.7203
O	-7.3289	5.3682	-7.0445
O	-8.9427	4.5532	-5.2676
H	-5.9323	0.7882	-5.6375
C	-5.5113	-0.9948	-3.5880
H	-4.7029	-1.7377	-3.5911
H	-6.0460	-1.1095	-2.6366
H	-6.2042	-1.2515	-4.3962
C	-8.6612	7.1888	-5.6177
H	-9.0246	7.3514	-4.6010
H	-7.8919	7.9186	-5.8805
H	-9.4869	7.2288	-6.3338
H	-2.9779	2.6546	-2.1311

3_Me-Me

Energy (POTENTIAL) = -1721.5487224 Eh

Atom	X	Y	Z
N	-7.1895	5.1067	-3.9620
H	-7.3207	5.0235	-2.9574
N	-3.6569	4.2312	-3.8593
N	-2.6969	6.8464	-3.8103
C	-5.8791	4.7704	-4.5014
H	-5.8535	5.1563	-5.5266
C	-5.6216	3.2758	-4.5242
C	-6.4647	2.2431	-4.8832
H	-7.4961	2.4585	-5.1553
C	-5.9866	0.9145	-4.8922
C	-4.6519	0.6927	-4.5318
C	-3.7841	1.7326	-4.1598
H	-2.7591	1.5196	-3.8718
C	-4.2825	3.0370	-4.1632
C	-2.3144	4.4422	-3.3672
H	-2.2990	4.5251	-2.2696
H	-1.6859	3.5953	-3.6558
C	-1.7576	5.7244	-3.9926
H	-1.5784	5.5526	-5.0685
H	-0.8017	5.9673	-3.5258
C	-2.1614	8.1435	-4.0081
C	-1.0745	8.5670	-3.2146
H	-0.6690	7.8947	-2.4638
C	-0.5354	9.8397	-3.3593
H	0.3011	10.1342	-2.7284
C	-1.0585	10.7600	-4.2844
C	-0.4696	12.1447	-4.4148
H	0.6015	12.1049	-4.6518
H	-0.9657	12.7185	-5.2048
H	-0.5673	12.7114	-3.4792
C	-2.1416	10.3410	-5.0615
H	-2.5704	11.0232	-5.7928
C	-2.6829	9.0560	-4.9395
H	-3.5038	8.7731	-5.5901
C	-4.0014	6.5602	-4.4021
H	-4.6479	7.4297	-4.2892
H	-3.9251	6.3415	-5.4808

C	-4.6223	5.3333	-3.7124
C	-4.9640	5.5878	-2.2310
C	-4.9908	4.5142	-1.3257
H	-4.7143	3.5201	-1.6600
C	-5.3648	4.7028	0.0068
H	-5.3746	3.8539	0.6854
C	-5.7209	5.9728	0.4655
H	-6.0097	6.1214	1.5025
C	-5.6974	7.0499	-0.4226
H	-5.9662	8.0463	-0.0815
C	-5.3252	6.8576	-1.7554
H	-5.3161	7.7166	-2.4163
S	-8.2341	6.1690	-4.6907
O	-8.1640	5.9181	-6.1374
O	-9.5032	6.0324	-3.9634
H	-4.2700	-0.3261	-4.5303
C	-6.9031	-0.2236	-5.2777
H	-7.7346	-0.3334	-4.5682
H	-7.3514	-0.0632	-6.2671
H	-6.3658	-1.1778	-5.3071
C	-7.6275	7.8392	-4.4114
H	-7.5546	8.0163	-3.3367
H	-6.6562	7.9524	-4.8962
H	-8.3504	8.5262	-4.8606

2_MeO-NO2

Energy (POTENTIAL) = -1010.0909183 Eh

Atom	X	Y	Z
N	-10.1116	3.6662	2.2621
C	-13.1056	2.4386	-0.4759
C	-13.4080	3.3470	0.5438
H	-14.4094	3.7466	0.6571
C	-12.4148	3.7653	1.4353
H	-12.6863	4.4757	2.2085
C	-11.0979	3.2830	1.3436
C	-10.8076	2.3668	0.3083
H	-9.8072	1.9619	0.1968
C	-11.7937	1.9552	-0.5806
H	-11.5583	1.2515	-1.3740
C	-10.2949	4.8522	3.0963
H	-11.1303	4.7217	3.7887
H	-10.4820	5.7540	2.4906
C	-8.9630	4.9517	3.8378
H	-8.6990	5.9896	4.0608
H	-8.9768	4.3838	4.7776
C	-8.7136	3.5866	1.8620
H	-8.5356	4.0157	0.8599
H	-8.3646	2.5457	1.8497
C	-6.6712	4.3639	3.0284
C	-6.0529	4.9997	4.1411
H	-6.6595	5.4759	4.9021
C	-4.6779	5.0100	4.2753
H	-4.2131	5.4919	5.1271
C	-3.8752	4.3868	3.3090
C	-4.4590	3.7519	2.2035
C	-5.8334	3.7381	2.0624
H	-6.2667	3.2522	1.1959
H	-3.8269	3.2770	1.4629
N	-8.0227	4.3590	2.8873
N	-2.4418	4.3999	3.4524
O	-1.7540	3.8393	2.5854
O	-1.9495	4.9719	4.4372
O	-13.9957	1.9719	-1.4051
C	-15.3352	2.4493	-1.3428
H	-15.3837	3.5392	-1.4716
H	-15.8654	1.9675	-2.1676
H	-15.8199	2.1748	-0.3959

A_-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4229785 Eh

Atom	X	Y	Z
S	-5.5820	2.0698	-0.2406
O	-6.9319	2.0213	-0.8297
O	-4.8250	0.8090	-0.0956
N	-10.1058	4.2810	1.7528
N	-5.7393	2.9021	1.2456
C	-13.1843	1.9021	0.2602
C	-13.4682	3.1904	0.7378
H	-14.4876	3.5564	0.7138
C	-12.4516	3.9829	1.2341
H	-12.6844	4.9780	1.5946
C	-11.1085	3.5091	1.2702
C	-10.8501	2.1956	0.7845
H	-9.8441	1.7975	0.8087
C	-11.8699	1.4112	0.2851
H	-11.6626	0.4129	-0.0800
C	-10.2868	5.5963	2.3717
H	-11.0630	5.5731	3.1451
H	-10.5661	6.3425	1.6172
C	-8.8863	5.8713	2.9603
H	-8.6245	6.9294	2.9575
H	-8.8255	5.4974	3.9879

C	-5.7763	2.7608	3.5954
C	-5.3723	2.2523	2.3019
H	-4.9006	1.2655	2.2602
C	-8.6920	3.8564	1.8792
H	-8.3326	3.3331	0.9958
H	-8.5850	3.1942	2.7479
C	-5.4558	4.0680	4.0498
C	-5.8905	5.9384	5.5513
H	-6.4667	6.3901	6.3530
C	-6.1883	4.6546	5.1207
H	-6.9995	4.0966	5.5679
C	-7.4134	5.7710	0.9913
C	-7.6933	5.4442	-0.3466
H	-8.3958	4.6559	-0.5912
C	-7.0653	6.1190	-1.3909
H	-7.2800	5.8575	-2.4231
C	-6.1549	7.1538	-1.1332
C	-5.8817	7.5022	0.1966
C	-6.5025	6.8074	1.2367
H	-6.2591	7.0601	2.2641
C	-4.4066	4.8186	3.4460
H	-3.8441	4.3860	2.6262
C	-4.0950	6.0882	3.9085
H	-3.2861	6.6505	3.4523
C	-4.8394	6.6504	4.9551
H	-5.1811	8.2942	0.4365
N	-7.9678	5.0871	2.1155
H	-4.5998	7.6503	5.3065
C	-4.5891	3.2568	-1.1476
H	-5.1128	4.2153	-1.1455
H	-3.6104	3.3381	-0.6690
H	-4.4875	2.8751	-2.1674
Rh	-6.6638	1.2903	4.6593
Rh	-7.4934	-0.5668	6.0484
O	-8.4316	2.2815	5.0770
O	-9.2051	0.5704	6.3431
O	-5.7194	-1.5716	5.6345
O	-4.9843	0.1255	4.3292
O	-7.5264	0.3544	3.0239
O	-8.2652	-1.3669	4.2958
O	-5.8458	2.0486	6.4051
O	-6.6378	0.3641	7.6970
C	-9.3086	1.7202	5.8259
C	-6.0209	1.4568	7.5257
C	-4.8947	-1.0502	4.8290
C	-8.0875	-0.7835	3.1836
C	-5.4350	2.1778	8.7471
C	-3.6944	-1.8752	4.3499
C	-8.6223	-1.4930	1.9334
C	-10.5853	2.5317	6.0789
N	-14.2451	1.0783	-0.2523
O	-15.4002	1.5342	-0.2635
O	-13.9675	-0.0595	-0.6645
O	-5.5978	7.7500	-2.2296
C	-4.6349	8.7769	-2.0167
H	-4.3141	9.0993	-3.0099
H	-5.0666	9.6341	-1.4831
H	-3.7640	8.4054	-1.4600
C	-3.5786	-3.1823	5.1467
H	-2.7207	-3.7592	4.7822
H	-3.4299	-2.9852	6.2139
H	-4.4777	-3.7961	5.0376
C	-2.4103	-1.0377	4.5078
H	-1.5478	-1.6108	4.1482
H	-2.4707	-0.1080	3.9344
H	-2.2332	-0.7816	5.5596
C	-3.9437	-2.1855	2.8555
H	-3.1106	-2.7748	2.4550
H	-4.8651	-2.7661	2.7251
H	-4.0333	-1.2670	2.2665
C	-8.1026	-0.8214	0.6553
H	-8.5010	-1.3449	-0.2220
H	-8.4001	0.2267	0.5923
H	-7.0094	-0.8482	0.6048
C	-8.1730	-2.9669	1.9716
H	-8.5335	-3.4695	2.8735
H	-8.5689	-3.4953	1.0965
H	-7.0794	-3.0454	1.9487
C	-10.1639	-1.4111	2.0026
H	-10.5035	-0.3705	2.0351
H	-10.6014	-1.8856	1.1163
H	-10.5442	-1.9242	2.8921
C	-3.9446	2.4667	8.4751
H	-3.8213	3.0945	7.5876
H	-3.5042	2.9873	9.3336
H	-3.3854	1.5361	8.3184
C	-5.5887	1.3209	10.0113
H	-5.1670	1.8557	10.8704
H	-6.6409	1.1061	10.2228
H	-5.0630	0.3655	9.9104
C	-6.2060	3.5066	8.9076
H	-7.2768	3.3254	9.0636
H	-5.8247	4.0539	9.7775
H	-6.0869	4.1378	8.0217

C	-10.1836	3.9209	6.6143
H	-9.5502	4.4522	5.8979
H	-11.0821	4.5223	6.7943
H	-9.6359	3.8366	7.5611
C	-11.4923	1.8182	7.0910
H	-12.3988	2.4133	7.2515
H	-11.7906	0.8285	6.7315
H	-10.9901	1.6908	8.0559
C	-11.3097	2.6805	4.7240
H	-11.5718	1.7022	4.3039
H	-12.2360	3.2519	4.8559
H	-10.6798	3.2030	4.0016

A-B-ts-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.423363 Eh

Atom	X	Y	Z
S	-5.2590	1.6955	-0.2305
O	-6.4522	1.2924	-0.9939
O	-4.3134	0.6478	0.2119
N	-10.1171	3.8941	1.6671
N	-5.8139	2.6584	1.0633
C	-13.4345	2.1199	-0.1266
C	-13.5849	3.3168	0.5895
H	-14.5651	3.7710	0.6728
C	-12.4872	3.9096	1.1824
H	-12.6169	4.8377	1.7267
C	-11.1947	3.3200	1.0788
C	-11.0693	2.1089	0.3395
H	-10.1046	1.6273	0.2417
C	-12.1714	1.5217	-0.2496
H	-12.0675	0.5960	-0.8028
C	-10.1598	5.0809	2.5251
H	-10.9397	5.0014	3.2894
H	-10.3420	5.9841	1.9291
C	-8.7480	5.0753	3.1382
H	-8.3957	6.0704	3.4021
H	-8.7180	4.4353	4.0204
C	-5.8953	2.9263	3.4572
C	-5.4036	2.3182	2.2366
H	-4.7166	1.4756	2.3895
C	-8.7463	3.3413	1.6429
H	-8.4575	2.9831	0.6594
H	-8.6583	2.5119	2.3507
C	-5.4070	4.1843	3.9175
C	-5.5382	6.0501	5.4800
H	-6.0179	6.5430	6.3204
C	-6.0137	4.8275	5.0310
H	-6.8614	4.3556	5.5095
C	-7.3580	5.3308	1.1276
C	-7.4994	5.1617	-0.2626
H	-8.1044	4.3602	-0.6691
C	-6.8670	6.0203	-1.1549
H	-6.9854	5.8838	-2.2260
C	-6.0761	7.0841	-0.6938
C	-5.9382	7.2741	0.6855
C	-6.5713	6.4032	1.5756
H	-6.4323	6.5600	2.6389
C	-4.3033	4.8196	3.2847
H	-3.8388	4.3512	2.4231
C	-3.8055	6.0228	3.7705
H	-2.9504	6.4898	3.2913
C	-4.4254	6.6416	4.8619
H	-5.3358	8.0823	1.0839
N	-7.9130	4.4438	2.0961
H	-4.0447	7.5895	5.2323
C	-4.3668	2.9419	-1.1643
H	-5.0410	3.7823	-1.3450
H	-3.4959	3.2596	-0.5862
H	-4.0570	2.4816	-2.1065
Rh	-6.7184	1.4509	4.6405
Rh	-7.3974	-0.4150	6.1049
O	-8.5223	2.3625	5.1244
O	-9.1578	0.6284	6.4362
O	-5.6142	-1.3655	5.6346
O	-5.0015	0.3427	4.2853
O	-7.6322	0.4433	3.0770
O	-8.2353	-1.2822	4.4156
O	-5.8440	2.2769	6.3275
O	-6.5034	0.5873	7.6851
C	-9.3582	1.7448	5.8750
C	-5.9302	1.6954	7.4624
C	-4.8460	-0.8239	4.7873
C	-8.1759	-0.6947	3.2933
C	-5.2891	2.4451	8.6381
C	-3.6477	-1.6155	4.2529
C	-8.8646	-1.3767	2.1049
C	-10.7284	2.4107	6.0564
N	-14.5811	1.5016	-0.7364
O	-15.6867	2.0543	-0.6201
O	-14.4228	0.4382	-1.3569
O	-5.4991	7.8630	-1.6550
C	-4.6731	8.9441	-1.2330
H	-4.3209	9.4273	-2.1470
H	-5.2347	9.6730	-0.6338

H	-3.8087	8.5896	-0.6559
C	-3.4154	-2.8832	5.0871
H	-2.5593	-3.4355	4.6824
H	-3.2007	-2.6375	6.1330
H	-4.2894	-3.5415	5.0672
C	-2.3929	-0.7220	4.2800
H	-1.5354	-1.2758	3.8803
H	-2.5351	0.1780	3.6749
H	-2.1512	-0.4135	5.3046
C	-3.9956	-1.9937	2.7935
H	-3.1799	-2.5857	2.3620
H	-4.9111	-2.5970	2.7521
H	-4.1433	-1.1046	2.1720
C	-8.3085	-0.8418	0.7776
H	-8.8311	-1.3164	-0.0615
H	-8.4281	0.2392	0.6928
H	-7.2396	-1.0582	0.6807
C	-8.6529	-2.8988	2.1894
H	-9.0532	-3.3069	3.1216
H	-9.1595	-3.3889	1.3498
H	-7.5868	-3.1512	2.1363
C	-10.3694	-1.0445	2.2352
H	-10.5412	0.0367	2.2112
H	-10.9225	-1.4941	1.4022
H	-10.7778	-1.4388	3.1723
C	-3.8213	2.7531	8.2769
H	-3.7573	3.3628	7.3708
H	-3.3432	3.2997	9.0984
H	-3.2553	1.8283	8.1098
C	-5.3536	1.6047	9.9210
H	-4.8874	2.1570	10.7454
H	-6.3878	1.3792	10.1996
H	-4.8221	0.6548	9.8006
C	-6.0716	3.7634	8.8259
H	-7.1299	3.5670	9.0384
H	-5.6544	4.3257	9.6695
H	-6.0089	4.3874	7.9295
C	-10.5308	3.8879	6.4483
H	-10.0006	4.4442	5.6719
H	-11.5066	4.3626	6.6029
H	-9.9595	3.9741	7.3810
C	-11.5455	1.6903	7.1389
H	-12.5237	2.1746	7.2410
H	-11.7073	0.6390	6.8837
H	-11.0409	1.7294	8.1105
C	-11.4503	2.3058	4.6933
H	-11.6433	1.2585	4.4327
H	-12.4132	2.8279	4.7367
H	-10.8495	2.7476	3.8958

B-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4429911 Eh

Atom	X	Y	Z
S	-4.7694	1.9298	0.3678
O	-5.0629	0.5093	0.0806
O	-3.4475	2.2494	0.9569
N	-10.1152	3.5235	1.7857
N	-6.0363	2.6122	1.2122
C	-12.5099	2.6430	-1.5176
C	-12.8784	3.6694	-0.6398
H	-13.7846	4.2339	-0.8234
C	-12.0848	3.9565	0.4563
H	-12.3868	4.7497	1.1298
C	-10.8937	3.2249	0.7004
C	-10.5511	2.1775	-0.1955
H	-9.6722	1.5695	-0.0240
C	-11.3466	1.8965	-1.2908
H	-11.0779	1.0967	-1.9702
C	-10.3587	4.6529	2.6859
H	-11.2501	4.5059	3.3041
H	-10.4706	5.5814	2.1157
C	-9.1004	4.6675	3.5502
H	-8.8425	5.6499	3.9287
H	-9.1642	3.9496	4.3633
C	-6.7002	3.6798	3.3005
C	-5.7731	3.0618	2.4200
H	-4.7688	2.9578	2.8343
C	-8.8171	2.9523	2.0559
H	-8.3145	2.5246	1.1992
H	-8.8404	2.2180	2.8547
C	-6.1678	4.7030	4.2596
C	-6.3328	5.9870	6.3258
H	-6.8426	6.1782	7.2665
C	-6.7944	4.9717	5.4905
H	-7.6272	4.3589	5.8112
C	-7.7305	5.1694	1.5481
C	-7.7912	4.8663	0.1834
H	-8.0808	3.8887	-0.1720
C	-7.4818	5.8383	-0.7588
H	-7.5308	5.6086	-1.8183
C	-7.1009	7.1292	-0.3605
C	-7.0543	7.4352	1.0058
C	-7.3735	6.4575	1.9490
H	-7.3252	6.7270	2.9955

C	-5.0238	5.4544	3.9284
H	-4.5302	5.2883	2.9753
C	-4.5332	6.4419	4.7856
H	-3.6472	7.0049	4.5040
C	-5.1980	6.7268	5.9800
H	-6.7751	8.4224	1.3530
N	-8.0231	4.1306	2.6055
H	-4.8305	7.5079	6.6402
C	-4.9128	2.8328	-1.1801
H	-5.9119	2.6752	-1.5913
H	-4.7375	3.8937	-0.9898
H	-4.1552	2.4343	-1.8605
Rh	-6.7661	1.5235	4.6060
Rh	-7.0107	-0.4763	5.9917
O	-8.6226	2.1149	5.3284
O	-8.7941	0.3250	6.6998
O	-5.2410	-1.1612	5.1863
O	-4.9361	0.7466	4.0065
O	-7.7147	0.4410	3.1165
O	-8.0578	-1.3631	4.4363
O	-5.7368	2.3790	6.1924
O	-5.9010	0.4983	7.4393
C	-9.2370	1.3967	6.1915
C	-5.4297	1.6537	7.1928
C	-4.5814	-0.4145	4.3940
C	-8.1829	-0.7227	3.3475
C	-4.3319	2.1733	8.1289
C	-3.2804	-0.9820	3.8144
C	-9.0127	-1.3478	2.2193
C	-10.6296	1.8907	6.6017
N	-13.3418	2.3455	-2.6605
O	-12.9967	1.4289	-3.4192
O	-14.3662	3.0201	-2.8365
O	-6.8114	7.9982	-1.3598
C	-6.4198	9.3280	-1.0126
H	-6.2446	9.8419	-1.9597
H	-7.2131	9.8469	-0.4601
H	-5.4958	9.3317	-0.4209
C	-3.0100	1.6255	7.5359
H	-2.1639	1.9385	8.1591
H	-3.0217	0.5302	7.4951
H	-2.8492	2.0077	6.5215
C	-4.5355	1.6313	9.5529
H	-3.7313	1.9924	10.2047
H	-5.4904	1.9719	9.9710
H	-4.5286	0.5380	9.5694
C	-4.3007	3.7084	8.1403
H	-5.2399	4.1196	8.5270
H	-3.4856	4.0562	8.7862
H	-4.1456	4.1118	7.1372
C	-8.3326	-1.0688	0.8662
H	-8.9528	-1.4623	0.0523
H	-8.1805	0.0010	0.7061
H	-7.3498	-1.5506	0.8138
C	-9.1719	-2.8605	2.4283
H	-9.6670	-3.0838	3.3779
H	-9.7760	-3.2826	1.6164
H	-8.1984	-3.3636	2.4262
C	-10.3971	-0.6600	2.2744
H	-11.0340	-1.0371	1.4659
H	-10.8991	-0.8637	3.2278
H	-10.3093	0.4248	2.1603
C	-2.6496	-1.9758	4.8040
H	-1.7240	-2.3808	4.3782
H	-2.4008	-1.4848	5.7525
H	-3.3234	-2.8097	5.0202
C	-3.6759	-1.7110	2.5077
H	-4.1324	-1.0213	1.7902
H	-2.7818	-2.1472	2.0456
H	-4.3841	-2.5233	2.7116
C	-2.2925	0.1550	3.5046
H	-2.0295	0.7046	4.4169
H	-1.3699	-0.2667	3.0872
H	-2.7076	0.8613	2.7822
C	-10.5053	3.3334	7.1334
H	-10.1161	4.0133	6.3697
H	-11.4908	3.6983	7.4455
H	-9.8368	3.3775	8.0019
C	-11.2354	0.9848	7.6828
H	-12.2333	1.3504	7.9515
H	-11.3304	-0.0470	7.3301
H	-10.6184	0.9773	8.5875
C	-11.5133	1.8653	5.3347
H	-11.6090	0.8459	4.9421
H	-12.5177	2.2338	5.5734
H	-11.0915	2.4929	4.5440

B_-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4471483 Eh

Atom	X	Y	Z
S	-5.9460	2.7510	1.2079
O	-5.3355	3.8795	0.4545
O	-7.1076	2.0844	0.5927
N	-9.2007	6.1402	3.9618

N	-6.4011	3.2882	2.7071
C	-13.1512	5.9755	2.6264
C	-12.8080	6.8148	3.6923
H	-13.5731	7.4085	4.1777
C	-11.4953	6.8727	4.1261
H	-11.2478	7.5171	4.9611
C	-10.4906	6.0890	3.5023
C	-10.8632	5.2508	2.4195
H	-10.1317	4.6225	1.9269
C	-12.1759	5.1981	1.9894
H	-12.4554	4.5484	1.1692
C	-8.7774	6.9284	5.1161
H	-9.2803	6.6174	6.0389
H	-8.9872	7.9886	4.9508
C	-7.2795	6.6258	5.2048
H	-6.6547	7.4715	5.4752
H	-7.0839	5.8011	5.8844
C	-5.6134	5.2817	3.9261
C	-5.4427	4.0827	3.3248
H	-4.4272	3.6906	3.4121
C	-8.1502	5.2442	3.5483
H	-8.1888	4.9767	2.5008
H	-8.0859	4.3481	4.1654
C	-4.5220	5.8512	4.7537
C	-2.9915	7.6189	5.4284
H	-2.6475	8.6450	5.3293
C	-4.0591	7.1762	4.6467
H	-4.5175	7.8586	3.9402
C	-6.7680	7.1448	2.7647
C	-6.9529	8.4961	3.0347
H	-7.1795	8.8604	4.0276
C	-6.8277	9.4390	2.0097
H	-6.9728	10.4860	2.2460
C	-6.5203	9.0215	0.7088
C	-6.3334	7.6518	0.4523
C	-6.4521	6.7193	1.4705
H	-6.2774	5.6721	1.2484
C	-3.8786	4.9890	5.6634
H	-4.2527	3.9772	5.7785
C	-2.7968	5.4291	6.4264
H	-2.3144	4.7428	7.1174
C	-2.3522	6.7487	6.3167
H	-6.0853	7.3346	-0.5556
N	-6.8932	6.0802	3.8299
H	-1.5171	7.0976	6.9180
C	-4.6184	1.5433	1.4029
H	-3.7733	2.0377	1.8859
H	-4.9794	0.7124	2.0035
H	-4.3308	1.2135	0.4010
Rh	-6.9421	1.6894	4.2998
Rh	-7.4261	-0.0752	5.9091
O	-8.9875	1.9706	4.1197
O	-9.4379	0.3166	5.6018
O	-5.3723	-0.3279	6.1086
O	-4.9306	1.3136	4.6105
O	-7.0118	0.2121	2.8725
O	-7.4663	-1.4371	4.3501
O	-6.9749	3.0448	5.9358
O	-7.3935	1.3541	7.3829
C	-9.7828	1.2494	4.8093
C	-7.2229	2.5788	7.1003
C	-4.5817	0.3973	5.4288
C	-7.2932	-0.9933	3.1721
C	-7.3771	3.5776	8.2585
C	-3.0715	0.1638	5.5709
C	-7.5102	-1.9477	1.9924
C	-11.2763	1.5791	4.6823
O	-6.3772	9.8474	-0.3553
C	-6.5388	11.2528	-0.1539
H	-6.3789	11.7131	-1.1307
H	-7.5501	11.4919	0.1984
H	-5.7999	11.6426	0.5574
N	-14.5257	5.9023	2.1865
O	-14.8052	5.1432	1.2485
O	-15.3690	6.6010	2.7663
C	-2.5383	-0.2719	4.1895
H	-2.7047	0.5074	3.4405
H	-1.4618	-0.4703	4.2504
H	-3.0344	-1.1888	3.8477
C	-2.4140	1.4945	5.9920
H	-2.8050	1.8375	6.9582
H	-1.3307	1.3592	6.0944
H	-2.5953	2.2773	5.2506
C	-2.7813	-0.9233	6.6150
H	-3.1622	-0.6394	7.6017
H	-3.2429	-1.8760	6.3367
H	-1.6987	-1.0765	6.6959
C	-6.5602	-1.5846	0.8376
H	-6.7441	-2.2508	-0.0138
H	-6.7103	-0.5509	0.5152
H	-5.5117	-1.7025	1.1381
C	-7.2986	-3.4057	2.4269
H	-7.9814	-3.6854	3.2345
H	-7.4788	-4.0729	1.5758

H	-6.2727	-3.5699	2.7774
C	-8.9771	-1.7314	1.5488
H	-9.2124	-2.3960	0.7090
H	-9.6729	-1.9538	2.3667
H	-9.1382	-0.6970	1.2267
C	-11.6480	1.6266	3.1871
H	-12.7041	1.8981	3.0740
H	-11.0430	2.3627	2.6529
H	-11.4957	0.6487	2.7141
C	-12.1358	0.5340	5.4070
H	-11.8901	0.4834	6.4722
H	-13.1953	0.7992	5.3103
H	-11.9930	-0.4644	4.9793
C	-11.4797	2.9687	5.3263
H	-12.5264	3.2794	5.2281
H	-11.2276	2.9469	6.3938
H	-10.8531	3.7197	4.8398
C	-6.1686	4.5302	8.2831
H	-6.0448	5.0655	7.3419
H	-6.2886	5.2664	9.0867
H	-5.2418	3.9745	8.4686
C	-7.4706	2.8453	9.6067
H	-7.6013	3.5784	10.4117
H	-8.3177	2.1537	9.6304
H	-6.5601	2.2719	9.8116
C	-8.6923	4.3467	8.0010
H	-9.5558	3.6771	8.0919
H	-8.8085	5.1548	8.7327
H	-8.7127	4.7770	6.9976

B-C-ts-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4326218 Eh

Atom	X	Y	Z
S	-5.7415	3.1645	1.4047
O	-5.1552	4.4183	0.8576
O	-6.8788	2.5808	0.6682
N	-9.4976	5.3923	4.4325
N	-6.2229	3.4126	2.9702
C	-12.2039	7.4708	1.9937
C	-12.4554	7.3554	3.3609
H	-13.3386	7.8085	3.7935
C	-11.5561	6.6529	4.1535
H	-11.7494	6.5479	5.2152
C	-10.4122	6.0797	3.5788
C	-10.1920	6.1760	2.1965
H	-9.3003	5.7632	1.7429
C	-11.0852	6.8803	1.4021
H	-10.9042	6.9932	0.3405
C	-9.1261	5.9336	5.7535
H	-9.4540	5.2479	6.5373
H	-9.6214	6.8904	5.9018
C	-7.5615	6.0644	5.7845
H	-7.2810	7.0149	6.2439
H	-7.1470	5.2627	6.3907
C	-5.6394	5.2963	4.4426
C	-5.3343	4.2039	3.6998
H	-4.2823	3.9123	3.7078
C	-8.6155	4.5027	4.0023
H	-8.6054	4.1722	2.9764
H	-8.1383	3.8701	4.7324
C	-4.6058	5.9400	5.2898
C	-3.5913	7.9183	6.2947
H	-3.5944	8.9953	6.4420
C	-4.5825	7.3317	5.5073
H	-5.3338	7.9634	5.0453
C	-7.1801	6.9863	3.5069
C	-7.9312	8.1176	3.8418
H	-8.2762	8.2870	4.8534
C	-8.2699	9.0734	2.8766
H	-8.8705	9.9251	3.1733
C	-7.8465	8.9090	1.5555
C	-7.0417	7.8017	1.2304
C	-6.7140	6.8552	2.1866
H	-6.1213	5.9975	1.8944
C	-3.6061	5.1603	5.9072
H	-3.6339	4.0802	5.8052
C	-2.6093	5.7502	6.6831
H	-1.8542	5.1225	7.1495
C	-2.5959	7.1335	6.8833
H	-6.7002	7.6869	0.2060
N	-6.9724	5.8994	4.4384
H	-1.8259	7.5925	7.4975
C	-4.3736	1.9837	1.3881
H	-3.5607	2.3921	1.9921
H	-4.7157	1.0322	1.7867
H	-4.0503	1.8833	0.3483
Rh	-6.6907	1.5068	4.1827
Rh	-7.1426	-0.5262	5.4546
O	-8.7479	1.7027	3.9627
O	-9.1608	-0.0586	5.3219
O	-5.0808	-0.8166	5.5014
O	-4.6809	1.1774	4.5037
O	-6.6712	0.2965	2.5173
O	-7.3103	-1.5458	3.6585

O	-6.7637	2.5405	6.0249
O	-6.9477	0.5967	7.1716
C	-9.5266	0.9268	4.6077
C	-6.7967	1.8549	7.1044
C	-4.3105	0.1072	5.0917
C	-7.0526	-0.9157	2.5860
C	-6.6682	2.6074	8.4389
C	-2.8079	-0.0218	5.3738
C	-7.2877	-1.6356	1.2529
C	-11.0244	1.2593	4.5693
N	-13.1218	8.2479	1.1638
O	-12.8228	8.4285	-0.0196
O	-14.1468	8.6916	1.6883
O	-8.1463	9.7479	0.5281
C	-9.0835	10.7968	0.7665
H	-9.2218	11.2982	-0.1937
H	-10.0476	10.3988	1.1093
H	-8.7039	11.5207	1.4991
C	-2.5265	0.8747	6.6030
H	-3.1049	0.5425	7.4734
H	-1.4621	0.8282	6.8624
H	-2.7843	1.9189	6.3946
C	-2.4337	-1.4777	5.6885
H	-2.6620	-2.1366	4.8430
H	-1.3589	-1.5453	5.8937
H	-2.9759	-1.8494	6.5628
C	-2.0029	0.4849	4.1633
H	-0.9296	0.4043	4.3724
H	-2.2193	-0.1091	3.2672
H	-2.2337	1.5305	3.9432
C	-7.0453	-3.1452	1.4087
H	-7.2308	-3.6510	0.4537
H	-6.0095	-3.3501	1.7050
H	-7.7063	-3.5801	2.1638
C	-8.7690	-1.3681	0.8936
H	-8.9555	-0.2942	0.7806
H	-9.0169	-1.8624	-0.0533
H	-9.4395	-1.7561	1.6694
C	-6.3731	-1.0535	0.1618
H	-6.5772	-1.5513	-0.7937
H	-6.5335	0.0212	0.0425
H	-5.3166	-1.2165	0.4076
C	-11.2832	2.1990	5.7709
H	-12.3436	2.4753	5.8058
H	-11.0242	1.7103	6.7170
H	-10.6946	3.1199	5.6843
C	-11.3857	1.9763	3.2579
H	-11.1601	1.3479	2.3888
H	-12.4582	2.2036	3.2463
H	-10.8359	2.9144	3.1474
C	-11.8571	-0.0250	4.7132
H	-12.9252	0.2217	4.6980
H	-11.6553	-0.7161	3.8862
H	-11.6353	-0.5439	5.6499
C	-5.5191	3.6255	8.3416
H	-5.6846	4.3483	7.5420
H	-5.4229	4.1727	9.2868
H	-4.5659	3.1223	8.1430
C	-6.3915	1.6248	9.5884
H	-6.2945	2.1813	10.5282
H	-7.2020	0.8990	9.7010
H	-5.4618	1.0702	9.4216
C	-8.0096	3.3278	8.6927
H	-8.8346	2.6089	8.7629
H	-7.9616	3.8841	9.6361
H	-8.2392	4.0343	7.8915

C-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4444489 Eh

Atom	X	Y	Z
S	-7.0386	2.8703	1.5443
O	-6.9043	4.1064	0.7286
O	-8.2207	2.0235	1.2793
N	-9.8422	5.0080	3.7136
N	-7.0729	3.2747	3.1600
C	-11.1221	7.5975	0.6782
C	-11.8310	7.5625	1.8806
H	-12.6742	8.2229	2.0380
C	-11.4241	6.6756	2.8687
H	-11.9614	6.6321	3.8096
C	-10.3117	5.8544	2.6435
C	-9.6365	5.8656	1.4220
H	-8.7559	5.2516	1.2663
C	-10.0460	6.7487	0.4281
H	-9.5063	6.8111	-0.5080
C	-9.6215	5.6086	5.0575
H	-10.1225	4.9810	5.7989
H	-10.0989	6.5838	5.0567
C	-8.1155	5.7043	5.4094
H	-8.0354	6.4292	6.2354
H	-7.7816	4.7397	5.7900
C	-6.0240	5.2659	4.1811
C	-5.9771	4.0711	3.5526
H	-4.9985	3.6093	3.4418

C	-9.4962	3.7738	3.5075
H	-9.6632	3.3163	2.5406
H	-9.2323	3.1521	4.3485
C	-4.8028	5.8157	4.8271
C	-3.4994	7.6933	5.6826
H	-3.4081	8.7631	5.8536
C	-4.6512	7.1936	5.0725
H	-5.4328	7.8835	4.7751
C	-7.4296	7.1433	3.4803
C	-8.2634	8.2060	3.8628
H	-8.6980	8.2314	4.8558
C	-8.5753	9.2443	2.9759
H	-9.2578	10.0213	3.3015
C	-8.0199	9.2615	1.6945
C	-7.1017	8.2583	1.3418
C	-6.8138	7.2178	2.2109
H	-6.1651	6.4132	1.8851
C	-3.7696	4.9557	5.2600
H	-3.8964	3.8820	5.1713
C	-2.6142	5.4583	5.8559
H	-1.8376	4.7690	6.1783
C	-2.4687	6.8327	6.0685
H	-6.6571	8.2853	0.3510
N	-7.2421	6.0119	4.2906
H	-1.5729	7.2250	6.5426
C	-5.5535	1.8979	1.2116
H	-4.6750	2.5078	1.4288
H	-5.5753	0.9986	1.8233
H	-5.5790	1.6499	0.1470
Rh	-6.8537	1.4698	4.6615
Rh	-6.5230	-0.3416	6.2620
O	-8.8830	1.3031	5.0489
O	-8.5817	-0.3663	6.5429
O	-4.4909	-0.1845	5.8941
O	-4.7994	1.4763	4.3888
O	-7.0389	0.0118	3.2204
O	-6.7432	-1.6793	4.6944
O	-6.7061	2.7919	6.2747
O	-6.3588	1.1017	7.7368
C	-9.3078	0.4492	5.8991
C	-6.5198	2.3277	7.4492
C	-4.0689	0.6701	5.0527
C	-6.9968	-1.2217	3.5354
C	-6.5479	3.3333	8.6092
C	-2.5504	0.7588	4.8540
C	-7.3651	-2.2212	2.4330
C	-10.8244	0.4315	6.1249
N	-11.4796	8.6008	-0.3264
O	-12.3228	9.4498	-0.0206
O	-10.9120	8.5604	-1.4188
O	-8.3061	10.1822	0.7236
C	-9.3253	11.1396	0.9882
H	-9.0379	11.8268	1.7956
H	-9.4530	11.7069	0.0636
H	-10.2779	10.6600	1.2490
C	-2.2042	1.6106	3.6227
H	-2.5567	2.6402	3.7302
H	-1.1163	1.6347	3.4891
H	-2.6502	1.1924	2.7134
C	-1.9738	1.4102	6.1322
H	-2.1894	0.7994	7.0152
H	-0.8861	1.5131	6.0393
H	-2.3978	2.4084	6.2945
C	-1.9845	-0.6645	4.6860
H	-2.4025	-1.1515	3.7963
H	-0.8956	-0.6204	4.5680
H	-2.2145	-1.2867	5.5553
C	-7.0133	-1.6483	1.0495
H	-7.3253	-2.3525	0.2692
H	-7.5106	-0.6900	0.8780
H	-5.9321	-1.4927	0.9508
C	-8.8968	-2.4151	2.5482
H	-9.2400	-3.1253	1.7866
H	-9.1696	-2.8100	3.5338
H	-9.4242	-1.4664	2.3971
C	-6.6454	-3.5597	2.6597
H	-6.9270	-4.2690	1.8726
H	-5.5567	-3.4323	2.6296
H	-6.9096	-3.9947	3.6276
C	-11.2660	1.8514	6.5399
H	-11.0626	2.5773	5.7465
H	-12.3429	1.8601	6.7435
H	-10.7446	2.1784	7.4481
C	-11.4890	0.0444	4.7859
H	-11.1768	-0.9570	4.4663
H	-12.5797	0.0419	4.8973
H	-11.2216	0.7529	3.9954
C	-11.2029	-0.5776	7.2174
H	-10.7271	-0.3271	8.1714
H	-12.2894	-0.5720	7.3636
H	-10.8977	-1.5925	6.9442
C	-5.6903	4.5603	8.2527
H	-6.0314	5.0358	7.3319
H	-5.7397	5.2962	9.0641

H	-4.6404	4.2793	8.1140
C	-6.0274	2.6884	9.9029
H	-6.0529	3.4259	10.7138
H	-6.6378	1.8301	10.1992
H	-4.9938	2.3446	9.7864
C	-8.0265	3.7470	8.7941
H	-8.6548	2.8732	9.0060
H	-8.1152	4.4417	9.6375
H	-8.4154	4.2429	7.8999

C-4-ts-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.440832 Eh

Atom	X	Y	Z
S	-7.1198	3.3596	1.5953
O	-6.9182	4.6702	0.9365
O	-8.3227	2.5898	1.2331
N	-9.5360	5.1670	4.1432
N	-7.1719	3.5704	3.2952
C	-11.3563	7.6902	1.3308
C	-11.9392	7.5375	2.5913
H	-12.8315	8.0935	2.8501
C	-11.3543	6.6665	3.4993
H	-11.8064	6.5314	4.4759
C	-10.1815	5.9708	3.1562
C	-9.6408	6.0996	1.8730
H	-8.7181	5.6019	1.6108
C	-10.2258	6.9652	0.9561
H	-9.7804	7.1140	-0.0194
C	-9.3438	5.7270	5.4987
H	-9.7833	5.0450	6.2335
H	-9.8894	6.6652	5.5484
C	-7.8478	5.9400	5.8343
H	-7.7822	6.6982	6.6290
H	-7.4437	5.0111	6.2349
C	-5.9128	5.4091	4.4389
C	-6.0147	4.2471	3.7636
H	-5.0974	3.6847	3.6174
C	-9.0473	3.9433	3.8876
H	-9.4489	3.4217	3.0299
H	-8.8578	3.3576	4.7718
C	-4.6122	5.7999	5.0467
C	-3.0713	7.5180	5.8281
H	-2.8437	8.5705	5.9771
C	-4.2950	7.1531	5.2655
H	-5.0033	7.9241	4.9818
C	-7.2878	7.3678	3.8561
C	-8.1706	8.3881	4.2480
H	-8.5946	8.3934	5.2453
C	-8.5526	9.4030	3.3627
H	-9.2693	10.1438	3.6989
C	-8.0268	9.4406	2.0690
C	-7.0664	8.4840	1.7040
C	-6.7028	7.4675	2.5747
H	-6.0153	6.7016	2.2383
C	-3.6791	4.8249	5.4547
H	-3.9323	3.7735	5.3677
C	-2.4547	5.1925	6.0116
H	-1.7547	4.4199	6.3194
C	-2.1415	6.5420	6.1980
H	-6.6424	8.5266	0.7047
N	-7.0294	6.2629	4.6785
H	-1.1904	6.8292	6.6385
C	-5.6451	2.3942	1.2174
H	-4.7618	2.9664	1.5034
H	-5.6933	1.4336	1.7238
H	-5.6649	2.2654	0.1314
Rh	-6.9553	1.4449	4.5001
Rh	-6.6589	-0.5513	5.8457
O	-8.9923	1.1863	4.7642
O	-8.7024	-0.5451	6.1880
O	-4.6327	-0.4164	5.4351
O	-4.8944	1.5242	4.3063
O	-7.0511	0.1912	2.8615
O	-6.9698	-1.6750	4.1354
O	-6.8792	2.5391	6.2739
O	-6.4115	0.6832	7.4819
C	-9.4244	0.2984	5.5719
C	-6.6129	1.9321	7.3665
C	-4.1840	0.5777	4.7830
C	-7.1113	-1.0726	3.0258
C	-6.5571	2.7868	8.6395
C	-2.6647	0.6646	4.5954
C	-7.4357	-1.8994	1.7775
C	-10.9438	0.2503	5.7662
N	-11.9112	8.6725	0.4050
O	-12.8474	9.3777	0.7973
O	-11.4113	8.7656	-0.7191
O	-8.3775	10.3422	1.1002
C	-9.4395	11.2456	1.3814
H	-9.1695	11.9551	2.1756
H	-9.6201	11.7968	0.4558
H	-10.3592	10.7206	1.6724
C	-11.4639	1.6858	5.9830
H	-11.2454	2.3231	5.1212

H	-12.5495	1.6686	6.1333
H	-11.0064	2.1403	6.8707
C	-11.5400	-0.3381	4.4673
H	-11.1742	-1.3573	4.2948
H	-12.6330	-0.3767	4.5445
H	-11.2754	0.2745	3.5991
C	-11.3134	-0.6335	6.9663
H	-10.8798	-0.2440	7.8943
H	-12.4032	-0.6589	7.0825
H	-10.9574	-1.6592	6.8319
C	-6.5735	-1.4060	0.5996
H	-6.8025	-1.9942	-0.2966
H	-6.7694	-0.3531	0.3802
H	-5.5043	-1.5212	0.8165
C	-8.9313	-1.6484	1.4734
H	-9.2314	-2.2209	0.5880
H	-9.5633	-1.9613	2.3134
H	-9.1168	-0.5867	1.2812
C	-7.1878	-3.3932	2.0304
H	-7.4334	-3.9649	1.1278
H	-6.1383	-3.5845	2.2806
H	-7.8048	-3.7671	2.8530
C	-2.1156	-0.7331	4.2536
H	-1.0268	-0.6842	4.1368
H	-2.3479	-1.4540	5.0422
H	-2.5419	-1.1049	3.3137
C	-2.3061	1.6585	3.4794
H	-2.6452	2.6710	3.7141
H	-1.2179	1.6845	3.3491
H	-2.7559	1.3606	2.5256
C	-2.0815	1.1441	5.9444
H	-0.9915	1.2323	5.8665
H	-2.4836	2.1243	6.2248
H	-2.3140	0.4356	6.7466
C	-5.5315	3.9191	8.4325
H	-5.7853	4.5442	7.5742
H	-5.4963	4.5546	9.3252
H	-4.5272	3.5117	8.2678
C	-6.1524	1.9327	9.8504
H	-6.1167	2.5627	10.7470
H	-6.8684	1.1238	10.0265
H	-5.1640	1.4837	9.7075
C	-7.9697	3.3705	8.8630
H	-8.7082	2.5688	8.9883
H	-7.9789	3.9848	9.7708
H	-8.2827	3.9956	8.0221

H-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4705662 Eh

Atom	X	Y	Z
S	-6.8593	3.7811	0.9192
O	-5.5299	4.2806	0.5445
O	-8.0179	4.0103	0.0419
N	-9.2176	5.1862	3.7196
N	-7.2266	4.4855	2.4167
C	-11.5314	8.0413	1.7033
C	-11.6081	7.9388	3.0971
H	-12.2487	8.6125	3.6530
C	-10.8525	6.9853	3.7543
H	-10.9154	6.9271	4.8338
C	-10.0040	6.1034	3.0380
C	-9.9746	6.2047	1.6256
H	-9.3134	5.5808	1.0399
C	-10.7193	7.1686	0.9696
H	-10.6510	7.2707	-0.1065
C	-8.7800	5.4606	5.0947
H	-8.2090	4.5927	5.4262
H	-9.6381	5.5469	5.7704
C	-7.9030	6.7327	5.2095
H	-8.5251	7.6241	5.2246
H	-7.3808	6.6960	6.1722
C	-6.0035	5.7427	4.1161
C	-6.1174	4.6827	3.2872
H	-5.3392	3.9310	3.2640
C	-8.5447	4.1250	3.0171
H	-9.1802	3.7586	2.2111
H	-8.3794	3.3108	3.7305
C	-4.9178	5.7977	5.1285
C	-3.3832	7.1099	6.4884
H	-3.0101	8.0804	6.8052
C	-4.4232	7.0409	5.5608
H	-4.8549	7.9512	5.1562
C	-7.1424	7.6361	2.9812
C	-8.0224	8.7317	3.0124
H	-8.5604	8.9881	3.9158
C	-8.2677	9.5162	1.8818
H	-8.9802	10.3295	1.9615
C	-7.6142	9.2429	0.6774
C	-6.6877	8.1930	0.6479
C	-6.4516	7.4102	1.7716
H	-5.7371	6.6024	1.6900
C	-4.3666	4.6273	5.6821
H	-4.7853	3.6651	5.4190
C	-3.3178	4.6981	6.5995

H	-2.9067	3.7807	7.0129
C	-2.8204	5.9397	7.0074
H	-6.1617	7.9835	-0.2792
N	-6.9224	6.8309	4.1277
H	-2.0117	5.9949	7.7311
C	-6.7434	2.0106	1.2107
H	-5.9551	1.8173	1.9384
H	-7.7034	1.6479	1.5824
H	-6.5092	1.5425	0.2506
Rh	-7.1917	1.3400	4.9335
Rh	-6.1233	-0.2668	6.3629
O	-8.9974	0.7970	5.7620
O	-7.9976	-0.7406	7.0838
O	-4.3102	0.2649	5.5251
O	-5.3119	1.7368	4.1390
O	-7.3710	-0.1515	3.5158
O	-6.3253	-1.6539	4.8449
O	-7.0105	2.7335	6.4609
O	-6.0022	1.2200	7.8013
C	-9.0219	-0.1237	6.6433
C	-6.5318	2.3574	7.5815
C	-4.2978	1.0740	4.5445
C	-6.8993	-1.3120	3.7609
C	-6.6623	3.2970	8.7850
C	-2.9897	1.1962	3.7576
C	-7.0905	-2.3759	2.6762
C	-10.3812	-0.5608	7.1964
N	-12.2584	9.0870	1.0246
O	-12.9982	9.8243	1.6913
O	-12.1081	9.2136	-0.2009
O	-7.7962	9.9282	-0.4938
C	-8.8237	10.9124	-0.5362
H	-8.6300	11.7362	0.1646
H	-8.8206	11.3063	-1.5554
H	-9.8094	10.4766	-0.3231
C	-11.4889	0.4101	6.7623
H	-11.5768	0.4568	5.6724
H	-12.4492	0.0743	7.1704
H	-11.2964	1.4233	7.1317
C	-10.2977	-0.6182	8.7343
H	-11.2619	-0.9406	9.1436
H	-9.5281	-1.3220	9.0637
H	-10.0624	0.3678	9.1531
C	-10.6572	-1.9711	6.6261
H	-11.6238	-2.3360	6.9922
H	-10.6936	-1.9521	5.5300
H	-9.8804	-2.6784	6.9337
C	-7.0237	4.7226	8.3455
H	-7.1092	5.3649	9.2297
H	-6.2542	5.1413	7.6907
H	-7.9784	4.7461	7.8129
C	-5.3462	3.3044	9.5842
H	-5.4641	3.9285	10.4774
H	-5.0681	2.2953	9.9017
H	-4.5273	3.7186	8.9860
C	-7.8015	2.7063	9.6508
H	-7.9577	3.3375	10.5332
H	-8.7429	2.6665	9.0889
H	-7.5556	1.6939	9.9869
C	-2.9477	2.4834	2.9208
H	-1.9975	2.5285	2.3765
H	-3.7554	2.5225	2.1850
H	-3.0163	3.3740	3.5536
C	-2.9592	-0.0387	2.8238
H	-2.0387	-0.0277	2.2293
H	-2.9891	-0.9697	3.4001
H	-3.8110	-0.0319	2.1328
C	-1.7938	1.1582	4.7261
H	-0.8593	1.2155	4.1566
H	-1.8221	2.0080	5.4185
H	-1.7846	0.2361	5.3138
C	-6.8433	-1.7473	1.2919
H	-6.9683	-2.5090	0.5139
H	-7.5446	-0.9327	1.0925
H	-5.8240	-1.3498	1.2165
C	-8.5579	-2.8518	2.7885
H	-8.7563	-3.6186	2.0307
H	-8.7557	-3.2871	3.7751
H	-9.2543	-2.0213	2.6293
C	-6.1347	-3.5576	2.8996
H	-6.2893	-4.3062	2.1141
H	-5.0885	-3.2340	2.8611
H	-6.3065	-4.0348	3.8688

H_-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4740178 Eh

Atom	X	Y	Z
S	-7.0249	3.1991	1.3050
O	-7.1893	2.0791	0.3312
O	-5.9069	3.1669	2.2514
N	-10.8998	3.3357	2.2338
N	-8.4371	3.3763	2.1770
C	-12.2863	0.2002	4.6570
C	-11.1078	0.0431	3.9193

H	-10.5616	-0.8906	3.9555
C	-10.6375	1.0919	3.1515
H	-9.7023	0.9548	2.6346
C	-11.3503	2.3137	3.0578
C	-12.5335	2.4491	3.8257
H	-13.1043	3.3684	3.8081
C	-12.9930	1.4064	4.6144
H	-13.8994	1.5208	5.1963
C	-11.4286	4.7009	2.3489
H	-12.5225	4.6864	2.3064
H	-11.0866	5.2403	1.4651
C	-10.9674	5.4331	3.6275
H	-11.3150	6.4709	3.5942
H	-11.4289	4.9664	4.5029
C	-9.0184	4.1750	4.3665
C	-8.3833	3.2708	3.5885
H	-7.8764	2.4088	4.0010
C	-9.7381	3.1440	1.4189
H	-9.7648	3.8623	0.5983
H	-9.7260	2.1382	1.0018
C	-9.2675	3.9315	5.8040
C	-9.7326	2.4176	7.6515
H	-9.9286	1.4102	8.0092
C	-9.5195	2.6362	6.2903
H	-9.5822	1.8082	5.5929
C	-8.6583	6.2803	3.1559
C	-9.0999	7.1692	2.1644
H	-10.1347	7.1749	1.8436
C	-8.2259	8.0834	1.5590
H	-8.6185	8.7502	0.7996
C	-6.8793	8.1225	1.9270
C	-6.4271	7.2396	2.9226
C	-7.2958	6.3431	3.5261
H	-6.9175	5.6753	4.2918
C	-9.2793	5.0085	6.7084
H	-9.1066	6.0139	6.3359
C	-9.4974	4.7885	8.0679
H	-9.4937	5.6287	8.7573
C	-9.7198	3.4921	8.5452
H	-5.3815	7.2730	3.2148
N	-9.5238	5.3951	3.8301
H	-9.8950	3.3234	9.6044
C	-6.9334	4.6757	0.2917
H	-7.8616	4.7814	-0.2739
H	-6.7736	5.5289	0.9508
H	-6.0902	4.5430	-0.3915
Rh	-7.4442	-0.2215	0.8207
Rh	-7.8532	-2.5788	1.1380
O	-9.4774	-0.0160	0.4579
O	-9.8726	-2.2029	0.8602
O	-5.8058	-2.8081	1.3469
O	-5.4332	-0.5930	1.0780
O	-7.2540	-0.5925	-1.1950
O	-7.6772	-2.7964	-0.9101
O	-7.5219	-0.0107	2.9068
O	-7.9324	-2.2153	3.1779
C	-10.2320	-1.0433	0.4797
C	-7.5828	-1.0707	3.6135
C	-5.0443	-1.7914	1.2719
C	-7.4008	-1.7814	-1.6277
C	-7.1654	-1.0154	5.0922
C	-3.5306	-2.0137	1.3690
C	-7.1706	-2.0310	-3.1224
C	-11.6590	-0.9058	-0.0642
C	-2.9094	-0.9169	2.2541
H	-1.8236	-1.0575	2.3105
H	-3.1100	0.0793	1.8504
H	-3.3110	-0.9580	3.2740
C	-2.9835	-1.9033	-0.0732
H	-1.8991	-2.0642	-0.0718
H	-3.4403	-2.6570	-0.7260
H	-3.1861	-0.9129	-0.4942
C	-3.2184	-3.4026	1.9464
H	-2.1324	-3.5420	2.0014
H	-3.6287	-3.5147	2.9563
H	-3.6359	-4.1985	1.3225
C	-5.7632	-2.6618	-3.2405
H	-5.5393	-2.8759	-4.2922
H	-4.9932	-1.9810	-2.8586
H	-5.7058	-3.5994	-2.6772
C	-8.2343	-3.0120	-3.6493
H	-9.2424	-2.5931	-3.5455
H	-8.0574	-3.2129	-4.7123
H	-8.2028	-3.9610	-3.1069
C	-7.2269	-0.7144	-3.9119
H	-7.0572	-0.9166	-4.9759
H	-8.2052	-0.2314	-3.8072
H	-6.4639	-0.0092	-3.5697
C	-11.6552	-1.6287	-1.4327
H	-11.3955	-2.6858	-1.3185
H	-12.6498	-1.5611	-1.8890
H	-10.9337	-1.1677	-2.1186
C	-12.0465	0.5669	-0.2585
H	-13.0571	0.6254	-0.6793

H	-12.0427	1.1080	0.6919
H	-11.3597	1.0735	-0.9434
C	-12.6475	-1.5969	0.8931
H	-12.6534	-1.1074	1.8731
H	-13.6612	-1.5430	0.4793
H	-12.3881	-2.6494	1.0381
C	-6.0694	-2.0895	5.2835
H	-5.7278	-2.0839	6.3249
H	-6.4461	-3.0876	5.0442
H	-5.2040	-1.8861	4.6406
C	-6.5990	0.3589	5.4709
H	-7.3656	1.1348	5.4346
H	-6.2156	0.3250	6.4975
H	-5.7814	0.6534	4.8054
C	-8.3861	-1.3547	5.9715
H	-8.0825	-1.3906	7.0243
H	-9.1696	-0.5959	5.8727
H	-8.8116	-2.3257	5.7005
N	-12.7665	-0.8888	5.4783
O	-13.8036	-0.7209	6.1340
O	-12.1184	-1.9442	5.4932
O	-5.9383	8.9606	1.3962
C	-6.3452	9.8459	0.3586
H	-5.4503	10.4010	0.0680
H	-6.7281	9.2984	-0.5135
H	-7.1104	10.5534	0.7052

4-MeO-NO2

Energy (POTENTIAL) = -1962.0048002 Eh

Atom	X	Y	Z
S	-6.3626	1.6660	-0.4658
O	-7.2444	1.1597	-1.5275
O	-5.5814	0.7242	0.3442
N	-9.6564	3.2056	1.0076
N	-7.3275	2.5840	0.5868
C	-11.0266	-0.3768	2.7006
C	-11.3646	0.8444	3.2939
H	-11.9695	0.8569	4.1924
C	-10.9099	2.0279	2.7400
H	-11.1640	2.9562	3.2349
C	-10.1070	2.0279	1.5694
C	-9.7743	0.7725	0.9936
H	-9.1665	0.7169	0.1000
C	-10.2299	-0.4091	1.5503
H	-9.9753	-1.3599	1.0976
C	-10.0886	4.5239	1.4851
H	-11.1278	4.4714	1.8174
H	-10.0733	5.1941	0.6221
C	-9.1955	5.0867	2.6074
H	-9.4442	6.1384	2.7856
H	-9.3893	4.5489	3.5392
C	-7.1890	3.7099	2.7617
C	-6.9192	2.6839	1.9235
H	-6.3638	1.8258	2.2822
C	-8.5765	3.1970	0.0457
H	-8.3852	4.2272	-0.2524
H	-8.8344	2.6188	-0.8425
C	-6.8991	3.6050	4.2106
C	-6.2818	4.6861	6.3039
H	-6.0338	5.5916	6.8520
C	-6.5844	4.7637	4.9449
H	-6.5678	5.7232	4.4368
C	-7.0868	5.7938	1.4436
C	-7.7301	6.8833	0.8151
H	-8.7835	7.0769	0.9798
C	-7.0299	7.7431	-0.0264
H	-7.5403	8.5757	-0.5022
C	-5.6668	7.5535	-0.2837
C	-5.0134	6.4816	0.3359
C	-5.7141	5.6224	1.1848
H	-5.1785	4.8073	1.6576
C	-6.9362	2.3717	4.8886
H	-7.2400	1.4750	4.3562
C	-6.6233	2.2956	6.2460
H	-6.6588	1.3338	6.7512
C	-6.2935	3.4512	6.9602
H	-3.9563	6.3019	0.1742
N	-7.7739	4.9299	2.3127
H	-6.0608	3.3919	8.0202
C	-5.2400	2.8711	-1.1807
H	-5.8265	3.6370	-1.6929
H	-4.6503	3.3115	-0.3748
H	-4.5952	2.3420	-1.8881
N	-11.4890	-1.6126	3.2896
O	-11.1610	-2.6808	2.7547
O	-12.1946	-1.5541	4.3066
O	-5.0800	8.4497	-1.1364
C	-3.6999	8.2769	-1.4372
H	-3.5085	7.3089	-1.9206
H	-3.4395	9.0807	-2.1298
H	-3.0742	8.3606	-0.5383

t-D-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4625573 Eh

Atom	X	Y	Z
S	-7.2298	3.4166	-1.4472
O	-8.0672	4.1342	-2.4294
O	-7.0369	1.9682	-1.6153
N	-12.2592	4.5665	1.8599
N	-7.8528	3.6131	0.1705
C	-13.4986	2.5248	5.3180
C	-13.0112	1.8078	4.2170
H	-12.9590	0.7267	4.2588
C	-12.6042	2.4821	3.0829
H	-12.2406	1.9015	2.2452
C	-12.6546	3.9002	3.0079
C	-13.1645	4.5964	4.1355
H	-13.2031	5.6777	4.1441
C	-13.5792	3.9201	5.2696
H	-13.9473	4.4675	6.1289
C	-12.3067	6.0263	1.7518
H	-13.1569	6.4337	2.2988
H	-12.4520	6.2655	0.6925
C	-10.9986	6.6359	2.2443
H	-10.9931	7.7026	2.0114
H	-10.9489	6.5409	3.3380
C	-9.7822	4.5462	1.4551
C	-8.9220	4.3109	0.2229
H	-9.3215	4.8047	-0.6693
C	-11.2168	4.0582	0.9838
H	-11.4122	4.4476	-0.0200
H	-11.2229	2.9732	0.9266
C	-9.4161	3.7345	2.7073
C	-9.1057	1.5658	3.7678
H	-8.9947	0.4897	3.6756
C	-9.2540	2.3421	2.6193
H	-9.2648	1.8543	1.6499
C	-8.6173	6.7589	1.6015
C	-8.5868	8.0198	0.9852
H	-9.4806	8.3938	0.4937
C	-7.4321	8.8051	0.9763
H	-7.4556	9.7750	0.4922
C	-6.2594	8.3197	1.5702
C	-6.2673	7.0508	2.1612
C	-7.4276	6.2851	2.1832
H	-7.3854	5.3163	2.6608
C	-9.3894	4.3256	3.9761
H	-9.4770	5.3995	4.0770
C	-9.2437	3.5498	5.1286
H	-9.2397	4.0333	6.1013
C	-9.1165	2.1647	5.0305
H	-5.3575	6.6562	2.5966
N	-9.8363	6.0125	1.5854
H	-9.0241	1.5581	5.9268
C	-5.6500	4.2454	-1.3399
H	-5.8148	5.2651	-0.9903
H	-5.0082	3.6938	-0.6574
H	-5.2403	4.2458	-2.3538
Rh	-4.9915	3.1242	2.2659
Rh	-2.8491	2.7720	3.3090
O	-5.6292	1.3944	3.2015
O	-3.6020	1.0390	4.1346
O	-2.1726	4.4863	2.3879
O	-4.1519	4.7954	1.3453
O	-4.3093	1.9979	0.6807
O	-2.2784	1.7037	1.6272
O	-5.5404	4.2377	3.9174
O	-3.5501	3.8586	4.9192
C	-4.8058	0.7059	3.8876
C	-4.7286	4.3420	4.8937
C	-2.9345	5.0942	1.5670
C	-3.1086	1.5687	0.6722
C	-5.2285	5.0391	6.1632
C	-2.3160	6.2790	0.8136
C	-2.6246	0.9076	-0.6213
C	-5.3199	-0.6059	4.4916
C	-4.0621	5.7446	6.8747
H	-4.4274	6.2278	7.7883
H	-3.2746	5.0370	7.1485
H	-3.6199	6.5170	6.2342
C	-6.3357	6.0505	5.8262
H	-7.1760	5.5677	5.3227
H	-6.7018	6.5118	6.7511
H	-5.9619	6.8463	5.1727
C	-5.7973	3.9142	7.0617
H	-5.0229	3.1795	7.3095
H	-6.1746	4.3444	7.9971
H	-6.6233	3.3940	6.5646
C	-4.1461	-1.5110	4.8971
H	-3.5084	-1.0294	5.6440
H	-4.5337	-2.4431	5.3245
H	-3.5230	-1.7651	4.0322
C	-6.2107	-1.3255	3.4616
H	-6.5995	-2.2546	3.8944
H	-7.0559	-0.7010	3.1616
H	-5.6413	-1.5824	2.5600
C	-6.1479	-0.2262	5.7397
H	-6.9832	0.4263	5.4723

H	-6.5499	-1.1329	6.2071
H	-5.5285	0.2938	6.4800
C	-0.9780	5.8162	0.2015
H	-0.5188	6.6451	-0.3499
H	-0.2794	5.4858	0.9756
H	-1.1306	4.9857	-0.4988
C	-3.2521	6.7780	-0.2965
H	-4.2221	7.0788	0.1030
H	-2.8000	7.6461	-0.7908
H	-3.4145	6.0026	-1.0530
C	-2.0623	7.4002	1.8458
H	-1.5711	8.2473	1.3522
H	-3.0020	7.7614	2.2750
H	-1.4123	7.0487	2.6536
C	-1.4533	-0.0449	-0.3362
H	-1.1143	-0.5016	-1.2733
H	-0.6083	0.4835	0.1146
H	-1.7550	-0.8486	0.3453
C	-3.7844	0.1493	-1.2913
H	-4.6285	0.8104	-1.5053
H	-3.4370	-0.2937	-2.2321
H	-4.1461	-0.6617	-0.6477
C	-2.1537	2.0673	-1.5326
H	-1.3289	2.6210	-1.0694
H	-1.8014	1.6656	-2.4898
H	-2.9712	2.7683	-1.7360
O	-5.0709	8.9936	1.6190
C	-4.9347	10.1858	0.8524
H	-3.8953	10.4998	0.9700
H	-5.1410	10.0050	-0.2106
H	-5.5944	10.9820	1.2212
N	-13.9083	1.8227	6.5088
O	-13.8051	0.5872	6.5321
O	-14.3474	2.4817	7.4632

t-D-E-ts-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4356007 Eh

Atom	X	Y	Z
N	-6.4287	0.5254	-7.7878
N	-3.3148	-1.0336	-6.7057
N	-2.0605	1.4828	-6.7345
C	-5.3089	-0.1936	-7.6044
H	-4.8035	-0.5075	-8.5195
C	-5.4664	-2.0038	-6.7571
C	-6.3291	-3.0124	-7.2628
H	-7.3979	-2.8675	-7.1746
C	-5.8204	-4.1749	-7.8067
C	-4.4156	-4.3874	-7.7834
C	-3.5387	-3.4192	-7.3172
H	-2.4731	-3.6135	-7.3558
C	-4.0407	-2.1793	-6.8646
C	-1.8533	-0.9722	-6.6215
H	-1.5373	-1.0330	-5.5728
H	-1.4264	-1.8238	-7.1540
C	-1.3239	0.3232	-7.2404
H	-1.4657	0.2993	-8.3258
H	-0.2544	0.4192	-7.0548
C	-1.7076	2.1245	-5.5607
C	-0.5340	1.7717	-4.8422
H	0.0933	0.9549	-5.1745
C	-0.1764	2.4348	-3.6815
H	0.7150	2.1440	-3.1389
C	-0.9786	3.4714	-3.1934
C	-2.1375	3.8498	-3.8847
H	-2.7529	4.6559	-3.5041
C	-2.4908	3.1940	-5.0471
H	-3.3902	3.5105	-5.5577
C	-3.4424	1.4056	-7.1952
H	-4.0094	2.3019	-6.9589
H	-3.4262	1.3150	-8.2854
C	-4.1676	0.1627	-6.5815
C	-4.5522	0.4587	-5.1313
C	-3.9264	-0.2134	-4.0722
H	-3.2352	-1.0229	-4.2740
C	-4.1792	0.1444	-2.7460
H	-3.6730	-0.3828	-1.9419
C	-5.0819	1.1690	-2.4590
H	-5.2837	1.4510	-1.4292
C	-5.7292	1.8249	-3.5092
H	-6.4502	2.6071	-3.2987
C	-5.4542	1.4866	-4.8327
H	-5.9573	2.0165	-5.6301
S	-6.6680	0.9102	-9.4396
O	-7.1843	2.2873	-9.4743
O	-5.4325	0.6293	-10.2122
H	-3.9993	-5.3163	-8.1567
C	-7.9081	-0.2283	-10.0676
H	-7.5323	-1.2435	-9.9299
H	-8.8404	-0.0805	-9.5315
H	-8.0225	-0.0033	-11.1315
H	-5.8708	-1.4634	-5.9036
Rh	-10.6401	0.3428	-5.3296
Rh	-8.5261	0.4353	-6.5249

O	-9.6764	-0.6964	-3.8381
O	-7.7211	-0.7162	-4.9687
O	-9.5568	1.4330	-8.0108
O	-11.5267	1.3345	-6.9108
O	-11.0109	-1.4598	-6.2837
O	-9.0628	-1.3590	-7.4265
O	-10.1769	2.1731	-4.4945
O	-8.2309	2.2916	-5.6395
C	-8.4836	-1.1016	-4.0246
C	-9.1292	2.7841	-4.8863
C	-10.8043	1.6616	-7.9041
C	-10.1809	-1.9025	-7.1381
C	-8.9777	4.2418	-4.4292
C	-11.4655	2.4443	-9.0446
C	-10.5450	-3.2145	-7.8483
C	-7.9688	-2.1372	-3.0139
C	-9.0299	4.2853	-2.8886
H	-8.9478	5.3229	-2.5444
H	-9.9716	3.8703	-2.5163
H	-8.2066	3.7148	-2.4431
C	-10.1762	5.0228	-5.0135
H	-10.1240	6.0715	-4.6980
H	-10.1649	4.9961	-6.1091
H	-11.1260	4.6027	-4.6687
C	-7.6676	4.8568	-4.9429
H	-6.7902	4.3281	-4.5600
H	-7.6218	4.8343	-6.0364
H	-7.6034	5.9016	-4.6171
C	-6.6208	-2.7269	-3.4464
H	-5.8564	-1.9536	-3.5418
H	-6.2825	-3.4516	-2.6961
H	-6.7048	-3.2469	-4.4061
C	-9.0173	-3.2660	-2.9194
H	-8.6728	-4.0298	-2.2124
H	-9.9833	-2.8847	-2.5767
H	-9.1653	-3.7469	-3.8943
C	-7.8321	-1.4306	-1.6484
H	-7.5059	-2.1519	-0.8894
H	-7.0901	-0.6263	-1.6963
H	-8.7885	-1.0032	-1.3300
C	-12.0630	-3.2459	-8.1074
H	-12.3323	-4.1835	-8.6074
H	-12.6277	-3.1766	-7.1738
H	-12.3703	-2.4146	-8.7535
C	-9.7861	-3.3481	-9.1794
H	-8.7060	-3.4099	-9.0298
H	-10.1069	-4.2645	-9.6889
H	-9.9973	-2.5005	-9.8409
C	-10.1540	-4.3675	-6.8946
H	-10.6740	-4.2762	-5.9347
H	-10.4326	-5.3272	-7.3460
H	-9.0748	-4.3861	-6.7094
C	-11.3318	3.9392	-8.6725
H	-11.7899	4.5578	-9.4534
H	-11.8353	4.1550	-7.7238
H	-10.2786	4.2272	-8.5805
C	-12.9495	2.0591	-9.1616
H	-13.4147	2.6264	-9.9762
H	-13.0629	0.9909	-9.3829
H	-13.4938	2.2724	-8.2373
C	-10.7370	2.1673	-10.3704
H	-10.8184	1.1095	-10.6486
H	-11.1927	2.7624	-11.1707
H	-9.6759	2.4201	-10.3014
N	-0.6171	4.1449	-1.9715
O	0.4124	3.7865	-1.3797
O	-1.3499	5.0564	-1.5592
O	-6.7278	-5.0792	-8.2842
C	-6.2540	-6.3184	-8.8054
H	-7.1441	-6.8623	-9.1286
H	-5.5909	-6.1679	-9.6674
H	-5.7314	-6.9067	-8.0396

D_-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4656726 Eh

Atom	X	Y	Z
S	-8.7621	4.9167	2.2049
O	-9.0111	6.3602	2.2426
O	-9.9137	4.0125	2.2229
N	-9.2502	7.0556	5.1242
N	-7.7388	4.3011	3.5007
C	-12.8076	4.8527	4.9422
C	-12.7689	6.1688	4.4653
H	-13.6672	6.6189	4.0600
C	-11.5929	6.8925	4.5315
H	-11.5939	7.9175	4.1830
C	-10.4072	6.3200	5.0665
C	-10.4746	4.9768	5.5295
H	-9.5916	4.4635	5.8876
C	-11.6533	4.2610	5.4726
H	-11.6819	3.2335	5.8124
C	-9.0827	8.3168	4.3902
H	-9.5172	9.1588	4.9480
H	-9.5884	8.2290	3.4302

C	-7.5813	8.5736	4.1552
H	-7.4685	9.2981	3.3507
H	-7.1303	9.0321	5.0465
C	-6.8550	6.3508	4.8800
C	-7.0538	4.9106	4.4008
H	-6.5285	4.2069	5.0416
C	-8.0758	6.6491	5.8466
H	-8.2679	5.7841	6.4770
H	-7.7602	7.4533	6.5194
C	-5.6003	6.4040	5.7898
C	-3.5261	7.4716	6.4685
H	-2.7733	8.2377	6.3035
C	-4.6243	7.3907	5.6084
H	-4.7131	8.0893	4.7840
C	-6.1192	7.1772	2.6477
C	-6.4297	7.8905	1.4760
H	-7.2725	8.5711	1.4620
C	-5.7078	7.7141	0.2941
H	-5.9950	8.2886	-0.5794
C	-4.6551	6.7916	0.2370
C	-4.3429	6.0617	1.3903
C	-5.0514	6.2556	2.5726
H	-4.7518	5.6797	3.4399
C	-5.4678	5.5219	6.8730
H	-6.2206	4.7619	7.0557
C	-4.3728	5.6016	7.7345
H	-4.2908	4.9006	8.5606
C	-3.3921	6.5753	7.5311
H	-3.5293	5.3435	1.3549
N	-6.8645	7.3458	3.8268
H	-2.5357	6.6375	8.1967
C	-7.7130	4.5311	0.8065
H	-6.8015	5.1250	0.8627
H	-7.4990	3.4623	0.8277
H	-8.2934	4.8011	-0.0810
Rh	-7.5121	2.0080	3.7121
Rh	-6.9605	-0.3090	4.1535
O	-9.4946	1.4325	3.6379
O	-8.9685	-0.7471	3.9516
O	-4.9688	0.2807	4.3100
O	-5.4903	2.4270	3.8292
O	-7.3140	1.5757	1.7028
O	-6.7269	-0.5682	2.1064
O	-7.6631	2.2900	5.7547
O	-7.2133	0.1118	6.1674
C	-9.7880	0.1963	3.7030
C	-7.4679	1.2999	6.5372
C	-4.6644	1.4989	4.1234
C	-6.9523	0.4095	1.3296
C	-7.4665	1.5879	8.0427
C	-3.1976	1.9280	4.2474
C	-6.7736	0.2144	-0.1804
C	-11.2386	-0.1800	3.3825
O	-3.8911	6.5350	-0.8679
C	-4.2009	7.2330	-2.0694
H	-4.0878	8.3189	-1.9489
H	-3.4855	6.8794	-2.8154
H	-5.2198	7.0121	-2.4150
N	-14.0394	4.1088	4.8946
O	-14.0749	2.9852	5.4198
O	-15.0215	4.6220	4.3363
C	-3.1201	3.0491	5.3052
H	-2.0822	3.3818	5.4220
H	-3.7268	3.9107	5.0144
H	-3.4750	2.6960	6.2809
C	-2.7541	2.4724	2.8721
H	-1.7152	2.8186	2.9255
H	-2.8134	1.6936	2.1019
H	-3.3834	3.3114	2.5598
C	-2.3117	0.7454	4.6619
H	-1.2697	1.0768	4.7406
H	-2.6171	0.3410	5.6327
H	-2.3597	-0.0650	3.9276
C	-8.1023	0.5845	-0.8730
H	-8.3847	1.6203	-0.6620
H	-8.0005	0.4667	-1.9582
H	-8.9174	-0.0665	-0.5348
C	-5.6524	1.1710	-0.6435
H	-4.7092	0.9520	-0.1281
H	-5.4858	1.0529	-1.7205
H	-5.9131	2.2160	-0.4475
C	-6.3943	-1.2375	-0.5030
H	-6.2734	-1.3537	-1.5864
H	-5.4532	-1.5200	-0.0203
H	-7.1686	-1.9352	-0.1674
C	-8.3640	2.7942	8.3652
H	-8.3426	2.9917	9.4432
H	-8.0306	3.6972	7.8468
H	-9.4032	2.6016	8.0748
C	-7.9474	0.3524	8.8222
H	-7.3157	-0.5169	8.6202
H	-7.9172	0.5603	9.8980
H	-8.9787	0.0942	8.5544
C	-5.9947	1.9016	8.4061

H	-5.6176	2.7535	7.8304
H	-5.9186	2.1452	9.4723
H	-5.3489	1.0399	8.2025
C	-12.1934	0.8467	4.0149
H	-11.9748	1.8578	3.6659
H	-13.2296	0.6050	3.7537
H	-12.1132	0.8401	5.1078
C	-11.5641	-1.5938	3.8863
H	-12.6043	-1.8401	3.6422
H	-10.9152	-2.3446	3.4258
H	-11.4442	-1.6639	4.9735
C	-11.3539	-0.1250	1.8404
H	-10.6647	-0.8361	1.3687
H	-12.3747	-0.3839	1.5350
H	-11.1243	0.8789	1.4686

D-MeO-NO2

Energy (POTENTIAL) = -1961.993306 Eh

Atom	X	Y	Z
N	-6.5680	5.4652	-4.5874
N	-3.1979	4.3711	-4.1395
N	-2.2928	7.0887	-3.8917
C	-5.3473	5.2229	-4.8678
H	-5.0212	4.9298	-5.8692
C	-3.4066	2.3227	-2.7317
C	-3.8485	1.0162	-2.5655
H	-3.6739	0.4831	-1.6355
C	-4.5521	0.3664	-3.5923
C	-4.7787	1.0393	-4.7999
C	-4.3045	2.3439	-4.9648
H	-4.4497	2.8352	-5.9213
C	-3.6352	3.0156	-3.9349
C	-1.9007	4.6957	-3.5383
H	-1.9515	4.8022	-2.4434
H	-1.2108	3.8787	-3.7663
C	-1.3592	5.9835	-4.1372
H	-1.2191	5.8583	-5.2223
H	-0.3899	6.1977	-3.6916
C	-1.8497	8.4001	-3.8459
C	-0.5654	8.7172	-3.3243
H	0.0889	7.9343	-2.9620
C	-0.1314	10.0256	-3.2284
H	0.8453	10.2499	-2.8169
C	-0.9643	11.0695	-3.6520
C	-2.2313	10.7931	-4.1731
H	-2.8628	11.6050	-4.5134
C	-2.6654	9.4815	-4.2727
H	-3.6374	9.3016	-4.7125
C	-3.6410	6.8020	-4.3717
H	-4.3311	7.5689	-4.0213
H	-3.6509	6.8101	-5.4728
C	-4.2149	5.4331	-3.8736
C	-4.6803	5.4585	-2.4105
C	-4.1543	6.3688	-1.4811
H	-3.4382	7.1173	-1.7968
C	-4.5329	6.3234	-0.1359
H	-4.1118	7.0430	0.5615
C	-5.4419	5.3629	0.3085
H	-5.7370	5.3273	1.3540
C	-5.9709	4.4478	-0.6056
H	-6.6814	3.6942	-0.2764
C	-5.5942	4.4944	-1.9478
H	-6.0218	3.7771	-2.6380
S	-7.6894	5.1982	-5.8727
O	-7.0082	4.9416	-7.1559
O	-8.6496	4.2046	-5.3700
H	-5.2976	0.5590	-5.6213
C	-8.4630	6.8130	-5.9277
H	-8.8745	7.0384	-4.9418
H	-7.7121	7.5519	-6.2173
H	-9.2586	6.7634	-6.6764
H	-2.8933	2.8125	-1.9114
N	-0.5103	12.4372	-3.5517
O	0.6246	12.6501	-3.1022
O	-1.2741	13.3416	-3.9173
O	-4.9586	-0.9048	-3.3214
C	-5.6865	-1.6089	-4.3257
H	-5.9131	-2.5883	-3.8990
H	-6.6249	-1.0973	-4.5763
H	-5.0899	-1.7415	-5.2375

E-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.4526439 Eh

Atom	X	Y	Z
N	-6.5288	0.3675	-7.4945
N	-3.4322	-1.2224	-6.2153
N	-1.8322	1.0155	-6.7508
C	-5.3581	-0.4746	-7.4228
H	-4.9336	-0.6721	-8.4154
C	-5.5802	-1.8571	-6.7606
C	-6.3824	-2.8888	-7.4474
H	-7.3288	-2.5866	-7.8765
C	-6.0153	-4.1963	-7.3867

C	-4.7879	-4.5673	-6.7160
C	-3.9038	-3.6491	-6.2069
H	-2.9683	-3.9750	-5.7676
C	-4.2181	-2.2720	-6.3582
C	-2.0466	-1.2217	-5.7321
H	-2.0404	-0.8671	-4.6969
H	-1.6537	-2.2387	-5.7612
C	-1.2040	-0.2934	-6.6112
H	-1.1187	-0.7264	-7.6145
H	-0.1961	-0.2071	-6.2048
C	-1.5079	2.0810	-5.9300
C	-0.6708	1.9244	-4.7957
H	-0.3139	0.9441	-4.5049
C	-0.3328	3.0068	-4.0009
H	0.2886	2.8697	-3.1241
C	-0.8190	4.2797	-4.3147
C	-1.6436	4.4674	-5.4328
H	-2.0057	5.4593	-5.6746
C	-1.9799	3.3880	-6.2255
H	-2.6030	3.5572	-7.0952
C	-3.1332	0.8962	-7.4109
H	-3.5636	1.8622	-7.6471
H	-2.9857	0.3826	-8.3645
C	-4.1252	0.0615	-6.5524
C	-4.5261	0.7951	-5.2717
C	-4.4924	0.1681	-4.0182
H	-4.2581	-0.8880	-3.9388
C	-4.7314	0.8886	-2.8453
H	-4.6821	0.3812	-1.8857
C	-5.0064	2.2549	-2.9081
H	-5.1618	2.8267	-1.9976
C	-5.0946	2.8782	-4.1551
H	-5.3264	3.9369	-4.2199
C	-4.8783	2.1522	-5.3254
H	-4.9640	2.6575	-6.2796
S	-6.5564	1.3287	-8.8160
O	-7.1957	2.6210	-8.4927
O	-5.2087	1.4061	-9.4530
H	-4.5289	-5.6172	-6.6317
C	-7.5942	0.4977	-10.0425
H	-7.1300	-0.4636	-10.2775
H	-8.5891	0.3530	-9.6275
H	-7.6308	1.1233	-10.9387
H	-6.1281	-1.6627	-5.8161
Rh	-10.8543	-0.4347	-5.5251
Rh	-8.6563	0.0048	-6.5075
O	-9.9179	-1.6480	-4.1339
O	-7.8914	-1.2946	-5.0641
O	-9.6512	1.2550	-7.8171
O	-11.6890	0.8195	-6.9366
O	-11.0504	-2.0268	-6.8438
O	-9.0851	-1.5374	-7.8483
O	-10.5676	1.2147	-4.3287
O	-8.4861	1.5645	-5.1476
C	-8.6608	-1.8101	-4.1875
C	-9.4841	1.8760	-4.4219
C	-10.9108	1.4084	-7.7544
C	-10.1747	-2.1920	-7.7492
C	-9.3594	3.1340	-3.5499
C	-11.5315	2.4452	-8.6992
C	-10.4619	-3.2819	-8.7926
C	-8.0090	-2.6362	-3.0709
C	-12.9300	1.9830	-9.1420
H	-13.5946	1.8444	-8.2845
H	-13.3747	2.7314	-9.8085
H	-12.8752	1.0327	-9.6871
C	-10.6291	2.6686	-9.9235
H	-11.0586	3.4524	-10.5591
H	-9.6204	2.9650	-9.6241
H	-10.5490	1.7542	-10.5233
C	-11.6369	3.7512	-7.8773
H	-10.6456	4.0906	-7.5548
H	-12.0879	4.5420	-8.4884
H	-12.2593	3.6055	-6.9874
C	-9.4483	-3.2368	-9.9464
H	-8.4367	-3.4747	-9.6062
H	-9.7291	-3.9772	-10.7049
H	-9.4288	-2.2506	-10.4222
C	-10.3776	-4.6444	-8.0696
H	-11.0952	-4.6962	-7.2444
H	-10.6038	-5.4528	-8.7756
H	-9.3700	-4.8140	-7.6730
C	-11.8863	-3.0580	-9.3400
H	-11.9675	-2.0834	-9.8378
H	-12.1282	-3.8353	-10.0743
H	-12.6289	-3.0934	-8.5379
C	-8.6102	4.2284	-4.3305
H	-8.4737	5.1120	-3.6954
H	-7.6302	3.8804	-4.6614
H	-9.1780	4.5330	-5.2181
C	-10.7493	3.6461	-3.1389
H	-11.2949	2.9022	-2.5512
H	-10.6397	4.5529	-2.5321
H	-11.3554	3.8949	-4.0174

C	-8.5602	2.7206	-2.2947
H	-7.5775	2.3302	-2.5698
H	-8.4178	3.5879	-1.6386
H	-9.0929	1.9472	-1.7282
C	-7.7362	-1.6449	-1.9157
H	-7.2512	-2.1680	-1.0828
H	-7.0781	-0.8324	-2.2434
H	-8.6698	-1.2045	-1.5483
C	-8.9695	-3.7430	-2.6036
H	-9.1918	-4.4428	-3.4182
H	-8.5101	-4.3083	-1.7843
H	-9.9152	-3.3258	-2.2476
C	-6.6883	-3.2566	-3.5536
H	-6.2661	-3.8895	-2.7643
H	-6.8432	-3.8758	-4.4441
H	-5.9527	-2.4866	-3.7979
O	-6.8435	-5.1142	-7.9704
C	-6.5672	-6.5073	-7.8282
H	-7.3886	-7.0207	-8.3316
H	-5.6218	-6.7859	-8.3111
H	-6.5474	-6.8103	-6.7736
N	-0.4782	5.4036	-3.4764
O	-0.9428	6.5166	-3.7625
O	0.2659	5.2120	-2.5031

C-D-ts-Piv-MeO-NO2

Energy (POTENTIAL) = -3567.430497 Eh

Atom	X	Y	Z
S	-8.2733	4.5433	2.0907
O	-8.6852	5.9631	2.1216
O	-9.3315	3.5630	1.7946
N	-9.3589	6.7306	4.9712
N	-7.5572	4.0354	3.5056
C	-12.9912	5.0130	3.7699
C	-12.8985	6.3987	3.8920
H	-13.7579	7.0260	3.6916
C	-11.6852	6.9548	4.2817
H	-11.6039	8.0298	4.3916
C	-10.5916	6.1198	4.5448
C	-10.6951	4.7317	4.4126
H	-9.8338	4.0885	4.5478
C	-11.9052	4.1763	4.0201
H	-11.9968	3.1098	3.8801
C	-8.9417	8.0005	4.2904
H	-9.4530	8.8364	4.7796
H	-9.2896	7.9042	3.2647
C	-7.4249	8.2178	4.3134
H	-7.2398	9.1510	3.7748
H	-7.0863	8.4005	5.3416
C	-6.3279	6.0366	4.5673
C	-6.7455	4.7338	4.3440
H	-6.3097	4.0429	5.0541
C	-8.6320	6.2022	5.9105
H	-8.9375	5.2626	6.3564
H	-7.8325	6.7623	6.3667
C	-5.3939	6.2934	5.6978
C	-3.6323	7.6585	6.7039
H	-2.9673	8.5161	6.6376
C	-4.5250	7.4034	5.6615
H	-4.5359	8.0596	4.7971
C	-5.9688	7.3166	2.5011
C	-6.5002	8.1117	1.4746
H	-7.4705	8.5796	1.6012
C	-5.8247	8.2844	0.2627
H	-6.2775	8.9049	-0.5027
C	-4.6022	7.6399	0.0389
C	-4.0667	6.8337	1.0538
C	-4.7314	6.6814	2.2653
H	-4.2906	6.0613	3.0385
C	-5.3532	5.4779	6.8505
H	-6.0325	4.6373	6.9397
C	-4.4549	5.7277	7.8857
H	-4.4473	5.0710	8.7522
C	-3.5844	6.8205	7.8207
H	-3.1159	6.3373	0.8813
N	-6.6379	7.1442	3.7265
H	-2.8884	7.0199	8.6308
C	-6.9910	4.3401	0.8463
H	-6.1476	4.9897	1.0793
H	-6.6964	3.2904	0.8596
H	-7.4256	4.6125	-0.1197
Rh	-7.3263	1.8259	3.8734
Rh	-6.8255	-0.4871	4.4502
O	-9.3410	1.3159	3.9570
O	-8.8533	-0.8695	4.3056
O	-4.8206	0.0689	4.5675
O	-5.2887	2.1735	3.8801
O	-7.2455	1.2595	1.8851
O	-6.6803	-0.8675	2.4154
O	-7.3828	2.2226	5.9131
O	-7.0512	0.0488	6.4452
C	-9.6621	0.0944	4.1190
C	-7.2575	1.2653	6.7461
C	-4.4921	1.2612	4.2794

C	-7.0056	0.0445	1.5906
C	-7.3025	1.6284	8.2373
C	-3.0303	1.6902	4.4634
C	-7.2186	-0.3726	0.1301
C	-11.1643	-0.2226	4.1028
C	-3.0006	2.6235	5.6958
H	-1.9734	2.9548	5.8892
H	-3.6234	3.5078	5.5322
H	-3.3662	2.1068	6.5916
C	-2.5715	2.4644	3.2130
H	-1.5364	2.8015	3.3427
H	-2.6124	1.8310	2.3182
H	-3.2027	3.3402	3.0391
C	-2.1224	0.4748	4.6969
H	-1.0856	0.8090	4.8226
H	-2.4159	-0.0788	5.5943
H	-2.1571	-0.2175	3.8483
C	-7.0294	0.8235	-0.8159
H	-7.2012	0.5052	-1.8512
H	-7.7301	1.6290	-0.5816
H	-6.0112	1.2247	-0.7489
C	-8.6847	-0.8652	0.0618
H	-8.9175	-1.2051	-0.9543
H	-8.8523	-1.6991	0.7529
H	-9.3778	-0.0570	0.3212
C	-6.2588	-1.5119	-0.2493
H	-5.2133	-1.1903	-0.1693
H	-6.3976	-2.3819	0.3984
H	-6.4407	-1.8197	-1.2859
C	-11.7891	0.4725	5.3323
H	-12.8747	0.3188	5.3402
H	-11.3791	0.0593	6.2626
H	-11.5904	1.5471	5.3262
C	-11.7617	0.3363	2.7954
H	-11.3632	-0.2050	1.9283
H	-12.8516	0.2201	2.7982
H	-11.5189	1.3935	2.6663
C	-11.4129	-1.7355	4.1837
H	-12.4917	-1.9315	4.1582
H	-10.9494	-2.2598	3.3413
H	-11.0088	-2.1595	5.1086
C	-5.8412	1.9116	8.6583
H	-5.8062	2.1914	9.7180
H	-5.2155	1.0233	8.5173
H	-5.4101	2.7298	8.0720
C	-8.1716	2.8777	8.4635
H	-9.2018	2.7062	8.1293
H	-8.1965	3.1212	9.5323
H	-7.7799	3.7453	7.9260
C	-7.8620	0.4492	9.0508
H	-7.8767	0.7081	10.1160
H	-8.8869	0.2088	8.7442
H	-7.2508	-0.4479	8.9215
N	-14.2641	4.4148	3.3566
O	-14.3309	3.1858	3.2867
O	-15.2054	5.1707	3.1056
O	-3.8645	7.7270	-1.1109
C	-4.3533	8.5577	-2.1575
H	-3.6146	8.4963	-2.9603
H	-5.3241	8.2090	-2.5352
H	-4.4468	9.6038	-1.8348

3-MeO-NO2

Energy (POTENTIAL) = -1962.0257581 Eh

Atom	X	Y	Z
N	-7.0551	5.2772	-4.3760
H	-7.2003	5.2810	-3.3714
N	-3.5361	4.2834	-4.5337
N	-2.5732	6.8509	-5.0158
C	-5.8173	4.7459	-4.9083
H	-5.8669	4.8644	-5.9966
C	-5.5917	3.2812	-4.5840
C	-6.4962	2.2446	-4.5075
H	-7.5617	2.4126	-4.6354
C	-6.0176	0.9410	-4.2551
C	-4.6455	0.7233	-4.0917
C	-3.7289	1.7905	-4.1621
H	-2.6702	1.6039	-4.0101
C	-4.2112	3.0718	-4.4108
C	-2.1221	4.5120	-4.3144
H	-1.8927	4.7283	-3.2599
H	-1.5667	3.6159	-4.6073
C	-1.6957	5.6903	-5.2003
H	-1.7832	5.3874	-6.2510
H	-0.6567	5.9677	-5.0226
C	-2.2244	7.9261	-4.2252
C	-1.1003	7.8853	-3.3584
H	-0.5253	6.9741	-3.2505
C	-0.7476	8.9802	-2.5895
H	0.0990	8.9254	-1.9157
C	-1.5034	10.1561	-2.6593
C	-2.6148	10.2309	-3.5107
H	-3.1832	11.1511	-3.5727
C	-2.9667	9.1383	-4.2780

H	-3.8118	9.2296	-4.9499
C	-3.9685	6.5327	-5.3345
H	-4.5949	7.4181	-5.2740
H	-4.0139	6.1633	-6.3647
C	-4.4772	5.4123	-4.3964
C	-4.6189	5.8882	-2.9373
C	-4.2729	5.0468	-1.8690
H	-3.8714	4.0595	-2.0659
C	-4.4385	5.4578	-0.5442
H	-4.1552	4.7873	0.2630
C	-4.9613	6.7200	-0.2573
H	-5.0850	7.0426	0.7729
C	-5.3254	7.5628	-1.3095
H	-5.7353	8.5483	-1.1048
C	-5.1590	7.1480	-2.6322
H	-5.4485	7.8258	-3.4262
S	-8.1811	6.1141	-5.2535
O	-8.0439	5.6890	-6.6539
O	-9.4547	5.9571	-4.5391
H	-4.2653	-0.2722	-3.8935
C	-7.7412	7.8562	-5.1744
H	-7.7354	8.1736	-4.1298
H	-6.7618	7.9997	-5.6341
H	-8.5018	8.4098	-5.7322
N	-1.1398	11.2927	-1.8511
O	-0.1482	11.2011	-1.1119
O	-1.8328	12.3187	-1.9269
O	-6.9794	-0.0332	-4.1896
C	-6.5587	-1.3719	-3.9593
H	-6.0514	-1.4778	-2.9905
H	-7.4684	-1.9771	-3.9544
H	-5.8917	-1.7308	-4.7552

15. References

1 (a) C. H. Yoder and J. J. Zuckerman, *Inorg. Chem.*, 1967, **6**, 103-107; (b) A. R. Katritzky, W. Fan and C. Fu, *J. Org. Chem.*, 1990, **55**, 3209-3213; (c) A. J. Arduengo, R. Krafczyk, R. Schmutzler, H. A. Craig, J. R. Goerlich, W. J. Marshall and M. Unverzagt, *Tetrahedron*, 1999, **55**, 14523-14534; (d) M. K. Denk, S. Gupta, J. Brownie, S. Tajammul and A. J. Lough, *Chem. Eur. J.*, 2001, **7**, 4477-4486.

2 L. S. Campbell-Verduyn, L. Mirfeizi, R. A. Dierckx, P. H. Elsinga and B. L. Feringa, *Chem. Commun.*, 2009, 2139-2141.

3 J. Raushel and V. V. Fokin, *Org. Lett.*, 2010, **12**, 4952-4955.

4 CrysalisPro Software system, Agilent Technologies UK Ltd., Oxford, UK.

5 G. M. Sheldrick, *Acta Crystallogr. A*, 2008, **64**, 112-122.

6 M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori and R. Spagna, *J. Appl. Crystallogr.*, 2005, **38**, 381-388.

7 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.

8 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Revision D.01 ed., Gaussian, Inc., Wallingford, CT, **2009**.

9 (a) A. D. Becke, *J. Chem. Phys*, 1993, **98**, 5648-5652; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789; (c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627; (d) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

10 (a) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654-3665; (b) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222; (c) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.

11 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283.

12 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.

13 R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650-654.

14 L. E. Roy, P. J. Hay and R. L. Martin, *J. Chem. Theory Comput.*, 2008, **4**, 1029-1031.