Guanidine Catalyzed Enantioselective Desymmetrization of *meso*-Aziridines

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Electronic Supplementary Information

General procedures and methods

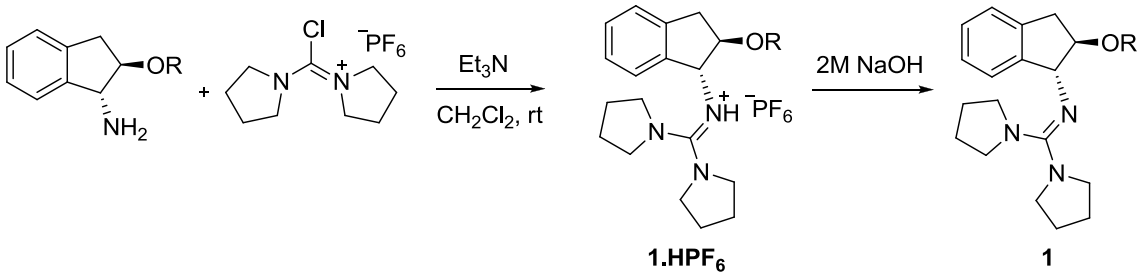
All reactions were performed in oven-dried round bottom flasks or glass vials. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen, unless otherwise noted. All solvent distillation was done at 760 Torr. Toluene, THF, diethyl ether and diisopropyl ether were distilled from sodium wire; CH_2Cl_2 was distilled from calcium hydride. Commercial reagents were purchased from Sigma Aldrich, Fluka, Alfa Aesar or Lancaster, and used as supplied without further purification. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25mm. Flash column chromatography was performed using Merck 60 (0.040 – 0.063 mm) mesh silica gel.

Instrumentation

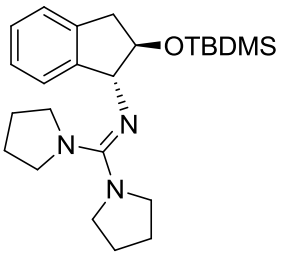
Proton nuclear magnetic resonance (^{1}H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AMX500 (500MHz) NMR spectrometer. The residual solvent peak was used as an internal reference. Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in ESI mode. High resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. Infrared spectra were recorded on a BIO-RAD FTS 165 FTIR spectrometer. Enantiomeric excesses were determined by chiral HPLC analysis on Jasco HPLC units, including a Jasco DG-980-50 Degasser, a LG-980-02 Ternary Gradient Unit, a PU-980 Intelligient HPLC Pump, UV-975 Intelligient UV/VIS Detectors, and an AS-950 Intelligient Sampler. Optical rotations were recorded on a Jasco DIP-1000 polarimeter. Melting points were determined on a BÜCHI B-540 melting point apparatus. Single crystal X-Ray diffraction studies were obtained on a Bruker-AXS Smart Apex CCD single-crystal diffractometer.

Preparation and characterization of the catalysts

General procedure for the synthesis of catalysts:

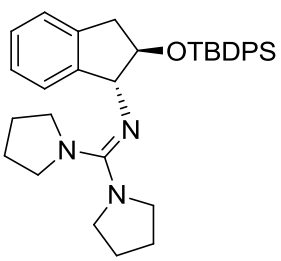


To a 10 mL flask containing O-protected 1-amino-2-indanol (1.1 mmol, 1.0 eq.) and 1-(Chloro-1-pyrrolidinylmethylene)pyrrolidinium hexafluorophosphate (366 mg, 1.1 mmol, 1.0 eq.) was added 5 mL of DCM, then Et_3N (0.77 mL, 5.5 mmol, 5.0 eq.). The reaction was stirred at room temperature for 36 hours and monitored by TLC (MeOH/DCM mixture 1/4). Most of the solvent was evaporated, and the residue was directly loaded onto a silica gel column, followed by flash column chromatography (MeOH/DCM mixture, 1/50 to 1/10). **1**·HPF_6 was obtained as white solid, and then it was dissolved in 5mL 2M NaOH, extracted three times with DCM, wash with brine, dried over Na_2SO_4, and concentrated to afford catalyst **1** as pale yellow oil.



(1a) (1R,2R)-2-(tert-butyldimethylsilyloxy)-N-(dipyrrolidin-1-ylmethylene)-2,3-dihydro-1H-inden-1-amine

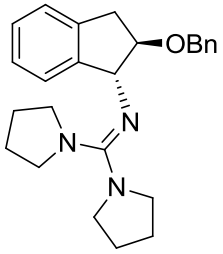
Pale yellow oil, 75% yield. $[\alpha]^{27}_D$ -112.4 (*c* 0.89, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 0.10 (d, 6H, *J* = 15.15 Hz), 0.90 (s, 9H), 1.86 (br, 8H), 2.79 (dd, 1H, *J* = 8.83, 15.10 Hz), 3.11 (dd, 1H, *J* = 6.95, 15.1 Hz), 3.31-3.39 (br, 8H), 4.42 (m, 1H), 4.74 (d, 1H, *J* = 7.55 Hz,), 7.09-7.13 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 18.9, 26.1, 26.6, 30.4, 40.0, 49.6, 70.3, 83.4, 124.5, 125.0, 127.3, 127.6, 139.9, 157.8. FTIR (film): 756, 1041, 1217, 1525, 3021 cm^{-1}. LRMS (ESI) m/z 414.2 ($M+H^+$), HRMS (ESI) m/z 414.2948 ($M+H^+$), calc. for $C_{24}H_{40}N_3OSi$ 414.2935



(1b) (1R,2R)-2-(tert-butyldiphenylsilyloxy)-N-(dipyrrolidin-1-ylmethylene)-2,3-dihydro-1H-inden-1-amine

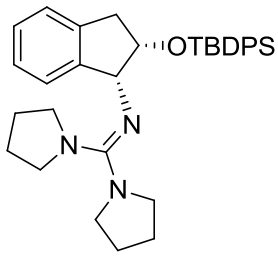
Pale yellow oil, 80% yield. $[\alpha]^{26}_D$ -92.6 (*c* 2.69, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.09 (d, 9H, *J* = 2.55 Hz), 1.87 (br, 8H), 2.70-2.80 (m, 2H), 3.33-3.40 (br, 8H), 4.58 (m, 1H), 4.98 (d, 1H, *J*

= 6.95 Hz), 6.98 (d, 1H, *J* = 6.95 Hz), 7.07-7.13 (m, 3H), 7.33-7.43 (m, 6H), 7.71-7.76 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 19.9, 26.1, 27.7, 39.8, 49.3, 70.4, 84.2, 124.5, 125.0, 127.2, 127.6, 128.0, 128.2, 130.0, 130.2, 134.9, 135.3, 136.5, 136.6, 139.9, 157.6. FTIR (film): 757, 1109, 1216, 1423, 1582, 3020 cm^{-1}. LRMS (ESI) m/z 538.3 ($M+H^+$), HRMS (ESI) m/z 538.3267 ($M+H^+$), calc. for calc. for $C_{34}H_{44}N_3OSi$ 538.3248



(1c) (1R,2R)-2-(benzyloxy)-N-(dipyrrolidin-1-ylmethylene)-2,3-dihydro-1H-inden-1-amine

Yellow oil, 75% yield. $[\alpha]^{27}_D$ -119.0 (*c* 1.25, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.80-1.88 (m, 8H), 2.90 (dd, *J* = 8.8, 15.15 Hz, 1H), 3.22 (dd, *J* = 6.95, 15.15 Hz, 1H), 3.27-3.42 (m, 8H), 4.29 (dd, 1H, *J* = 7.55, 15.75 Hz), 4.70 (dd, 2H, *J* = 11.95, 23.35 Hz), 5.01 (d, 1H, *J* = 6.9 Hz,), 7.11–7.17 (m, 4H), 7.25-7.27 (m, 1H), 7.31-7.37 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 26.1, 37.3, 49.2, 69.2, 72.7, 90.2, 124.6, 125.1, 127.3, 127.6, 128.0, 128.3, 128.9, 139.8, 139.9, 145.2, 157.5. FTIR (film): 758, 929, 1047, 1216, 1422, 1525, 3020 cm^{-1}. LRMS (ESI) m/z 390.2 ($M+H^+$), HRMS (ESI) m/z 390.2533 ($M+H^+$), calc. for $C_{25}H_{32}N_3O$ 390.2540

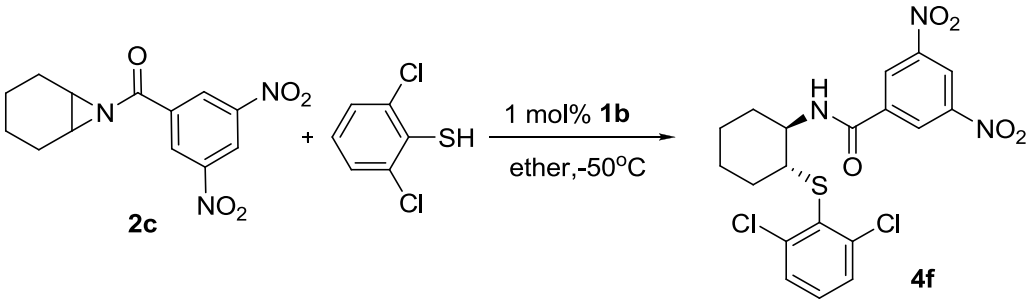


(1d) (1R,2S)-2-(tert-butyldiphenylsilyloxy)-N-(dipyrrolidin-1-ylmethylene)-2,3-dihydro-1H-inden-1-amine

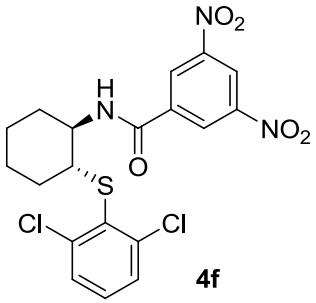
Yellow oil, 70% yield. $[\alpha]^{27}_D$ +7.9 (*c* 1.31, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.04 (s, 9H), 1.83 (br, 8H), 2.66 (d, 1H, *J* = 11.3 Hz), 3.12 (dd, 1H, *J* = 6.35, 14.45 Hz), 3.27-3.38 (br, 8H), 4.48 (br, 1H), 4.81 (d, 1H, *J* = 5.05 Hz), 7.07 (t, 1H, *J* = 4.1 Hz), 7.12 (s, 2H), 7.21-7.23 (m, 1H), 7.34 (t, 4H, *J* = 7.25 Hz), 7.38-7.42 (m, 2H), 7.66-7.71 (m, 4H). FTIR (film): 760, 928, 1045, 1215, 1427, 1521, 3019 cm^{-1}. LRMS (ESI) m/z 538.3 ($M+H^+$), HRMS (ESI) m/z 538.3237 ($M+H^+$), calc. for $C_{34}H_{44}N_3OSi$ 538.3248

Desymmetrization of N-3,5-dinitrobenzoyl aziridines with thiols

General procedure for the desymmetrization of *meso* N-3,5-dinitrobenzoyl aziridines with thiols:



To a 10 mL flask containing catalyst **1b** (0.27 mg, 0.0005 mmol, 1 mol %) and a stirring bar, aziridine **2c** (14.6 mg, 0.05 mmol, 1.0 eq.) was added, followed by 5 mL of ether. The reaction mixture was placed in a cryobath preset at -50 ^{o}C and allowed to stir for 0.5h before 2,6-dichlorobenzenethiol (17.9 mg, 0.1 mmol, 2.0 eq.) was added. The reaction was stirred at -50 ^{o}C and monitored by TLC for 48 hours. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (silica gel, gradient elution with hexane/EA mixture, 8/1 to 4/1 and then DCM) to afford the product **4f** (21.6 mg) as a white solid in 92% yield and 94% ee.

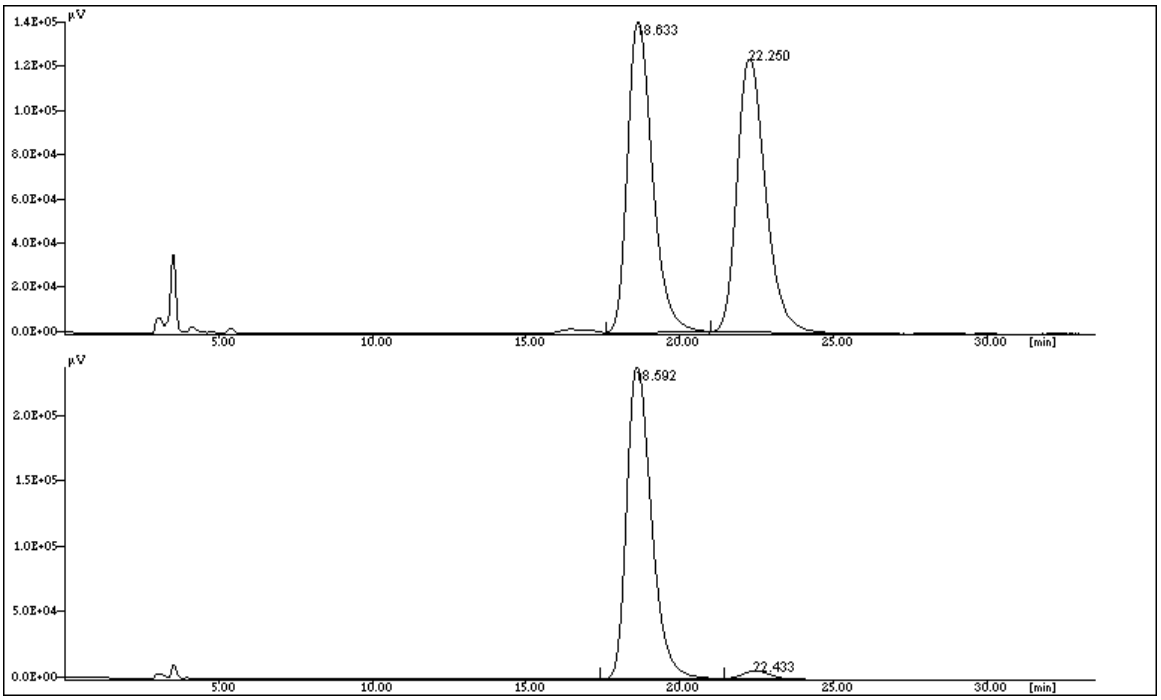


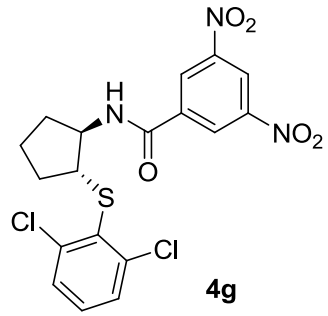
4f

(4f) N-((1R,2R)-2-(2,6-dichlorophenylthio)cyclohexyl)-3,5-dinitrobenzamide

White solid, 92% yield, 94% ee. Mp = 210.9-212.0 ^{o}C. $[\alpha]^{26}_{D}$ -33.3 (*c* 1.0, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.27-1.32 (m, 1H), 1.40-1.54 (m, 2H), 1.63-1.83 (m, 3H), 2.12-2.14 (m, 1H), 2.36-2.39 (m, 1H), 3.30-3.35 (m, 1H), 4.04-4.10 (m, 1H), 6.65 (d, 1H, *J* = 6.95 Hz), 7.20 (t, 1H, *J* = 8.2 Hz), 7.38 (d, 2H, *J* = 7.55 Hz), 8.90 (d, 2H, *J* = 1.9 Hz), 9.17 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 24.5, 25.8, 32.4, 33.4, 52.9, 55.3, 120.9, 127.1, 128.9, 130.2, 132.2, 138.1, 141.5, 148.5, 162.1. FTIR (film): 929, 1045, 1215, 1424, 1520, 1633, 3020, 3428 cm^{-1}. LRMS (ESI) m/z 468.1 (M-H^{+}), HRMS (ESI) m/z 468.0201 (M-H^{+}), calc. for $C_{19}H_{16}Cl_2N_3O_5S$ 468.0193.

The enantiomeric excess was determined by chiral HPLC; Phenomenex Lux 5u Cellulose-2 (4.6 mm i.d. x 250 mm); hexane/2-propanol 80/20; flow rate 1.0 ml/min; temp 25°C; detection UV 230 nm; retention time: 18.6 min (major) and 22.4 min (minor).



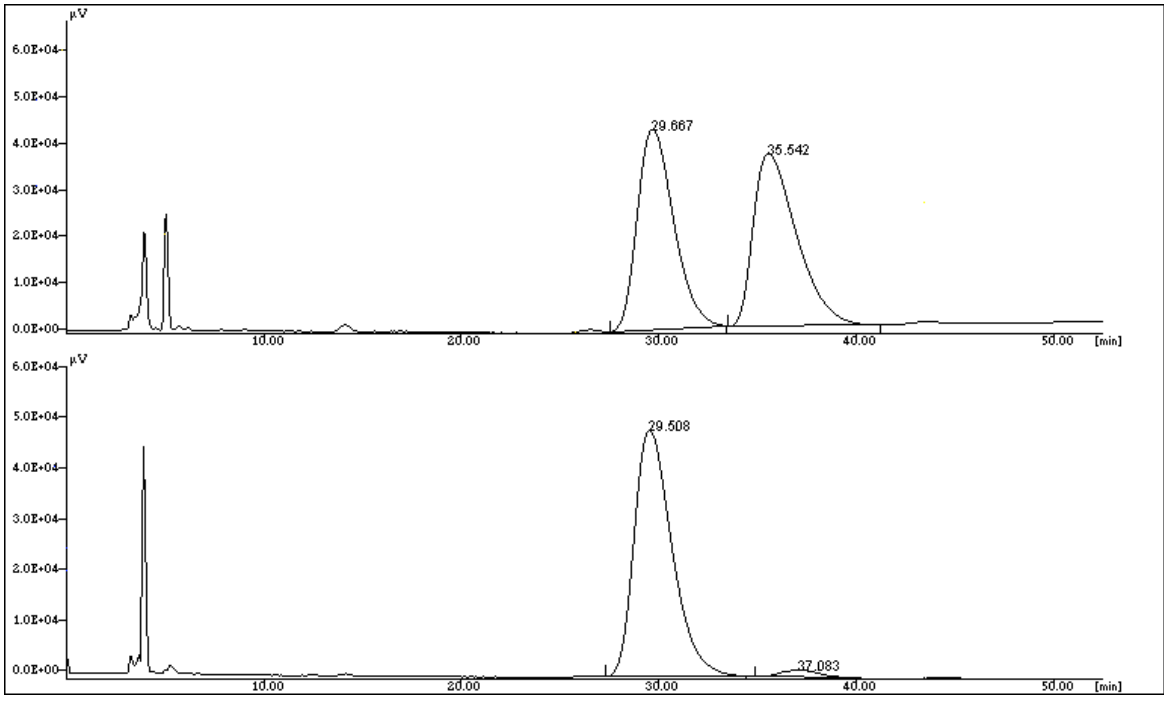


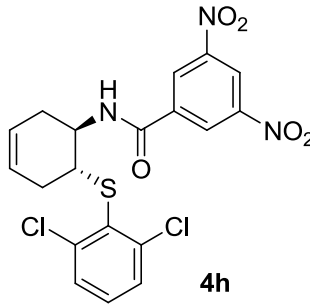
4g

(4g) N-((1R,2R)-2-(2,6-dichlorophenylthio)cyclopentyl)-3,5-dinitrobenzamide

White solid, 94% yield, 94% ee. Mp = 183.7-185.2 ^{o}C. $[\alpha]^{27}_{D}$ -30.1 (*c* 1.0, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.59-1.69 (m, 1H), 1.77-1.95 (m, 3H), 2.20-2.28 (m, 1H), 2.41-2.48 (m, 1H), 3.65 (q, 1H, *J* = 7.7 Hz), 4.29-4.36 (m, 1H), 6.35 (d, 1H, *J* = 5.7 Hz), 7.15 (t, 1H, *J* = 8.2 Hz), 7.36 (d, 2H, *J* = 8.2 Hz), 8.75 (d, 2H, *J* = 1.9 Hz), 9.12 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.6, 31.8, 32.3, 53.0, 59.9, 121.7, 127.7, 129.5, 131.0, 132.9, 138.5, 142.3, 149.2, 163.0. FTIR (film): 928, 1046, 1216, 1425, 1520, 1633, 3020, 3459 cm-1. LRMS (ESI) m/z 454.2 (M-H^+), HRMS (ESI) m/z 454.0019 (M-H^+), calc. for $C_{18}H_{14}Cl_2N_3O_5S$ 454.0037.

The enantiomeric excess was determined by chiral HPLC; CHIRALCEL OD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 80/20; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 29.5 min (major) and 37.1 min (minor).



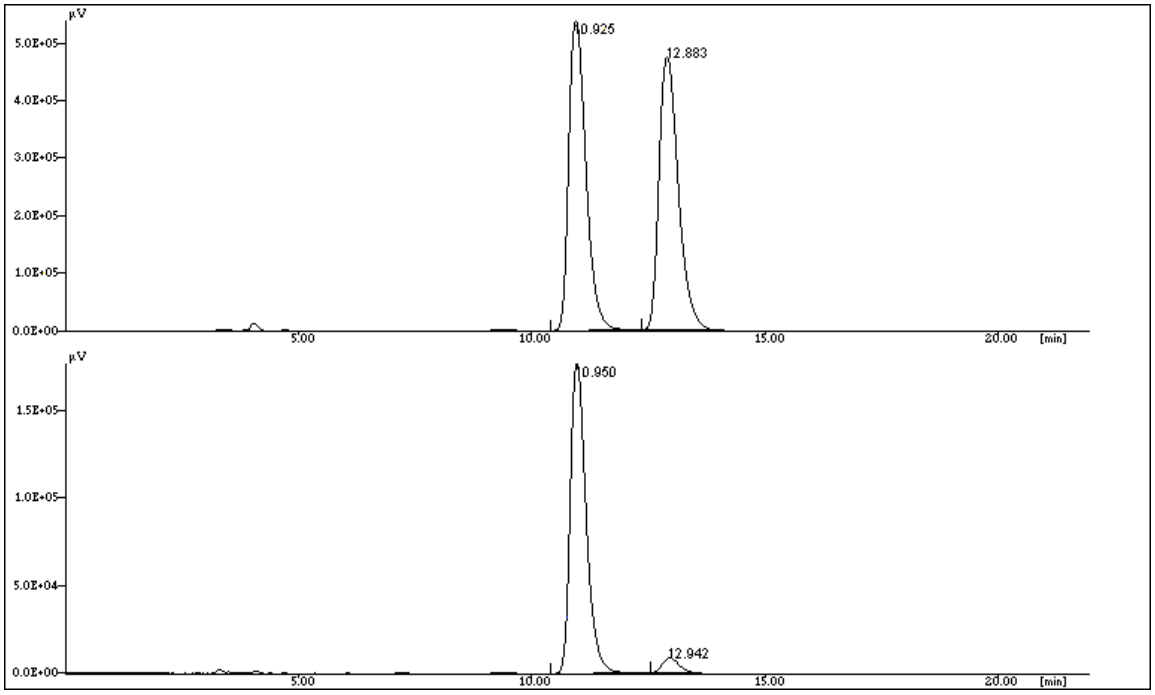


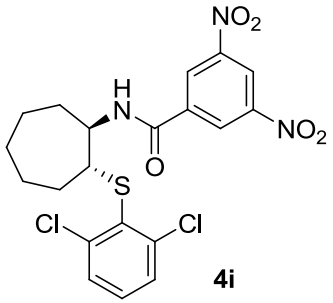
4h

(4h) N-((1R,6R)-6-(2,6-dichlorophenylthio)cyclohex-3-enyl)-3,5-dinitrobenzamide

White solid, 93% yield, 90% ee. Mp = 207.5-209.1 ^{o}C. $[\alpha]^{28}_{D}$ -44.5 (*c* 0.53, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 2.19-2.24 (m, 1H), 2.45-2.60 (m, 2H), 2.90-2.95 (m, 1H), 2.41-2.48 (m, 1H), 3.69-3.75 (m, 1H), 4.29-4.36 (m, 1H), 5.69 (t, 2H, *J* = 11.5 Hz), 6.69 (d, 1H, *J* = 7.0 Hz), 7.19 (t, 1H, *J* = 8.2 Hz), 7.37 (d, 2H, *J* = 7.6 Hz), 8.88 (d, 2H, *J* = 1.9 Hz), 9.15 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 32.03, 34.5, 48.5, 51.7, 121.7, 125.0, 126.0, 127.8, 129.6, 131.0, 132.6, 138.6, 142.1, 149.3, 163.0. FTIR (film): 929, 1046, 1216, 1426, 1519, 1602, 2976, 3020, 3443 cm^{-1}. LRMS (ESI) m/z 466.3 ($M\text{-}H^+$), HRMS (ESI) m/z 466.0031 ($M\text{-}H^+$), calc. for $C_{19}H_{14}Cl_2N_3O_5S$ 466.0037.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 10.9 min (major) and 12.9 min (minor).



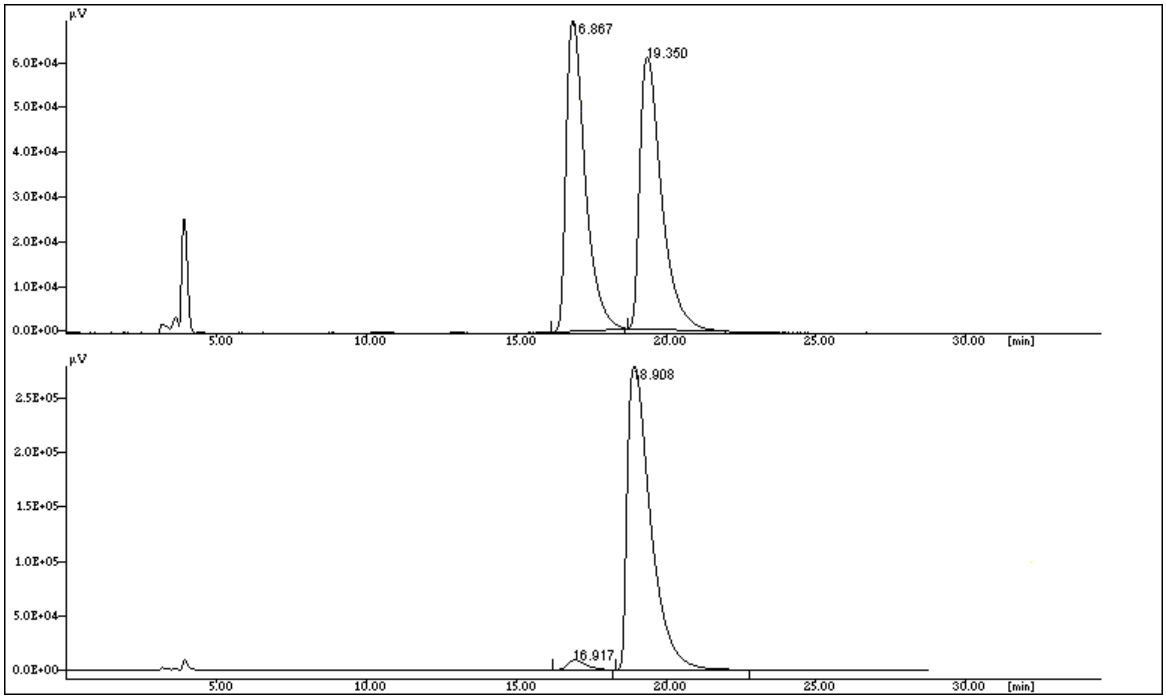


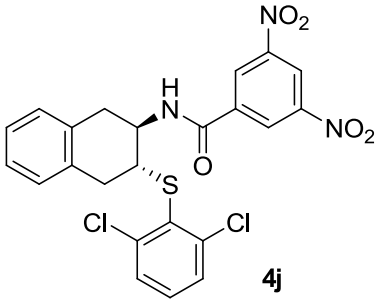
4i

(4i) N-((1R,2R)-2-(2,6-dichlorophenylthio)cycloheptyl)-3,5-dinitrobenzamide

White solid, 91% yield, 95% ee. Mp = 222.5-225.0 ^{o}C. $[\alpha]^{29}_{D}$ +14.2 (*c* 0.57, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.53-1.94 (m, 11H), 2.09-2.14 (m, 1H), 3.44-3.49 (m, 1H), 4.13-4.15 (m, 1H), 6.65 (d, 1H, *J* = 6.4 Hz), 7.19 (t, 1H, *J* = 7.6 Hz), 7.38 (d, 2H, *J* = 7.6 Hz), 8.89 (d, 2H, *J* = 1.9 Hz), 9.15 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 24.6, 25.0, 28.2, 32.2, 33.0, 55.4, 57.8, 120.9, 127.1, 128.9, 130.4, 132.3, 138,2, 141.7, 148.6, 162.0. FTIR (film): 928, 1045, 1216, 1425, 1520, 1631, 2978, 3020, 3435 cm^{-1}. LRMS (ESI) m/z 482.0 ($M\text{-}H^+$), HRMS (ESI) m/z 482.0327 ($M\text{-}H^+$), calc. for $C_{20}H_{18}Cl_2N_3O_5S$ 482.0350.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 16.9 min (minor) and 18.9 min (major).



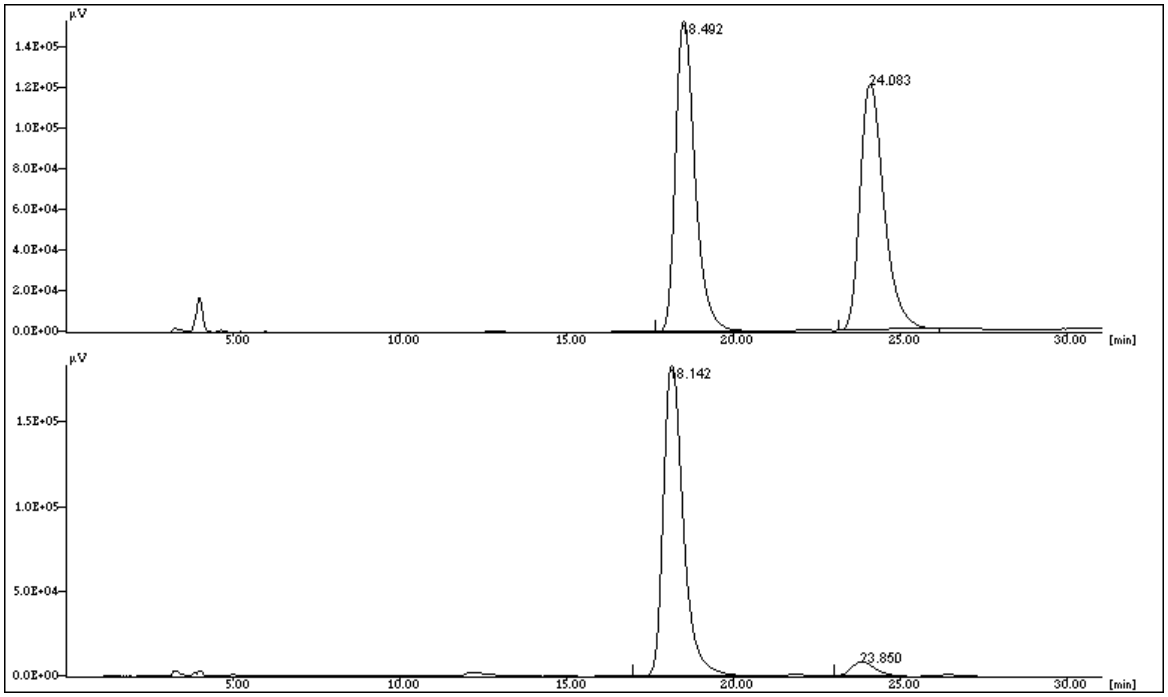


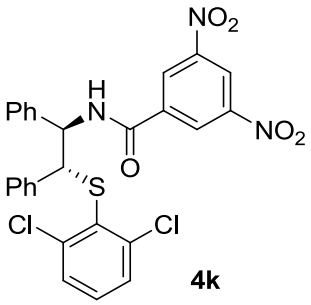
4j

(4j) N-((2R,3R)-3-(2,6-dichlorophenylthio)-1,2,3,4-tetrahydronaphthalen-2-yl)-3,5-dinitrobenzamide

White solid, 90% yield, 90% ee. Mp = 231.7-234.0 ^{o}C. $[\alpha]^{29}_{D}$ -62.7 (*c* 0.47, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 2.95 (dd, 1H, *J* = 8.2, 16.4 Hz), 3.19 (dd, 1H, *J* = 8.83, 17.0 Hz), 3.29 (dd, 1H, *J* = 5.68, 17.0 Hz), 3.65 (dd, 1H, *J* = 5.05, 17.0 Hz), 3.85-3.90 (m, 1H), 4.46-4.52 (m, 1H), 6.79 (d, 1H, *J* = 6.9 Hz), 7.09-7.17 (m, 4H), 7.23 (t, 1H, *J* = 7.7 Hz), 7.37 (d, 2H, *J* = 8.2 Hz), 8.88 (s, 2H), 9.15 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 35.0, 35.4, 48.5, 51.8, 121.1, 126.7, 127.2, 128.6, 129.0, 129.0, 130.6, 131.7, 132.8, 133.5, 137.8, 141.5, 148.6, 162.5. FTIR (film): 757, 928, 1046, 1215, 1424, 1519, 1631, 2977, 3019, 3460 cm^{-1}. LRMS (ESI) m/z 516.2 (M-H^{+}), HRMS (FAB) m/z 517.0271 (M), calc. for $C_{23}H_{17}Cl_2N_3O_5S$ 517.0266.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 18.1 min (major) and 23.9 min (minor).



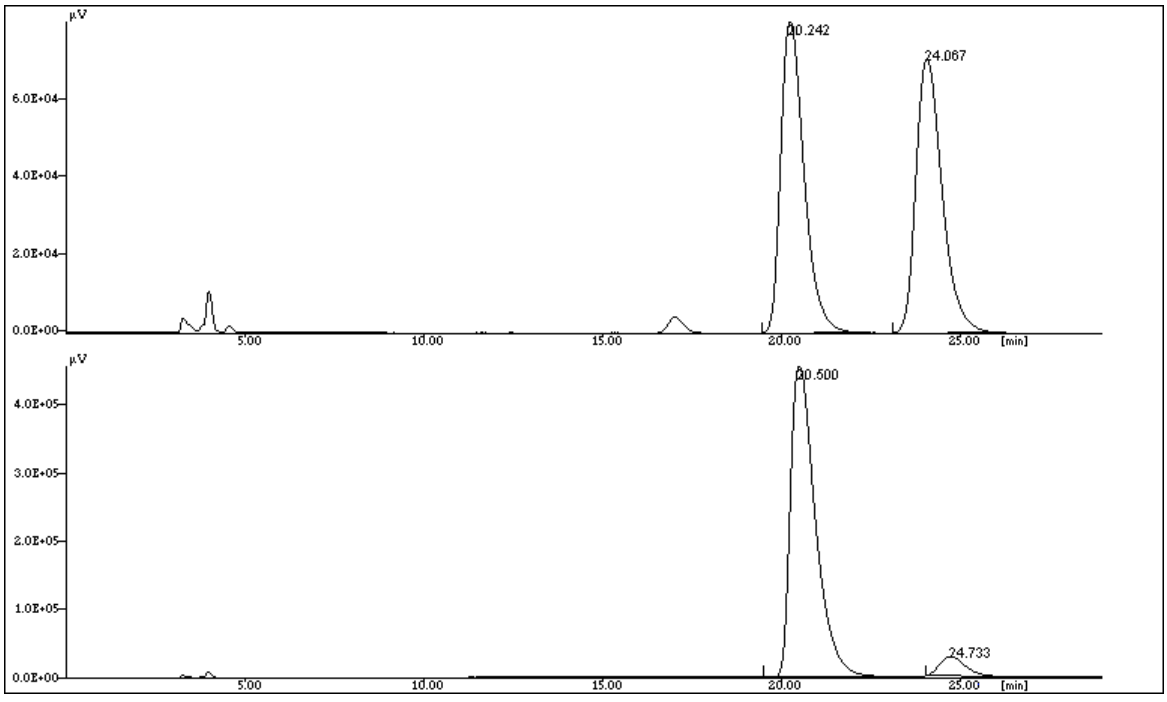


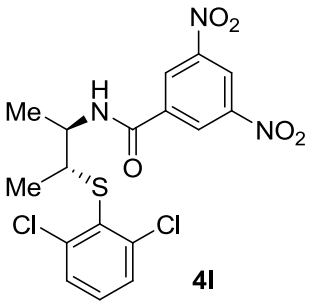
4k

(4k) N-((1R,2R)-2-(2,6-dichlorophenylthio)-1,2-diphenyl-ethyl)-3,5-dinitrobenzamide

White solid, 93% yield, 88% ee. Mp = 213.5-215.2 ^{o}C. $[\alpha]^{29}_{D}$ +4.7 (*c* 1.60, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 5.14 (d, 1H, *J* = 8.2 Hz), 5.77 (t, 1H, *J* = 8.2 Hz), 7.02-7.21 (m, 15H), 7.84 (d, 1H, *J* = 8.2 Hz), 9.09 (d, 2H, *J* = 1.9 Hz), 9.17 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 58.7, 59.4, 121.9, 127.3, 128.1, 128.5, 128.7, 128.9, 129.0, 129.1, 129.4, 131.0, 131.7, 138.1, 138.2, 139.3, 141.7, 149.4, 162.8. FTIR (film): 746, 919, 1046, 1215, 1425, 1527, 1642, 2977, 3020, 3431 cm^{-1}. LRMS (ESI) m/z 566.3 ($M\text{-}H^{+}$), HRMS (FAB) m/z 566.0349 ($M\text{-}H^{+}$), calc. for $C_{27}H_{18}Cl_2N_3O_5S$ 566.0344.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 20.5 min (major) and 24.7 min (minor).



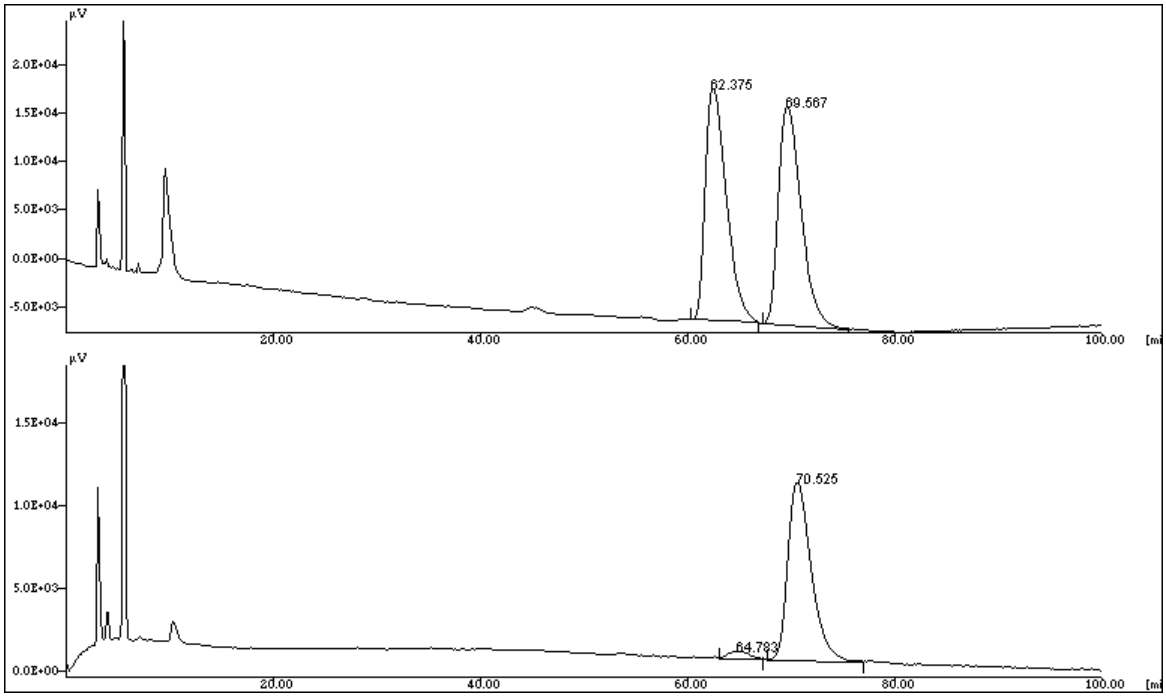


4l

(4l) N-((2R,3R)-3-(2,6-dichlorophenylthio)butan-2-yl)-3,5-dinitrobenzamide

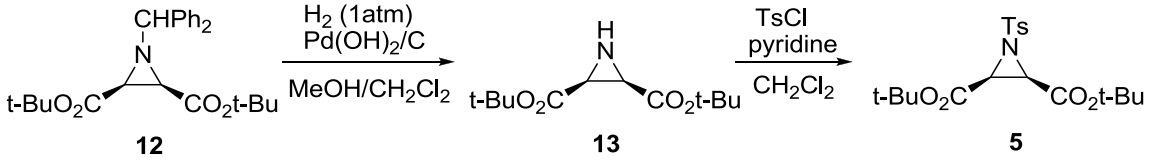
White solid, 91% yield, 93% ee. Mp = 184.1-186.1°C. $[\alpha]^{29}_{D}$ +53.5 (*c* 0.40, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.29-1.33 (m, 6H), 3.84-3.90 (m, 1H), 4.45-4.52 (m, 1H), 7.06 (d, 1H, *J* = 8.2 Hz), 7.29 (d, 1H, *J* = 9.5 Hz), 7.47 (d, 2H, *J* = 8.2 Hz), 9.04 (d, 2H, *J* = 1.9 Hz), 9.21 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 18.5, 19.1, 48.9, 51.1, 121.1, 127.1, 128.9, 130.5, 131.6, 138.0, 141.4, 148.7, 162.1. FTIR (film): 928, 1045, 1216, 1425, 1520, 1643, 2977, 3020, 3446 cm^{-1}. LRMS (ESI) m/z 442.1 ($M\text{-}H^+$), HRMS (ESI) m/z 442.0044 ($M\text{-}H^+$), calc. for $C_{17}H_{14}Cl_2N_3O_5S$ 442.0037.

The enantiomeric excess was determined by chiral HPLC; Phenomenex Lux 5u Cellulose-1 (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 64.8 min (minor) and 70.5 min (major).



Preparation and desymmetrization of *cis*-aziridine-2,3-dicaboxylate 5

Procedure for the synthesis of ***cis*-di-*tert*-butyl 1-tosylaziridine-2,3-dicarboxylate 5**:



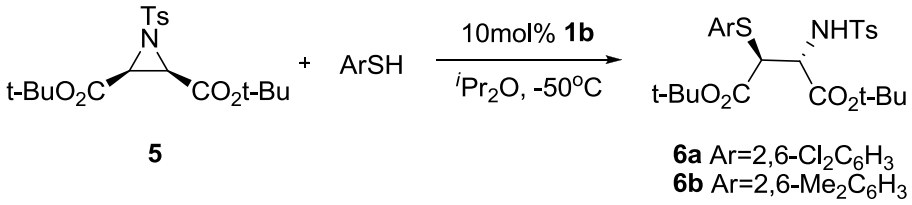
***cis*-di-*tert*-butyl 1-benzhydrylaziridine-2,3-dicarboxylate (12)** was prepared by literature procedure.[1] White solid, 60% yield. Mp = 198.0-202.2 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.46 (s, 18H), 2.52 (s, 2H), 3.83 (s, 1H), 7.22-7.26 (m, 2H), 7.28-7.44 (m, 4H), 7.57 (d, 4H, J = 6.95 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 28.0, 44.4, 76.7, 81.6, 127.3, 127.4, 128.4, 142.0, 166.1. FTIR (film): 929, 1046, 1216, 1477, 1633, 2977, 3020, 3452 cm^{-1}. LRMS (ESI) m/z 432.1 (M+Na^{+}), HRMS (ESI) m/z 432.2162 (M+Na^{+}), calc. For $C_{25}H_{31}NO_4Na$ 432.2145.

***cis*-di-*tert*-butyl 1-tosylaziridine-2,3-dicarboxylate (5)** To a solution of **12** (409 mg, 1.0 mmol) in MeOH/DCM mixture 1/1 (20 mL) was added $Pd(OH)_2/C$ (170mg). Bubbling of hydrogen gas for 15 minutes, the reaction was stirred for a further 4 hours under a positive atmosphere of hydrogen gas (balloon). The reaction mixture was filtered through a thin layer of celite and the solvent was evaporated under reduced pressure, affording aziridine **13** as colorless oil, which was used for next step without purification.

The crude azirdine **13** was dissolved in DCM (5 mL) and cooled to 0^{o}C. TsCl (381 mg, 2 mmol, 2.0 eq.) was added in one portion, followed by pyridine (237 mg, 3 mmol, 3.0 eq.). The reaction mixture was stirred at 0 ^{o}C for 1 hour. Most of the solvent was evaporated, and the residue was directly loaded onto a silica gel column, followed by flash column chromatography (hexane/EA mixture, 8/1 to 4/1) to afford **5** (277.9 mg, 0.7 mmol) as a white solid in 70% yield (2 steps). Mp = 94.8-96.9 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.40 (s, 18H), 2.42 (s, 3H), 3.43 (s, 2H), 7.33 (d, 2H, J = 8.2 Hz), 7.88 (d, 2H, J = 8.2 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.4, 28.5, 42.0, 84.0, 128.9, 130.4, 134.8, 145.8, 163.6. FTIR (film): 771, 928, 1045, 1216, 1370, 1477, 1643, 1749, 2980, 3020, 3430 cm^{-1}. LRMS (ESI) m/z 419.9 (M+Na^{+}), HRMS (ESI) m/z 420.1448 (M+Na^{+}), calc. For $C_{19}H_{27}NO_6SNa$ 420.1451.

[1] Williams, A. L.; Johnston, J. N. *J. Am. Chem. Soc.* **2004**, *126*, 1612

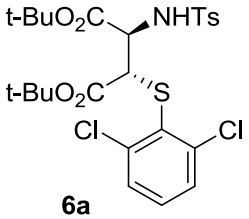
General procedure for the desymmetrization of *cis*-aziridine **5** with thiols:



5

6a Ar=2,6-$Cl_2C_6H_3$
6b Ar=2,6-$Me_2C_6H_3$

To a 10 mL flask containing catalyst **1b** (2.7 mg, 0.005 mmol, 10 mol %) and a stirring bar, aziridine **5** (19.9 mg, 0.05 mmol, 1.0 eq.) was added, followed by 10 mL of diisopropyl ether. The reaction mixture was placed in a cryobath preset at -50 ^{o}C and allowed to stir for 0.5h before thiol (0.25 mmol, 5.0 eq.) was added. The reaction was stirred at -50 ^{o}C and monitored by TLC for 48 hours. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (silica gel, gradient elution with hexane/EA mixture, 8/1 to 4/1).

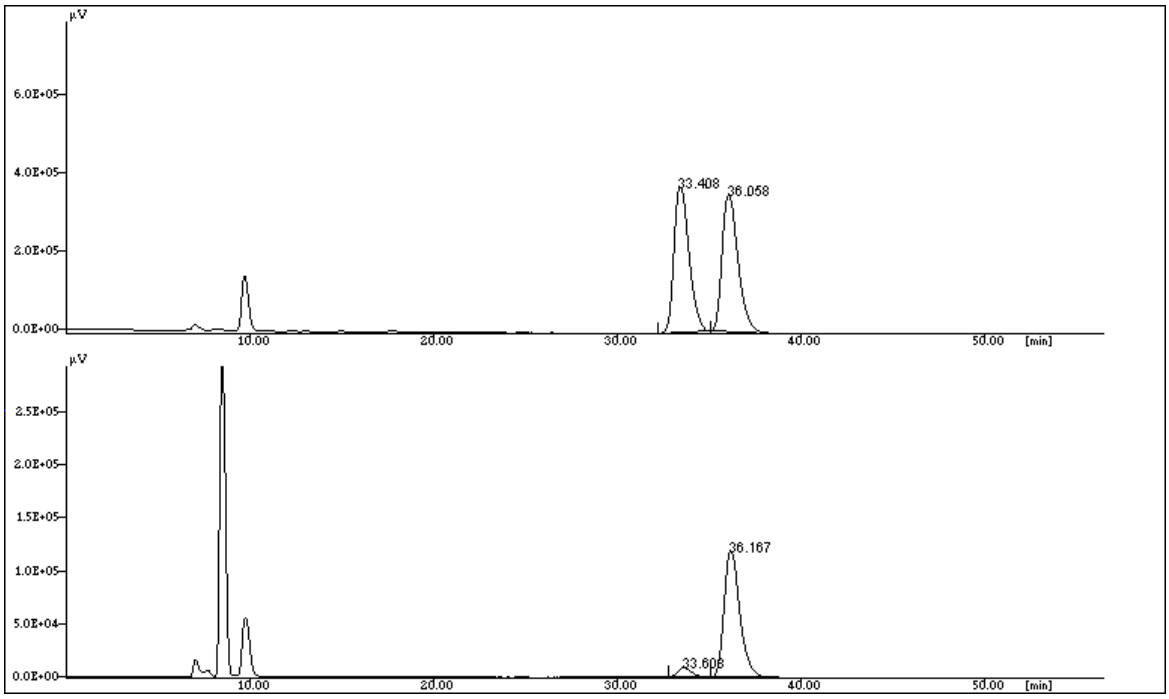


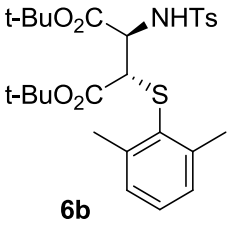
6a

(6a) (2R,3R)-di-*tert*-butyl 2-(2,6-dichlorophenylthio)-3-(4-methylphenylsulfonamido)succinate

White solid, 91% yield, 88% ee. Mp = 117.0-119.0 ^{o}C. $[\alpha]^{29}_{D}$ -33.5 (*c* 1.30, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.35 (s, 18H), 2.40 (s, 3H), 4.08 (d, 1H, *J* = 3.8 Hz), 4.26 (dd, 1H, *J* = 3.8, 7.6 Hz), 5.65 (d, 1H, *J* = 7.55 Hz), 7.20 (t, 1H, *J* = 8.2 Hz), 7.27 (d, 2H, *J* = 8.2 Hz), 7.39 (d, 2H, *J* = 8.2 Hz), 7.75 (d, 2H, *J* = 8.2 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 22.2, 28.2, 28.4, 54.0, 57.6, 83.5, 84.7, 128.1, 129.4, 130.3, 130.9, 133.4, 137.2, 141.7, 144.3, 168.1, 169.1. FTIR (film): 758, 928, 1045, 1159, 1216, 1349, 1424, 1522, 1642, 1731, 2980, 3020, 3436 cm^{-1}. LRMS (ESI) m/z 574.0 ($M-H^+$), HRMS (ESI) m/z 598.0860 ($M+Na^+$), calc. for $C_{25}H_{31}Cl_2NO_6S_2Na$ 598.0862.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 95/05; flow rate 0.5 mL/min; temp 25°C; detection UV 210 nm; retention time: 33.6 min (minor) and 36.2 min (major).



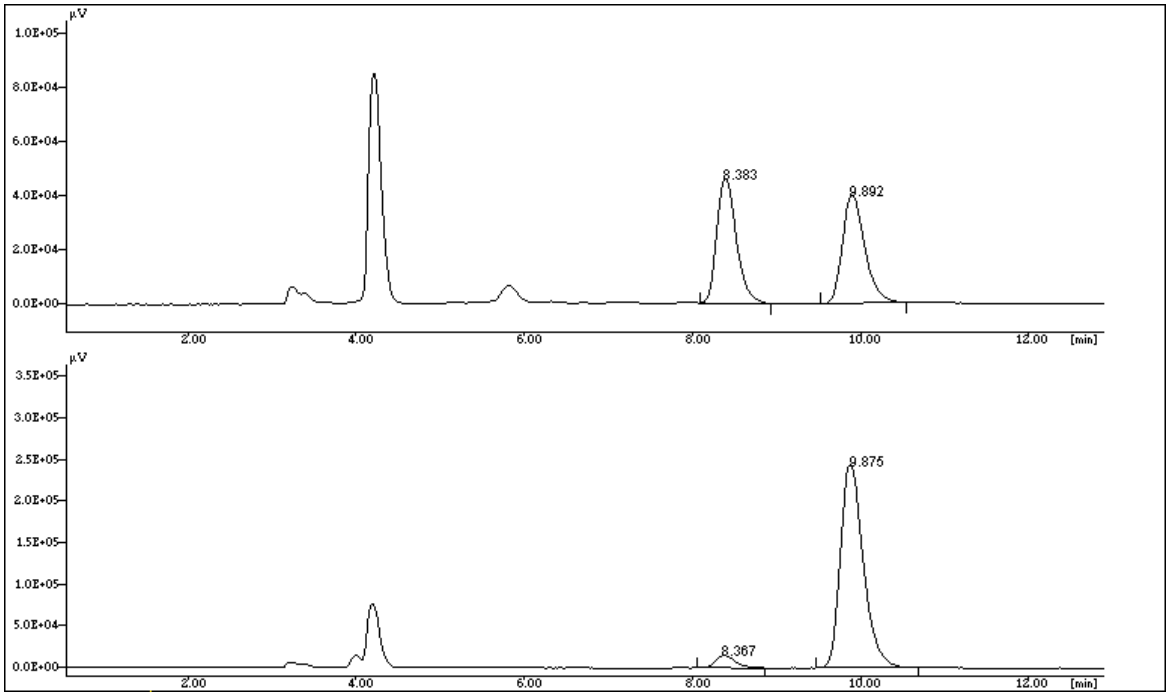


6b

(6b) (2R,3R)-di-tert-butyl 2-(2,6-dimethylphenylthio)-3-(4-methylphenylsulfonamido)succinate

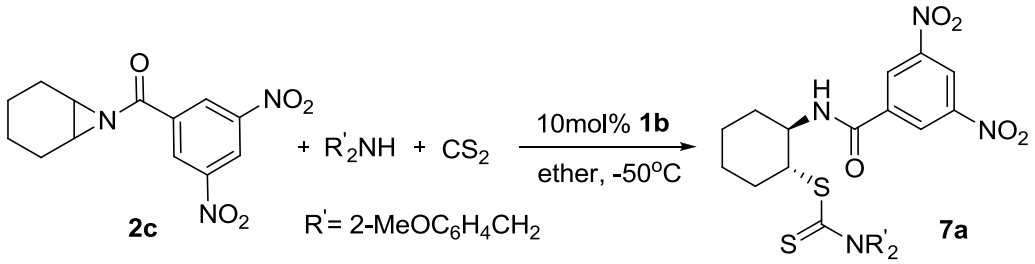
White solid, 97% yield, 90% ee. Mp = 131.5-133.0 ^{o}C. $[\alpha]^{29}_{D}$ -33.6 (*c* 1.41, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.33 (d, 18H, *J* = 13.9 Hz), 2.40 (s, 3H), 2.52 (s, 6H), 3.76 (d, 1H, *J* = 4.4 Hz), 4.27 (dd, 1H, *J* = 4.45, 7.6 Hz), 5.58 (d, 1H, *J* = 7.55 Hz), 7.07-7.15 (m, 3H), 7.27(d, 2H, *J* = 8.2 Hz), 7.68 (d, 2H, *J* = 8.8 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.5, 22.0, 27.6, 27.7, 53.7, 57.4, 82.6, 83.7, 127.4, 128.3, 128.8, 129.6, 132.2, 136.5, 143.2, 143.6, 167.7, 168.6. FTIR (film): 759, 928, 1045, 1159, 1216, 1426, 1522, 1642, 1733, 2980, 3020, 3436 cm^{-1}. LRMS (ESI) m/z 534.1 ($M-H^+$), HRMS (ESI) m/z 558.1965 ($M+Na^+$), calc. for $C_{27}H_{37}NO_6S_2Na$ 558.1955.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 210 nm; retention time: 8.4 min (minor) and 9.9 min (major).

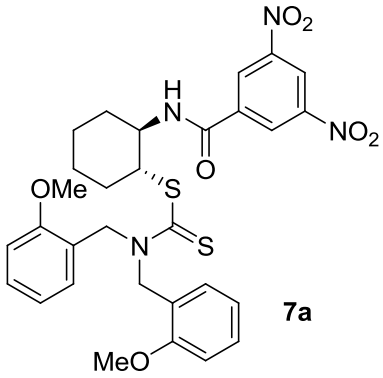


Desymmetrization of N-3,5-dinitrobenzoyl aziridines with carbamodithioic acids

General procedure for the desymmetrization of *meso* N-3,5-dinitrobenzoyl Aziridines with carbamodithioic acids:



To a 10 mL flask containing catalyst **1b** (2.7 mg, 0.005 mmol, 10 mol %) and a stirring bar, aziridine **2c** (14.6 mg, 0.05 mmol, 1.0 eq.) was added, followed by 2.5 mL of ether, and CS_2 (7.2 μL, 0.12 mmol, 2.4 eq.). The reaction mixture was placed in a cryobath preset at -50^{o}C and allowed to stir for 0.5h before bis(2-methoxybenzyl)amine (15.4 mg, 0.06 mmol, 1.2 eq.) was added. The reaction was stirred at -50^{o}C and monitored by TLC for 24 hours. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (silica gel, gradient elution with hexane/EA mixture, 8/1 to 4/1 and then DCM) to afford the product **7a** (30.7 mg) as a white solid in 98% yield and 89% ee.

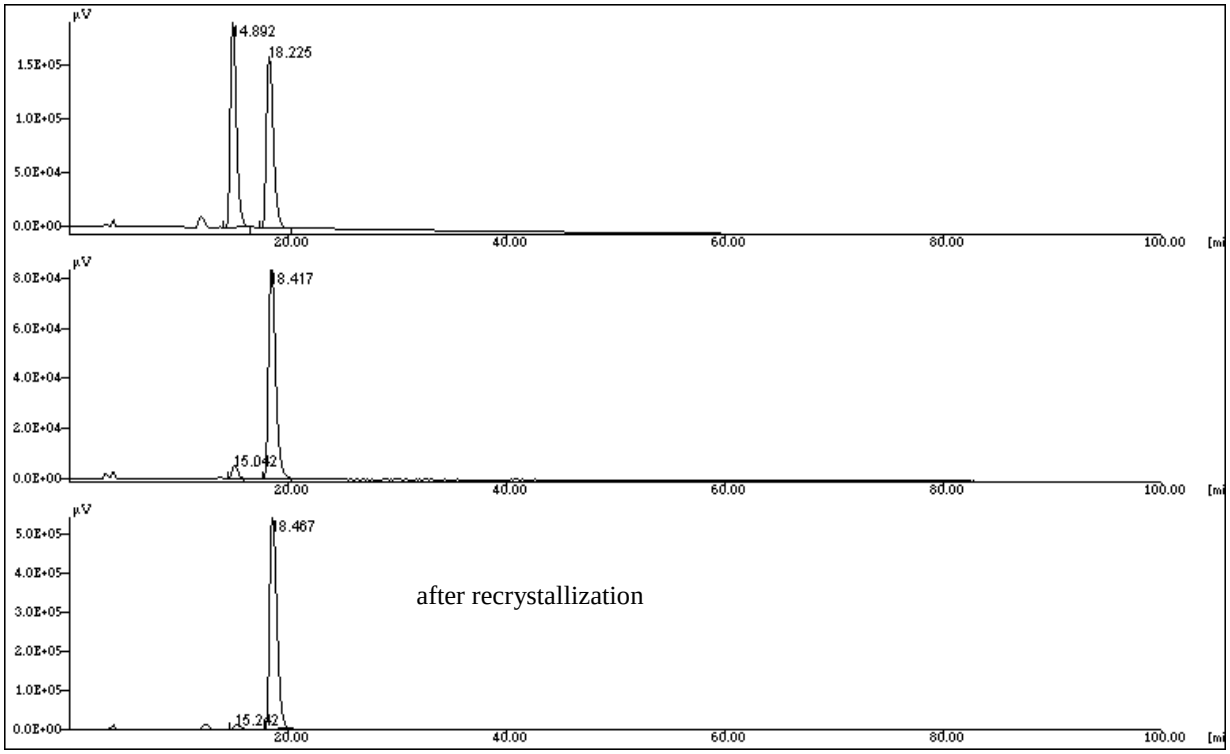


7a

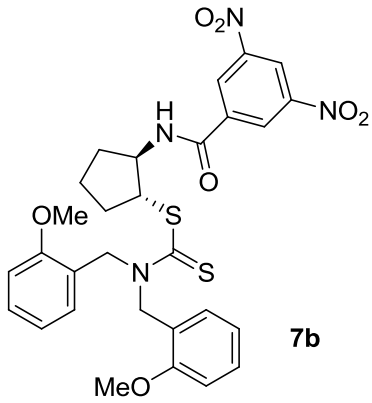
(7a) (1R,2R)-2-(3,5-dinitrobenzamido)cyclohexyl bis(2-methoxybenzyl)carbamodithioate

White solid, 98% yield, 89% ee. 96% ee was obtained after recrystallization from DCM/Hexane. Mp = 185.7-188.0 ^{o}C. $[\alpha]^{29}_{D}$ -22.4 (*c* 0.54, $CHCl_3$) (96% ee). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.42-1.48 (m, 3H), 1.50-1.71 (m, 1H), 1.82-1.89 (m, 2H), 2,21 (d, 1H, *J* = 13.3 Hz), 2,41 (d, 1H, *J* = 7.6 Hz), 3.74 (s, 6H), 3.97-3.99 (m, 1H), 3.36-4.41 (m, 1H), 5.00 (dd, 2H, *J* = 17.0, 34.1 Hz), 5.25 (d, 1H, *J* = 15.8 Hz), 5.44 (d, 1H, *J* = 15.8 Hz), 6.44 (t, 1H, *J* = 7.6 Hz), 6.68 (t, 1H, *J* = 7.6 Hz), 6.77 (d, 1H, *J* = 8.2 Hz), 6.82 (t, 2H, *J* = 9.2 Hz), 6.90 (d, 1H, *J* = 7.6 Hz), 7.09 (t, 1H, *J* = 7.6 Hz), 7.20 (t, 1H, *J* = 7.6 Hz), 8.71 (d, 1H, *J* = 6.9 Hz), 9.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 24.5, 26.6, 32.2, 33.9, 51.6, 53.9, 54.0, 55.2, 55.2, 57.6, 110.3, 110.3, 119.8, 120.4, 120.7, 122.2, 123.2, 126.5, 126.8, 127.7, 128.4, 128.9, 137.8, 148.4, 156.9, 157.2, 161.7, 200.7. FTIR (film): 756, 927, 1030, 1110, 1216, 1344, 1437, 1467, 1493, 1544, 1664, 2977, 3020, 3456 cm^{-1}. LRMS (ESI) m/z 647.1 (M+Na^{+}), HRMS (ESI) m/z 647.1607 (M+Na^{+}), calc. for $C_{30}H_{32}N_4O_7S_2Na$ 647.1605.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 15.0 min (minor) and 18.4 min (major).



after recrystallization

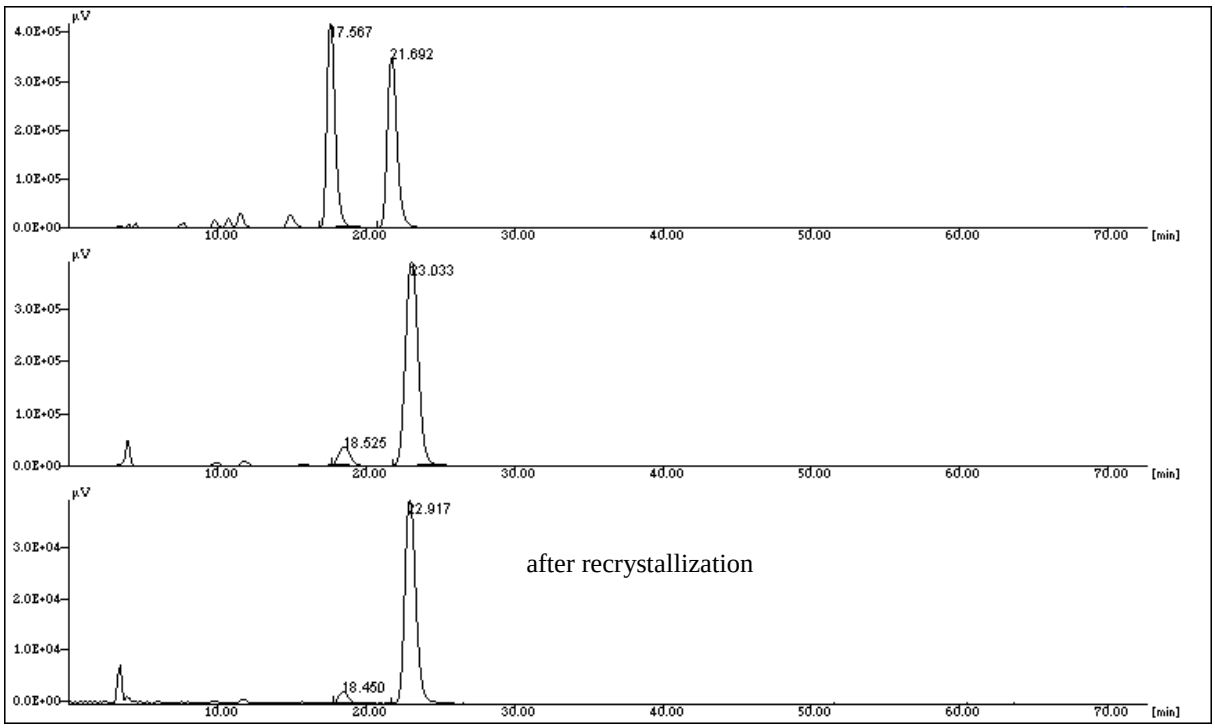


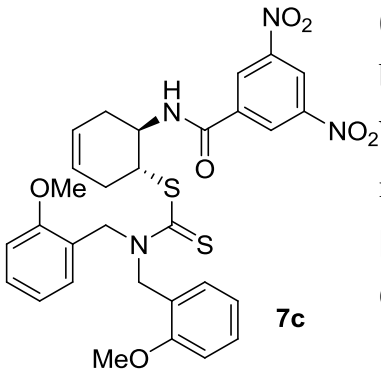
7b

(7b) (1R,2R)-2-(3,5-dinitrobenzamido)cyclopentyl bis(2-methoxybenzyl)carbamodithioate

White solid, 98% yield, 85% ee. 91% ee was obtained after recrystallization from DCM/Hexane. Mp = 146.2-148.0 ^{o}C. $[\alpha]^{29}_{D}$ -55.7 (*c* 2.14, $CHCl_3$) (85% ee). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.59-1.65 (m, 1H), 1.77-1.92 (m, 3H), 2.21-2.27 (m, 1H), 2.53-2.49 (m, 1H), 3.76 (d, 6H, *J* = 12.6 Hz), 4.11-4.18 (m, 1H), 4.64-4.70 (m, 1H), 4.93 (d, 1H, *J* = 17.0 Hz), 5.10 (d, 2H, *J* = 17.8 Hz), 5.56 (d, 1H, *J* = 15.8 Hz), 6.46 (t, 1H, *J* = 7.6 Hz), 6.77 (d, 1H, *J* = 8.2 Hz), 6.84-6.90 (m, 3H), 6.99 (d, 1H, *J* = 7.6 Hz), 7.05 (t, 1H, *J* = 7.6 Hz), 7.25 (m, 1H), 8.74 (d, 1H, *J* = 5.1 Hz), 9.05-9.08 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 21.0, 27.7, 31.7, 51.9, 52.4, 54.0, 55.2, 55.2, 62.1, 110.2, 110.3, 119.9, 120.6, 120.7, 122.2, 123.1, 126.6, 126.8, 127.6, 128.3, 129.0, 137.5, 148.5, 156.9, 156.9, 162.6, 199.9. FTIR (film):759, 928, 1046, 1216, 1424, 1476, 1530, 1640, 2977, 3020, 3451 cm^{-1}. LRMS (ESI) m/z 609.0 ($M\text{-}H^+$), HRMS (ESI) m/z 609.1481 ($M\text{-}H^+$), calc. for $C_{29}H_{29}N_4O_7S_2$ 609.1483.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 18.5 min (minor) and 23.0 min (major).



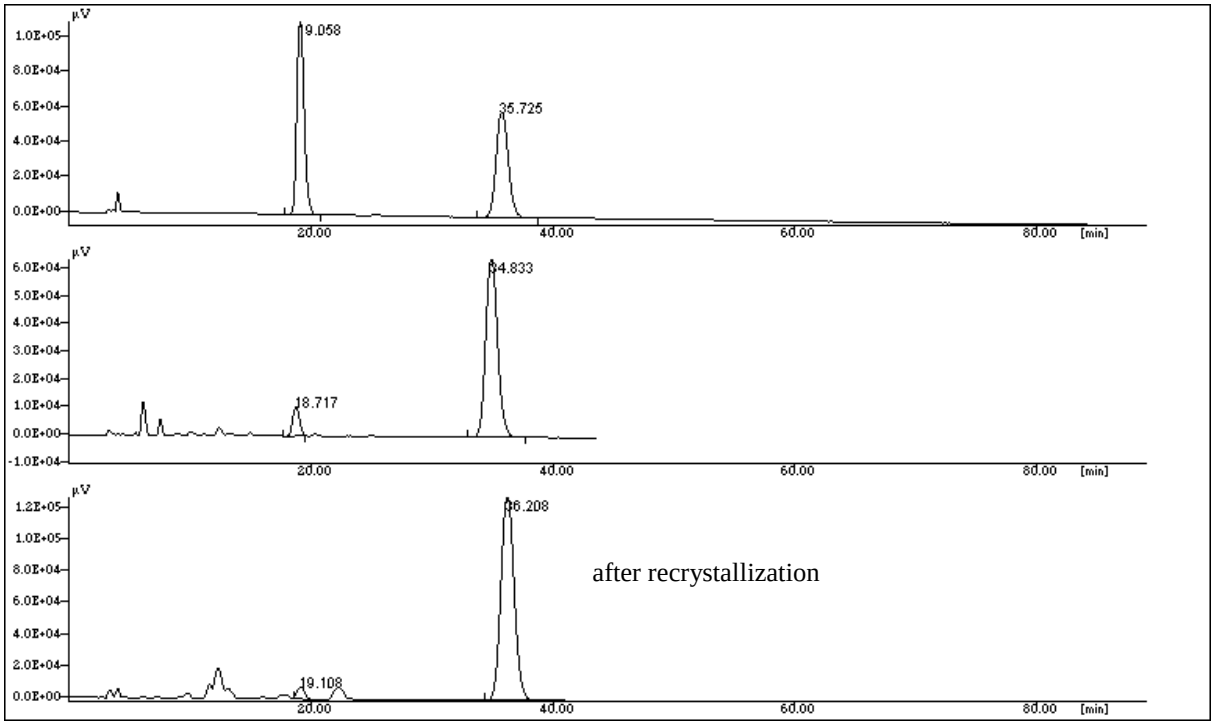


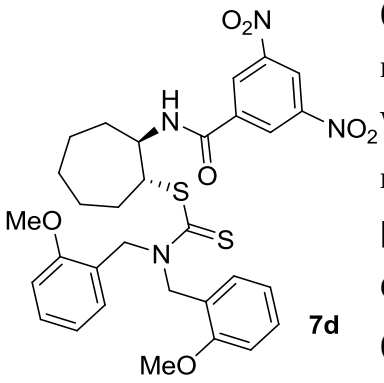
7c

(7c) (1R,6R)-6-(3,5-dinitrobenzamido)cyclohex-3-enyl bis(2-methoxybenzyl)carbamodithioate

White solid, 80% yield, 84% ee. 95% ee was obtained after recrystallization from DCM/Hexane. Mp = 175.2-177.1 ^{o}C. $[\alpha]^{31}_{D}$ -7.1 (*c* 0.53, $CHCl_3$) (84% ee). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 2,26 (t, 1H, *J* = 12.0 Hz), 2,51 (t, 1H, *J* = 13.3 Hz), 2.63 (d, 1H, *J* = 17.0 Hz), 2.84 (d, 1H, *J* = 17.0 Hz), 3.73 (s, 3H), 3.74 (s, 3H), 4.26-4.34 (m, 1H), 4.59-4.65 (m, 1H), 4.99 (s, 2H), 5.37 (s, 2H), 5.71 (d, 2H, *J* = 10.7 Hz), 6.50 (t, 1H, *J* = 7.6 Hz), 6.64 (t, 1H, *J* = 7.6 Hz), 6.80 (t, 2H, *J* = 8.2 Hz), 6.90 (t, 2H, *J* = 6.3 Hz), 7.12 (t, 1H, *J* = 7.6 Hz), 7.19 (t, 1H, *J* = 8.2 Hz), 8.85 (d, 1H, *J* = 7.6 Hz), 9.09 (s, 2H), 9.10 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 31.4, 33.5, 50.4, 51.7, 53.5, 54.0, 55.2, 55.2, 110.3, 110.3, 119.9, 120.4, 120.8, 122.1, 123.1, 125.3, 126.5, 127.1, 127.7, 128.5, 129.0, 137.69, 148.5, 150.0, 156.9, 156.9, 161.9, 200.5. FTIR (film): 771, 928, 1031, 1218, 1344, 1433, 1470, 1532, 1665, 2975, 3020, 3443 cm^{-1}. LRMS (ESI) m/z 645.0 ($M+Na^+$), HRMS (ESI) m/z 645.1430 ($M+Na^+$), calc. for $C_{30}H_{30}N_4O_7S_2Na$ 647.1448.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 18.7 min (minor) and 34.8 min (major).



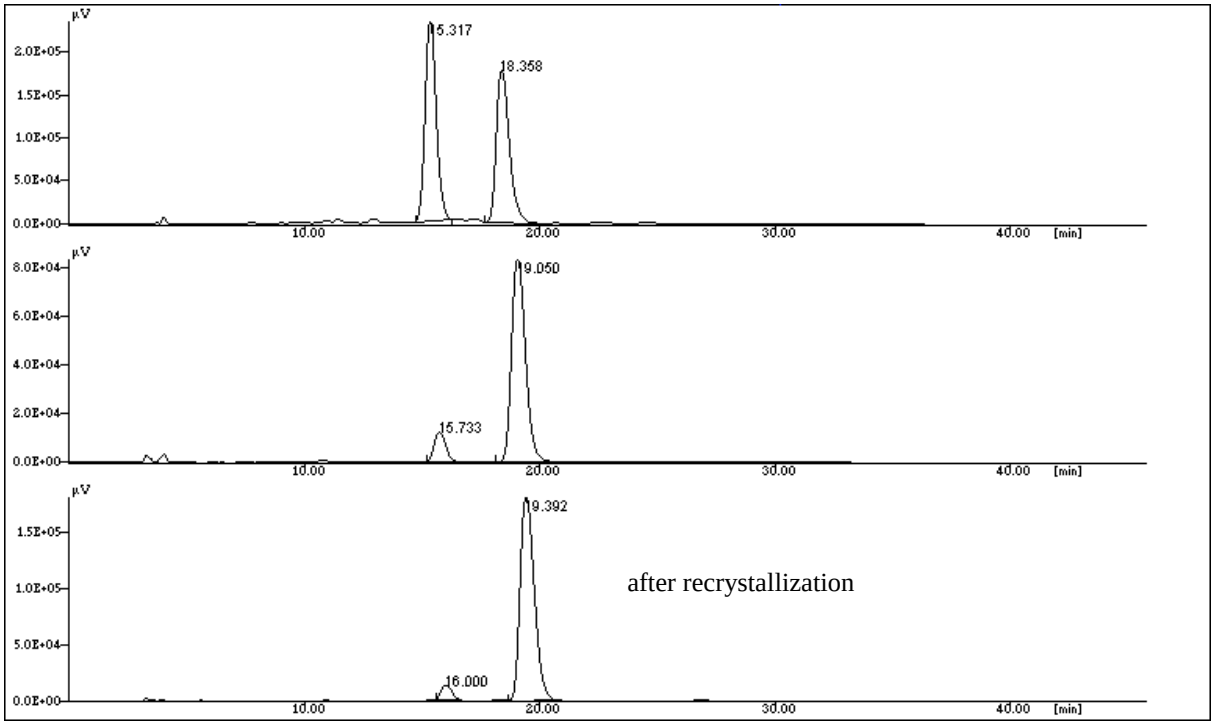


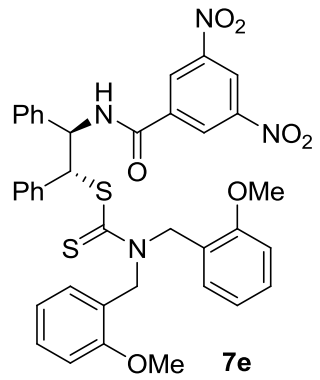
7d

(7d) (1R,2R)-2-(3,5-dinitrobenzamido)cycloheptyl bis(2-methoxybenzyl)carbamodithioate

White solid, 67% yield, 80% ee. 90% ee was obtained after recrystallization from DCM/Hexane. Mp = 127.9-129.7 ^{o}C. $[\alpha]^{30}_{D}$ -8.4 (*c* 0.45, $CHCl_3$) (90% ee). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 1.66 (m, 3H), 1.78-1.92 (m, 4H), 1.93-1.97 (m, 1H), 2.13-2.23 (m, 2H), 3.74 (s, 6H), 4.20-4.23 (m, 1H), 4.53-4.58 (m, 1H), 4.97 (dd, 2H, *J* = 17.0, 32.2 Hz), 5.29 (d, 1H, *J* = 15.8 Hz), 5.40 (d, 1H, *J* = 15.8 Hz), 6.48 (t, 1H, *J* = 7.6 Hz), 6.64 (t, 1H, *J* = 7.0 Hz), 6.80 (dd, 2H, *J* = 8.2, 12.7 Hz), 6.87 (t, 2H, *J* = 7.6 Hz), 7.10 (t, 1H, *J* = 8.2 Hz), 7.18 (t, 1H, *J* = 7.6 Hz), 8.68 (d, 1H, *J* = 7.0 Hz), 9.06 (s, 2H), 9.07(s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 24.7, 27.0, 27.9, 30.4, 33.6, 34.6, 52.2, 54.7, 55.9, 55.9, 57.5, 60.0, 110.9, 111.0, 120.5, 121.0, 121.4, 122.9, 123.9, 127.2, 127.7, 128.4, 129.1, 129.6, 138.5, 149.1, 157.6, 157.9, 162.2, 201.4. FTIR (film): 771, 927, 1030, 1109, 1216, 1344, 1436, 1465, 1493, 1545, 1663, 2974, 3019, 3431 cm^{-1}. LRMS (ESI) m/z 661.1 ($M+Na^+$), HRMS (ESI) m/z 661.1773 ($M+Na^+$), calc. for $C_{31}H_{34}N_4O_7S_2Na$ 661.1761.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 15.7 min (minor) and 19.0 min (major).



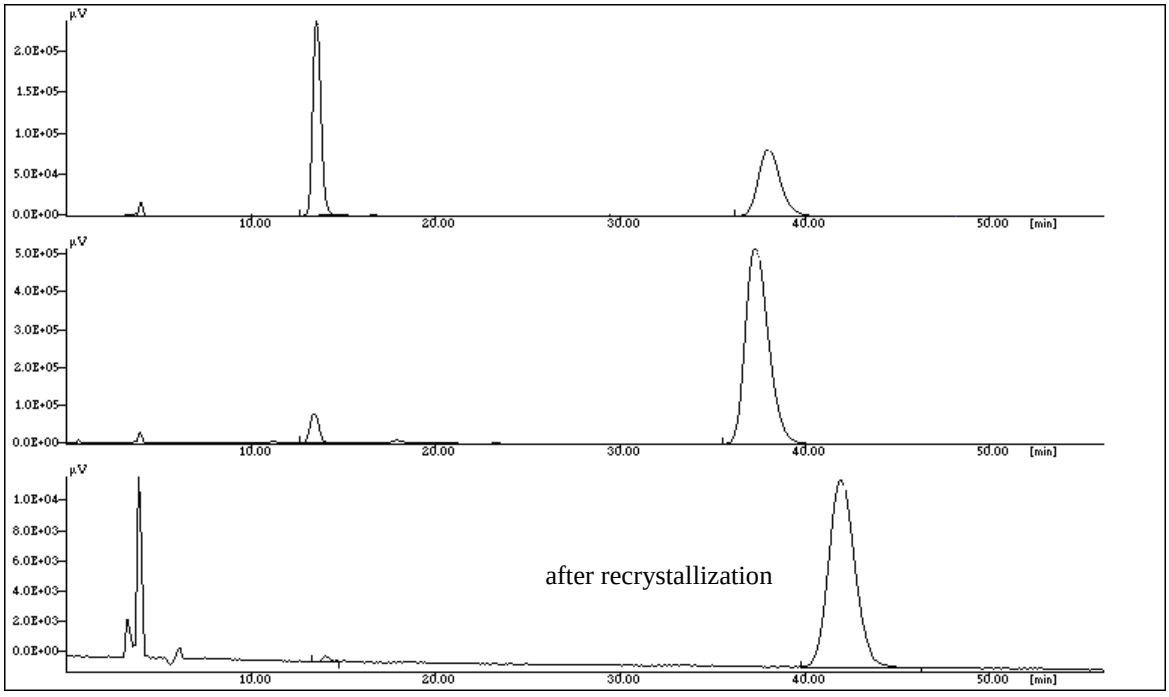


7e

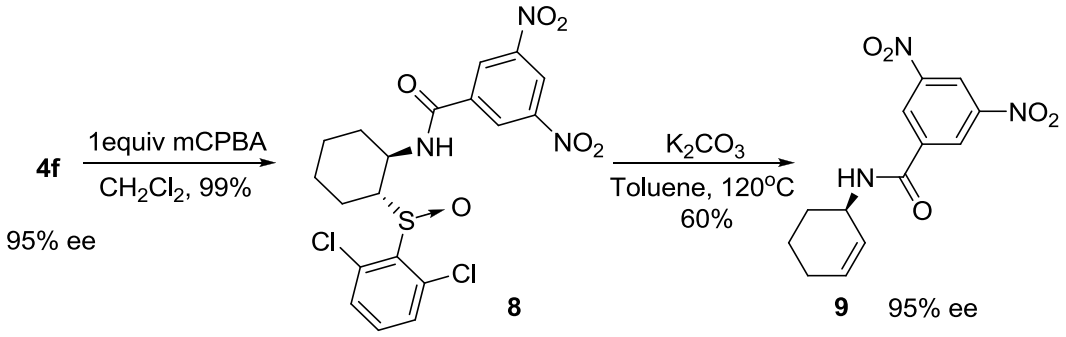
(7e) (1R,2R)-2-(3,5-dinitrobenzamido)cycloheptyl bis(2-methoxybenzyl)carbamodithioate

White solid, 91% yield, 90% ee. 98% ee was obtained after recrystallization from DCM/Hexane. Mp = 195.5-197.0 ^{o}C. $[\alpha]^{29}_{D}$ -30.1 (*c* 0.66, $CHCl_3$) (90% ee). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 3.70 (s, 3H), 3.76 (s, 3H), 4.93 (d, 1H, *J* = 17.0 Hz), 5.08 (d, 1H, *J* = 17.0 Hz), 5.26 (d, 1H, *J* = 15.8 Hz), 5.58 (dd, 1H, *J* = 7.6, 11.4 Hz), 5.65 (d, 1H, *J* = 15.8 Hz), 6.00 (d, 1H, *J* = 11.9 Hz), 6.51 (t, 1H, *J* = 7.6 Hz), 6.60 (t, 1H, *J* = 7.6 Hz), 6.80 (dd, 2H, *J* = 8.2, 20.2 Hz), 6.90 (d, 1H, *J* = 7.6 Hz), 6.99 (d, 1H, *J* = 7.6 Hz), 7.13-7.20 (m, 10H), 7.34 (d, 1H, *J* = 7.0 Hz), 9.11 (s, 3H), 9.56 (d, 1H, *J* = 7.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 51.5, 54.1, 55.1, 55.3, 60.9, 61.6, 110.3, 110.4, 120.0, 120.3, 120.8, 122.1, 123.1, 126.7, 127.4, 127.7, 127.8, 128.1, 128.5, 128.6, 128.7, 128.8, 129.1, 136.9, 137.6, 139.8, 148.5, 157.0, 157.4, 161.7, 200.47. FTIR (film): 771, 1092, 1218, 1452, 1642, 3435 cm^{-1}. LRMS (ESI) m/z 721.0 ($M\text{-}H^+$), HRMS (ESI) m/z 723.1973 ($M+H^+$), calc. for $C_{38}H_{35}N_4O_7S_2$ 723.1953.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 13.3 min (minor) and 37.2 min (major).



Preparation of chiral allylic amide from chiral compound 4f

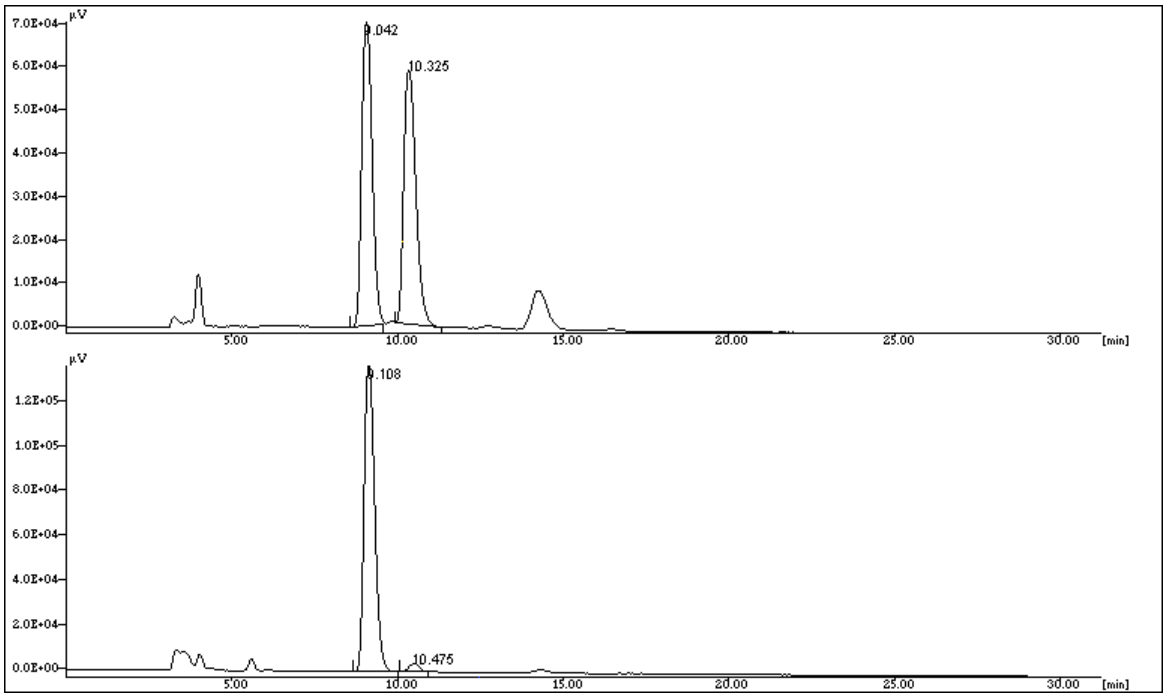


N-((1R,2R)-2-(2,6-dichlorophenylsulfinyl)cyclohexyl)-3,5-dinitrobenzamide (8) To a solution of **4f** (94.0 mg, 0.20 mmol, 1.0 eq.) in CH_2Cl_2 2 mL was added **mCPBA** (70% W/W, 49.3 mg, 0.20 mmol, 1.0 eq.). The reaction mixture was stirred at room temperature for 15 minutes. Most of the solvent was evaporated, and the residue was directly loaded onto a silica gel column, followed by flash column chromatography (hexane/EA mixture, 8/1 to 1/1) to afford **8** (97.0 mg, 0.2 mmol) as a white solid in quantitative yield. Mp = 139.9-142.6 ^oC. $[\alpha]^{28}_D$ +24.2 (*c* 0.50, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$, ppm): δ 1.32-1.50 (m, 5H), 1.82-1.85 (m, 2H), 2.65 (d, 1H, *J* = 10.1 Hz), 3.90-3.96 (m, 1H), 4.39-4.42 (m, 1H), 7.41 (d, 2H, *J* = 4.5 Hz), 7.87 (s, 1H), 9.07 (d, 2H, *J* = 2.5 Hz), 9.10 (d, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 24.7, 26.0, 26.8, 34.0, 55.5, 64.1, 121.6, 128.3, 134.0, 135.6, 139.1, 149.3, 163.7. FTIR (film): 753, 1045, 1215, 1344, 1427, 1543, 1669, 2976, 3020, 3442 cm^{-1}. LRMS (ESI) m/z 508.0 ($M+Na^+$), HRMS (ESI) m/z 508.0108 ($M+Na^+$), calc. for $C_{19}H_{17}Cl_2N_3O_6SNa$ 508.0107.

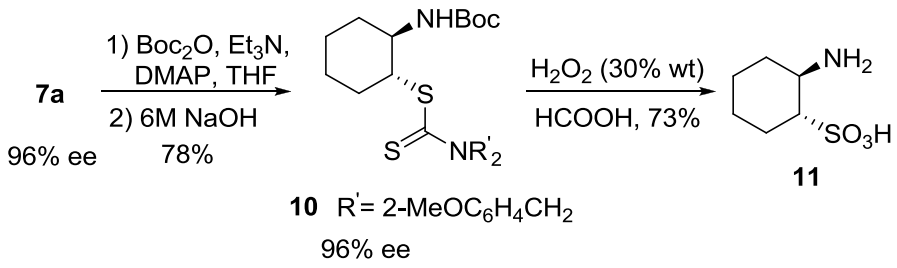
(R)-N-(cyclohex-2-enyl)-3,5-dinitrobenzamide (9) To a 5 mL flask containing **8** (38.8 mg, 0.08 mmol, 1.0 eq.) was added 1 mL of toluene, then K_2CO_3 (331 mg, 2.4 mmol, 30.0 eq.). The reaction was stirred under N_2 and heated under reflux for 3 days. The reaction mixtue was filtered and most of the solvent was evaporated under reduced pressure. The residue was directly loaded onto a silica gel column, followed by flash column chromatography (hexane/EA mixture, 20/1 to 8/1) to afford **9** (13.9 mg, 0.048 mmol) as a white solid in 60% yield and 95% ee. Mp = 154.2-155.8 ^oC. $[\alpha]^{29}_D$ +58.3 (*c* 0.30, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$, ppm): δ 1.69-1.77 (m, 3H), 2.04-2.10 (m, 3H), 4.74 (br, 1H), 5.69 (dd, 1H, *J* = 2.5, 9.5 Hz), 6.00-6.02 (m, 1H), 6.25 (d, 1H, *J* = 5.7 Hz), 8.93 (d, 2H, *J* = 2.5 Hz), 9.16 (t, 1H, *J* = 1.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ

20.3, 25.5, 29.9, 46.8, 121.7, 127.0, 127.8, 133.3, 138.9, 149.3, 162.7. FTIR (film): 767, 928, 1045, 1216, 1344, 1424, 1528, 1643, 2976, 3020, 3434 cm^{-1}. LRMS (ESI) m/z 290.2 ($M-H^+$), HRMS (ESI) m/z 290.0773 ($M-H^+$), calc. for $C_{13}H_{12}N_3O_5$ 290.0782.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK AD-H (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 9.1 min (major) and 10.5 min (minor).

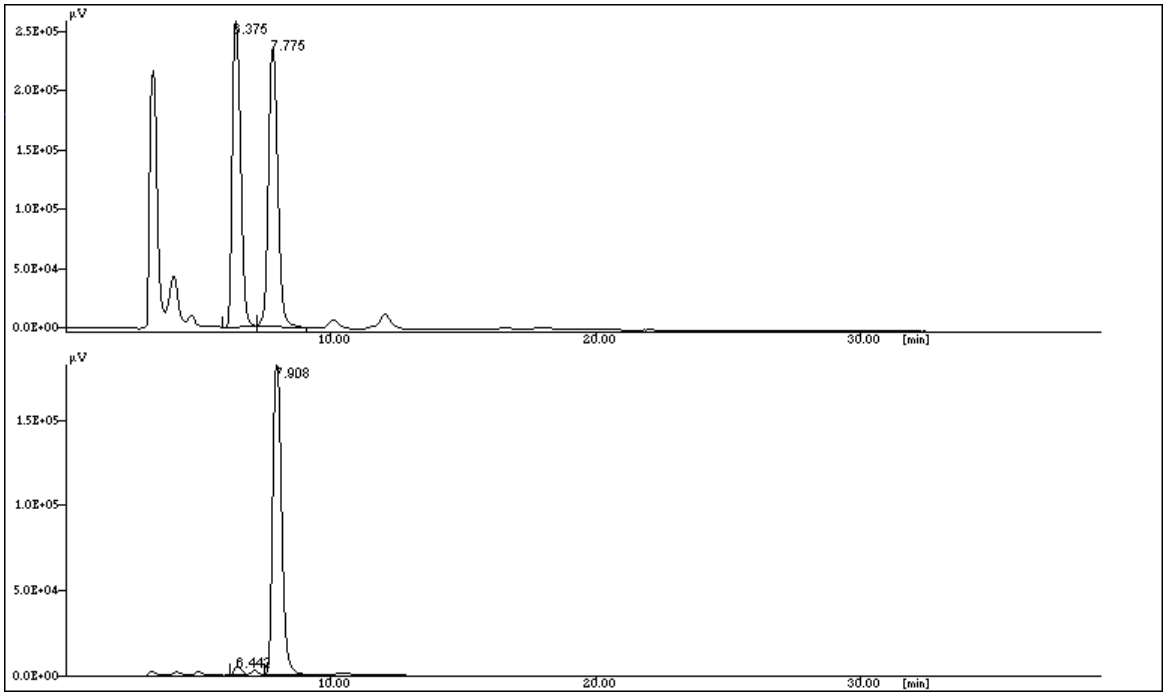


Preparation of chiral *β*-amino sulfonic acid from chiral compound 7a



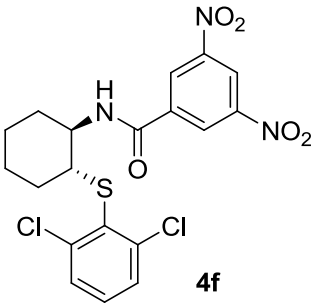
(1R,2R)-2-(bis(2-methoxybenzyl)carbamothioylthio)cyclohexylcarbamate (10) To a solution of **7a** (62.4 mg, 0.1 mmol, 1.0 eq.) in THF (1 mL), Boc_2O (47 μL, 0.2 mmol, 2.0 eq.), Et_3N (42 μL, 0.3 mmol, 3.0 eq.) and DMAP (2.5mg, 0.02 mmol, 20 mol%) were added and the mixture was stirred at room temperature for 48 hours. 6M NaOH (1 mL) was added and the mixture was stirred at room temperature for 2 hours. Water was added and the mixture was extracted with ethyl acetate three times. Combined organic layer was washed with brine, dried over $NaSO_4$ and concentrated. The residue was purified by flash column chromatography (silica gel, hexane/EA mixture, 8/1 to 4/1) to afford **10** (41.1 mg, 0.078 mmol) as a white solid in 78% yield (2 steps) and 96% ee. Mp = 142.8-145.2 ^oC. $[\alpha]^{29}_D$ +30.5 (*c* 0.35, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$, ppm): δ 1.27-1.32 (m, 3H), 1.43 (s, 9H), 1.48-1.53 (m, 1H), 1.74 (m, 2H), 2.25 (m, 2H), 3.50 (m, 1H), 3.74 (s, 3H), 3.76 (s, 3H), 4.09-4.15 (m, 1H), 4.99 (dd, 2H, *J* = 17.7, 30.3 Hz), 5.30 (d, 1H, *J* = 15.8 Hz), 5.42 (d, 1H, *J* = 15.8 Hz), 5.56 (d, 1H, *J* = 7.6 Hz), 6.84 (d, 2H, *J* = 8.2 Hz), 6.92-6.96 (m, 2H), 7.03 (d, 1H, *J* = 7.0 Hz), 7.18 (d, 1H, *J* = 7.0 Hz), 7.23-7.26 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 25.5, 27.0, 27.5, 29.1, 33.9, 35.6, 51.5, 53.7, 55.3, 55.7, 56.6, 79.4, 110.7, 110.8, 121.2, 123.4, 124.1, 127.2, 128.2, 129.0, 129.1, 156.3, 157.5, 157.8, 201.2. FTIR (film): 760, 928, 1046, 1217, 1424, 1473, 1518, 1603, 1696, 2977, 3020, 3443 cm^{-1}. LRMS (ESI) m/z 553.1 ($M+Na^+$), HRMS (ESI) m/z 553.2173 ($M+Na^+$), calc. for $C_{28}H_{38}N_2O_4S_2Na$ 553.2165.

The enantiomeric excess was determined by chiral HPLC; CHIRALPAK IA (4.6 mm i.d. x 250 mm); hexane/2-propanol 90/10; flow rate 1.0 mL/min; temp 25°C; detection UV 230 nm; retention time: 6.4 min (minor) and 7.9 min (major).



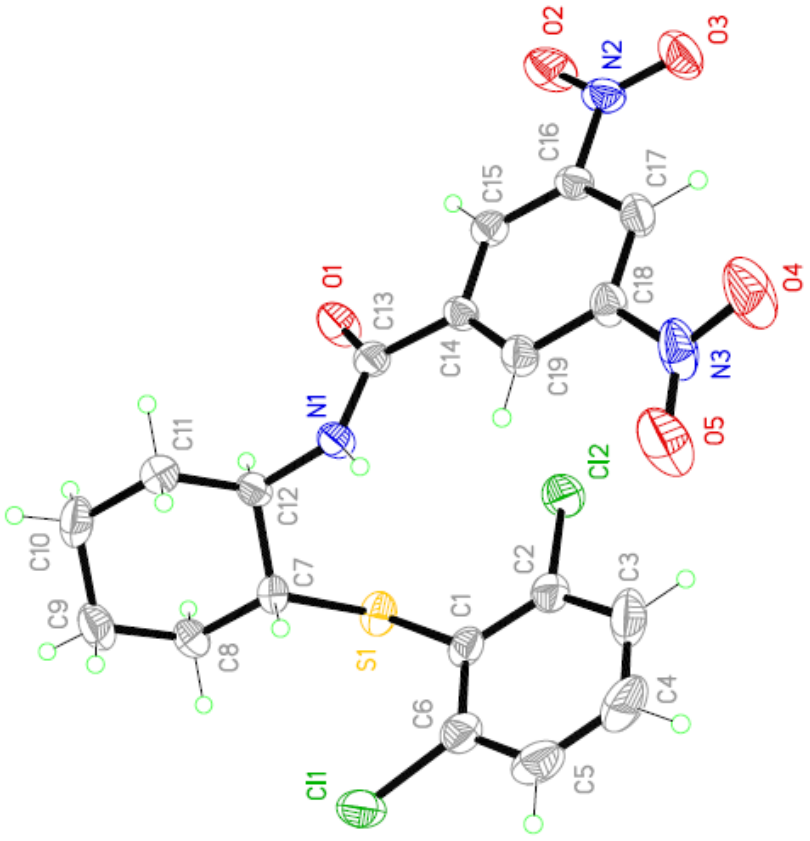
(1R,2R)-2-aminocyclohexane-1-sulfonic acid (11) To a 10 mL flask containing **10** (77.0 mg, 0.145 mmol) was added 98% formic acid (5.25 mL). H_2O_2 (30% W/W, 2.25 mL) was added dropwise. The reaction mixture was stirred at room temperature for 3 days. After removal of the solvent under reduced pressure, the crude product was further purified via recrystallization from methanol and diethyl ether, to afford **11** (23.8 mg, 0.133 mmol) as a white solid in 92% yield. Mp = 410 ^{o}C dec. $[\alpha]^{32}_{D}$ -21.4 (*c* 1.14, H_2O). ^{1}H NMR (500 MHz, D_2O, ppm): δ 1.26-1.39 (m, 2H), 1.43-1.53 (m, 2H), 1.80-1.84 (m, 2H), 2.12-2.26 (m, 2H), 2.93 (dt, 1H, *J* = 3.8, 11.4 Hz), 3.38 (dt, 1H, *J* = 3.8, 11.4 Hz). ^{13}C NMR (125 MHz, D_2O, ppm): δ 23.5, 23.6, 26.4, 30.2, 50.4, 60.0. FTIR (KBr): 1039, 1184, 1385, 1447, 1509, 1531, 1595, 1617, 2854, 2926,3139, 3443 cm^{-1}. LRMS (ESI) m/z 178.2 (M-H^{+}), HRMS (ESI) m/z 180.0697 (M+H^{+}), calc. for $C_6H_{14}NO_3S$ 180.0689.

Determination of the absolute configuration of chiral compound 4f by X-ray Crystallographic analysis



4f

The crystal is monoclinic, space group P2(1). The asymmetric unit contains one molecule of the compound C19H17Cl2N3O5S. The H atom H1N was located from different map and refined with restraints in bond length and thermal parameters. Final R values are R1= 0.0459 and wR2= 0.1160 for 2-theta max of 55º.

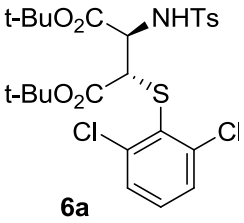


Crystal data and structure refinement for 9440.

Identification code	9440
Empirical formula	C19 H17 Cl2 N3 O5 S
Formula weight	470.32
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)

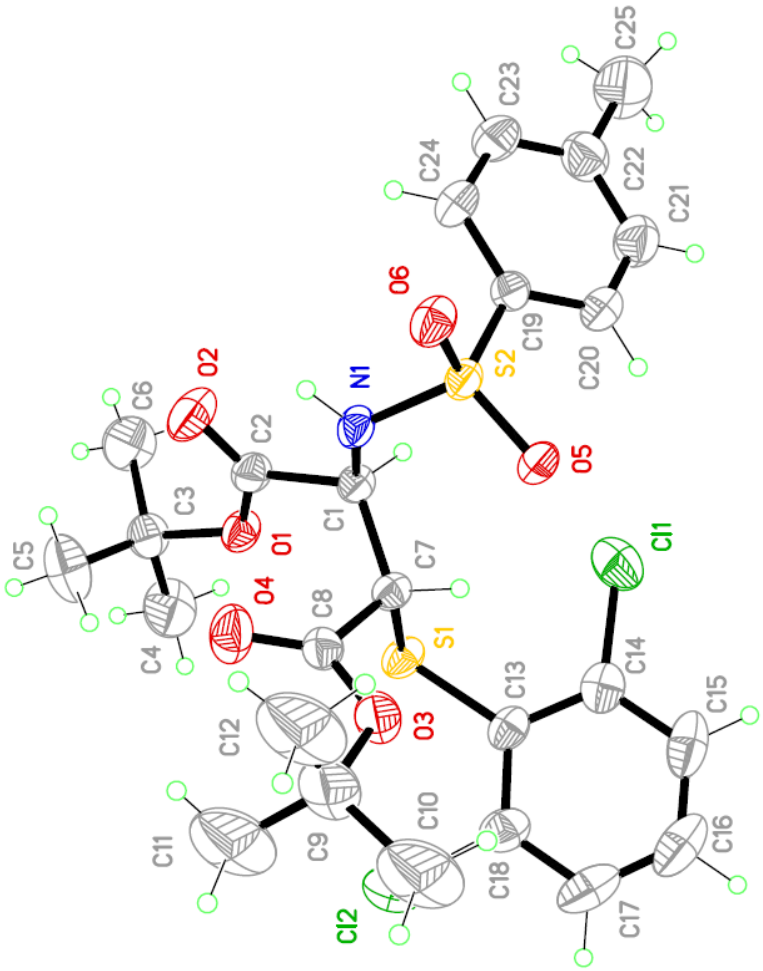
Unit cell dimensions	a = 8.4505(6) Å	α= 90°.
	b = 6.8838(5) Å	β= 101.790(2)°.
	c = 17.8060(13) Å	γ = 90°.
Volume	1013.95(13) $Å^3$	
Z	2	
Density (calculated)	1.540 Mg/m^3	
Absorption coefficient	0.461 mm^{-1}	
F(000)	484	
Crystal size	0.26 x 0.24 x 0.04 mm^3	
Theta range for data collection	1.17 to 27.49°.	
Index ranges	-10<=h<=10, -8<=k<=7, -22<=l<=23	
Reflections collected	7133	
Independent reflections	3546 [R(int) = 0.0265]	
Completeness to theta = 27.49°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9818 and 0.8895	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3546 / 2 / 274	
Goodness-of-fit on F^2	1.141	
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.1160	
R indices (all data)	R1 = 0.0494, wR2 = 0.1334	
Absolute structure parameter	0.01(9)	
Largest diff. peak and hole	0.371 and -0.280 $e.Å^{-3}$	

Determination of the absolute configuration of chiral compound 6a by X-ray Crystallographic analysis



6a

The crystal is triclinic, space group P-1. The asymmetric unit contains one molecule of the compound C25H31NO6S2Cl2. Final R values are R1= 0.0660 and wR2= 0.1672 for 2-theta max of 55º.



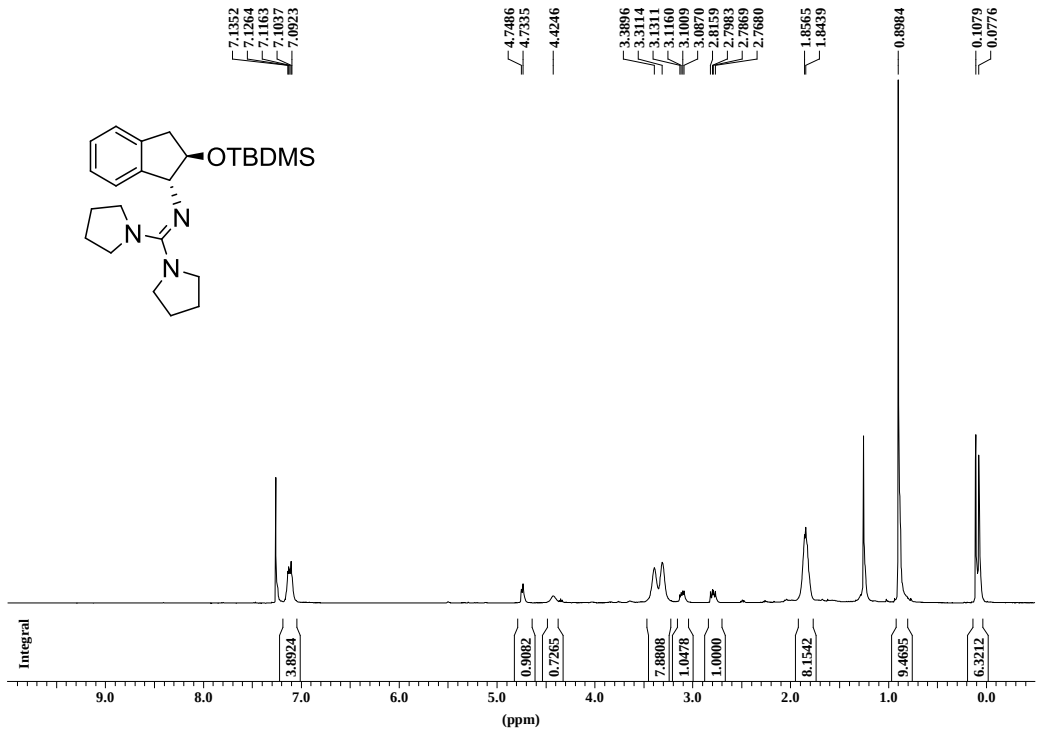
Crystal data and structure refinement for A106.

Identification code	a106
Empirical formula	C25 H31 Cl2 N O6 S2
Formula weight	576.53
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1

Unit cell dimensions	a = 9.3366(10) Å	α= 105.126(2)°.
	b = 10.2792(11) Å	β= 101.706(2)°.
	c = 16.2940(17) Å	γ = 99.829(2)°.
Volume	1436.2(3) $Å^3$	
Z	2	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	0.410 mm^{-1}	
F(000)	604	
Crystal size	0.56 x 0.18 x 0.08 mm^3	
Theta range for data collection	1.34 to 27.49°.	
Index ranges	-12<=h<=12, -13<=k<=13, -21<=l<=21	
Reflections collected	18790	
Independent reflections	6589 [R(int) = 0.0314]	
Completeness to theta = 27.49°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9680 and 0.8031	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6589 / 27 / 342	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0660, wR2 = 0.1672	
R indices (all data)	R1 = 0.0763, wR2 = 0.1800	
Largest diff. peak and hole	0.707 and -0.671 $e.Å^{-3}$	

Copy of NMR spectrum

1H AMX500 zhy1031 3 1 cat TBS



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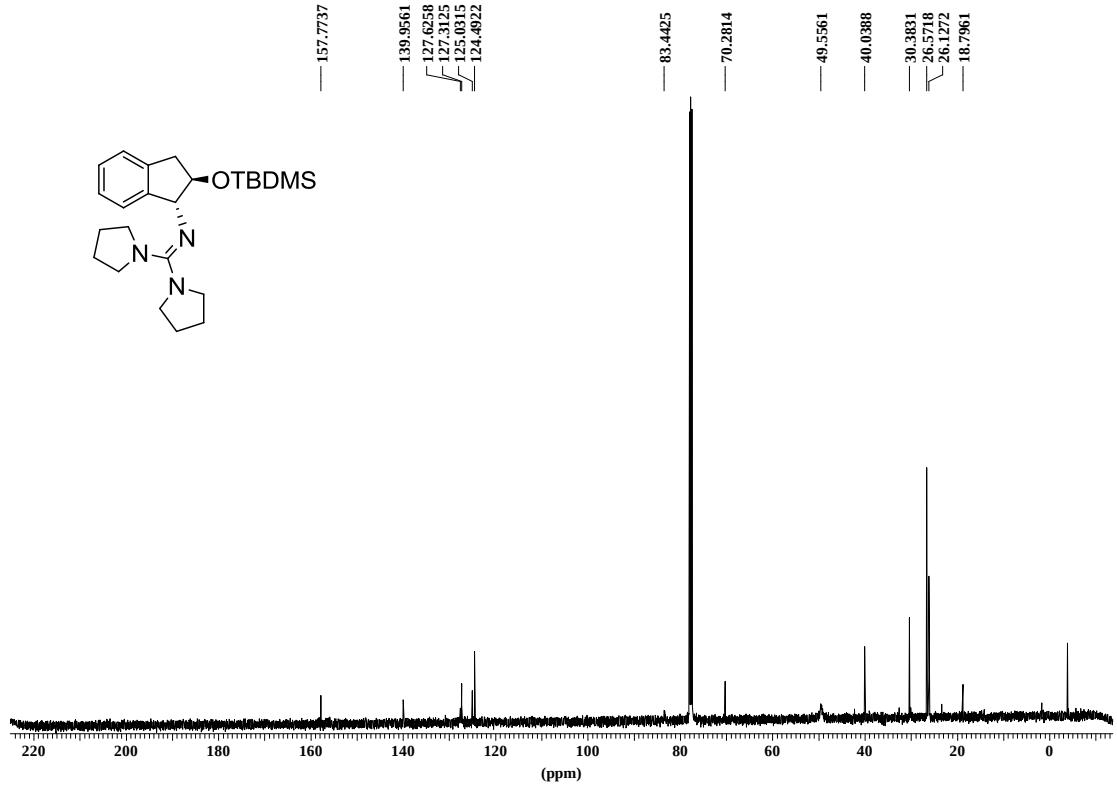

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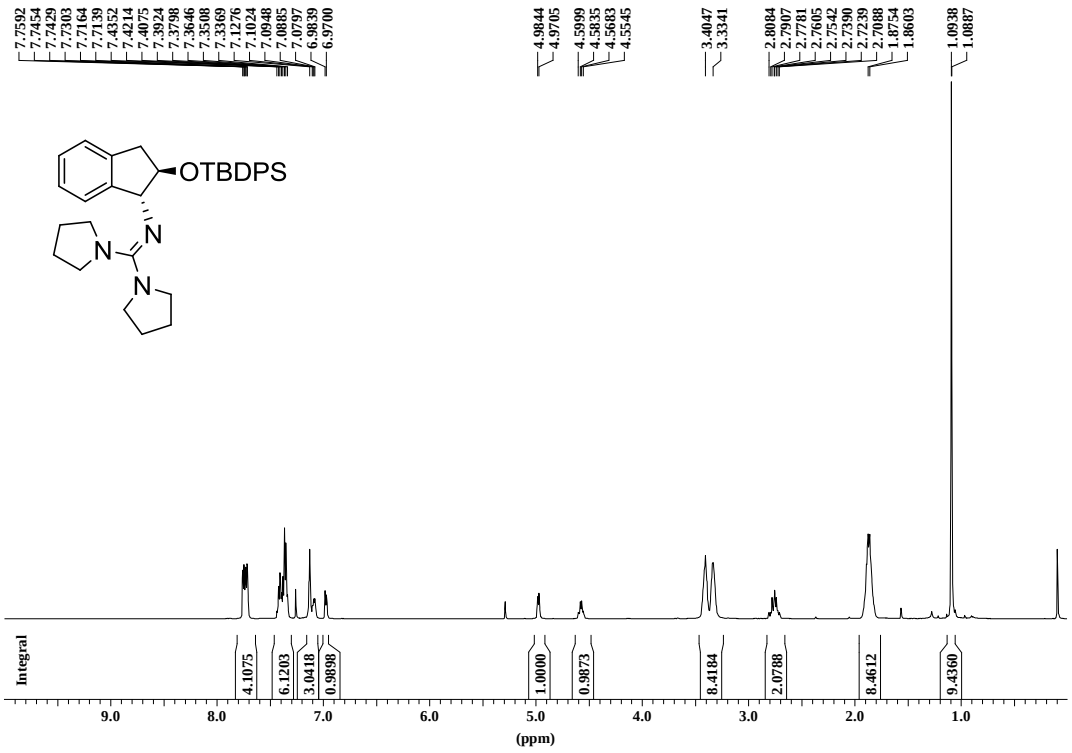

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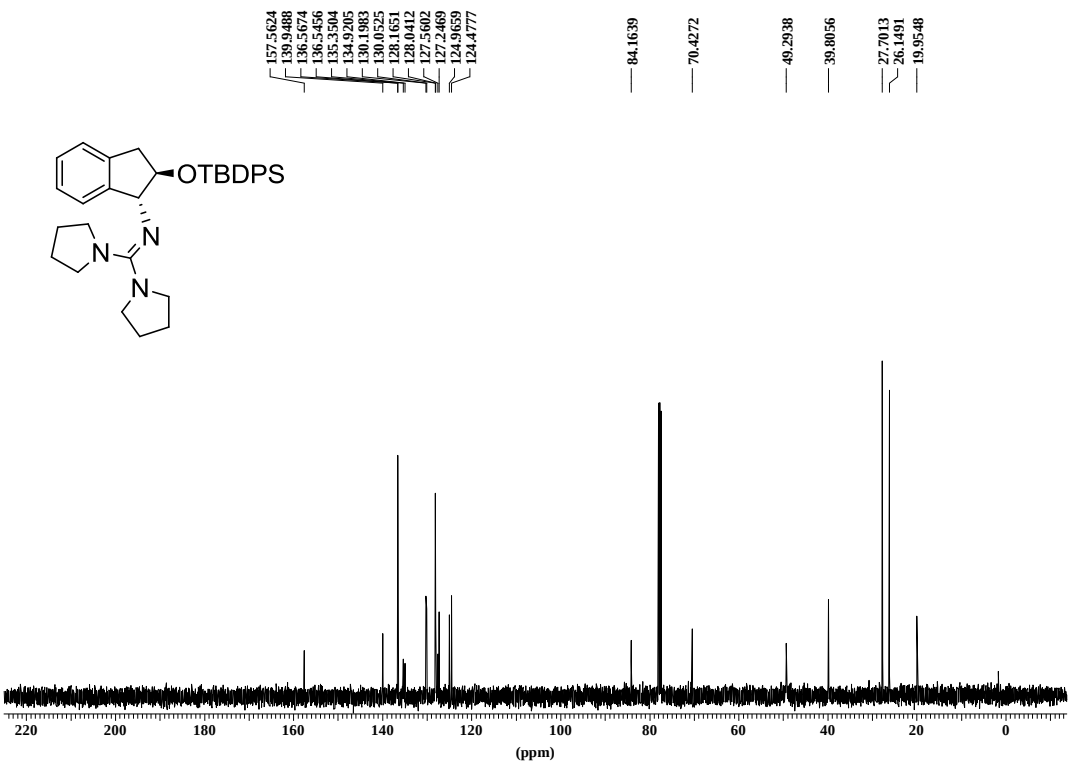

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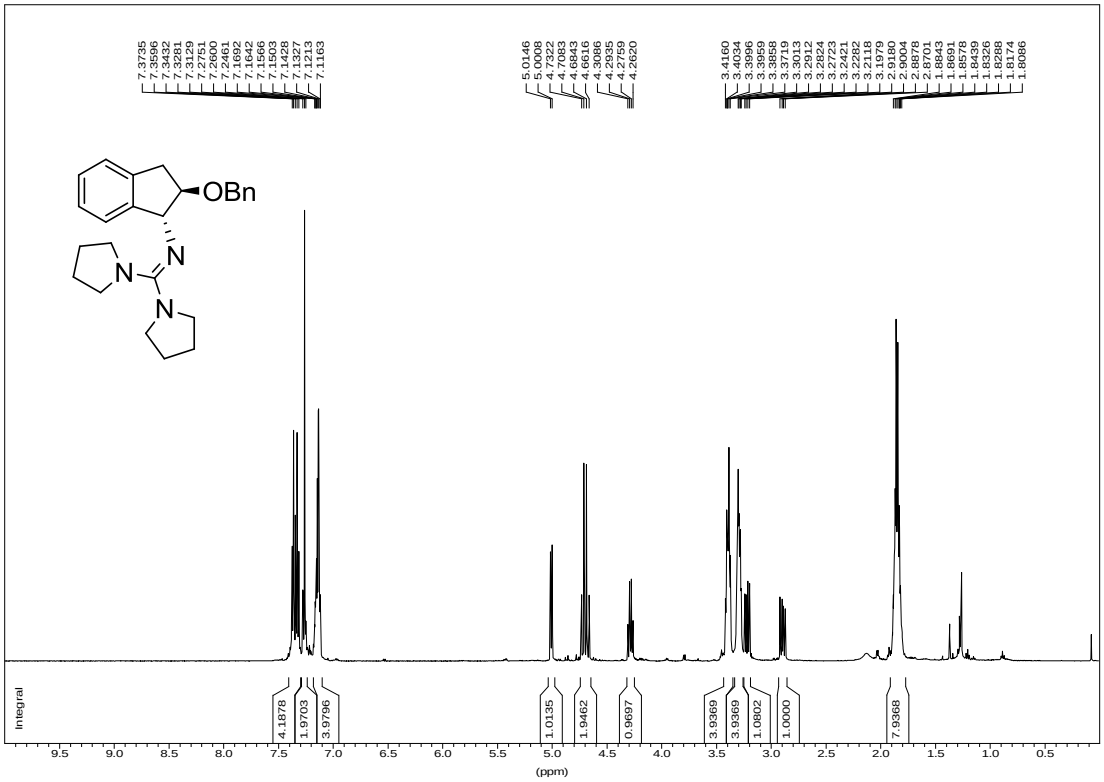

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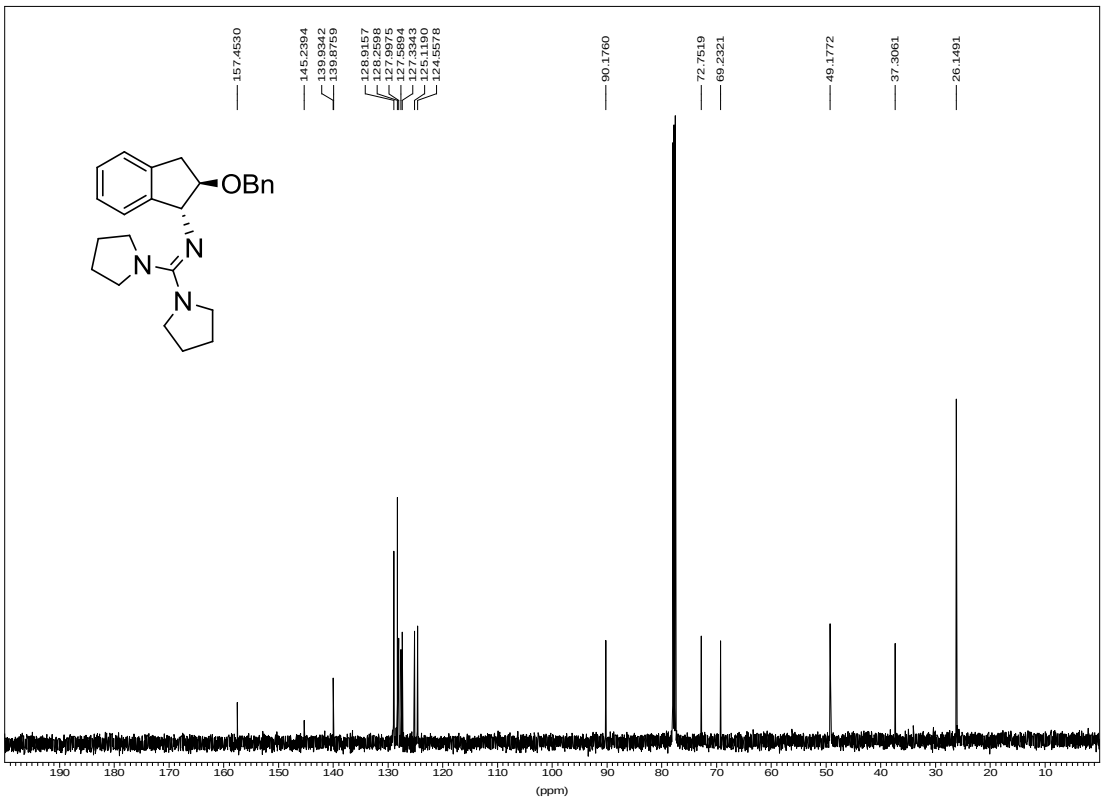

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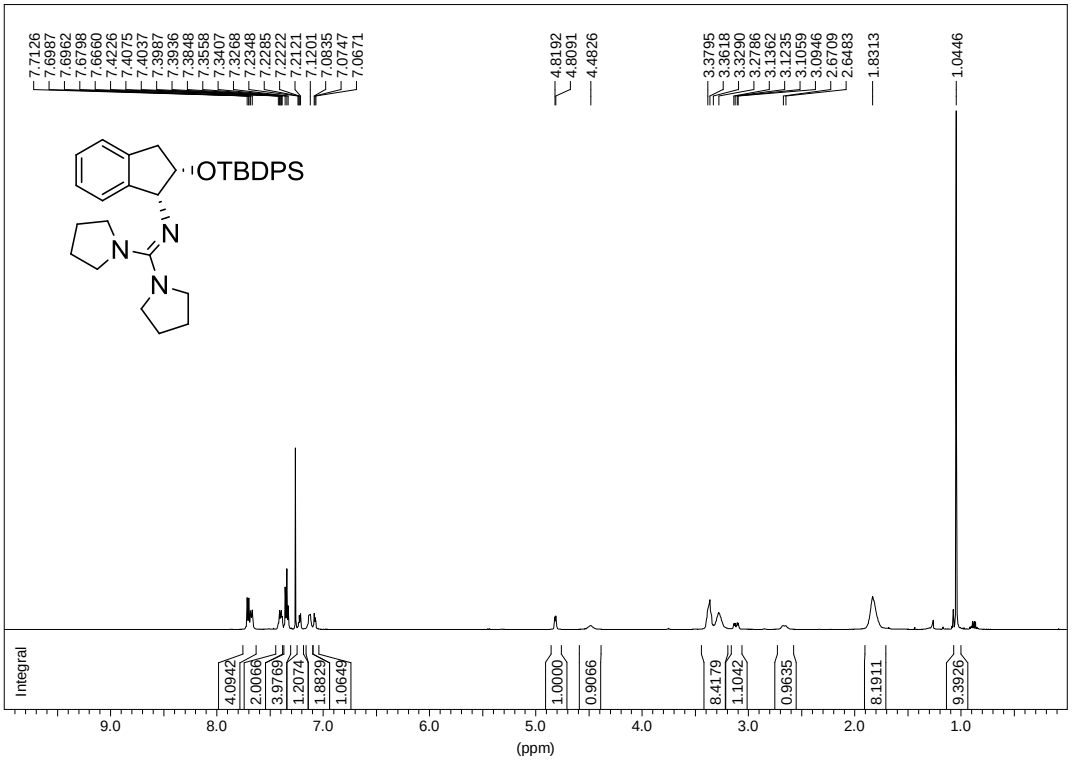

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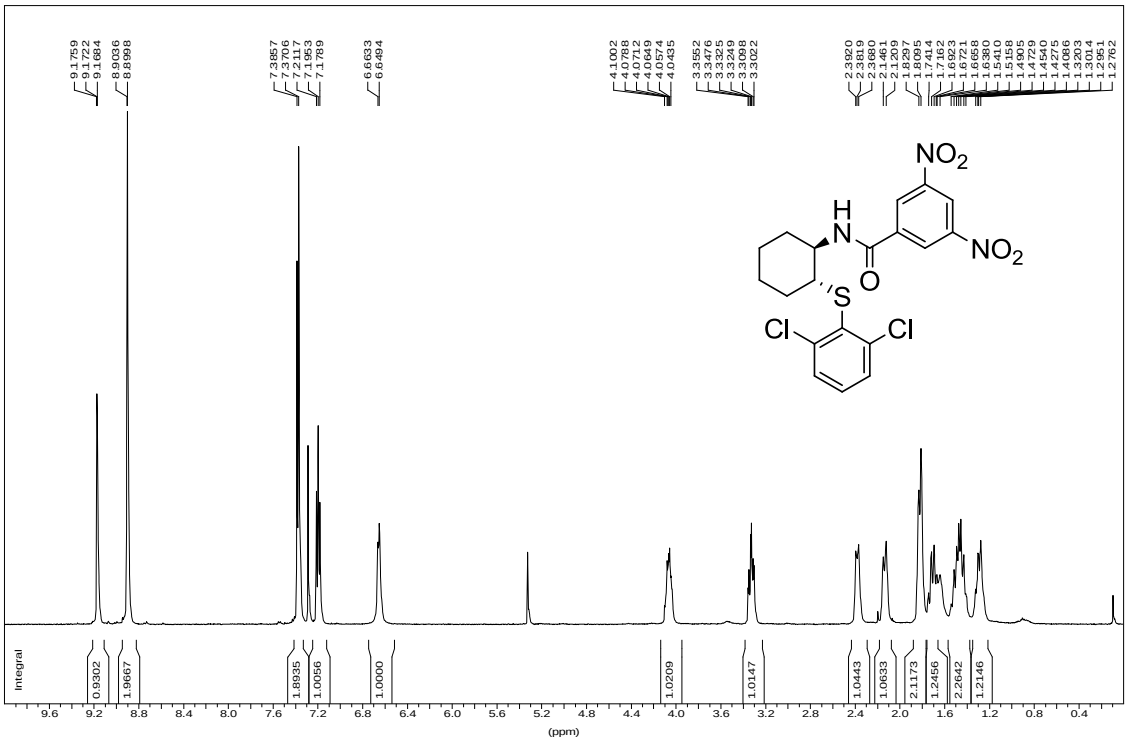

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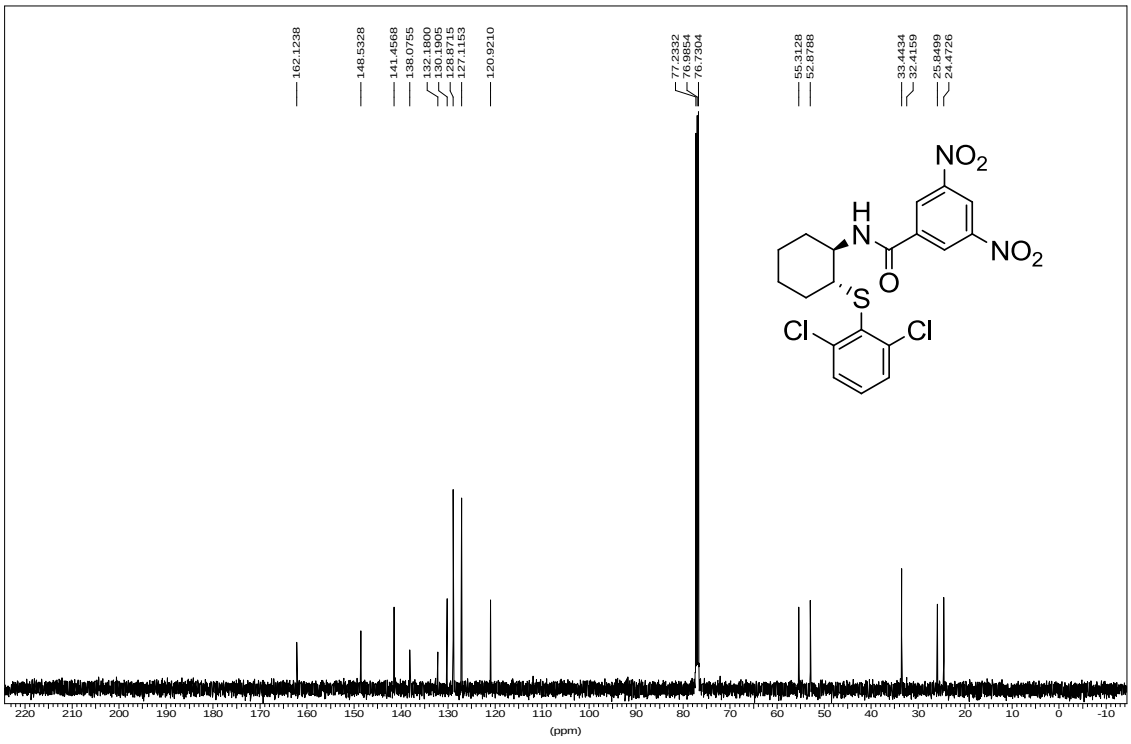

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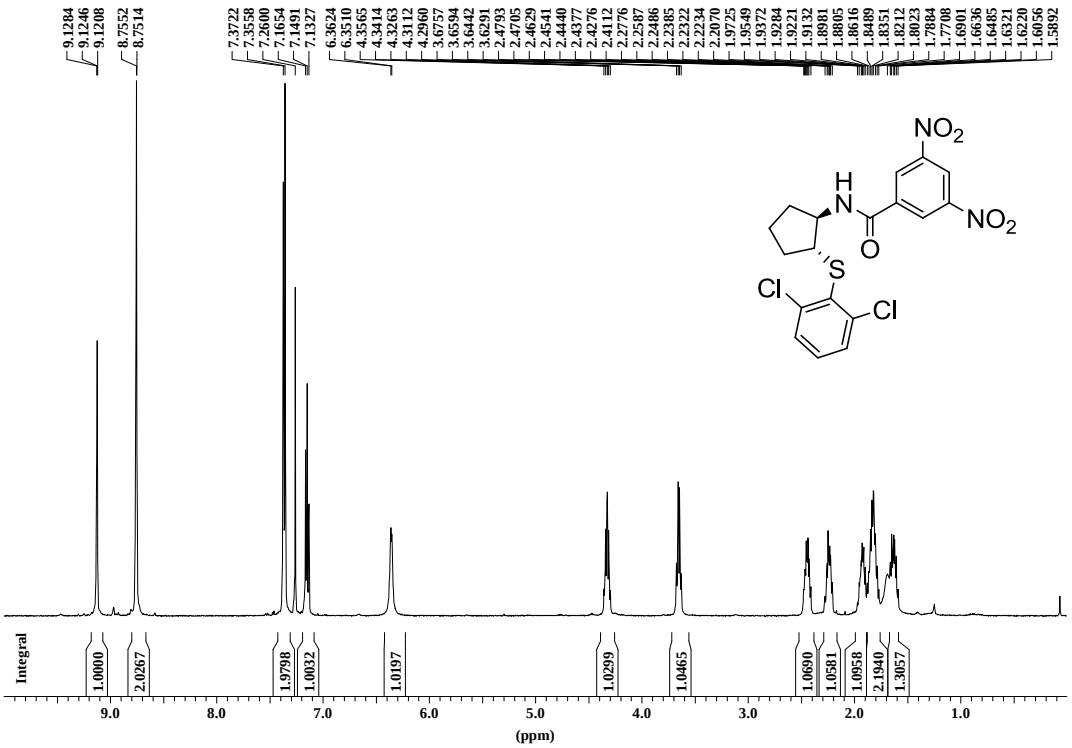

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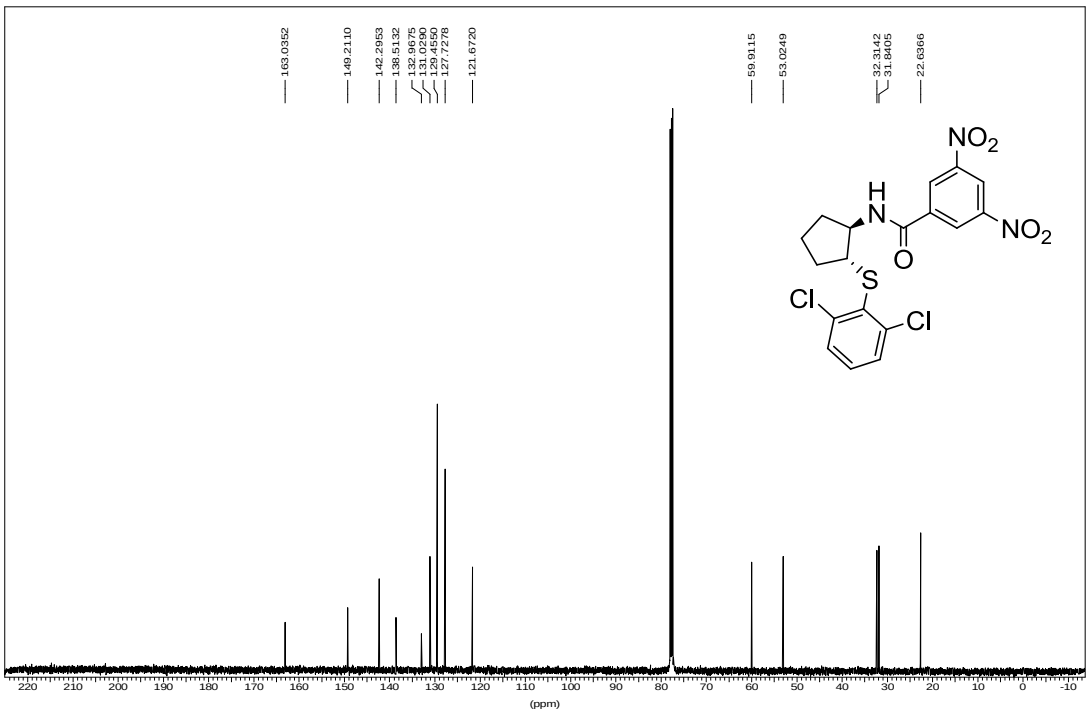

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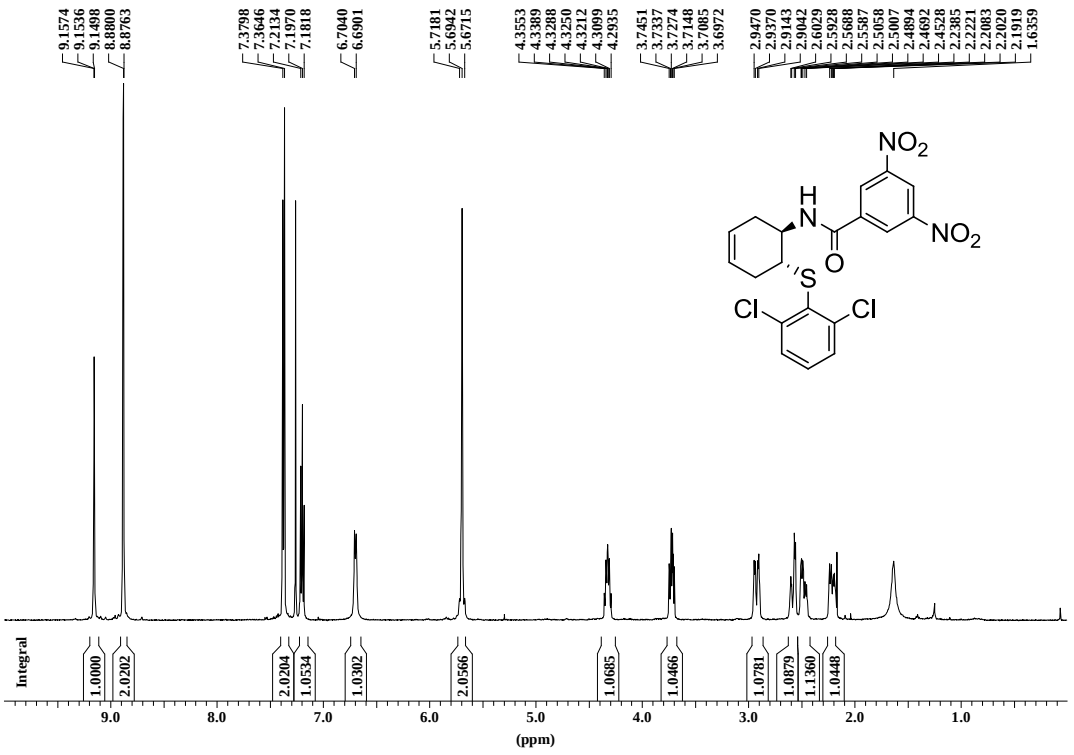

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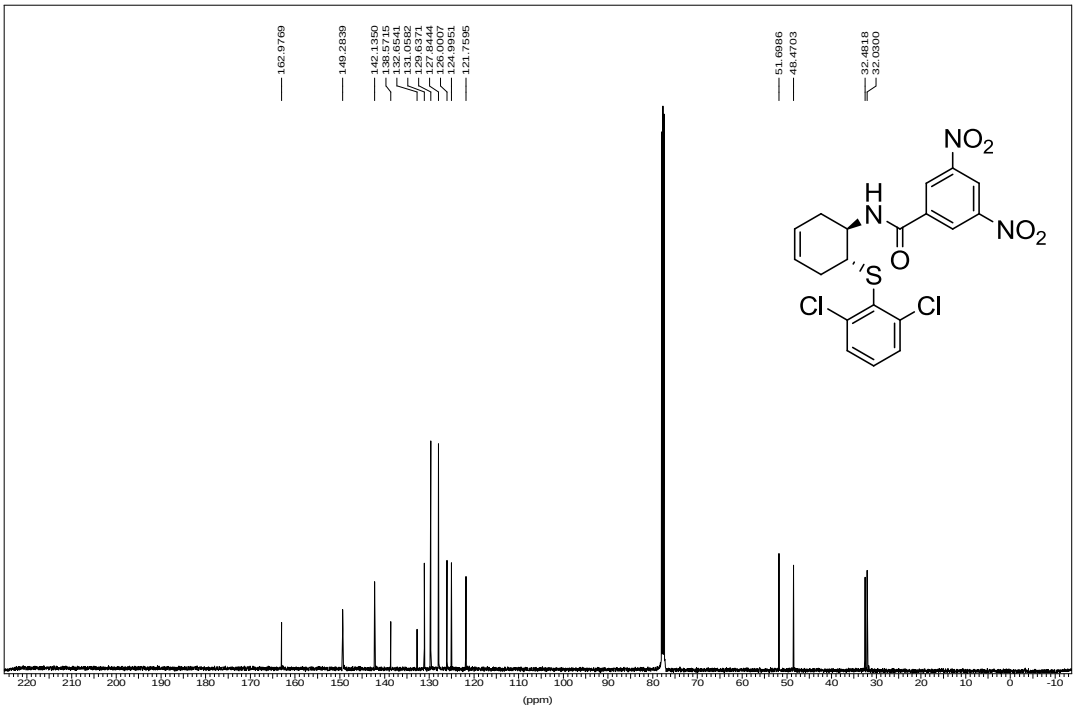

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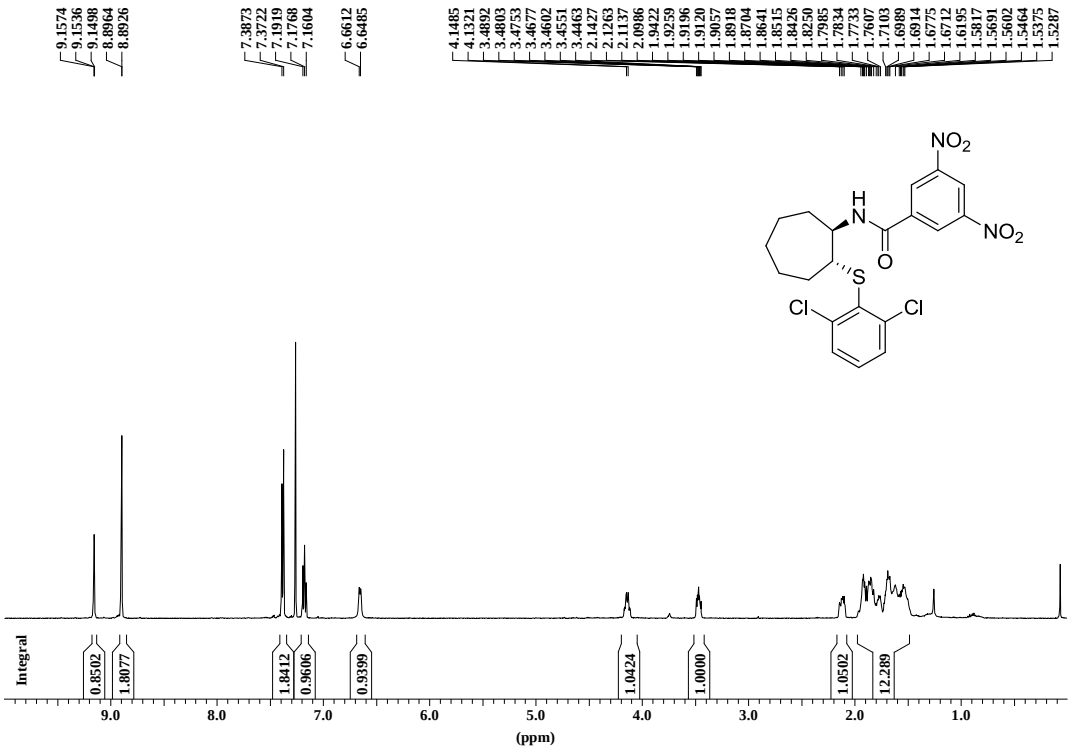

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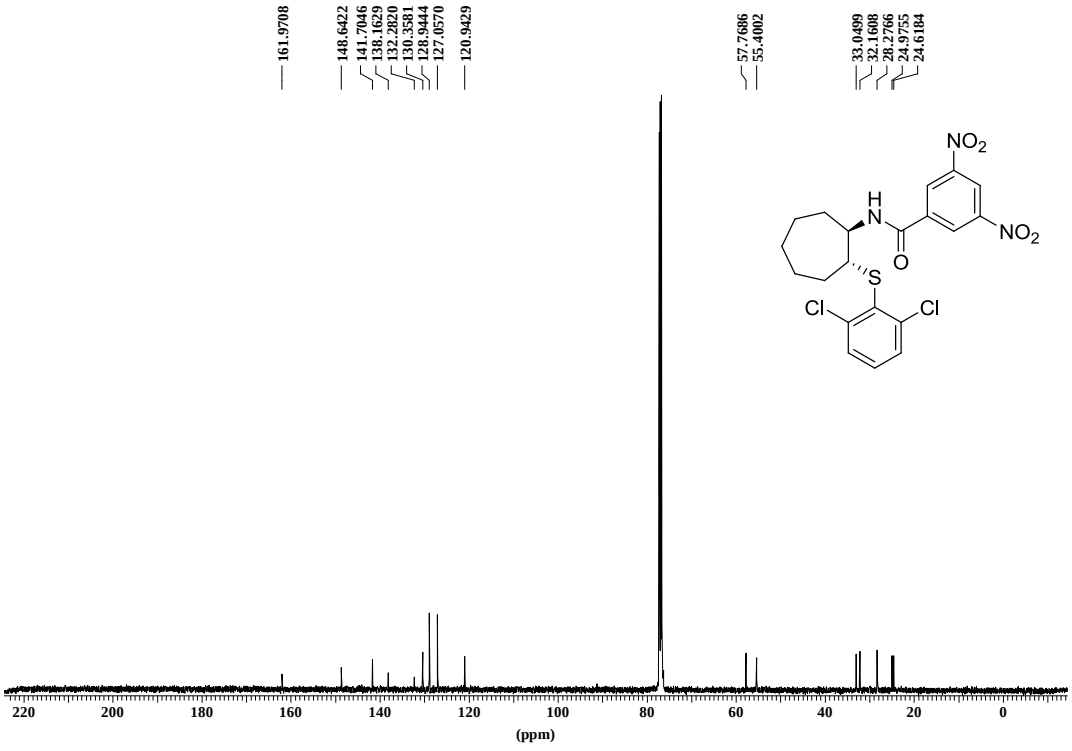

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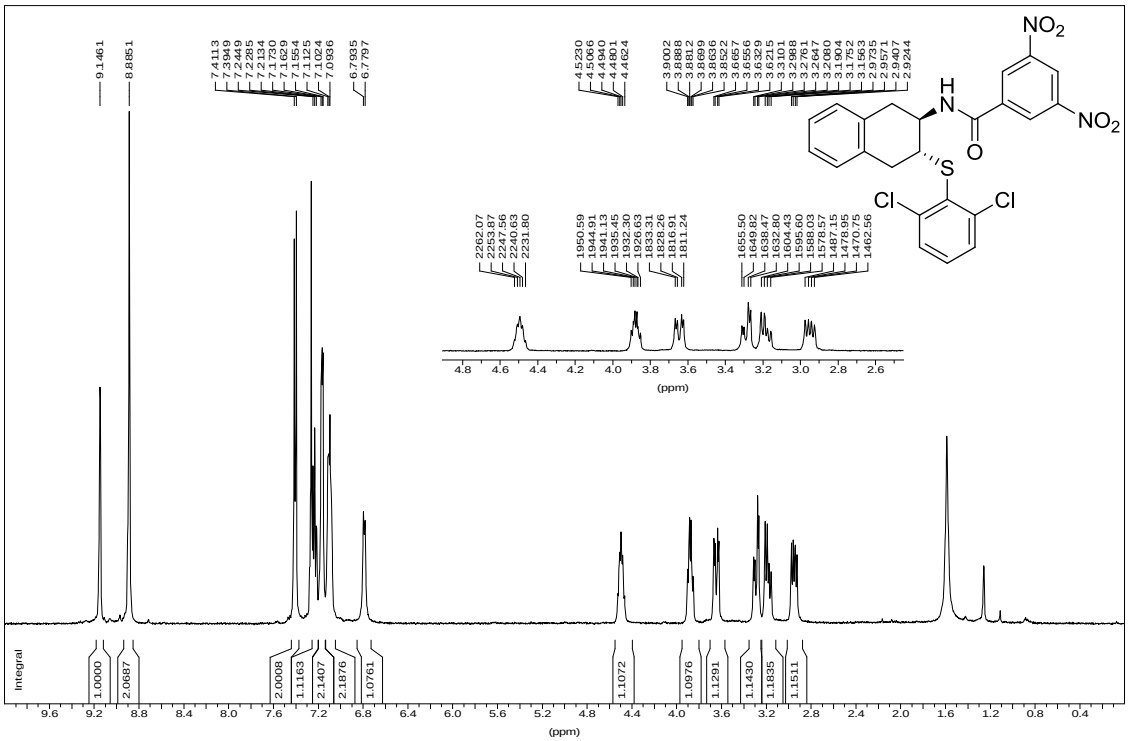

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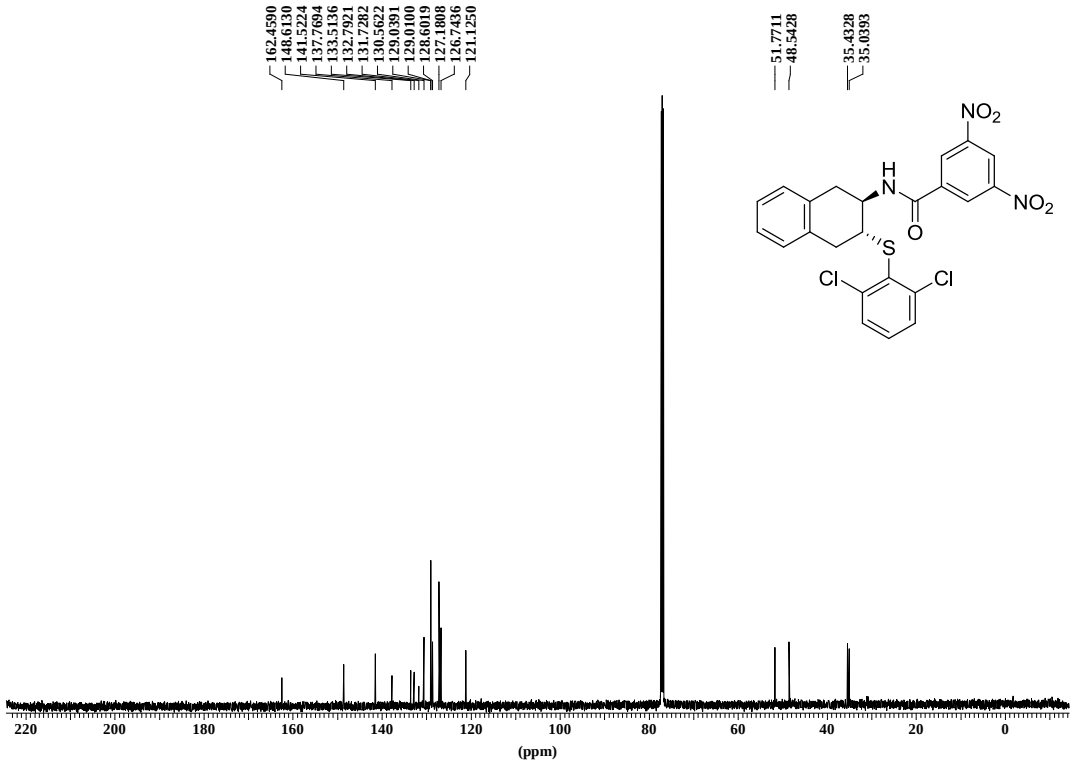

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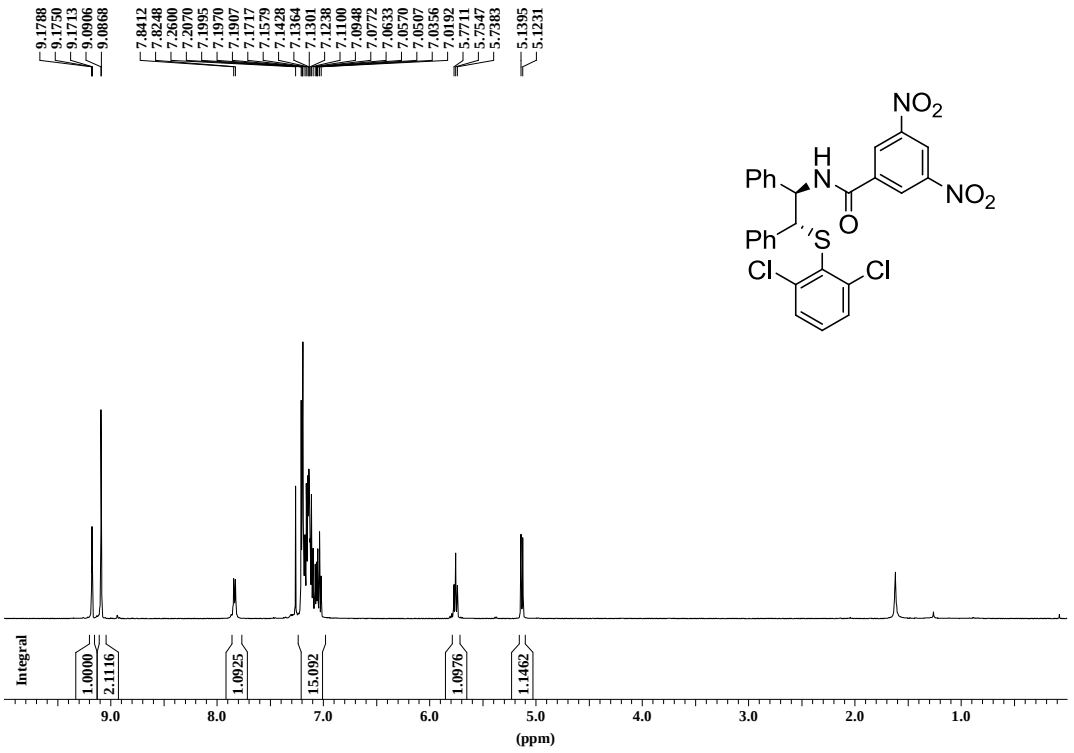

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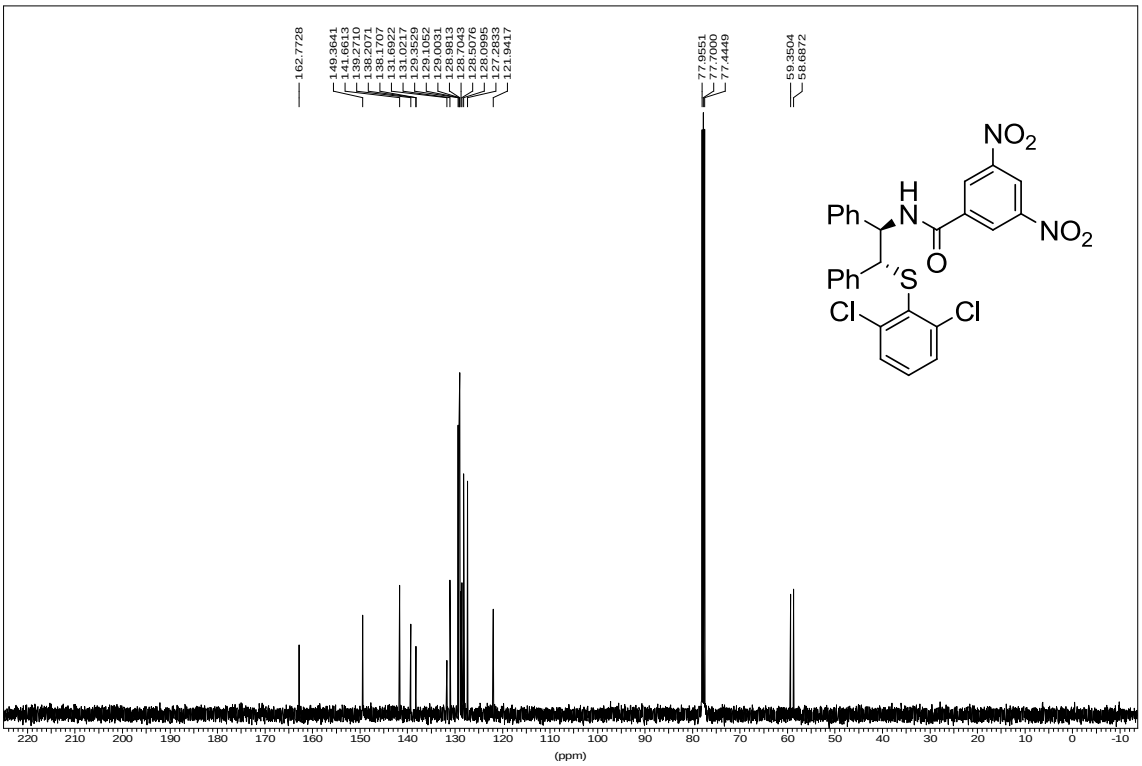

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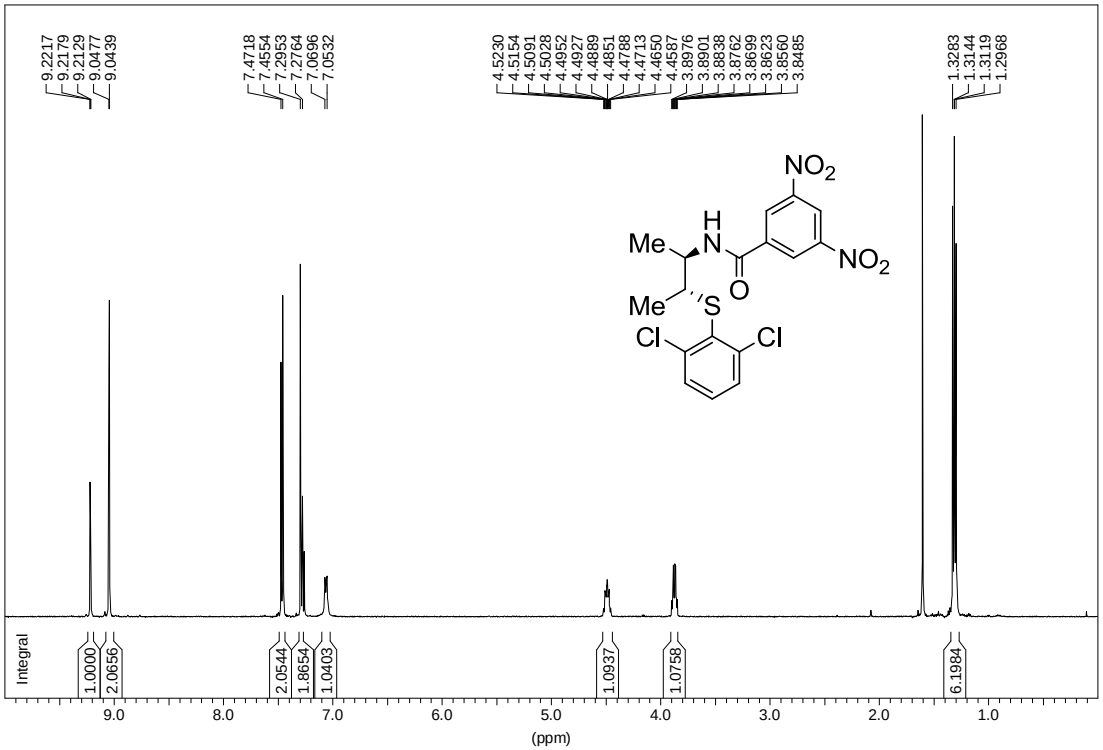

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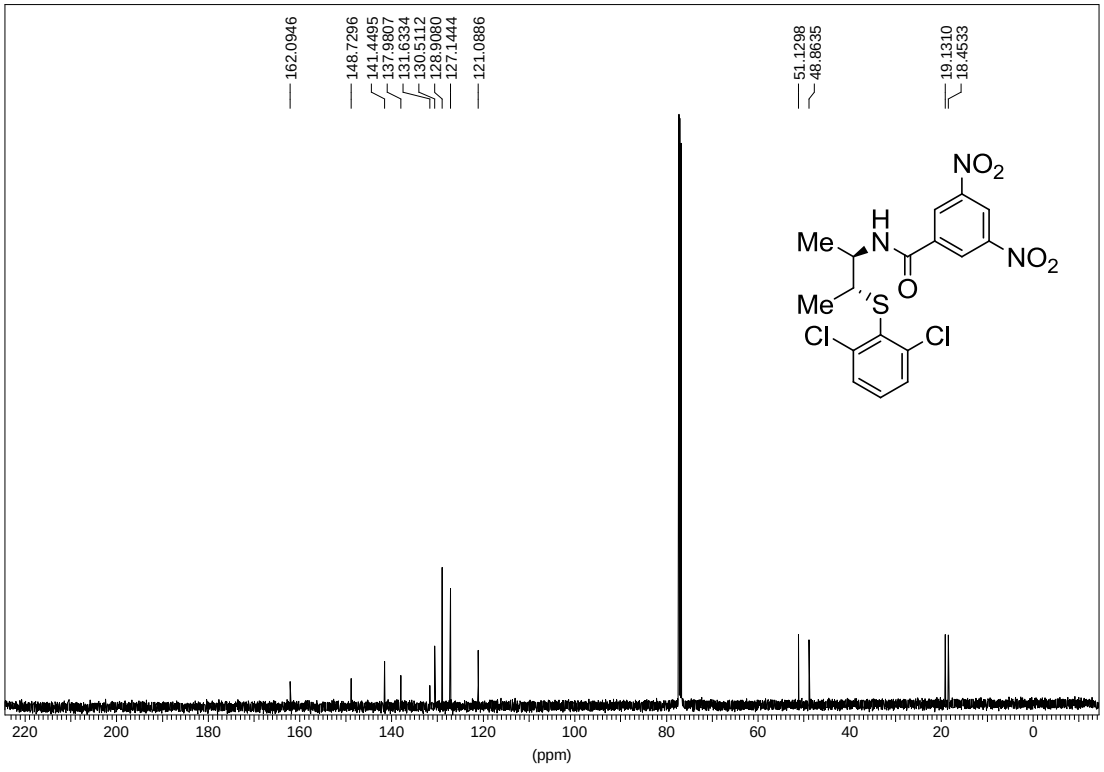

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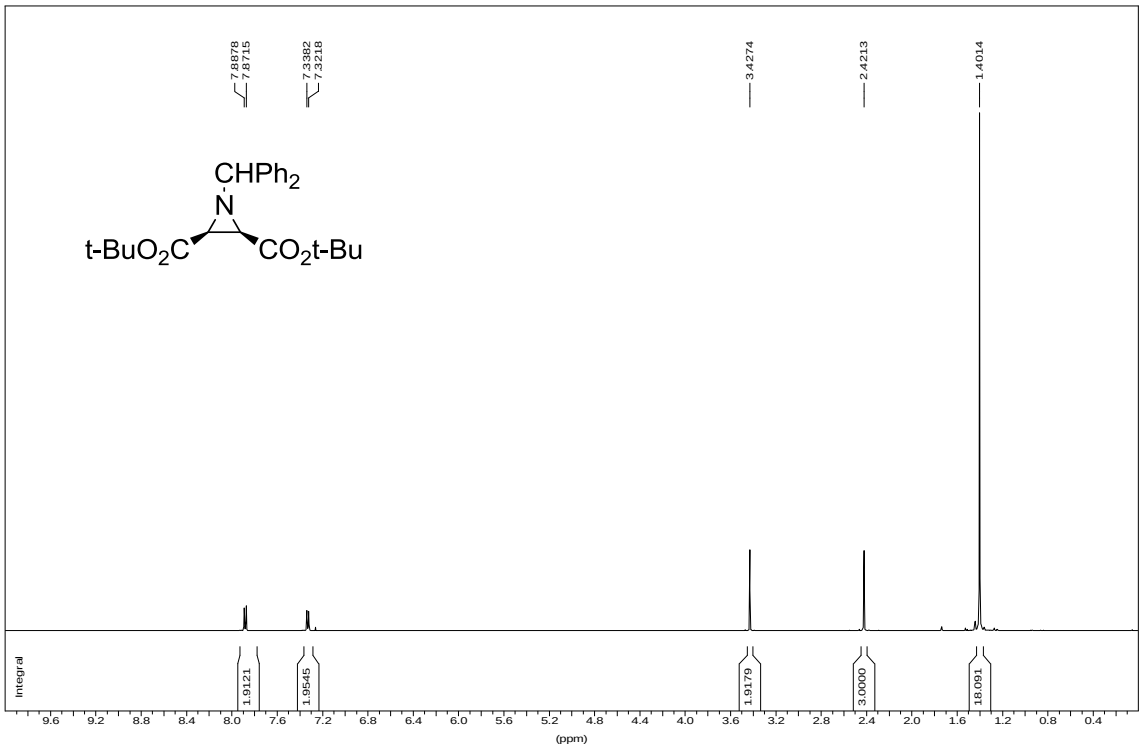

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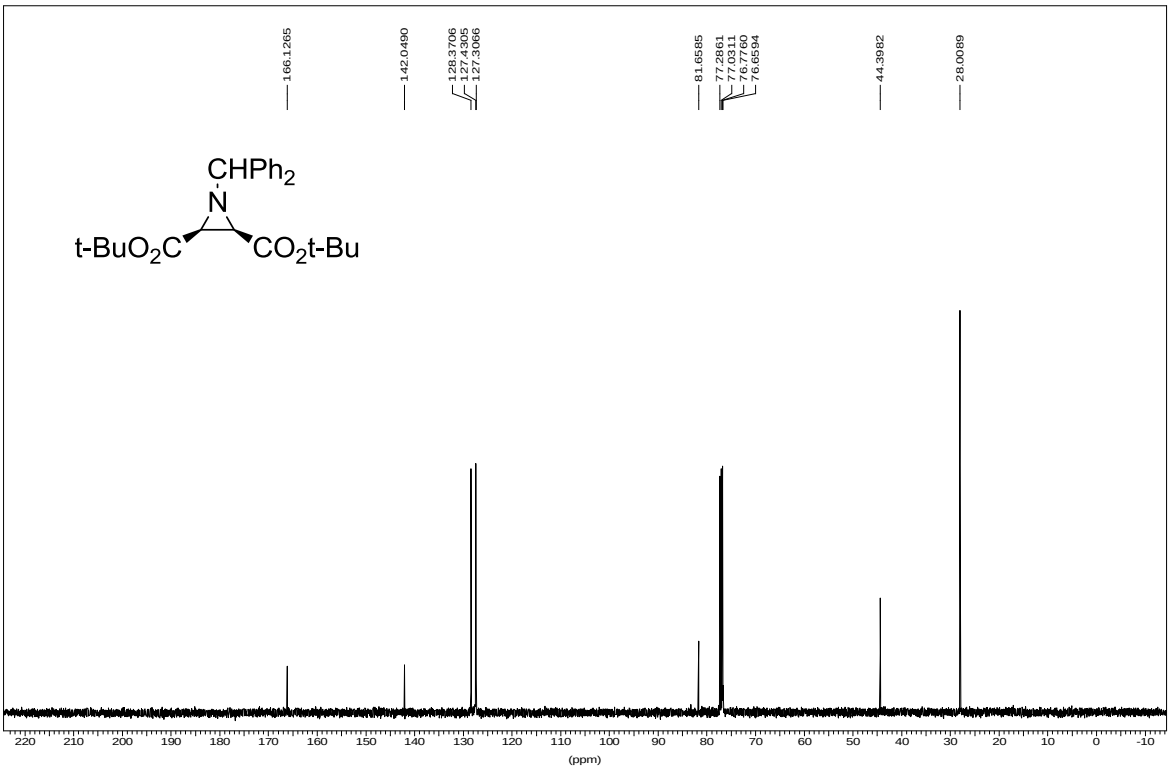

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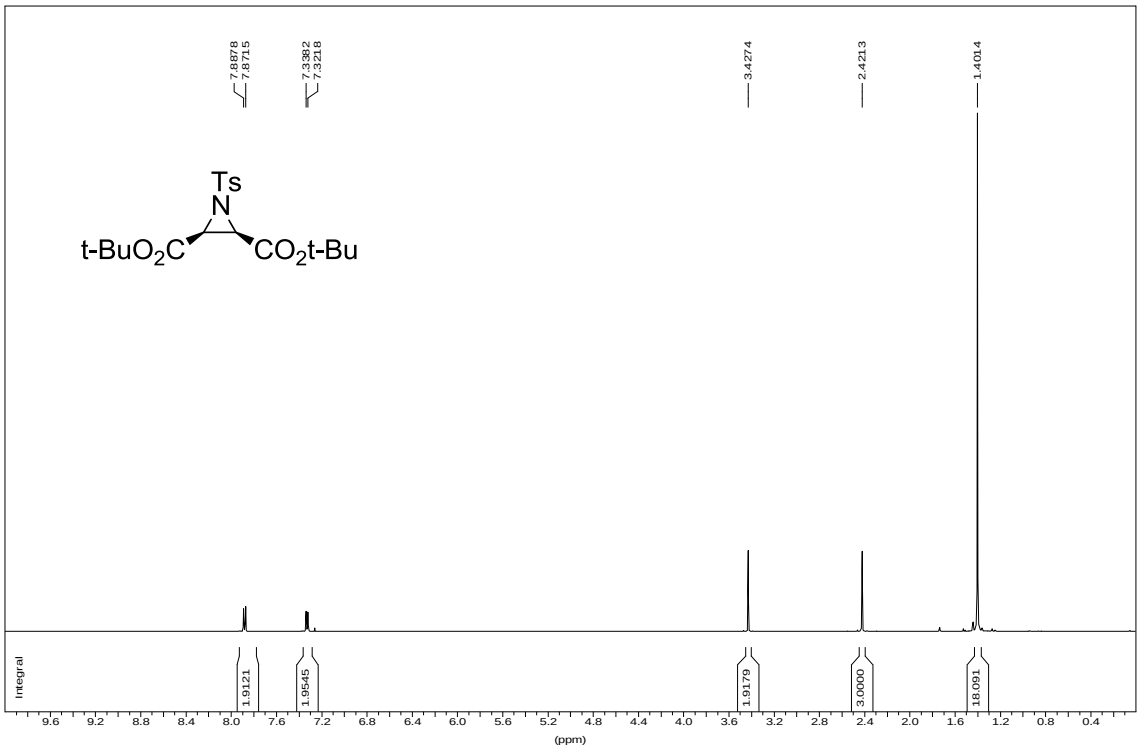

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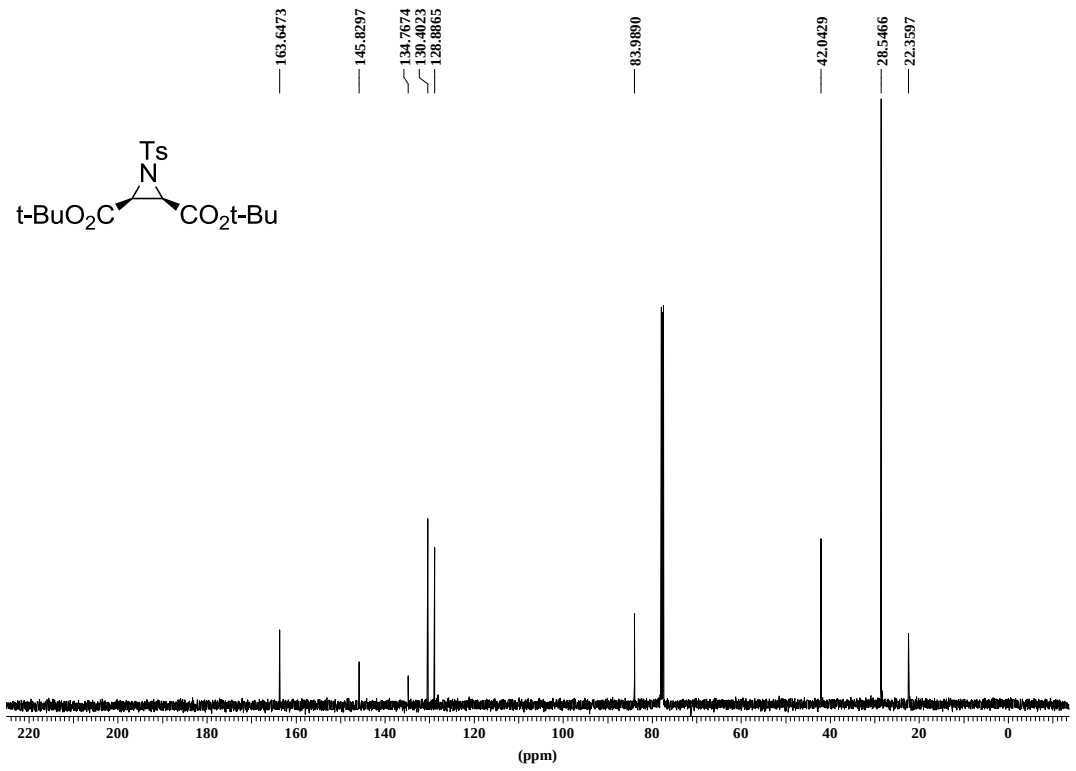

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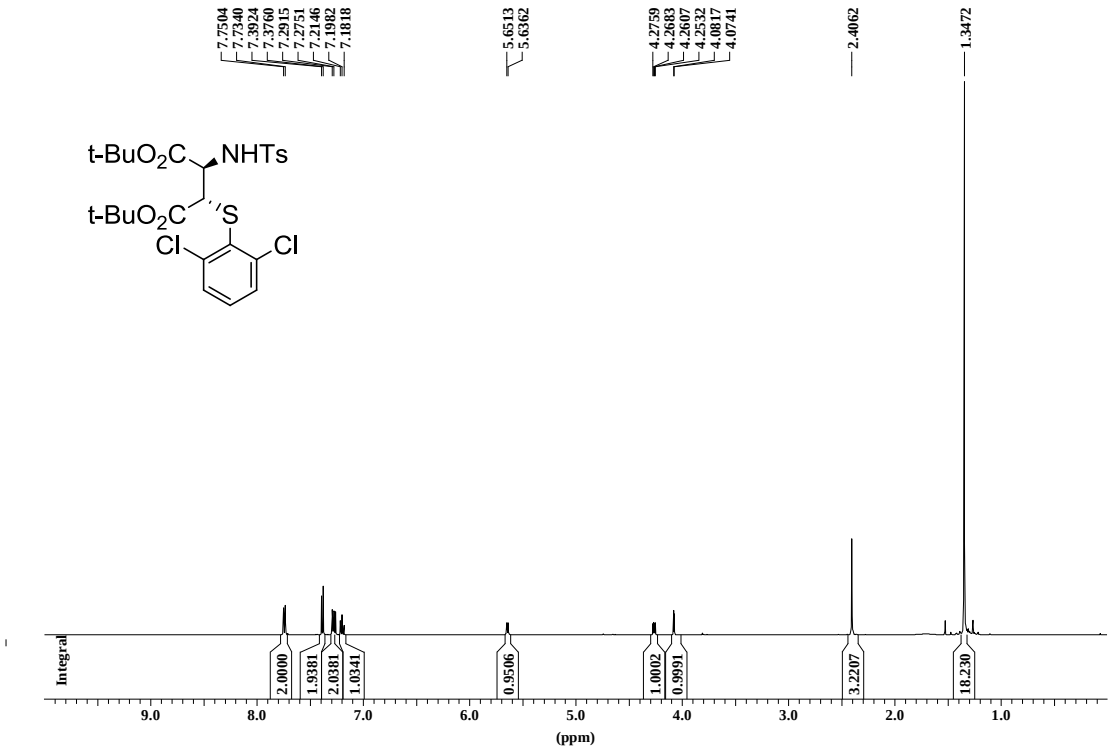

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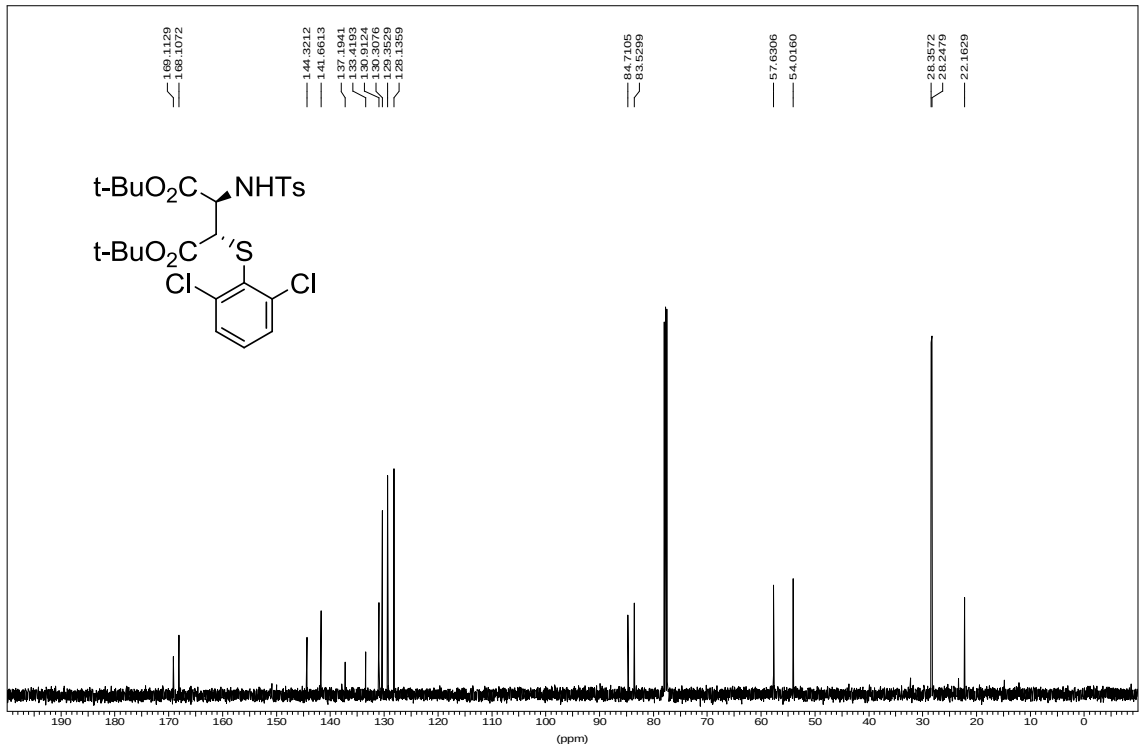

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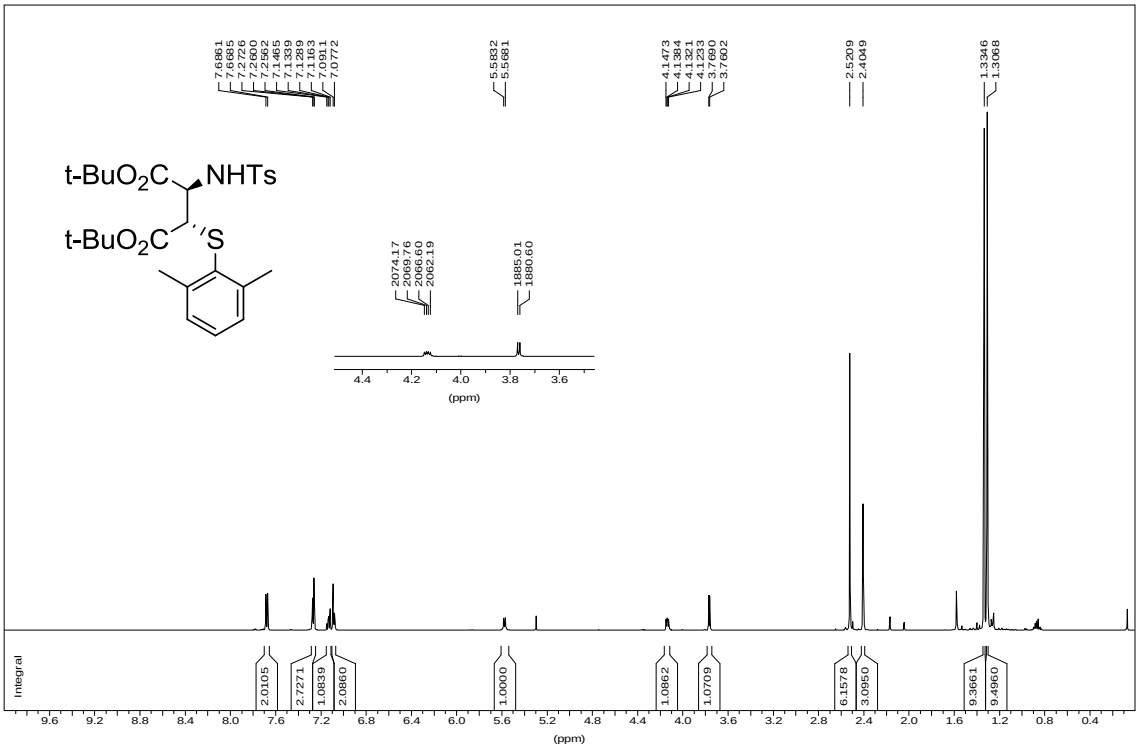

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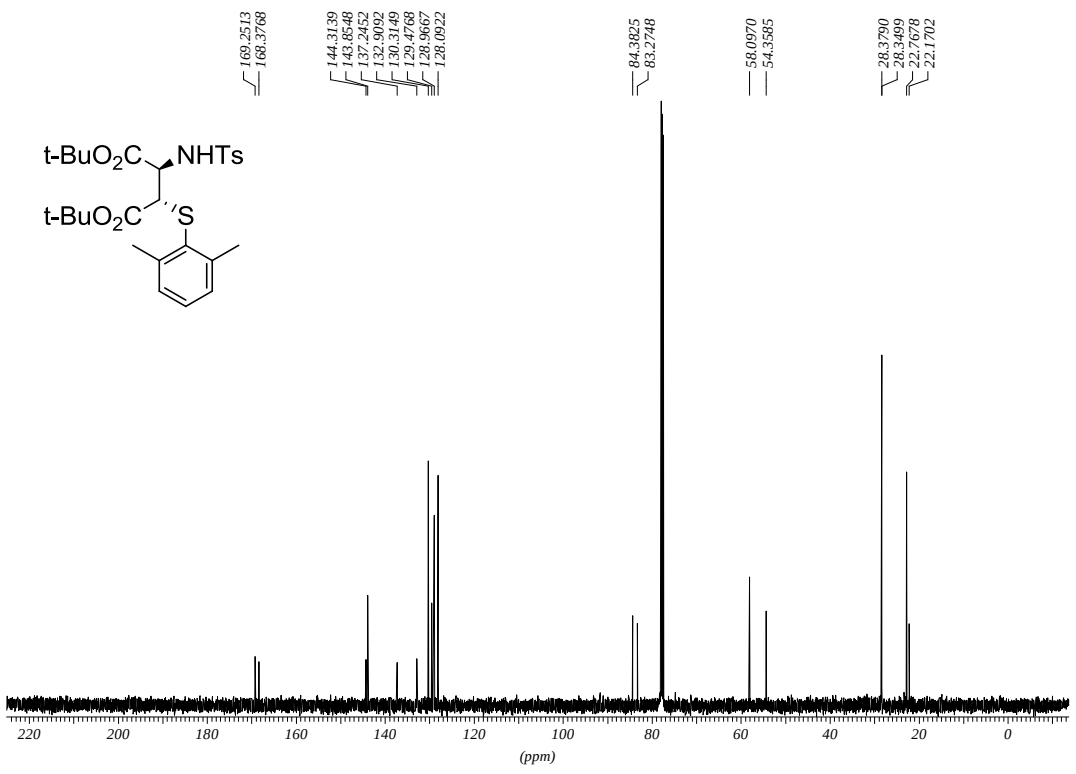

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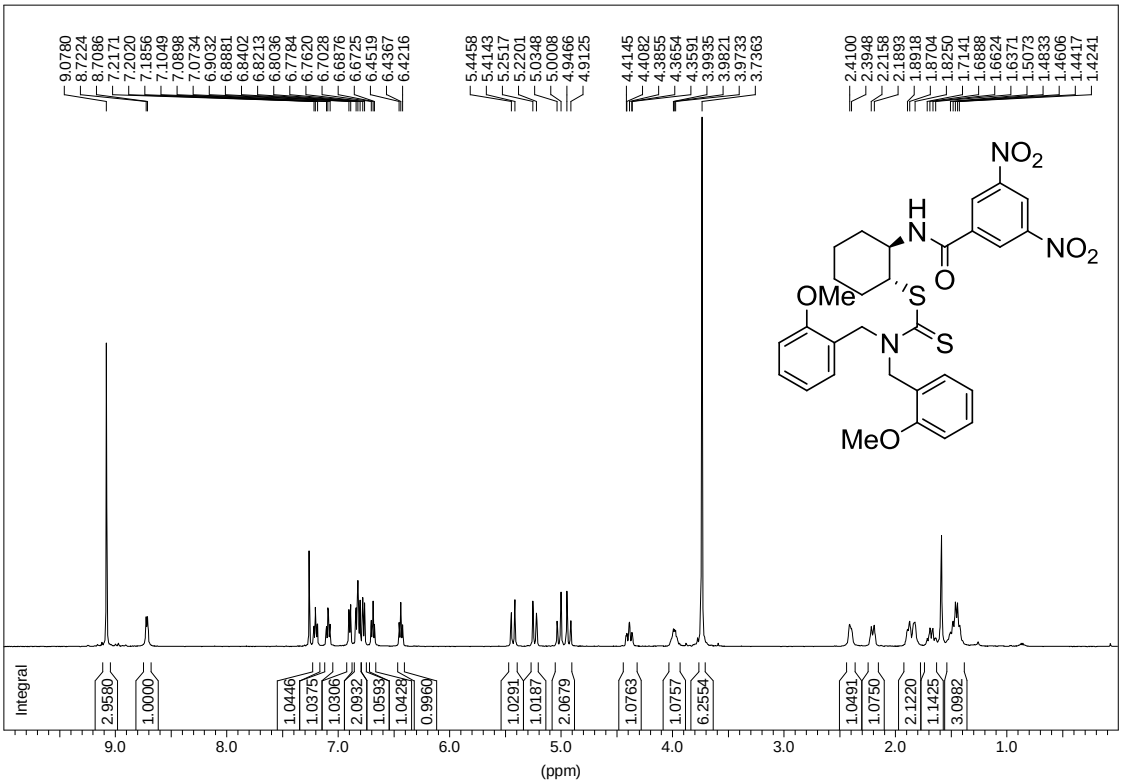

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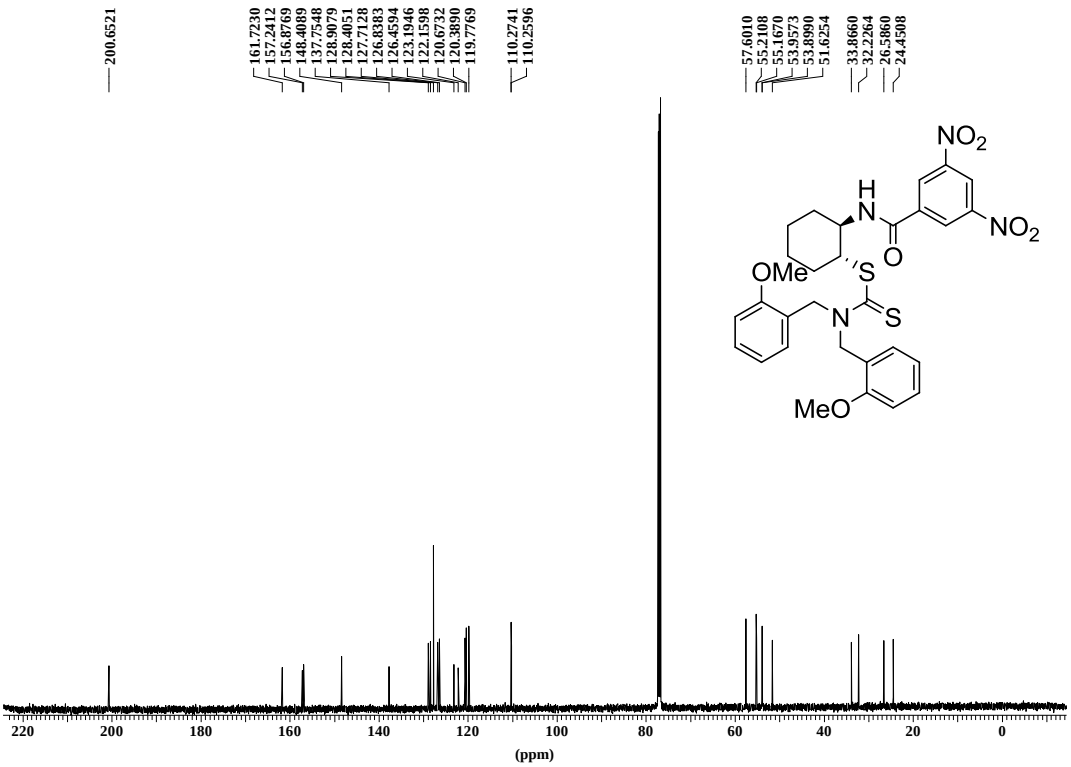

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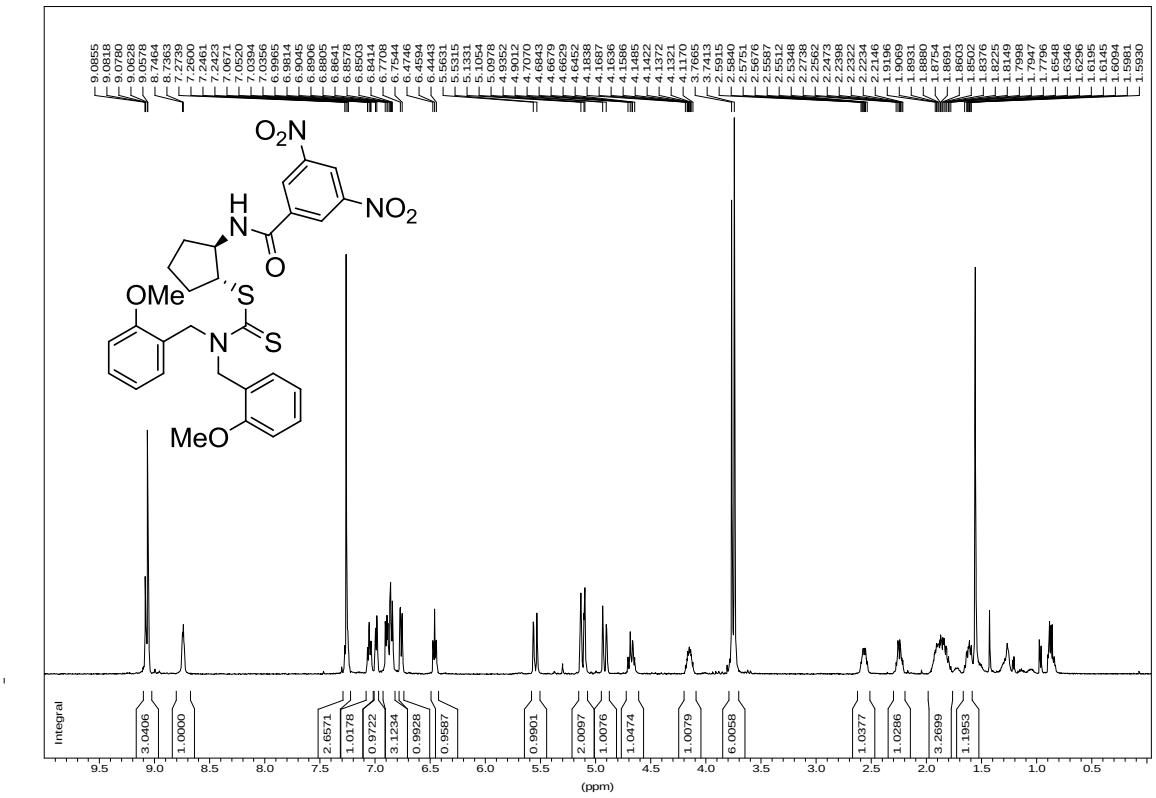

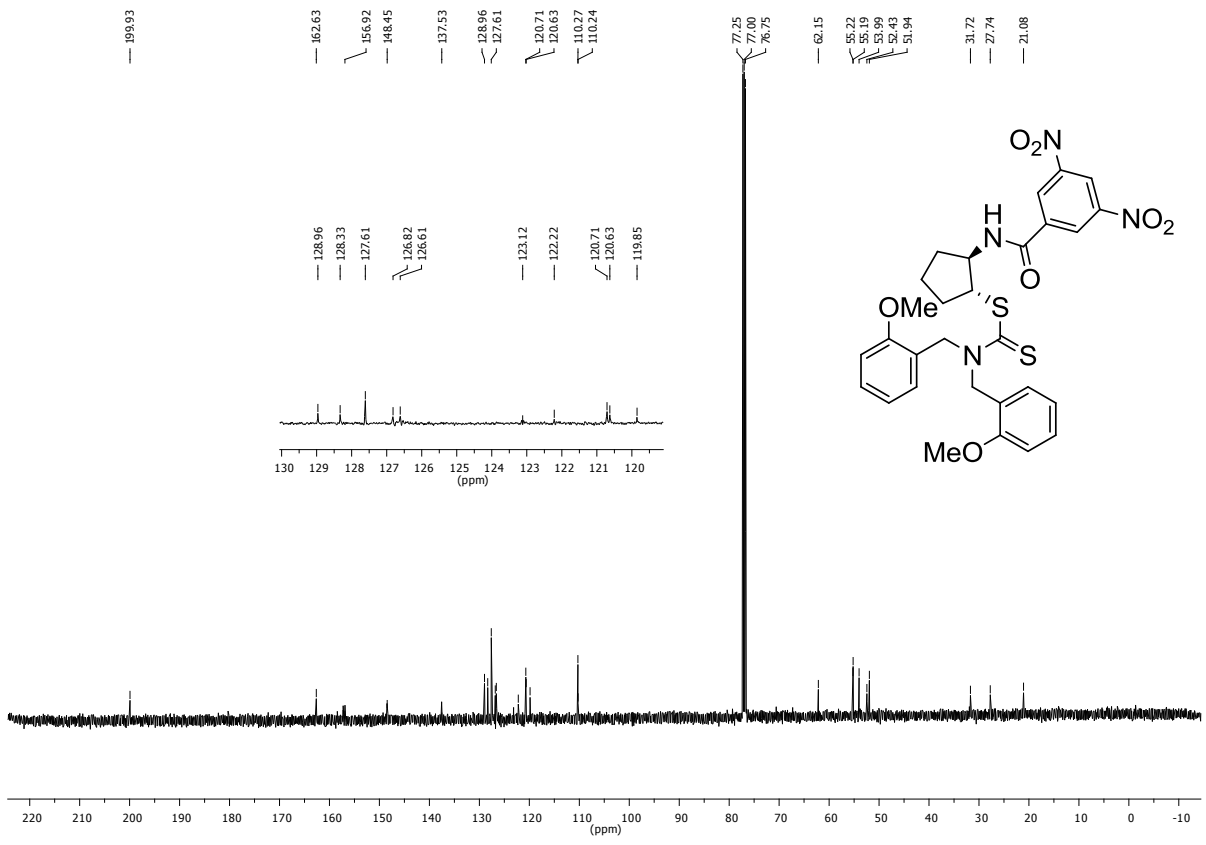

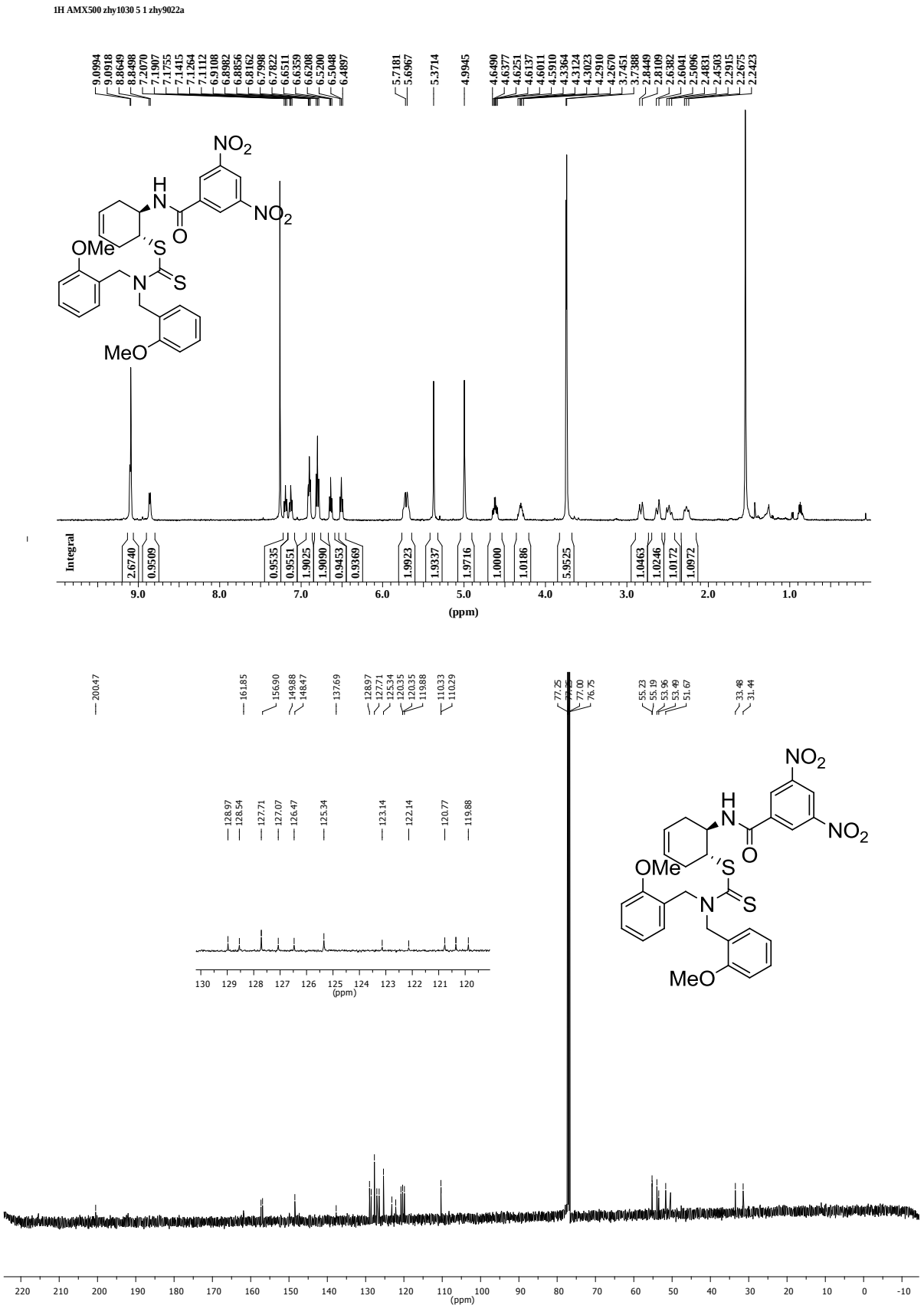
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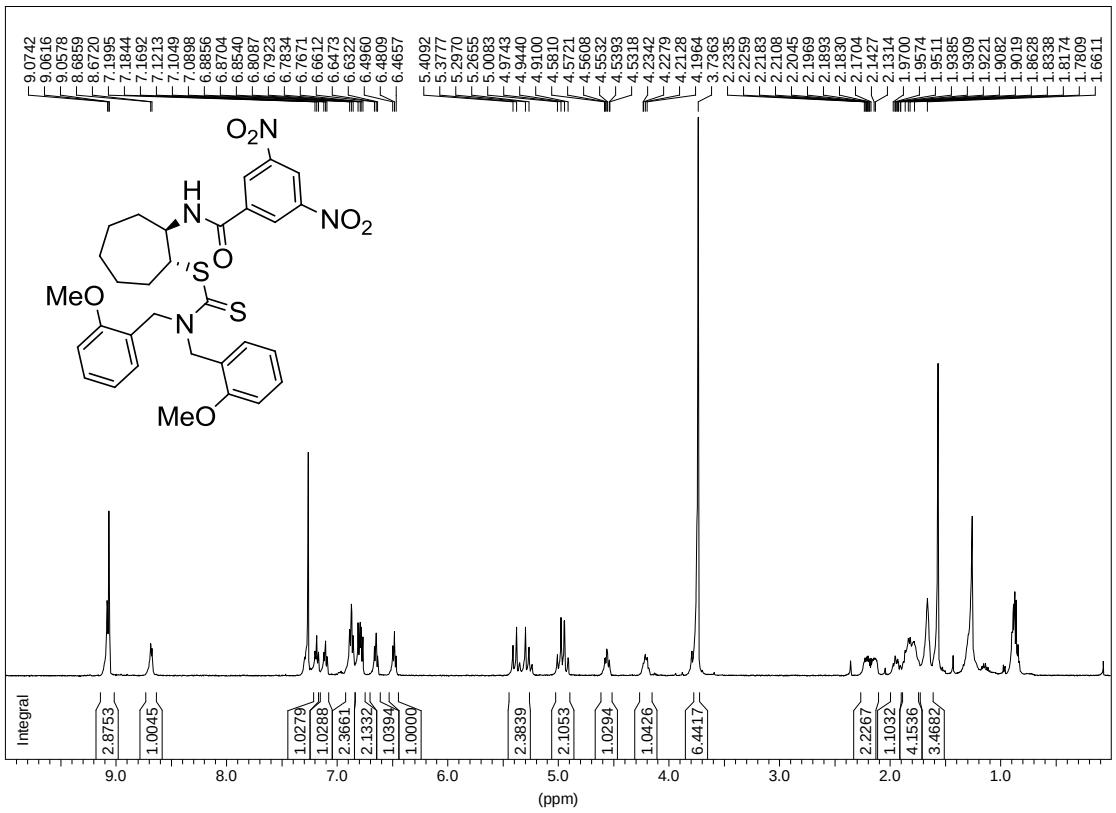

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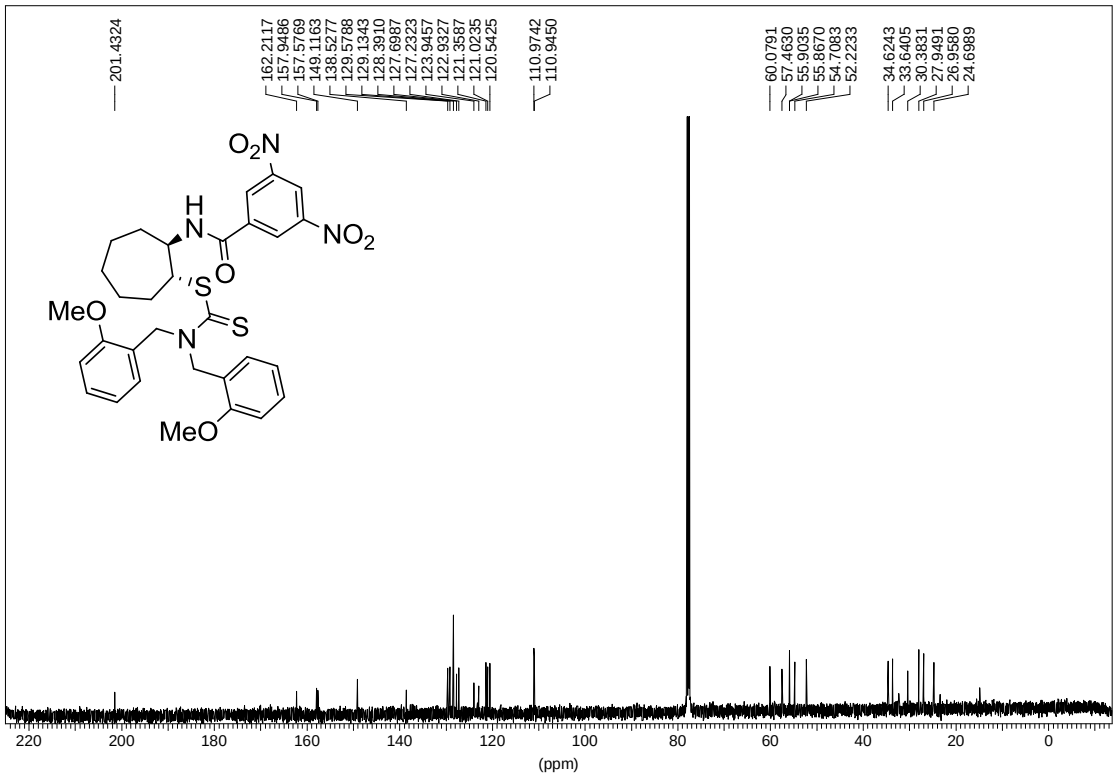

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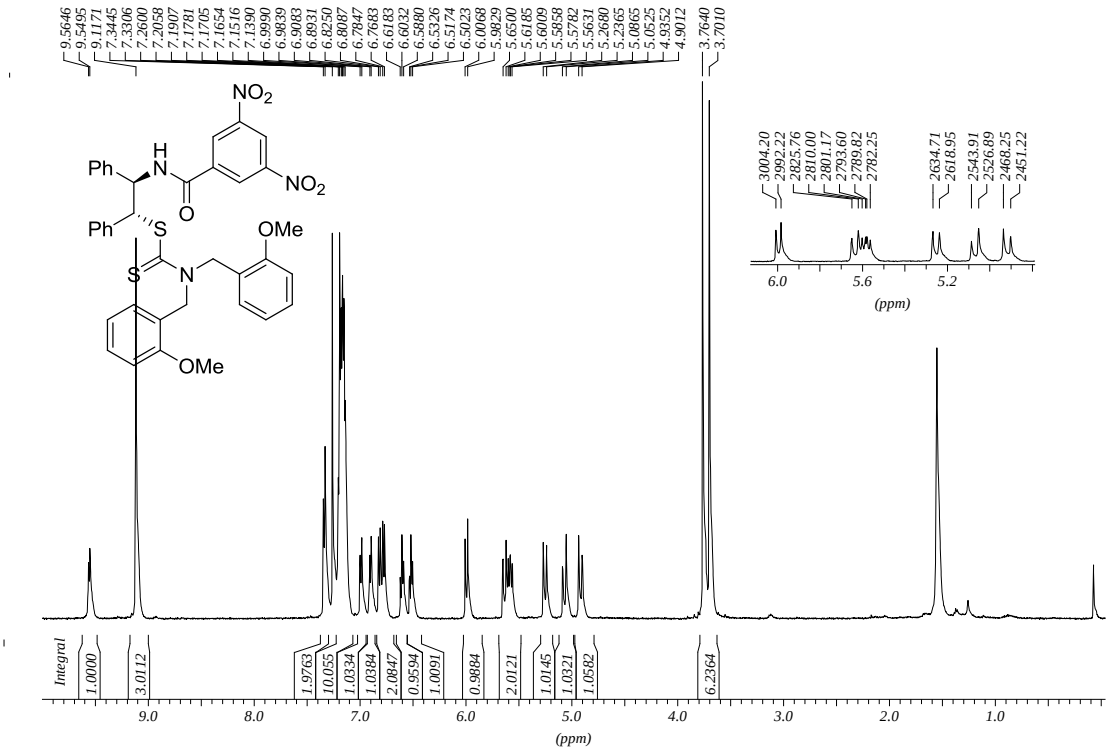

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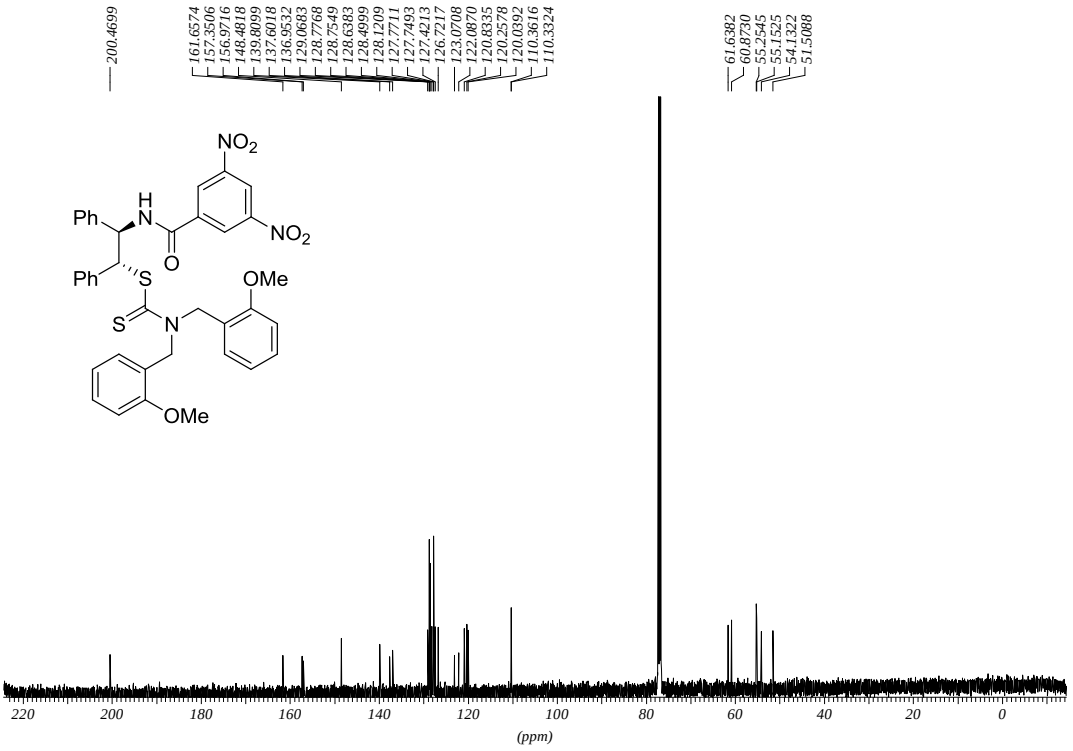

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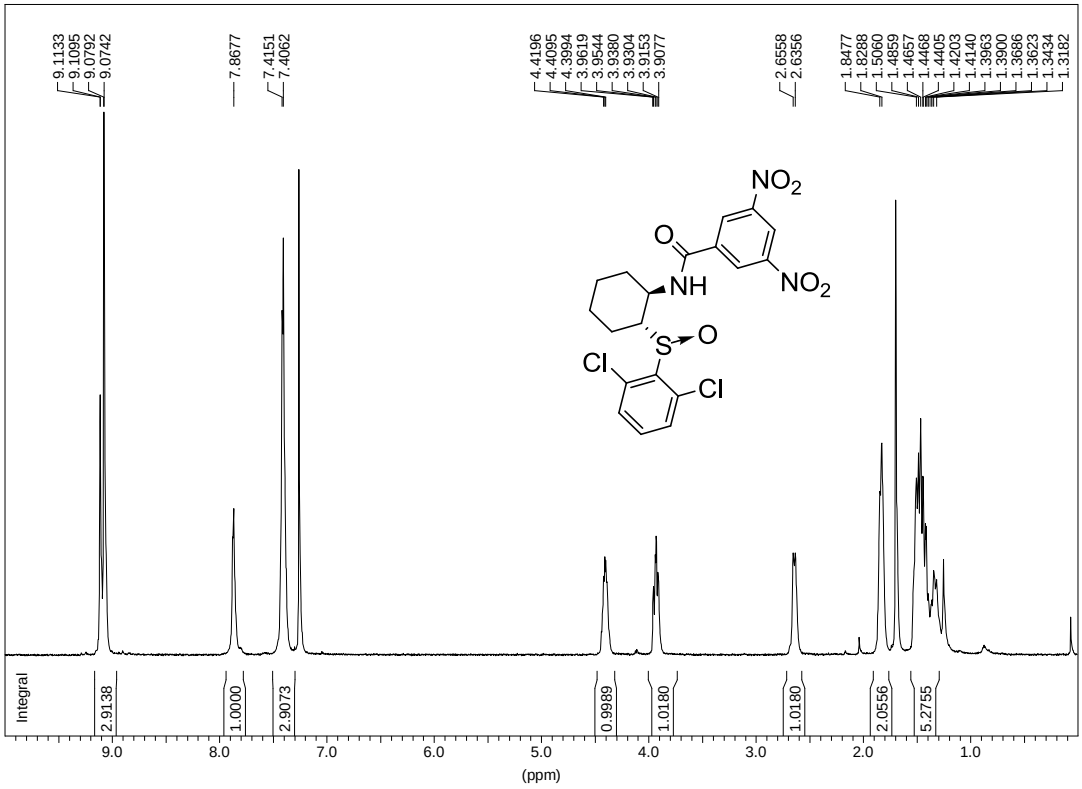

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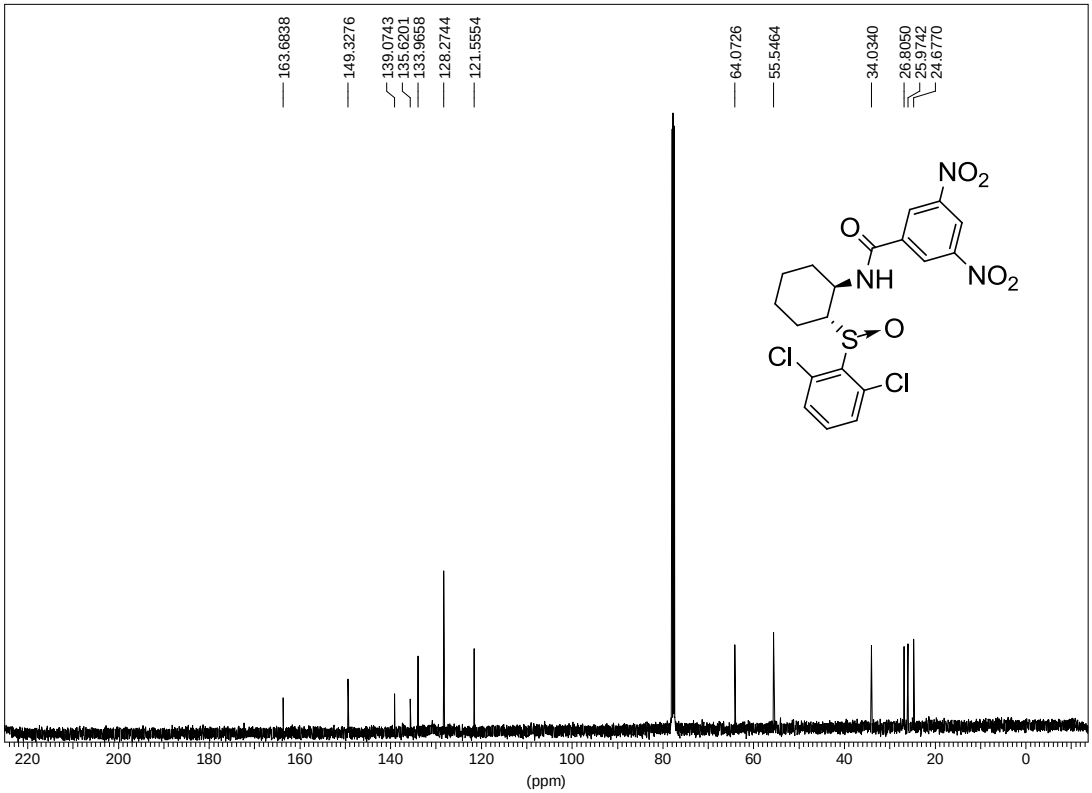

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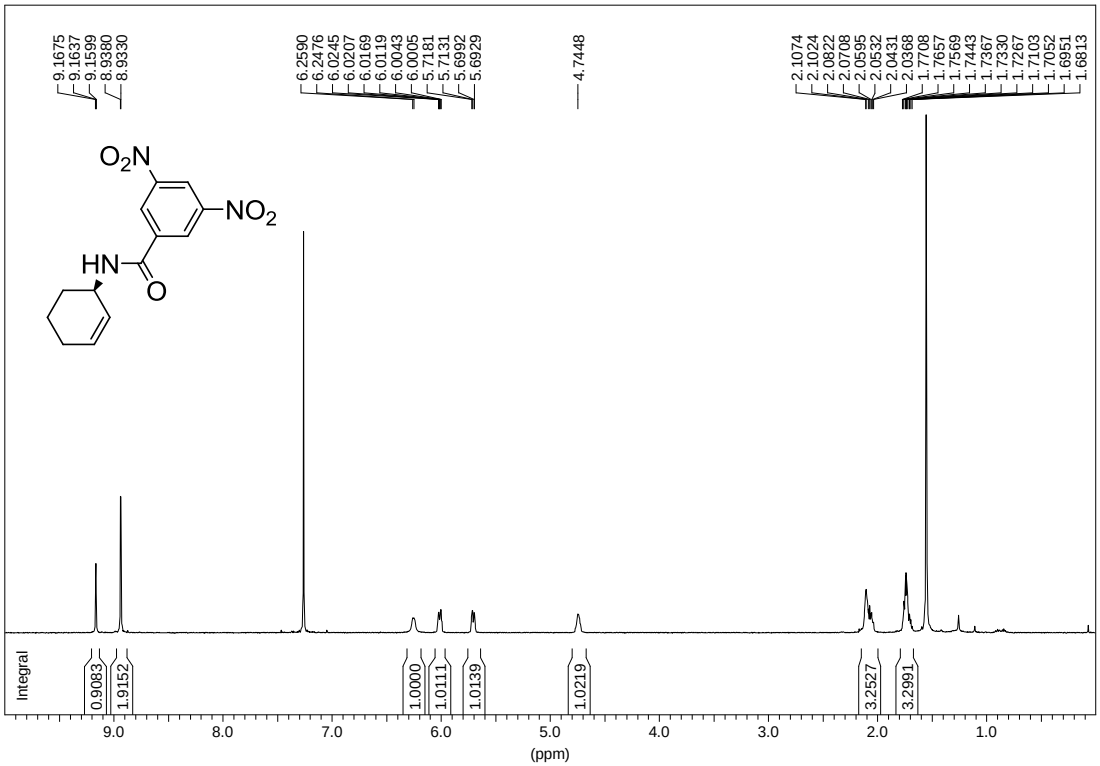

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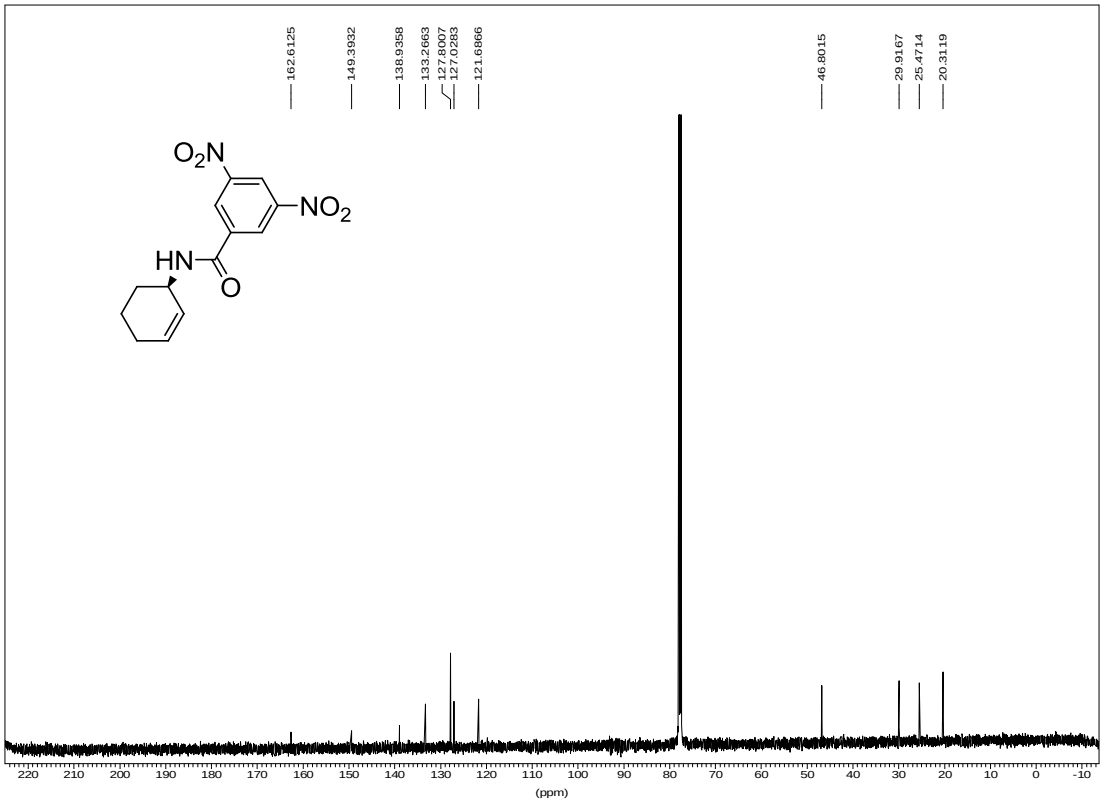

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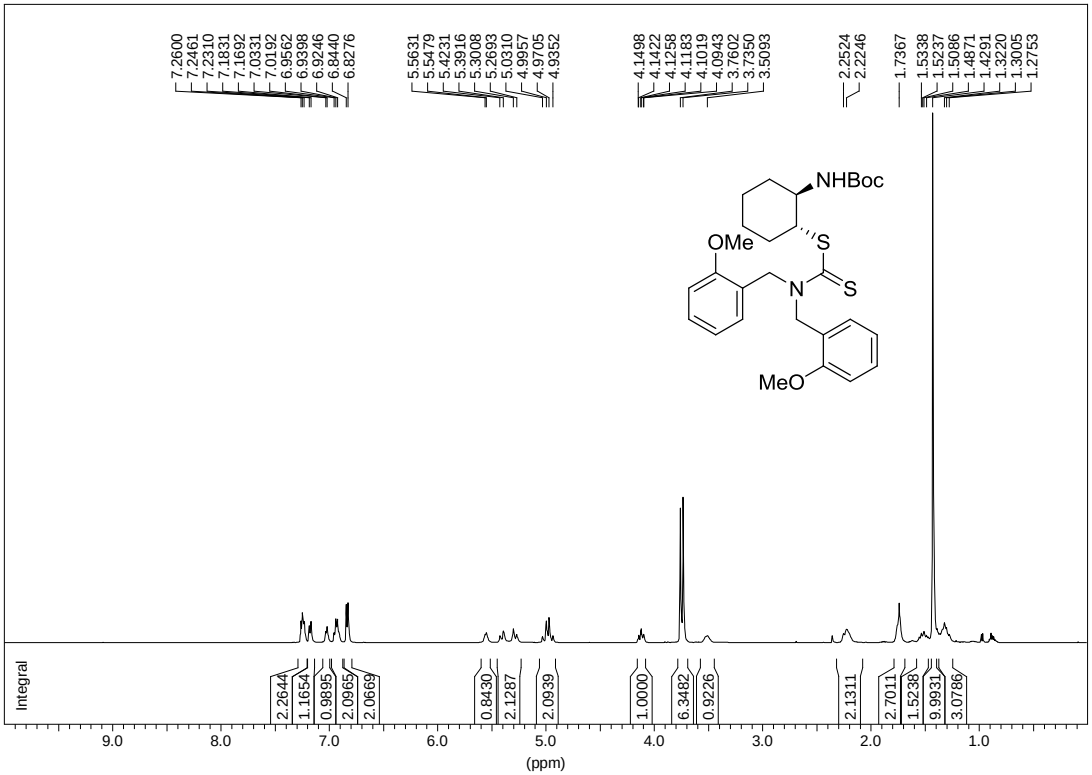

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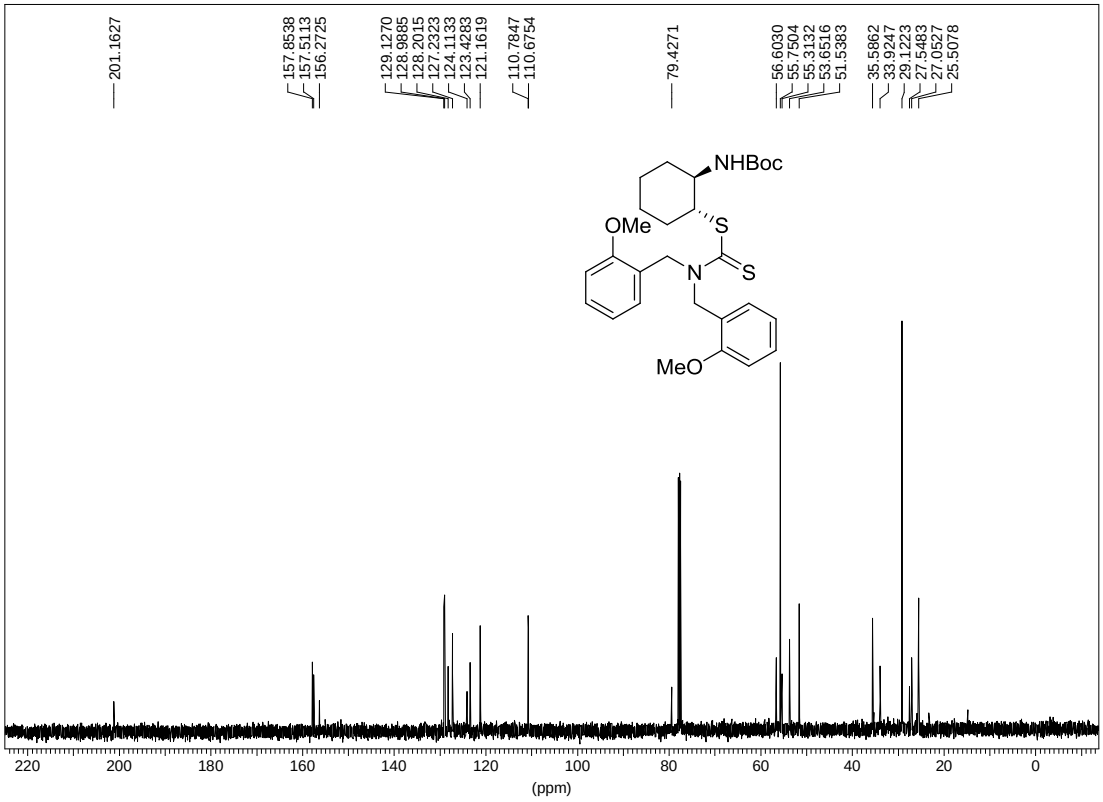

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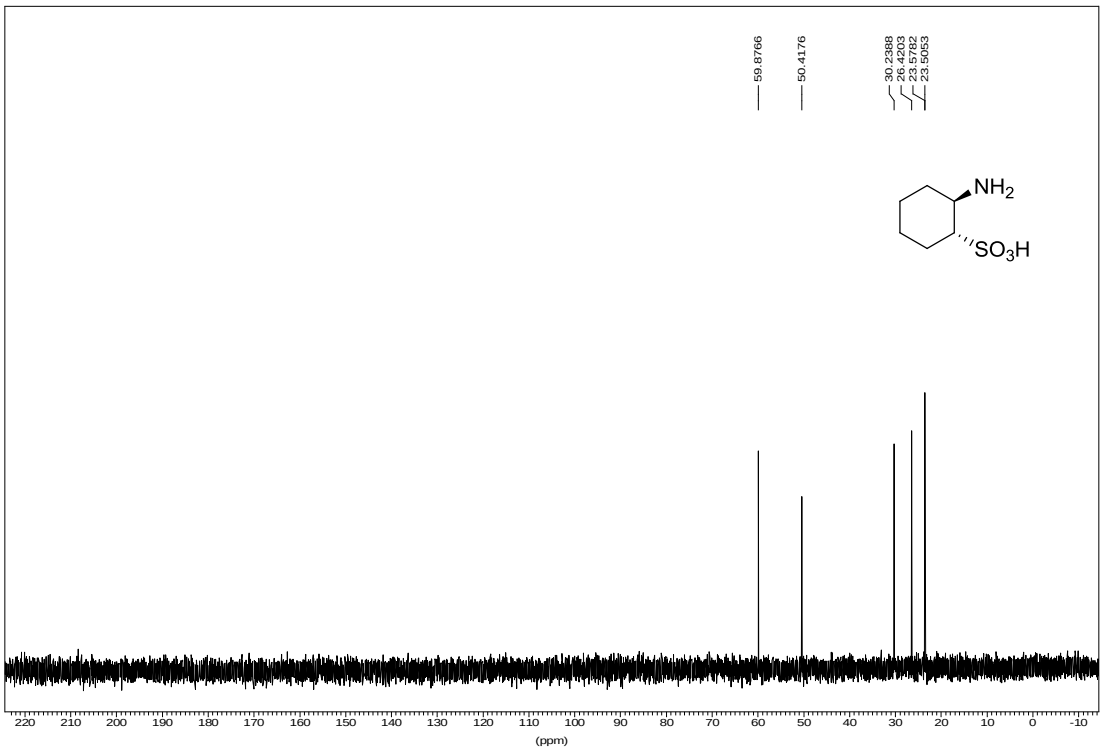

Computational Study

Full citation for Gaussian 09:

Gaussian 09, Revision **A.2**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Methodology

Geometry optimization was performed with RB3LYP[1]/6-31G(d,p)[2] using the default option in Gaussian 09 (default convergence criteria, integration grid, use of symmetry in two-electron integral symmetry). Frequency calculations were performed at 253.15K on RB3LYP/6-31G(d,p) optimized TS structures in the gas phase. All energies reported in the paper are the potential energy (electronic energy) that is not correct by zero-point energy. Inclusion of zero-point correction and thermal corrections do not change the conclusion derived (refer to SI), but due to the large number of low frequency vibrational modes, the entropy contribution from the vibrational partition function might be significantly overestimated.[3]

At RB3LYP/6-31G(d,p), neither mechanism 1 nor mechanism 2 is able to predict the correct absolute configuration as determined by single crystal diffraction. Calculation with a more flexible basis sets (6-311+G(2df,2p))[4] and simulation of solvent effect by CPCM[5] predicts the same stereo-chemical outcome as RB3LYP/6-31G(d,p). CPCM calculation performed with the following keywords: SCRF=(CPCM,solvent=diethylether).

Table 1: $\Delta X=X_{SS}-X_{RR}$ where X=E(electronic energy), E_{ZPE}(electronic energy+ZPE), H(enthalpy at 253.15K) and G(Gibbs energy at 253.15K) for B3LYP/6-31G(d,p)

	Mechanism 1	Mechanism 2
ΔE_{ZPE}(kcal/mol)	-0.7	-4.2
ΔH(kcal/mol)	-0.7	-4.1
ΔG(kcal/mol)	-1.5	-4.9

Table 2: RB3LYP/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) results performed with CPCM to simulate the effect of Et_2O as solvent($\Delta E=E_{SS}-E_{RR}$)

	Mechanism 1	Mechanism 2
ΔE(kcal/mol)	-1.7	-2.4
ΔE_{ZPE}(kcal/mol)	-1.7	-2.7
ΔH(kcal/mol)	-1.7	-2.7
ΔG(kcal/mol)	-2.5	-3.6

The use of RM06-2X[6]/6-311+G(2df,2p) single point calculation with CPCM on RB3LYP/6-31G(d,p) optimized TS structures results in both mechanisms being able to predict the absolute configuration as determined for single crystal diffraction.

Table 3: RM06-2X/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) results performed with CPCM to simulate the effect of Et_2O as solvent ($\Delta E=E_{SS}-E_{RR}$)

	Mechanism 1	Mechanism 2
ΔE(kcal/mol)	+1.2	+2.3
ΔE_{ZPE}(kcal/mol)	+1.3	+2.0
ΔH(kcal/mol)	+1.2	+2.0
ΔG(kcal/mol)	+0.5	+1.2

For comparison purpose single point calculations at RM06-2x/6-311+G(2df,2p) on RB3LYP optimized TS structures have been performed and the results are tabulated in Table 4. Without modeling the effect of solvent, the opposite enantiomer is predicted with a reverse in trend of enantioselectivity (Unsubstituted thiols give the best enantioselectivity and 2,6-dichloro gives the lowest)

Table 4: RM06-2X/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) results ($\Delta E=E_{SS}-E_{RR}$)

		Mechanism 1	Mechanism 2
Ar=Ph	ΔE(kcal/mol)	1.7	-3.0
Ar = 2,6-$Cl_2C_6H_3$	ΔE(kcal/mol)	0.9	-0.3
Ar=4-BrC_6H_4	ΔE(kcal/mol)	1.5	-1.9

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1. (a) Becke, A. D., *J. Chem. Phys.* **1993,** *98* (2), 1372-1377. (b) Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B* **1988,** *37* (2), 785.
2. (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A., *J. Chem. Phys.* **1971,** *54* (2), 724-728. (b) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A., *J. Chem. Phys.* **1982,** *77* (7), 3654-3665.(c) Hehre, W. J.; Ditchfield, R.; Pople, J. A., *J. Chem. Phys.* **1972,** *56* (5), 2257-2261.
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Cartesian Coordinates for TS structures

TS structures for Mechanism 1: Ar = 2,6-$Cl_2C_6H_3$

Table 5

	TS_{RR} conformation 1	TS_{RR} conformation 2	TS_{SS} conformation 1	TS_{SS} conformation 2
E[RB3LYP/6-31G(d,p)]	-4443.61289718	-4443.62357469	-4443.61858961	-4443.62472903
Zero-point correction	1.052485	1.052646	1.052589	1.05253
Thermal correction to Energy	1.102726	1.10276	1.102722	1.102769
Thermal correction Enthalpy	1.103528	1.103562	1.103524	1.103571
Thermal correction to Gibbs Free Energy	0.963616	0.962541	0.962854	0.963805
E[CPCM/RB3LYP/6 311+G(2df,2p)]	-4444.60398174	-4444.60293568	-4444.59763360	-4444.60570226
E[CPCM/RM06-2X/6-311+G(2df,2p)	-4443.32859307	-4443.33304246	-4443.32694864	-4443.33115198
E[CPCM/RM06-2X/6-311+G(2df,2p	-4443.2976274	-4443.30922534	-4443.30407005	-4443.30773991

TS_{RR} conformation 1

Si	-4.88328800	-2.19934000	0.76801300
O	-4.08428300	-0.84826800	1.36707100
N	-2.16225600	1.86803300	-0.15928500
N	-1.68209500	3.90472500	-1.20469700
N	-3.54322400	2.65214200	-1.86726700
C	-2.84224900	-0.23105500	1.06395200
C	-1.92607000	-0.25067900	2.31085300
C	-2.27741600	1.02907700	3.03296700
C	-2.95807000	1.90619700	2.18085100
C	-3.12149400	1.28392300	0.80486300
C	-1.99921300	1.40896600	4.34535000
C	-2.41145700	2.66758200	4.79081700
C	-3.09450000	3.54051200	3.93697800
C	-3.37093000	3.16300800	2.62079300
C	-2.46490500	2.81676900	-1.06694600
C	-1.39970600	4.55556900	-2.50938800
C	-0.08505600	5.33671200	-2.28536600
C	0.50490900	4.75814800	-0.98841900
C	-0.73650300	4.40158300	-0.17385400
C	-4.03528100	1.31621200	-2.30053800
C	-5.09294900	1.66037100	-3.35538900
C	-5.65034300	3.00433500	-2.86248300
C	-4.38447300	3.74061400	-2.40860100
C	-4.27716800	-3.78339900	1.67116500
C	-4.46498400	-3.57886400	3.19151100
C	-5.10737800	-5.00695600	1.22342600
C	-2.78774300	-4.07641900	1.38488700
H	-2.37039000	-0.68680500	0.18856500
H	-2.09835800	-1.15065700	2.90632000
H	-0.87186200	-0.24400700	2.00625900
H	-4.12690700	1.41501700	0.40540800
H	-1.47240300	0.73630200	5.01624400
H	-2.20396200	2.97030700	5.81300800
H	-3.41570400	4.51166400	4.30162500
H	-3.90840500	3.83841600	1.95894100
H	-2.20856900	5.23145500	-2.80128900
H	-1.30537400	3.77725600	-3.27087500
H	0.58967200	5.23488000	-3.13818700
H	-0.30461700	6.40240600	-2.16362700
H	1.15183100	5.46679200	-0.46601300
H	1.07197800	3.84454400	-1.18604200
H	-0.55461200	3.65608700	0.59619500
H	-1.17745900	5.28884200	0.29978800
H	-4.49058300	0.76933500	-1.47181700
H	-3.20529200	0.71721300	-2.68069000
H	-5.84687100	0.87523100	-3.43338900
H	-4.62717300	1.78184700	-4.33957000
H	-6.32572400	2.84932200	-2.01398300
H	-6.19257900	3.56056500	-3.63083800
H	-3.90784500	4.22430300	-3.26845400
H	-4.55899000	4.50136000	-1.64252900
H	-5.51377900	-3.40601900	3.45376500
H	-3.88593300	-2.72761400	3.56381600
H	-4.12934800	-4.47225100	3.73468900
H	-4.73331600	-5.91299900	1.71848900
H	-5.04243700	-5.17607000	0.14253400
H	-6.16383100	-4.90657300	1.49094100
H	-2.13170400	-3.23325500	1.62579200
H	-2.61777100	-4.34872500	0.33872300

H	-2.45293200	-4.92631200	1.99444100
C	-4.66472300	-2.30257800	-1.11613000
C	-3.40164700	-2.50107100	-1.71371600
C	-5.76584500	-2.15468800	-1.98359800
C	-3.24561500	-2.55011200	-3.10039300
H	-2.51426500	-2.62236600	-1.10012500
C	-5.61902800	-2.21877200	-3.37142100
H	-6.75664200	-1.99097600	-1.57129100
C	-4.35689400	-2.41440200	-3.93410600
H	-2.25521500	-2.69473800	-3.52149400
H	-6.49166300	-2.11948100	-4.01167300
H	-4.24027700	-2.46465100	-5.01307900
C	-6.68422300	-1.82882000	1.20471600
C	-6.99613200	-0.70205900	1.98876300
C	-7.75288700	-2.65441300	0.80231400
C	-8.31236500	-0.41176200	2.35221600
H	-6.19339700	-0.05086200	2.32038600
C	-9.07095200	-2.36652100	1.16041400
H	-7.56296500	-3.53497100	0.19427700
C	-9.35380800	-1.24282400	1.93821400
H	-8.52400700	0.46258900	2.96174200
H	-9.87503900	-3.02001200	0.83373200
H	-10.37848800	-1.01850800	2.22080600
H	-1.16225000	1.74058200	0.05636000
S	1.03436000	0.96210800	0.02567700
C	0.90841800	-0.32971200	-1.16895100
C	0.76192400	-0.09356600	-2.55904100
C	0.96375600	-1.70634600	-0.82637300
C	0.69207900	-1.10435900	-3.51397400
C	0.89886000	-2.73743700	-1.76106700
C	0.76619700	-2.43601100	-3.11392100
H	0.59879300	-0.84192000	-4.56147700
H	0.96559600	-3.76537300	-1.42375200
H	0.73646100	-3.23165300	-3.85123000
Cl	1.12718000	-2.19933000	0.86019500
Cl	0.66202400	1.55852500	-3.17877400
H	3.12315400	3.57271100	0.27385000
C	4.07578700	3.13877400	0.60574100
C	3.44818500	0.67789000	0.72626600
C	3.09707000	2.17683300	2.73656400
C	3.29588600	0.74195900	2.22292200
H	3.41772800	-0.28593300	0.23436400
H	2.08675500	2.51603700	2.46854500
H	4.21571300	0.32489500	2.65185000
H	3.14936000	2.18295400	3.83159900
H	2.47689000	0.08734500	2.53006300
C	5.86844000	0.15884400	-0.51876000
O	5.29585200	-0.22786600	-1.55292600
C	7.22692600	-0.43081100	-0.18618500
C	9.75397100	-1.58009100	0.34834300
C	7.77880800	-1.36422900	-1.06882500
C	7.93591800	-0.06997900	0.96406200
C	9.17897500	-0.65021600	1.20859500
C	9.02547100	-1.91792300	-0.78718700
H	7.22560400	-1.64101200	-1.95729400
H	7.51501100	0.65443300	1.64792500
H	10.72002300	-2.01860000	0.55312100
N	9.92153100	-0.26983300	2.42392200
N	9.60364900	-2.90242500	-1.72031000
O	10.70794500	-3.37144600	-1.44372000
O	9.39769200	0.54455700	3.18260200
O	11.02178100	-0.79048500	2.60811600
O	8.94853400	-3.19666800	-2.71832400
H	4.87785900	3.75972700	0.19074800
C	4.13607400	3.13818500	2.14051400
H	5.13941100	2.83166000	2.45621400
H	3.97381600	4.15350400	2.52265100
C	4.19247900	1.73651200	0.01022000
H	4.01044900	1.71859500	-1.06842900
N	5.44293000	1.07182600	0.38932300

TS_{RR} conformation 2

Si	-5.39245600	-0.38046900	0.27482100
O	-4.20018100	0.29277700	1.25785500
N	-1.25944100	1.29747300	0.20157700
N	0.06413900	2.67563500	-1.12427100
N	-2.06033500	3.40593100	-0.44833700
C	-2.87145400	-0.08001700	1.58759400
C	-2.75547500	-0.59306100	3.04479300
C	-1.41902400	-0.07647000	3.51498100
C	-0.93353600	0.90975400	2.65069000
C	-1.91227700	1.14812700	1.51248000
C	-0.69318700	-0.43162100	4.65090200
C	0.51699600	0.21461700	4.91383800
C	0.99572200	1.20741600	4.05246600
C	0.26937400	1.56151000	2.91299600
C	-1.08108000	2.45850800	-0.45940600
C	0.19860400	3.52613500	-2.33096100
C	1.71199000	3.70646200	-2.46485500
C	2.26321500	2.34988500	-2.00832200
C	1.33332200	1.92408100	-0.86513900
C	-3.51432700	3.09866400	-0.54204400
C	-4.18442700	4.47914900	-0.41842800
C	-3.14721400	5.33052500	0.33147800
C	-1.82867200	4.85169500	-0.28402900
C	-5.99889900	-2.08170100	0.93838900
C	-6.46605000	-1.90914600	2.40113700
C	-7.19511800	-2.56297200	0.08641300
C	-4.89889400	-3.16286100	0.88562300
H	-2.48212600	-0.84153300	0.90211300
H	-3.57455100	-0.15923400	3.63310800
H	-2.84423300	-1.68155600	3.11111400
H	-2.48909200	2.05689100	1.70349300
H	-1.05896900	-1.20507900	5.32059700
H	1.09397400	-0.05862800	5.79229900
H	1.94003600	1.69932600	4.26408300
H	0.64983900	2.32609800	2.24179000
H	-0.33249700	4.47050500	-2.23018500
H	-0.21809000	2.98898200	-3.19260700
H	2.00110500	3.97345800	-3.48431200
H	2.05069000	4.50702200	-1.79760300
H	3.29550900	2.38193100	-1.65914200
H	2.20132500	1.62820600	-2.82909700
H	1.16341700	0.84604000	-0.86108600
H	1.73759300	2.21345500	0.10722200
H	-3.83518300	2.42634100	0.25290900
H	-3.72920600	2.60620600	-1.49463300
H	-5.14490900	4.41048600	0.09697700
H	-4.36809800	4.90585800	-1.41045000
H	-3.16503100	5.10883400	1.40421700
H	-3.29548600	6.40579000	0.20359400
H	-1.67231000	5.35854900	-1.24655000
H	-0.94783100	5.02685900	0.33905700
H	-7.25732000	-1.15792600	2.49212900
H	-5.64513300	-1.61129100	3.06115700
H	-6.86499400	-2.85921000	2.78082800
H	-7.53536100	-3.54429300	0.44314700
H	-6.92874400	-2.67449000	-0.97063300
H	-8.04814000	-1.88058000	0.15402800
H	-3.99152100	-2.87491700	1.42567400
H	-4.61254100	-3.40871700	-0.14065100
H	-5.26579300	-4.08957200	1.34700700
C	-4.77854200	-0.45988700	-1.51617100
C	-3.73034800	-1.32133200	-1.90035700
C	-5.31821600	0.37794900	-2.51298100
C	-3.25424600	-1.35475700	-3.21213600
H	-3.26213200	-1.97801700	-1.17405600
C	-4.84849500	0.34708700	-3.82759400
H	-6.11785500	1.06830700	-2.26301500
C	-3.81615900	-0.52236000	-4.18072400
H	-2.44512000	-2.02993100	-3.47171200
H	-5.29142600	1.00052800	-4.57458800
H	-3.44991100	-0.55022000	-5.20316500
C	-6.77780300	0.90032700	0.44904600
C	-6.70259400	1.89289300	1.44519200
C	-7.93201500	0.88523400	-0.35877900
C	-7.72346500	2.82954400	1.62109100
H	-5.83221200	1.92454900	2.09315900
C	-8.95516300	1.82010500	-0.18926000
H	-8.03955100	0.13775600	-1.14015200

C	-8.85279600	2.79691500	0.80174500
H	-7.64032500	3.58006800	2.40274200
H	-9.83146700	1.78397900	-0.83038700
H	-9.64868600	3.52374500	0.93707500
H	-0.68247300	0.49024800	-0.07272200
S	0.35250100	-1.68268400	-0.03854000
C	-0.00224600	-2.80951300	-1.33779400
C	0.36718500	-2.60499100	-2.69313100
C	-0.67169500	-4.04393000	-1.11179500
C	0.10739200	-3.51467200	-3.71642800
C	-0.94902500	-4.96653900	-2.11769000
C	-0.55705600	-4.70384300	-3.42806400
H	0.42910700	-3.28622900	-4.72622400
H	-1.46441100	-5.88633800	-1.86569800
H	-0.76322200	-5.42087600	-4.21586100
Cl	-1.20447800	-4.47636900	0.51111300
Cl	1.20485300	-1.12390000	-3.17087300
H	1.98676500	-2.26222800	2.88675200
C	3.05584000	-2.14989500	2.66973300
C	3.03990600	-1.62440300	0.17672900
C	3.08848300	-4.02986900	0.97486200
C	3.35822300	-3.04841900	-0.17720400
H	2.95723700	-0.88938000	-0.61067600
H	2.00579100	-4.16802200	1.07436200
H	4.41921500	-3.08142800	-0.45787600
H	3.51753200	-5.00672400	0.72445900
H	2.79725500	-3.32571900	-1.07507000
C	4.84895600	0.35077700	0.68166900
O	4.04271700	1.28366700	0.48637600
C	6.31449000	0.59835600	0.38836700
C	9.02916100	1.14515500	-0.18242800
C	6.70699800	1.87515600	-0.02347100
C	7.27888100	-0.40703800	0.51998100
C	8.60951500	-0.11563700	0.22937600
C	8.04888400	2.12447800	-0.29868500
H	5.96378500	2.65528400	-0.12041900
H	6.98527400	-1.39513800	0.84748700
H	10.06698800	1.35280100	-0.40070600
N	9.62208300	-1.18087200	0.36238300
N	8.45281900	3.47429400	-0.73370700
O	9.64646500	3.66801900	-0.95888300
O	9.23675700	-2.29105200	0.72301100
O	10.78952100	-0.89169300	0.10294600
O	7.57076000	4.32452500	-0.84639300
H	3.53155100	-1.74695000	3.57142300
C	3.65899100	-3.51425200	2.30350700
H	4.74849700	-3.41975800	2.22885600
H	3.45322300	-4.23484300	3.10361600
C	3.19800100	-1.12238900	1.55049700
H	2.65046000	-0.19814300	1.75017400
N	4.59583400	-0.89540200	1.15124400

TS_{SS} conformation 1

Si	-3.19362200	-2.10598400	-1.93242500
O	-1.65925500	-2.01022000	-1.26360600
N	-1.27830000	0.40547300	1.48052600
N	-0.61942400	1.48467200	3.44426300
N	-2.78296900	0.60980200	3.25789500
C	-0.94022400	-1.06972900	-0.48364400
C	0.46555300	-1.65461700	-0.22223000
C	0.29049800	-2.43672300	1.05915000
C	-0.88157600	-2.04217100	1.71929500
C	-1.57728600	-0.94230500	0.93506500
C	1.10940500	-3.41817800	1.61509200
C	0.74026800	-4.00173900	2.83098000
C	-0.43678800	-3.61807700	3.48055000
C	-1.25889100	-2.63317200	2.92435700
C	-1.55251100	0.82343500	2.73317900
C	-0.91728300	2.63443400	4.33685300
C	0.45275900	3.28931800	4.60365300
C	1.34907300	2.78766300	3.46293100
C	0.85016900	1.36274100	3.23174400
C	-4.01386300	0.49246500	2.43715900
C	-5.13444400	0.58825000	3.47642200
C	-4.51508100	-0.11009800	4.69663400
C	-3.08005600	0.43159300	4.69608000
C	-2.93472100	-2.30143500	-3.82446100
C	-2.08973600	-3.57065700	-4.07469000
C	-4.28491100	-2.43457400	-4.55898300
C	-2.17647400	-1.08082800	-4.38665100
H	-0.90364200	-0.09727400	-0.98696500
H	0.78234500	-2.26597300	-1.07133800
H	1.21373500	-0.86557600	-0.07537900
H	-2.65604200	-1.08186900	0.86092700
H	2.02119300	-3.73599500	1.11829800
H	1.37281600	-4.76892700	3.26752500
H	-0.71858700	-4.09432700	4.41522900
H	-2.18526400	-2.35186400	3.41874000
H	-1.37934700	2.31545600	5.27425200
H	-1.60845300	3.30646800	3.81959400
H	0.37277600	4.37832200	4.63856100
H	0.84075800	2.95357100	5.57140300
H	2.41149200	2.81257400	3.71611600
H	1.18604700	3.37719800	2.55610400
H	1.10282900	0.96204500	2.25328700
H	1.24649500	0.67276600	3.98772400
H	-4.06454400	-0.47899600	1.93661600
H	-4.03344300	1.26709400	1.66863100
H	-6.05337100	0.11490100	3.12411000
H	-5.35837300	1.63539100	3.70878800
H	-4.51710700	-1.19643000	4.55345800
H	-5.03098900	0.10738000	5.63491700
H	-3.05193100	1.38786600	5.22856300
H	-2.34589000	-0.23743200	5.15310900
H	-2.59150700	-4.47444300	-3.71377700
H	-1.11435600	-3.50875900	-3.58158100
H	-1.91175100	-3.69691100	-5.15125100
H	-4.11738600	-2.50977900	-5.64182800
H	-4.93379600	-1.56803800	-4.38851600
H	-4.82935700	-3.33428500	-4.25480000
H	-1.21999300	-0.92322700	-3.87756800
H	-2.76093700	-0.15934200	-4.30419000
H	-1.95968200	-1.23341800	-5.45258300
C	-4.23366100	-0.57915900	-1.48784800
C	-3.76637300	0.72564600	-1.74984300
C	-5.50344500	-0.69911200	-0.88869700
C	-4.52951400	1.85293900	-1.43776800
H	-2.79241700	0.87740500	-2.20501900
C	-6.27692100	0.42350300	-0.58391600
H	-5.89774900	-1.68339000	-0.65531700
C	-5.79132100	1.70316600	-0.85861600
H	-4.13863800	2.84287200	-1.65304200
H	-7.25931400	0.29733000	-0.13611700
H	-6.39230000	2.57815900	-0.62626300
C	-3.97181300	-3.66088900	-1.18549700
C	-3.23161000	-4.44109200	-0.27755400
C	-5.26780200	-4.10601700	-1.51623800
C	-3.76061900	-5.60788100	0.27793200
H	-2.22692100	-4.13179600	-0.00792300
C	-5.80132900	-5.27111100	-0.96320400
H	-5.87808300	-3.53882000	-2.21419800
C	-5.04711700	-6.02587000	-0.06307800
H	-3.16469900	-6.19070000	0.97484300
H	-6.80329600	-5.59023900	-1.23682200
H	-5.45935200	-6.93471100	0.36642700
H	-0.63460600	1.00386300	0.94751600
S	0.35680200	2.88336900	-0.22419000
C	-0.81463300	3.87452100	-1.08158300
C	-1.50616700	4.94564300	-0.45681900
C	-1.16294300	3.68927900	-2.44404800
C	-2.42653000	5.75869400	-1.11315900
C	-2.07349200	4.49242500	-3.12676100
C	-2.70837500	5.53730400	-2.45920900
H	-2.90956100	6.56182300	-0.56818200
H	-2.27970500	4.29222500	-4.17206000
H	-3.41559600	6.17220200	-2.98272100
Cl	-0.44850600	2.36489500	-3.36824500
Cl	-1.22971100	5.30571400	1.25005700
H	2.27306100	2.80104300	-2.96212400

C	3.12732400	2.89028100	-2.28705200
C	3.49076500	2.59137000	0.25841100
C	4.63018300	4.48760000	-1.01772800
C	4.06652800	4.00309700	0.32498000
C	2.78699500	2.23101900	-0.98602200
H	2.93109900	2.33192400	1.15847100
H	4.95316900	5.53125000	-0.92941700
H	4.83997800	4.02428900	1.10117800
H	5.51750900	3.89682300	-1.27442900
H	3.26012400	4.67492400	0.64595200
H	2.27229300	1.28251200	-0.99738400
N	4.48145900	1.56451100	-0.09980900
C	4.16514600	0.34534000	0.39465700
O	3.13397900	0.01323600	1.02314800
C	5.20885100	-0.71830000	0.13638300
C	7.09102200	-2.77905500	-0.30620800
C	6.38284400	-0.45641900	-0.57786400
C	4.97573100	-2.00520000	0.62934900
C	5.91315800	-3.00757700	0.39743800
C	7.29586500	-1.48841900	-0.78363600
H	6.57134000	0.53777700	-0.96051300
H	4.06810400	-2.19993500	1.18518600
H	7.81212300	-3.56574900	-0.47659500
N	5.65194100	-4.36524400	0.90801300
N	8.53315600	-1.21120700	-1.53895500
O	9.32456800	-2.14014800	-1.69471600
O	4.57079400	-4.57049300	1.46206600
O	6.52696000	-5.21385400	0.75001300
O	8.69579600	-0.07006900	-1.96573400
H	3.93834400	2.29814600	-2.73470100
C	3.57888500	4.34974100	-2.12700100
H	3.97141300	4.71435500	-3.08280900
H	2.70567000	4.96771900	-1.88254600

TS_{SS} conformation 2

Si	-5.61603600	0.07318300	-1.16368400
O	-4.12476500	-0.65439000	-1.42696200
N	-1.09104100	-1.18496800	0.52247300
N	0.22055000	-2.10523200	2.20075500
N	-2.11648800	-2.14857800	2.39378900
C	-2.78525000	-0.27154400	-1.13397800
C	-2.01965100	0.06776300	-2.43654800
C	-1.34648500	-1.22905600	-2.81739400
C	-1.35559200	-2.12889700	-1.74766800
C	-2.05480600	-1.52383200	-0.54358900
C	-0.74323400	-1.58673100	-4.02335500
C	-0.15641000	-2.84845400	-4.14293200
C	-0.17051100	-3.74791200	-3.07091100
C	-0.77227700	-3.39046000	-1.86283600
C	-0.99345100	-1.81535800	1.70865000
C	0.55617000	-2.18663700	3.64246000
C	2.08385500	-2.03974400	3.66450900
C	2.51332800	-2.67070700	2.33213000
C	1.45748500	-2.13627400	1.36484300
C	-3.35737100	-1.32891100	2.37295100
C	-4.22204900	-1.98138300	3.45874400
C	-3.79252000	-3.45535100	3.40808000
C	-2.27267200	-3.35100400	3.23731200
C	-6.11026800	1.17590800	-2.66088900
C	-6.00920700	0.32858400	-3.94902900
C	-7.56531100	1.66859100	-2.49689100
C	-5.19554800	2.41245300	-2.79716300
H	-2.76296100	0.55023400	-0.41288400
H	-2.70498700	0.43802300	-3.20307800
H	-1.26922000	0.84489400	-2.24490700
H	-2.78957200	-2.20739900	-0.11821400
H	-0.72878800	-0.89469000	-4.86073400
H	0.31330400	-3.13677400	-5.07879000
H	0.28425900	-4.72775200	-3.18135600
H	-0.78992800	-4.09231600	-1.03211300
H	0.26629800	-3.16210800	4.04912800
H	0.02438000	-1.40715900	4.19457600
H	2.36313000	-0.98152900	3.68114400
H	2.52318700	-2.52241300	4.54104800
H	2.46274100	-3.76454500	2.39372100
H	3.51133500	-2.37172600	2.01180300
H	1.72391200	-1.12622600	1.03956300
H	1.29092900	-2.75999400	0.48379500
H	-3.85789000	-1.38487000	1.40411400
H	-3.12091600	-0.28052100	2.56841200
H	-5.28604600	-1.83073100	3.26801300
H	-3.99048900	-1.55376600	4.44048900
H	-4.24066200	-3.95294200	2.54104900
H	-4.06574200	-4.02032300	4.30261300
H	-1.79610600	-3.22282800	4.21604100
H	-1.81848600	-4.21803200	2.74917400
H	-6.66350900	-0.54870700	-3.91179100
H	-4.98904200	-0.02654600	-4.12611900
H	-6.30853000	0.92867200	-4.81873000
H	-7.83268600	2.32690900	-3.33418700
H	-7.70315500	2.24421700	-1.57422000
H	-8.28129400	0.84121500	-2.49413200
H	-4.13548300	2.15016300	-2.87550000
H	-5.31191600	3.10201600	-1.95556500
H	-5.45588000	2.96915100	-3.70748500
C	-5.57412500	1.04031900	0.46946600
C	-4.70204800	2.13382500	0.65650500
C	-6.37643400	0.66733300	1.56609600
C	-4.62874400	2.81441600	1.87341100
H	-4.06131000	2.46898400	-0.15341300
C	-6.31950800	1.35342700	2.78139900
H	-7.05835700	-0.17231500	1.47256500
C	-5.44196600	2.42686400	2.93937900
H	-3.93336900	3.64098700	1.98435600
H	-6.96089800	1.04871000	3.60409200
H	-5.39294200	2.95864500	3.88543900
C	-6.77707000	-1.41476300	-1.03142100
C	-6.29454300	-2.70528100	-1.32120900
C	-8.13564200	-1.29670700	-0.67639400
C	-7.12656500	-3.82456900	-1.25670900
H	-5.25484700	-2.82753200	-1.60876900
C	-8.97065700	-2.41312600	-0.60582100
H	-8.55637000	-0.32168200	-0.44548000
C	-8.46705500	-3.68169300	-0.89677000
H	-6.72859000	-4.80811900	-1.49149100
H	-10.01344600	-2.29155700	-0.32621100
H	-9.11594200	-4.55149300	-0.84609700
H	-0.32999000	-0.53775900	0.26775600
S	0.79146400	1.44650300	-0.30136900
C	0.02382400	2.78990400	0.53429200
C	-0.11337900	2.87101000	1.94446000
C	-0.52496400	3.90516900	-0.15693100
C	-0.70885100	3.94188400	2.60670700
C	-1.12731800	4.98684900	0.48139300
C	-1.21710900	5.01002400	1.87155300
H	-0.76386400	3.93473100	3.68936800
H	-1.51496800	5.80539200	-0.11439900
H	-1.67165000	5.85599400	2.37702400
Cl	-0.46737000	3.97409000	-1.91666500
Cl	0.49045800	1.56700200	2.97437800
H	2.79147900	2.56759000	-2.30443100
C	3.56409300	2.69315000	-1.54148700
C	3.94211100	1.76808400	0.85012900
C	4.42446000	4.21157300	0.30716900
C	4.00878200	3.19717900	1.38267200
C	3.41214500	1.60764300	-0.51421100
H	3.50619000	1.06778500	1.56631500
H	4.37760100	5.22678300	0.71807000
H	4.70946400	3.21960100	2.22520400
H	5.46679200	4.02720300	0.02300500
H	3.01926700	3.45947400	1.77760000
H	3.22830200	0.59188200	-0.83798600
N	5.22623400	1.30791100	0.29922600
C	5.39919500	-0.03344100	0.36096800
O	4.57585900	-0.90031900	0.72163900
C	6.77935100	-0.48947800	-0.06473300
C	9.33394100	-1.42478300	-0.83266900

C	7.75763200	0.41112100	-0.50027700
C	7.07698300	-1.85427500	-0.01265400
C	8.34178200	-2.29453300	-0.39354900
C	9.00843300	-0.07300300	-0.87621700
H	7.53651000	1.46921700	-0.53845600
H	6.31997200	-2.55134300	0.32131900
H	10.31099700	-1.78122500	-1.12612000
N	8.64835500	-3.73576000	-0.33341900
N	10.03642200	0.87916500	-1.33860200
O	11.13288800	0.42185700	-1.65899700
O	7.76070300	-4.49148200	0.05908200
O	9.77314300	-4.09461300	-0.67922200
O	9.73424400	2.07018900	-1.37605500
H	4.52981200	2.52930100	-2.03868900
C	3.52367900	4.10323300	-0.93147400
H	3.82236300	4.83433000	-1.69113500
H	2.48943200	4.33957700	-0.65479500

TS structures for Mechanism 1: Ar = C_6H_5

Table 6

	TS_{RR} conformation 2	TS_{SS} conformation 1	TS_{SS} conformation 2
E[RB3LYP/6-31G(d,p)]	-3524.43933185	-3524.43933185	-3524.43933185
Zero-point correction	1.052646	1.052589	1.05253
Thermal correction to Energy	1.10276	1.102722	1.102769
Thermal correction Enthalpy	1.103562	1.103524	1.103571
Thermal correction to Gibbs Free Energy	0.962541	0.962854	0.963805
E[CPCM/RB3LYP/6-311+G(2df,2p)]	-3525.3513829	-3525.34604401	-3525.3486387
E[CPCM/RM06-2X/6-311+G(2df,2p)]	-3524.12004858	-3524.11526177	-3524.11618422
E[RM06-2X/6-311+G(2df,2p)]	-3524.09654554	-3524.09136714	-3524.09384538

TS_{RR} conformation 1: Attempt to derive the TS structures for Ar=C_6H_5 from Ar= 2,6-$Cl_2C_6H_3$ transition was not successfully.

TS_{RR} conformation 2

Si	5.26827200	-0.83016900	-0.06401100
O	4.20369600	-0.16240700	-1.18666000
N	1.34371000	1.15347800	-0.37226000
N	0.05432600	2.74152300	0.74297600
N	2.23358000	3.27860100	0.06427700
C	2.87290200	-0.45954100	-1.57253500
C	2.79627700	-1.06759800	-2.99460200
C	1.49516200	-0.53850000	-3.54596700
C	1.03319400	0.53608500	-2.77814100
C	2.00323300	0.83006900	-1.64470300
C	0.77912400	-0.95755800	-4.66629000
C	-0.39745000	-0.28726100	-5.01093400
C	-0.85321500	0.79050000	-4.24464700
C	-0.13709300	1.20909900	-3.12041800
C	1.20434700	2.38956500	0.14120800
C	-0.03819800	3.72409500	1.85259500
C	-1.54104200	3.80484100	2.14932900
C	-2.05666400	2.40700600	1.78887700
C	-1.24894300	2.03327500	0.54585600
C	3.66721700	2.89998200	0.21610400
C	4.41280400	4.23045000	0.01807900
C	3.45430200	5.06275700	-0.84820600
C	2.08932000	4.71194800	-0.24764500
C	5.55304100	-2.70894300	-0.37157800
C	6.07385500	-2.91341200	-1.81167300
C	6.61698600	-3.23365800	0.61970300
C	4.26456900	-3.53785800	-0.17710300
H	2.38468300	-1.13756100	-0.86273700
H	3.65171900	-0.70298000	-3.57873400
H	2.84985600	-2.16058700	-2.98440900
H	2.64272000	1.67318600	-1.92040500
H	1.12645200	-1.79749600	-5.26171000
H	-0.96638100	-0.60887400	-5.87821300
H	-1.77202700	1.29941700	-4.51942400
H	-0.50053300	2.04010200	-2.52240100
H	0.37195100	4.69551700	1.57688100
H	0.52942400	3.34620100	2.71143500
H	-1.73174500	4.08955300	3.18702000
H	-2.00686900	4.55902500	1.50544300

H	-3.12473500	2.36512900	1.57434100
H	-1.84007500	1.70519200	2.60254800
H	-1.11433400	0.95578700	0.44892600
H	-1.73114100	2.40483400	-0.36290000
H	3.97162400	2.16301000	-0.52694300
H	3.83209300	2.45751800	1.20178200
H	5.39042500	4.07432300	-0.44349700
H	4.57377200	4.72852300	0.98041400
H	3.50064900	4.74160000	-1.89469600
H	3.65672700	6.13614100	-0.81191600
H	1.92452600	5.31521900	0.65529600
H	1.24446800	4.87093300	-0.92283800
H	6.99939300	-2.35741400	-1.99324300
H	5.34313100	-2.59792700	-2.56333000
H	6.28540900	-3.97684100	-1.98637700
H	6.76146600	-4.31225800	0.47208500
H	6.31773800	-3.08376200	1.66287300
H	7.58983900	-2.75501400	0.46993700
H	3.44975900	-3.22006700	-0.83537500
H	3.89907200	-3.49364100	0.85283000
H	4.46654400	-4.59370500	-0.40307500
C	4.66438400	-0.46563500	1.69444100
C	3.44914000	-0.99258500	2.17908700
C	5.39125200	0.37638300	2.56003500
C	2.99177000	-0.70924700	3.46757500
H	2.82845000	-1.62623200	1.55292000
C	4.93908300	0.66386800	3.84959900
H	6.32332400	0.82051200	2.22499300
C	3.73969900	0.11729500	4.30746900
H	2.05283600	-1.13506500	3.80655400
H	5.52603900	1.31170300	4.49546300
H	3.38884200	0.33439800	5.31274300
C	6.84909600	0.14588600	-0.43451200
C	6.91086300	0.98909800	-1.56041300
C	8.00737300	0.04931800	0.36200100
C	8.06753300	1.70618500	-1.87269400
H	6.03890700	1.07616200	-2.20091300
C	9.16695200	0.76354900	0.05478400
H	8.01099000	-0.58681200	1.24288200
C	9.19963100	1.59604700	-1.06450000
H	8.08664400	2.34641500	-2.75071000
H	10.04360700	0.66903700	0.68950000
H	10.10127400	2.15174100	-1.30611800
H	0.74226900	0.39244300	-0.00636500
S	-0.23080700	-1.68081100	0.31261000
C	-0.19674600	-2.28359500	1.98183200
C	-0.71293900	-1.53703100	3.06180500
C	0.32512500	-3.56219100	2.27125500
C	-0.70503000	-2.04077500	4.36296800
C	0.34017600	-4.06031900	3.57370800
C	-0.17427000	-3.30494700	4.63030500
H	-1.11623000	-1.44164000	5.17186000
H	0.75229500	-5.04824800	3.76311300
H	-0.16674600	-3.69669900	5.64308900
H	-1.81123300	-2.38093800	-2.75158400
C	-2.88768300	-2.31155200	-2.55242200
C	-2.96316300	-1.72741300	-0.07317600
C	-2.86594600	-4.14697400	-0.81061500
C	-3.21183900	-3.15705600	0.31330300
H	-2.89069800	-0.97008500	0.69368000
H	-1.77450100	-4.22270100	-0.88179700
H	-4.27248100	-3.24779000	0.58139600
H	-3.24441800	-5.14116800	-0.54726300
H	-2.64361500	-3.37796700	1.22207200
C	-4.80225700	0.15129500	-0.61467600
O	-4.03496200	1.11752800	-0.43725900
C	-6.27561900	0.33931000	-0.32223200
C	-9.01096200	0.77727700	0.24124500
C	-6.71909000	1.59887500	0.09155100
C	-7.19897500	-0.70333300	-0.45884000
C	-8.54094100	-0.46499700	-0.17225600
C	-8.07039300	1.79421100	0.36331900
H	-6.00787800	2.40778600	0.19284500
H	-6.86599400	-1.67853700	-0.78736600
H	-10.05690800	0.94355100	0.45627300
N	-9.51061300	-1.56865900	-0.31267100
N	-8.52873100	3.12604200	0.80037400
O	-9.72973500	3.27150500	1.02222300
O	-9.08098900	-2.66088000	-0.67788200
O	-10.68894900	-1.32656900	-0.05476800
O	-7.68120300	4.01000600	0.91751600
H	-3.36475100	-1.95125100	-3.47129100
C	-3.43443800	-3.69276600	-2.16238600
H	-4.52836400	-3.64755300	-2.10888500
H	-3.18134300	-4.42186900	-2.94109000
C	-3.08615200	-1.26629500	-1.46026600
H	-2.57407300	-0.32502100	-1.66932200
N	-4.49339400	-1.09496400	-1.06252600
H	0.71857600	-4.16037900	1.45507400
H	-1.12452300	-0.55051800	2.86890000

TS_{SS} conformation 1

Si	2.91089300	1.83600000	-1.98529700
O	1.52527300	1.80337100	-1.03821300
N	1.36987200	-0.79531100	1.54752800
N	0.78153100	-2.04691100	3.42315900
N	2.90182200	-1.06312600	3.30060700
C	0.86840500	0.81882500	-0.25862000
C	-0.47692700	1.41347500	0.21344400
C	-0.11787800	2.10418500	1.50864700
C	1.11605900	1.64123100	1.98801700
C	1.66797400	0.57170400	1.05859500
C	-0.83080900	3.06848900	2.21860600
C	-0.29144300	3.57367700	3.40592300
C	0.94858300	3.12857300	3.87216500
C	1.66204200	2.15779800	3.16179800
C	1.68041200	-1.28989600	2.75954500
C	1.13230500	-3.25922800	4.20378500
C	-0.20926400	-3.98945000	4.41942300
C	-1.13910400	-3.41930900	3.33857700
C	-0.69294100	-1.96224900	3.23321500
C	4.12080300	-0.80897900	2.49514200
C	5.24899100	-0.95912800	3.51915400
C	4.61000400	-0.39777600	4.79866100
C	3.19023000	-0.97812400	4.74941200
C	2.33983800	1.80653800	-3.82025600
C	1.48434100	3.06658700	-4.08239800
C	3.54711600	1.80075700	-4.78088100
C	1.47357000	0.55901900	-4.09877100
H	0.74113200	-0.11208600	-0.82328300
H	-0.87863300	2.08990600	-0.54588300
H	-1.22417000	0.63146300	0.39891100
H	2.73396300	0.68039500	0.85382500
H	-1.79004900	3.43128000	1.86001500
H	-0.83803700	4.32881100	3.96307600
H	1.36487800	3.54585300	4.78456800
H	2.63562000	1.83165900	3.51708900
H	1.59201100	-3.01199700	5.16426500
H	1.84595700	-3.85450300	3.62553700
H	-0.08802300	-5.07345000	4.35444800
H	-0.59730100	-3.75912600	5.41745300
H	-2.19597800	-3.50489900	3.60191800
H	-0.97074000	-3.91702400	2.37866200
H	-0.96630400	-1.48563000	2.29605000
H	-1.10786900	-1.35827400	4.05056500
H	4.12423300	0.21036700	2.09549600
H	4.17192500	-1.50013100	1.65194700
H	6.14964100	-0.42325000	3.21174400
H	5.51012500	-2.01474800	3.65365200
H	4.58072800	0.69670900	4.75846400
H	5.13454300	-0.68587600	5.71281500
H	3.18528500	-1.96958000	5.21326600
H	2.43710800	-0.36199400	5.24800800
H	2.05683700	3.98753800	-3.93332700
H	0.61034600	3.10577600	-3.42380100
H	1.11983800	3.06499800	-5.11861300
H	3.19957900	1.75540900	-5.82180600
H	4.20064000	0.93730600	-4.61493100
H	4.15055600	2.70913300	-4.68416100

H	0.61276000	0.49968200	-3.42349100
H	2.04489500	-0.37018800	-4.00982300
H	1.08007800	0.59883300	-5.12361200
C	4.08183800	0.40498400	-1.55230800
C	3.68619800	-0.94133500	-1.69047700
C	5.38444600	0.64576900	-1.07064600
C	4.54718100	-1.99594600	-1.37909800
H	2.69158600	-1.19359100	-2.04222600
C	6.25304800	-0.40328600	-0.76082100
H	5.72913800	1.66685000	-0.93734700
C	5.83753300	-1.72717200	-0.91748800
H	4.20496800	-3.01873900	-1.50615900
H	7.25632300	-0.18520600	-0.40389900
H	6.51598100	-2.54394400	-0.68591300
C	3.72025600	3.48753900	-1.55164100
C	3.10797200	4.34542200	-0.61896400
C	4.92195600	3.92418700	-2.14470600
C	3.66810200	5.58250200	-0.29453500
H	2.18131600	4.03789600	-0.14488300
C	5.48628200	5.15927900	-1.82236100
H	5.43573000	3.29283200	-2.86527000
C	4.85826600	5.99307100	-0.89563000
H	3.17278700	6.22583600	0.42753700
H	6.41394700	5.47022000	-2.29494600
H	5.29418000	6.95609600	-0.64478200
H	0.79947000	-1.41708800	0.94477000
S	-0.11247600	-3.18300700	-0.26187700
C	0.92782800	-3.90222500	-1.50646500
C	1.64894700	-5.08558200	-1.24445900
C	1.05652900	-3.33672300	-2.79198100
C	2.46325900	-5.66638200	-2.21579300
C	1.86540500	-3.92490500	-3.76576100
C	2.57798000	-5.09224500	-3.48529400
H	3.00571500	-6.57948900	-1.98235100
H	1.93878900	-3.46574500	-4.74851700
H	3.20782200	-5.54935900	-4.24269700
H	-1.87731100	-2.61888900	-2.91534600
C	-2.81451300	-2.77080600	-2.37159600
C	-3.39321300	-2.89815300	0.15498600
C	-4.43099200	-4.52850100	-1.50965900
C	-3.98954500	-4.28457400	-0.05969600
C	-2.61909000	-2.32485900	-0.95216700
H	-2.92731200	-2.78038400	1.13401500
H	-4.76392900	-5.56636900	-1.62464700
H	-4.83203400	-4.41228800	0.62992900
H	-5.28983500	-3.88753500	-1.74086200
H	-3.22419700	-5.02036900	0.21824000
H	-2.04725500	-1.43507300	-0.74643900
N	-4.31179000	-1.79748300	-0.18473200
C	-4.05900300	-0.66015000	0.51750900
O	-3.12828400	-0.45145100	1.32315000
C	-5.03510500	0.46202900	0.25053800
C	-6.79074200	2.62907000	-0.19905900
C	-6.11620400	0.32008100	-0.62589300
C	-4.83198600	1.68197700	0.90257100
C	-5.70496600	2.73890200	0.66343000
C	-6.96857400	1.40268000	-0.83123000
H	-6.28181800	-0.62138500	-1.13243500
H	-3.99739800	1.78493400	1.58353400
H	-7.46374700	3.45671900	-0.37239300
N	-5.47243100	4.02771600	1.34017900
N	-8.10827600	1.25235700	-1.75720400
O	-8.84545300	2.22463200	-1.91340500
O	-4.46130400	4.13455200	2.03549800
O	-6.30012500	4.91997300	1.16908100
O	-8.24884900	0.16588400	-2.31432000
H	-3.55431800	-2.10153700	-2.83085900
C	-3.28296300	-4.23028000	-2.48366500
H	-3.58745700	-4.43494300	-3.51614700
H	-2.43547600	-4.89034900	-2.26235400
H	0.51495000	-2.42388100	-3.02268900
H	1.55511100	-5.54637400	-0.26572700

TS_{SS} conformation 2

Si	5.81653700	0.56590000	0.08580800
O	4.50457500	0.00623000	0.96746800
N	0.99385900	-0.98013600	0.52567600
N	-0.83708700	-2.18178000	-0.20162100
N	1.18955400	-2.32335500	-1.38833000
C	3.11650100	0.30688000	1.02209900
C	2.77578000	0.98811200	2.36875100
C	2.54157600	-0.17837600	3.30128700
C	2.30570200	-1.34885400	2.57173200
C	2.35712400	-1.05939400	1.08008700
C	2.51555300	-0.20938400	4.69463500
C	2.25655100	-1.42009400	5.34309800
C	2.02481600	-2.58875800	4.61001000
C	2.04624500	-2.55811600	3.21327700
C	0.44836800	-1.82633800	-0.36447800
C	-1.82831800	-2.49727700	-1.25345700
C	-2.76796900	-3.46491100	-0.53562000
C	-2.87313800	-2.85183900	0.87464800
C	-1.52057600	-2.14068500	1.11952400
C	2.22745000	-1.53125600	-2.09991500
C	2.62054700	-2.44361900	-3.26924800
C	2.39690700	-3.85460300	-2.70306000
C	1.08471800	-3.69373000	-1.92672600
C	6.44564800	2.25205800	0.76991900
C	6.79232700	2.07955800	2.26573700
C	7.71734600	2.68762900	0.00887300
C	5.38696900	3.36666100	0.62321700
H	2.79553900	0.89409800	0.15636300
H	3.58062300	1.65266800	2.69165600
H	1.85783700	1.58364100	2.26733100
H	2.90803600	-1.82025100	0.52721400
H	2.69662600	0.69292700	5.27202300
H	2.23983100	-1.45552500	6.42855300
H	1.83386100	-3.52340400	5.12900400
H	1.87290700	-3.46731000	2.64208600
H	-1.35889800	-2.90408400	-2.14652100
H	-2.36778100	-1.57976200	-1.51528100
H	-3.73770900	-3.53213600	-1.03189900
H	-2.32348000	-4.46634600	-0.50206500
H	-3.08062900	-3.59954600	1.64390800
H	-3.68020000	-2.11737000	0.87683700
H	-1.66099100	-1.10537000	1.43986000
H	-0.88691700	-2.64488700	1.85439200
H	3.09342800	-1.33730700	-1.46292300
H	1.81626400	-0.56726000	-2.40959400
H	3.64631600	-2.25813600	-3.59228200
H	1.95920900	-2.27352000	-4.12614200
H	3.21097900	-4.12641000	-2.02200500
H	2.32551400	-4.62709400	-3.47270300
H	0.23652300	-3.80327600	-2.61378300
H	0.95253100	-4.41170000	-1.11238600
H	7.56251300	1.31702800	2.41975600
H	5.91868000	1.78988700	2.85839000
H	7.17267500	3.02458100	2.67612500
H	8.05994700	3.66327500	0.37919400
H	7.53837900	2.79149300	-1.06721800
H	8.54141200	1.98188700	0.15144400
H	4.43470300	3.11111200	1.09938700
H	5.18739400	3.60584500	-0.42557300
H	5.74793700	4.28802400	1.09990200
C	5.38116700	0.66931900	-1.75959100
C	4.39458200	1.55433700	-2.24391300
C	6.02406900	-0.15267400	-2.70679300
C	4.07503600	1.62236300	-3.60119000
H	3.85293800	2.20542100	-1.56413500
C	5.71868500	-0.07897900	-4.06793400
H	6.77821300	-0.86171100	-2.37983400
C	4.74296300	0.81097800	-4.51943900
H	3.30159900	2.30860500	-3.93139900
H	6.24498800	-0.71561100	-4.77424300
H	4.50421100	0.87103600	-5.57763600
C	7.09977000	-0.78898400	0.39164000
C	6.82417600	-1.81798700	1.31204700
C	8.35668400	-0.80875100	-0.24516800
C	7.75789400	-2.81983800	1.58246000

H	5.86635600	-1.82659700	1.82261300
C	9.29246800	-1.80998800	0.01983200
H	8.61529700	-0.03773800	-0.96607700
C	8.99464600	-2.81917500	0.93650900
H	7.51959800	-3.60041100	2.29989400
H	10.25280400	-1.80080200	-0.48819400
H	9.72214500	-3.59827800	1.14623800
H	0.35906900	-0.26317600	0.93158700
S	-0.75308400	1.70651200	1.16072700
C	-0.16029200	2.33759900	-0.38962000
C	-0.36462400	1.65357000	-1.60720200
C	0.52946300	3.56740800	-0.44835200
C	0.07678600	2.18230700	-2.82120300
C	0.97676400	4.09080500	-1.66138700
C	0.74945900	3.40635900	-2.85905400
H	-0.11953500	1.64137000	-3.74398900
H	1.49374300	5.04716200	-1.67238900
H	1.07430700	3.82880200	-3.80567300
H	-3.14187600	2.46650200	2.85771900
C	-3.77697500	2.72760400	2.00660000
C	-3.74263500	2.12596500	-0.51625600
C	-4.25359900	4.50284800	0.25325000
C	-3.69990700	3.60957000	-0.86702300
C	-3.50181800	1.76531400	0.88497500
H	-3.21720200	1.49619400	-1.23630400
H	-4.10476600	5.55637300	-0.01016500
H	-4.26267500	3.76156200	-1.79530300
H	-5.33456100	4.34471200	0.34401800
H	-2.65652600	3.87636000	-1.07234200
H	-3.34412700	0.71853900	1.09539700
N	-5.10318200	1.64628500	-0.20735300
C	-5.31071400	0.33380800	-0.48439700
O	-4.47511800	-0.51913100	-0.84955400
C	-6.75200700	-0.09788800	-0.31832400
C	-9.42164200	-0.98622600	-0.04214400
C	-7.74272600	0.77898700	0.13808800
C	-7.09609700	-1.41417700	-0.63890000
C	-8.41603200	-1.83231200	-0.49639800
C	-9.05031400	0.31780100	0.26934300
H	-7.48796300	1.80173000	0.38082800
H	-6.33331200	-2.09236500	-0.99664000
H	-10.44254000	-1.32458600	0.06411000
N	-8.76661000	-3.22452300	-0.83359900
N	-10.09116700	1.24366000	0.75737400
O	-11.23810700	0.80937000	0.85353300
O	-7.85954000	-3.96402600	-1.21335800
O	-9.94302500	-3.56167100	-0.71263400
O	-9.74701800	2.38964100	1.03843100
H	-4.81542500	2.57053700	2.32758800
C	-3.57148000	4.19350700	1.59328400
H	-3.95536500	4.84977600	2.38260900
H	-2.49475400	4.38291200	1.50955600
H	0.69604900	4.11482800	0.47433400
H	-0.90089900	0.70913300	-1.59301700

TS structures for Mechanism 1: Ar = 4-BrC_6H_4

Table 7

	TS_{RR} conformation 2	TS_{SS} conformation 1	TS_{SS} conformation 2
E[RB3LYP/6-31G(d,p)]	-6095.54371289	-6095.53857681	-6095.54598442
Zero-point correction	1.061663	1.061791	1.062407
Thermal correction to Energy	1.127990	1.111297	1.111679
Thermal correction Enthalpy	1.128934	1.112099	1.112480
Thermal correction to Gibbs Free Energy	0.946111	0.972615	0.974944
E[CPCM/RB3LYP/6 311+G(2df,2p)]	-6098.89375254	-6098.88773337	-6098.89125038
E[CPCM/RM06-2X/6-311+G(2df,2p)	-6097.69337829	-6097.68767884	-6097.68923931
E[RM06-2X/6-311+G(2df,2p)]	-6097.66954935	-6097.66450967	-6097.66711533

TS_{RR} conformation 1: As attempt to derive the TS structures for Ar=C_6H_5 from Ar= 2,6-$Cl_2C_6H_3$ transition was not successfully, and all the TS structures for Ar=4-BrC_6H_4 are derived from Ar=C_6H_5, this TS structure was not included

TS_{RR} conformation 2

Si	5.28871300	0.11822100	0.67601700
O	4.25222400	-1.16101900	1.04130000
N	1.37633600	-1.56250000	-0.41782500
N	0.05407100	-1.97601800	-2.29926300
N	2.24717700	-2.79015600	-2.21285400
C	2.93143300	-1.23344700	1.54863100
C	2.88751300	-1.79961900	2.98910800
C	1.58844100	-2.56566200	3.03740200
C	1.10258400	-2.79603700	1.74566800
C	2.05410600	-2.21162300	0.71399400
C	0.89447500	-3.05204800	4.14409900
C	-0.28407600	-3.77517500	3.94298700
C	-0.76396100	-4.00902700	2.65009300
C	-0.07029400	-3.51893700	1.54064600
C	1.21596900	-2.11229000	-1.63767900
C	-0.05160200	-1.96905100	-3.78187200
C	-1.52567800	-1.62917500	-4.05739200
C	-1.97060000	-0.85567100	-2.81058700
C	-1.24061100	-1.56863600	-1.67469700
C	3.67578700	-2.38311000	-2.08744800
C	4.43159100	-3.48082200	-2.85588300
C	3.49188800	-4.69494000	-2.78503200
C	2.11476400	-4.04916200	-2.96832300
C	5.59304000	1.24719000	2.20515100
C	6.15321500	0.38707800	3.35972700
C	6.63167200	2.33311000	1.84266800
C	4.30587500	1.95518400	2.68331400
H	2.43346900	-0.25714800	1.52945000
H	3.74772600	-2.46816100	3.12743100
H	2.95803700	-1.01531500	3.74895400
H	2.69284400	-3.00487600	0.31541300
H	1.26030200	-2.86852100	5.15063900
H	-0.83597100	-4.15462900	4.79777100
H	-1.68395600	-4.56766700	2.50774700
H	-0.45225000	-3.69434600	0.53871700
H	0.21859900	-2.93431300	-4.21298100
H	0.63348500	-1.21378500	-4.18305600
H	-1.63999000	-1.06625000	-4.98695900
H	-2.10780000	-2.55172300	-4.15464600
H	-3.04723200	-0.86914700	-2.63963400
H	-1.63717300	0.18673100	-2.87200700
H	-1.09145800	-0.92595500	-0.80778800
H	-1.79047000	-2.45970000	-1.35689400
H	3.99186600	-2.33701800	-1.04554100
H	3.81682300	-1.38740700	-2.51570500
H	5.41532300	-3.66737000	-2.41931400
H	4.58033900	-3.18542900	-3.90015800
H	3.55531700	-5.17755500	-1.80349200
H	3.69816500	-5.44867300	-3.54906000
H	1.93582200	-3.86888700	-4.03637700
H	1.28381000	-4.64174000	-2.57677900
H	7.08952400	-0.10778800	3.08269400
H	5.44719200	-0.38877000	3.67255300
H	6.35728600	1.01873500	4.23461600
H	6.79130200	2.99654600	2.70305200
H	6.30008100	2.95755700	1.00581400
H	7.60368100	1.90180800	1.58415700
H	3.51224200	1.25429400	2.96133700
H	3.90359400	2.63578900	1.92709900
H	4.52670100	2.55796100	3.57462700
C	4.63547200	1.07683400	-0.82150300
C	3.40854500	1.77037400	-0.77454000
C	5.33834800	1.09393600	-2.04302800
C	2.91691400	2.46092100	-1.88381400
H	2.80876000	1.77521000	0.13018900
C	4.85152600	1.78243400	-3.15619500
H	6.27926700	0.56012600	-2.13172700
C	3.64082100	2.47131500	-3.07708100
H	1.97090400	2.98757700	-1.81042000
H	5.42072600	1.78302400	-4.08203200
H	3.26325000	3.01445000	-3.93903000
C	6.87274900	-0.81492300	0.21899300
C	6.95846800	-2.20622100	0.41820000
C	8.01197200	-0.16782300	-0.29996300
C	8.11974800	-2.91771800	0.11000000
H	6.10242600	-2.73385500	0.82674100
C	9.17578400	-0.87374300	-0.61015800
H	7.99739100	0.90457800	-0.47452600
C	9.23250500	-2.25294400	-0.40655900
H	8.15755300	-3.99061600	0.27914900
H	10.03700500	-0.34600800	-1.01021300
H	10.13756000	-2.80403200	-0.64580700
H	0.76096000	-0.77918200	-0.14073600
S	-0.27654900	0.90064300	1.12017000
C	-0.22075200	2.51876600	0.40038200
C	-0.80169800	2.80870200	-0.85201300
C	0.39065900	3.58986800	1.08630300
C	-0.76595200	4.09074500	-1.40015200
C	0.44196200	4.87394400	0.54635700
C	-0.13632300	5.11659700	-0.69824300
H	-1.22265100	4.29047400	-2.36362500
H	0.92296500	5.67978300	1.09019200
H	-1.86389000	-0.85288500	3.71497900
C	-2.93882700	-0.75279000	3.52065600
C	-2.99223500	0.66568300	1.40527000
C	-2.91187300	1.77237700	3.68115700
C	-3.24524400	1.92199300	2.18803800
H	-2.92747100	0.70956700	0.32779000
H	-1.82144900	1.76949400	3.79641400
H	-4.30522900	2.17915500	2.06389400
H	-3.29365900	2.64295200	4.22634200
H	-2.67571600	2.73899800	1.73448500
C	-4.83631300	-1.01074700	0.38959000
O	-4.06127200	-1.53376800	-0.43569300
C	-6.30712100	-0.92876100	0.04192100
C	-9.03668100	-0.82270300	-0.68403800
C	-6.73967900	-1.48767400	-1.16425200
C	-7.23810300	-0.31801600	0.88950800
C	-8.57727100	-0.27480300	0.50920000
C	-8.08841400	-1.42578600	-1.50306500
H	-6.02178900	-1.96370100	-1.81876900
H	-6.91314800	0.10937700	1.82841100
H	-10.08070900	-0.78197800	-0.96021100
N	-9.55594800	0.37364700	1.40370500
N	-8.53529500	-2.01751800	-2.77796300
O	-9.73411200	-1.95642300	-3.04574800
O	-9.13489800	0.85874300	2.45167500
O	-10.73232100	0.38832500	1.04405700
O	-7.68091800	-2.53523000	-3.49591800
H	-3.41982900	-1.67003600	3.87978100
C	-3.48889600	0.47408400	4.26293300
H	-4.58205700	0.48565900	4.18341700
H	-3.24541600	0.39904700	5.32921300
C	-3.13014800	-0.66456300	2.01038100
H	-2.61660600	-1.45961000	1.46553800
N	-4.53612400	-0.49316100	1.60991700
H	0.83186600	3.40268600	2.06022400
H	-1.29287200	2.01319000	-1.40391300
Br	-0.06704400	6.87639800	-1.45299800

TS_{SS} conformation 1

Si	0.59645900	3.84003700	-1.83406600
O	-0.32357500	3.10803800	-0.62942000
N	1.27196000	0.40115300	1.23827500
N	1.72206000	-1.36411900	2.68810500
N	2.91605500	0.64187300	2.89117400
C	-0.27123900	1.79582700	-0.09348800
C	-1.64329700	1.47047500	0.53630600
C	-1.50420800	1.96440200	1.95731500
C	-0.15439800	2.16007100	2.28325200
C	0.72795500	1.77502900	1.10620000
C	-2.49984000	2.21811800	2.89894600
C	-2.13327600	2.68626600	4.16440600

C	-0.79027200	2.90799900	4.48089400
C	0.20891900	2.64605100	3.53832000
C	1.96084400	-0.10036400	2.28000400
C	2.77828600	-2.31041100	3.13136400
C	2.09226800	-3.69057700	3.13220600
C	0.87734400	-3.51792800	2.20937900
C	0.43329400	-2.08202000	2.48003300
C	3.67437200	1.72296000	2.21638400
C	4.82808900	1.99290800	3.18603000
C	4.16682500	1.77225000	4.55495000
C	3.30220400	0.52739200	4.31590600
C	-0.20406400	3.46760100	-3.54543200
C	-1.57411800	4.18096800	-3.60225000
C	0.68962900	3.99135100	-4.69005000
C	-0.43990400	1.95454600	-3.74626200
H	0.02434300	1.06888300	-0.85723100
H	-2.44245800	1.96723100	-0.02086300
H	-1.84538100	0.39145200	0.52960300
H	1.53010300	2.48808500	0.90773900
H	-3.54758200	2.05874500	2.65997900
H	-2.90260300	2.89110900	4.90302600
H	-0.52189600	3.29340800	5.46031300
H	1.24894100	2.83988400	3.78460100
H	3.15512700	-2.06784600	4.12776200
H	3.60987000	-2.26397800	2.42197200
H	2.77734400	-4.47362300	2.79955100
H	1.76547300	-3.94146500	4.14706200
H	0.08101700	-4.23642700	2.41664000
H	1.17358800	-3.61918700	1.16155500
H	-0.16335900	-1.65545600	1.67888800
H	-0.14981700	-2.01407500	3.40725100
H	3.06404200	2.62618300	2.11246500
H	3.98258900	1.40920400	1.21713800
H	5.23931200	2.99682500	3.05912000
H	5.63806700	1.27140700	3.03182000
H	3.54078500	2.63233800	4.81624700
H	4.88211800	1.61901600	5.36643500
H	3.90098600	-0.37152300	4.49200800
H	2.40959200	0.47560000	4.94498300
H	-1.47569000	5.26713200	-3.51637200
H	-2.23987600	3.84184300	-2.80116400
H	-2.07025800	3.96510100	-4.55812400
H	0.22053100	3.77940000	-5.66032700
H	1.67710600	3.51790400	-4.69151600
H	0.83387300	5.07567800	-4.63470900
H	-1.09160300	1.53697900	-2.97157300
H	0.48927000	1.37739300	-3.75701200
H	-0.93542500	1.78232300	-4.71148000
C	2.41445300	3.29707600	-1.71823100
C	2.83925000	1.99257100	-2.04555000
C	3.39938300	4.20029400	-1.26918500
C	4.18038800	1.61498700	-1.94306200
H	2.12920100	1.23935900	-2.37260300
C	4.74133300	3.82797200	-1.16415100
H	3.11599100	5.21337000	-1.00083800
C	5.13696400	2.53364800	-1.50552000
H	4.47178600	0.60352600	-2.21069800
H	5.47734400	4.55181100	-0.82420900
H	6.18227300	2.24442800	-1.43728700
C	0.45484800	5.67557400	-1.41459000
C	-0.36736700	6.09521200	-0.35256600
C	1.12668300	6.67103400	-2.15132600
C	-0.51577400	7.44830000	-0.04246000
H	-0.89292100	5.34902900	0.23492300
C	0.98214300	8.02473500	-1.84412200
H	1.78311200	6.39255600	-2.97209800
C	0.15746700	8.41647800	-0.78820200
H	-1.15786900	7.74589100	0.78203600
H	1.51244100	8.77198800	-2.42799200
H	0.04198300	9.46976300	-0.54823800
H	1.03375500	-0.27317800	0.49207500
S	1.10707600	-1.58696700	-1.51535800
C	2.52603500	-2.60505300	-1.22216200
C	3.68065700	-2.07092200	-0.60868800
C	2.57035500	-3.96510900	-1.59053100
C	4.81111800	-2.84991200	-0.36528300
C	3.69142400	-4.75687700	-1.34374500
C	4.80688500	-4.19600500	-0.72645400
H	5.69150900	-2.41352900	0.09541000
H	3.69747300	-5.80202400	-1.63420200
H	-1.02849700	-1.78424800	-3.64247100
C	-1.61730900	-2.57193100	-3.16425300
C	-1.62501600	-3.63569100	-0.79855700
C	-1.89141300	-5.08065400	-2.88735100
C	-1.42644700	-5.01298200	-1.42495100
C	-1.43059000	-2.47388700	-1.67922700
H	-1.13288500	-3.53482400	0.17039400
H	-1.63401600	-6.05782800	-3.31160600
H	-1.96189300	-5.74970000	-0.81544500
H	-2.98345100	-4.99356000	-2.92279300
H	-0.35911100	-5.26184900	-1.36402800
H	-1.44313100	-1.50710400	-1.20049300
N	-3.03618000	-3.21559600	-0.77690300
C	-3.31944300	-2.33687500	0.21599000
O	-2.52316800	-1.80725900	1.02187400
C	-4.78239800	-1.96873600	0.31736200
C	-7.48976400	-1.20160000	0.57111100
C	-5.75243800	-2.52477600	-0.52352800
C	-5.16333900	-1.03318700	1.28392400
C	-6.50111900	-0.66393900	1.38859500
C	-7.08113000	-2.13260300	-0.37826600
H	-5.46667700	-3.24995900	-1.27364800
H	-4.41160900	-0.60945300	1.93673600
H	-8.52588600	-0.90915800	0.66612500
N	-6.89100400	0.33928300	2.39606200
N	-8.10326100	-2.72083200	-1.26615000
O	-9.26849600	-2.36009700	-1.10826100
O	-5.99449200	0.86017300	3.06102100
O	-8.08688800	0.59800500	2.51117800
O	-7.72573900	-3.53340400	-2.10750400
H	-2.67238900	-2.34839900	-3.37305200
C	-1.25816000	-3.95775200	-3.72138200
H	-1.58042000	-4.02437400	-4.76636200
H	-0.16591500	-4.06643400	-3.71922500
H	1.71162400	-4.40634200	-2.08484400
H	3.69335300	-1.01936500	-0.33875900
Br	6.34959900	-5.27768000	-0.37295100

TS_{SS} conformation 2

Si	-5.73600800	-0.06862300	-0.52047000
O	-4.39877100	-0.99633700	-0.93396600
N	-0.87489200	-1.46285200	-0.00855800
N	0.97935100	-2.03237200	1.24391500
N	-1.05879800	-1.57771700	2.32744200
C	-3.01838400	-0.72704800	-1.13347400
C	-2.65995900	-0.87755200	-2.63170400
C	-2.37464800	-2.35512500	-2.77614200
C	-2.13414000	-2.93231000	-1.52444100
C	-2.22488100	-1.87826300	-0.43319200
C	-2.31254600	-3.13843300	-3.92755800
C	-2.01467100	-4.49882000	-3.80900700
C	-1.78085900	-5.07323400	-2.55509800
C	-1.83766400	-4.28813300	-1.40067100
C	-0.31769100	-1.68413100	1.19497200
C	1.96411400	-1.70207300	2.29728500
C	2.93362300	-2.88041600	2.21771100
C	3.04420800	-3.12373400	0.69974100
C	1.67585600	-2.70213300	0.11198500
C	-2.13656800	-0.56832500	2.50748900
C	-2.52322100	-0.73088400	3.98367300
C	-2.23963600	-2.21559800	4.25904800
C	-0.91779200	-2.44154900	3.51642500
C	-6.31431200	1.02785900	-1.99601500
C	-6.63459100	0.11126100	-3.19809400
C	-7.59535100	1.79868000	-1.60478600
C	-5.24288800	2.05706500	-2.41820600
H	-2.73352100	0.24832200	-0.72651300

H	-3.47303700	-0.52543700	-3.27055100
H	-1.76085100	-0.29070000	-2.86592300
H	-2.76616600	-2.23022100	0.44472400
H	-2.49668800	-2.70174400	-4.90516800
H	-1.97002900	-5.11868600	-4.69978100
H	-1.56085000	-6.13396700	-2.47918500
H	-1.66358900	-4.73501700	-0.42449800
H	1.49256700	-1.57040900	3.26864600
H	2.48166600	-0.77708200	2.01809100
H	3.89775200	-2.64551900	2.67214400
H	2.51030800	-3.75205300	2.73016300
H	3.28508600	-4.16116100	0.45585600
H	3.83022300	-2.48147600	0.29891100
H	1.79232000	-2.01021000	-0.72607900
H	1.06458600	-3.54513100	-0.22180100
H	-2.99561600	-0.77654200	1.86575800
H	-1.76281500	0.42720000	2.25614200
H	-3.56141400	-0.44286100	4.15708400
H	-1.88715700	-0.10252400	4.61695500
H	-3.02951100	-2.84209800	3.83003300
H	-2.15724600	-2.45360800	5.32237600
H	-0.08153000	-2.13024200	4.15461500
H	-0.74198000	-3.47739500	3.21314200
H	-7.41742800	-0.61495300	-2.95761500
H	-5.75676400	-0.44982000	-3.53429200
H	-6.98769800	0.71282700	-4.04637800
H	-7.91357100	2.44032300	-2.43732000
H	-7.43731200	2.44557700	-0.73475100
H	-8.42739600	1.12347800	-1.38237100
H	-4.28150800	1.59450800	-2.66431500
H	-5.06839300	2.80768500	-1.64174800
H	-5.57875100	2.59568900	-3.31466500
C	-5.37650600	0.96440400	1.03109800
C	-4.44235200	2.02212200	1.02829700
C	-6.03419800	0.69564300	2.24830000
C	-4.18845500	2.78277300	2.17153200
H	-3.89450300	2.26881200	0.12379300
C	-5.79271400	1.45764300	3.39401200
H	-6.75077200	-0.11772000	2.30419000
C	-4.87094100	2.50485500	3.35714800
H	-3.46384200	3.59017500	2.13022600
H	-6.32895600	1.23492700	4.31279500
H	-4.68527100	3.10253300	4.24520100
C	-7.02726400	-1.39704600	-0.14589300
C	-6.74437700	-2.74794900	-0.42259300
C	-8.30052300	-1.09521200	0.37673300
C	-7.68755100	-3.75003900	-0.18816400
H	-5.77278200	-3.01138400	-0.82836500
C	-9.24620000	-2.09391700	0.61475300
H	-8.56328600	-0.06740500	0.61241800
C	-8.94127700	-3.42591400	0.33136600
H	-7.44319500	-4.78466200	-0.41319900
H	-10.21931200	-1.83158100	1.02049000
H	-9.67617400	-4.20491100	0.51392300
H	-0.25143500	-1.07398900	-0.74063100
S	0.84072400	0.50259300	-2.02112400
C	0.24445400	1.83222300	-1.01249600
C	0.51206000	1.90472500	0.37158500
C	-0.52102800	2.87707500	-1.57324800
C	0.05422600	2.96417300	1.15539900
C	-0.99276100	3.93777800	-0.80051300
C	-0.69732100	3.97466400	0.56092000
H	0.28876900	3.00973400	2.21366900
H	-1.57357200	4.73381900	-1.25397000
H	3.21814200	0.08929600	-3.84027300
C	3.84999500	0.80549700	-3.30716200
C	3.82645100	1.81636900	-0.91995100
C	4.32955100	3.27495900	-2.95060300
C	3.77982000	3.21855500	-1.51733700
C	3.57312100	0.69743400	-1.83410500
H	3.30357700	1.73834300	0.03496300
H	4.17847200	4.27934000	-3.36252100
H	4.34046700	3.89416400	-0.86131600
H	5.41082400	3.09575800	-2.93202800
H	2.73475400	3.55089300	-1.50830000
H	3.42083900	-0.27017800	-1.38081600
N	5.18694500	1.24713800	-0.88218200
C	5.38594900	0.34165500	0.10845800
O	4.54220200	-0.14291900	0.89195300
C	6.82612700	-0.10540700	0.23833300
C	9.49143400	-0.99248600	0.55489700
C	7.82445300	0.33715200	-0.63702100
C	7.16036600	-0.98606200	1.27090900
C	8.47830400	-1.41119300	1.41026200
C	9.12974400	-0.11643600	-0.46356900
H	7.57699500	1.02511600	-1.43407600
H	6.39157500	-1.32520400	1.95180400
H	10.51087500	-1.33090000	0.67414800
N	8.81750100	-2.34533900	2.49987700
N	10.17868000	0.34592600	-1.39370100
O	11.32363500	-0.06336500	-1.20749700
O	7.90247500	-2.72460400	3.22985800
O	9.99258600	-2.69011500	2.61035000
O	9.84226800	1.10899400	-2.29655300
H	4.88895200	0.48854800	-3.46884100
C	3.64681900	2.23078400	-3.84554300
H	4.03167700	2.28955900	-4.86994400
H	2.57023200	2.43409500	-3.89153600
H	1.10926800	1.12472800	0.83363900
H	-0.73661600	2.85464900	-2.63683800
Br	-1.32479900	5.43924700	1.62940200

TS structures for Mechanism 2: Ar = 2,6-$Cl_2C_6H_3$

7 conformations for both (*R*,*R*) and (*S*,*S*) transition state were located. Their electronic energies and relative electronic energies are given in Table 7

Table 8: CPCM/RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Relative energy (kcal/mol)	Conformation	Electronic energy (hartree)	Relative energy (kcal/mol)
TS_{RR} conformation 1	-4443.326602	7.7	TS_{SS} conformation 1	-4443.328913	3.9
TS_{RR} conformation 2	-4443.324719	8.8	TS_{SS} conformation 2	-4443.325530	3.1
TS_{RR} conformation 3	-4443.325534	8.3	TS_{SS} conformation 3	-4443.328913	3.9
TS_{RR} conformation 4	-4443.326602	7.7	TS_{SS} conformation 4	-4443.325670	6.0
TS_{RR} conformation 5	-4443.327339	7.2	TS_{SS} conformation 5	-4443.325671	6.0
TS_{RR} conformation 6	-4443.327339	7.2	TS_{SS} conformation 6	-4443.328913	3.9
TS_{RR} conformation 7	-4443.338798	0.0	TS_{SS} conformation 7	-4443.335179	0.0

Table 9: RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)	Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)
TS_{RR} conformation 7	-4443.31310491	0	TS_{SS} conformation 7	-4443.31361401	0.

Table 10: Correction to zero-point energy, thermal correction to electronic energy, enthalpy and Gibbs derived from RB3LYP/6-31G(d,p) for (R,R) TS structures

Conformation	Zero-point correction	Thermal correction to Energy	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
1	1.052568	1.119688	1.120632	0.938360

2	1.053258	1.120052	1.120996	0.941685
3	1.053004	1.119892	1.120837	0.940479
4	1.052568	1.119688	1.120632	0.938360
5	1.052794	1.119883	1.120827	0.938606
6	1.052794	1.119883	1.120827	0.938602
7	1.053665	1.120534	1.121478	0.942341

Table 11 Correction to zero-point energy, thermal correction to electronic energy, enthalpy and Gibbs derived from RB3LYP/6-31G(d,p) for (S,S) TS structures

Conformation	Zero-point correction	Thermal correction to Energy	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
1	1.053027	1.120086	1.121030	0.939922
2	1.052856	1.120028	1.120972	0.939560
3	1.053027	1.120086	1.121030	0.939922
4	1.053293	1.120178	1.121122	0.942487
5	1.053293	1.120178	1.121122	0.942488
6	1.053027	1.120086	1.121030	0.939922
7	1.053163	1.120151	1.121095	0.940386

TS_{RR} conformation 1

Si	-4.10535200	1.15055100	-0.86363500
O	-3.75109600	-0.43059100	-1.33471400
N	-1.56111100	-2.04715100	0.32883000
N	-0.70298400	-2.70617800	2.37686400
N	-2.96610600	-3.08244800	1.91505900
C	-2.56687400	-1.07631300	-1.75478700
C	-2.66344000	-1.60569300	-3.20596100
C	-1.71966800	-2.78406500	-3.20671500
C	-1.46537300	-3.20623100	-1.89556500
C	-2.25799700	-2.35164300	-0.91881700
C	-1.13241400	-3.44794600	-4.28200800
C	-0.29217300	-4.53667900	-4.03078400
C	-0.04135500	-4.95526500	-2.72043300
C	-0.63039100	-4.29033100	-1.64137200
C	-1.75136400	-2.60903500	1.53084700
C	0.71820100	-2.60926300	1.93244600
C	1.50388300	-2.70460400	3.24303600
C	0.57096200	-2.02149100	4.25350000
C	-0.80889200	-2.55391600	3.84792400
C	-3.15467300	-4.26806700	2.78170100
C	-4.66848800	-4.50695700	2.72373300
C	-5.22736700	-3.08270000	2.59022700
C	-4.26412500	-2.43447500	1.59080200
C	-4.05370800	1.26008400	1.03343100
C	-2.79731900	1.22533200	1.67712100
C	-2.68992400	1.28342500	3.06868900
C	-3.83849700	1.37116700	3.85888500
C	-5.09226700	1.40237900	3.24779900
C	-5.19363000	1.35054700	1.85523800
C	-2.83474100	2.38258200	-1.53098600
C	-2.21926400	2.23194300	-2.78882000
C	-1.32088500	3.17938100	-3.28192200
C	-1.02511100	4.31932700	-2.53239100
C	-1.63601100	4.50229500	-1.29077500
C	-2.52241700	3.54395500	-0.79719700
C	-5.83410200	1.46567300	-1.63838700
C	-6.83566100	0.35505800	-1.24994100
C	-6.38137700	2.84936000	-1.22510800
C	-5.68040200	1.44473400	-3.17739200
H	-0.79494600	-1.35461500	0.23902800
H	-1.70041600	-0.40806800	-1.67350600

H	-3.69874900	-1.92085400	-3.39460900
H	-2.41283300	-0.84514200	-3.95153300
H	-3.20160400	-2.85045600	-0.68962400
H	-1.31689400	-3.12145100	-5.30183400
H	0.17801600	-5.05669000	-4.85993700
H	0.62269900	-5.79487700	-2.53987300
H	-0.42741400	-4.61333700	-0.62382100
H	0.89408000	-1.64675200	1.44639100
H	0.95009800	-3.40742800	1.22357300
H	1.66230500	-3.75283800	3.52029600
H	2.48312100	-2.22952500	3.15830200
H	0.60904200	-0.93274900	4.13908000
H	0.80709000	-2.25814000	5.29386500
H	-0.98855100	-3.52492000	4.32480800
H	-1.63579900	-1.88446600	4.09827200
H	-2.85133600	-4.06763600	3.81439900
H	-2.55992000	-5.10789300	2.41076000
H	-5.03065600	-5.03804200	3.60719800
H	-4.92830600	-5.10115300	1.84080800
H	-5.18392300	-2.56282700	3.55356900
H	-6.26061300	-3.05394100	2.23660200
H	-4.58381900	-2.65605800	0.56790800
H	-4.17749200	-1.35216500	1.68778300
H	-1.88363200	1.15013200	1.09316400
H	-1.70785800	1.28713400	3.53509800
H	-3.75552600	1.42747100	4.94076100
H	-5.99213500	1.47846300	3.85200700
H	-6.18363900	1.38775400	1.41359600
H	-2.44043500	1.36258900	-3.40084400
H	-0.85221600	3.02743000	-4.24996300
H	-0.32012300	5.05529100	-2.90765000
H	-1.41861000	5.38987500	-0.70312300
H	-2.97100900	3.70080600	0.17951100
H	-7.04122000	0.32230700	-0.17554300
H	-6.46754100	-0.63165000	-1.54782400
H	-7.79553900	0.52059100	-1.75768300
H	-7.33977800	3.04068200	-1.72615200
H	-5.69723400	3.65532600	-1.51200200
H	-6.55504300	2.93204700	-0.14786700
H	-5.29740300	0.48251600	-3.53309600
H	-5.00840500	2.23127000	-3.53397900
H	-6.65779100	1.60582000	-3.65136300
O	0.07904000	0.14736300	0.32203600
C	0.96781600	0.80997200	-0.28739700
N	1.46237800	0.47504200	-1.47790100
C	1.39187100	2.08961900	0.39816400
C	2.67755900	-0.82807200	-1.76378400
C	2.86460500	0.64257900	-1.84887100
C	1.80732700	3.22634900	-0.30179700
C	1.26519900	2.15862500	1.78945800
C	2.09702600	4.39338000	0.40302900
H	1.87377900	3.22720100	-1.38105800
C	1.57797100	3.33685400	2.45603600
H	0.91156900	1.29834800	2.33910200
C	2.00387000	4.48027800	1.78765200
N	2.48720000	5.60011700	-0.35158700
N	1.42351000	3.38280900	3.92131500
H	2.23605100	5.39520700	2.31444700
O	2.80483600	6.59577100	0.29438700
O	2.46012300	5.53452800	-1.57986600
O	0.97195500	2.38025900	4.47914800
O	1.74862000	4.41723000	4.49697700
H	2.75304500	-1.30003100	-0.79638600
H	3.51959900	1.06457300	-1.08215000
S	5.24768500	-1.59150300	-1.78857200
C	5.50175600	-1.57222700	-0.06187500
C	5.01187400	-2.57460900	0.82161500
C	6.24267200	-0.55503200	0.60878600
C	5.25536000	-2.59820300	2.19316700
C	6.49412300	-0.55089100	1.97791800
C	6.00363300	-1.57966500	2.77963700
H	4.87272000	-3.42057200	2.78790300
H	7.07634800	0.25717900	2.40660200
H	6.20734500	-1.59058000	3.84559100
C	2.24641300	-1.65258800	-2.95394200
C	2.66926000	-1.02895500	-4.29418700
H	1.15687100	-1.75905500	-2.91984000
C	2.38351700	0.47916700	-4.34505900
H	2.15115400	-1.54599900	-5.11026000
H	3.74296700	-1.19422300	-4.44223400
C	3.14234800	1.21609100	-3.23194700
H	1.30629100	0.66007300	-4.23772100
H	2.68128200	0.88669700	-5.31800800
H	2.90500800	2.28741800	-3.24186000
H	4.22214600	1.12345700	-3.39578600
H	2.67416800	-2.65096900	-2.84294100
Cl	4.03303000	-3.90934900	0.18501100
Cl	6.90000200	0.79938100	-0.30735500

TS_{RR} conformation 2

Si	-4.18579900	-0.48176600	-1.43172600
O	-3.17340100	-1.83014400	-1.32963700
N	-0.85763000	-1.78194000	0.87157300
N	-0.21880100	-1.48064200	3.08133200
N	-2.04812800	-2.85218600	2.60212500
C	-1.77353900	-1.97799000	-1.46395100
C	-1.38761000	-2.88588000	-2.65667800
C	-0.05564800	-3.45908100	-2.23501800
C	0.11627600	-3.32305000	-0.85162800
C	-1.12526100	-2.69019600	-0.24268400
C	0.93833900	-4.05555000	-3.00814100
C	2.10682900	-4.50291000	-2.38434800
C	2.27815300	-4.35819000	-1.00420600
C	1.27635900	-3.77034000	-0.22657100
C	-1.04673000	-2.03697700	2.17467700
C	1.12053600	-0.92264600	2.74302000
C	1.64418400	-0.42437700	4.09319800
C	0.36646200	0.01964200	4.82043400
C	-0.63435100	-1.08115200	4.44761000
C	-1.91382800	-3.79721100	3.72974700
C	-3.09600000	-4.74697600	3.51656800
C	-4.18651400	-3.79915000	2.99558400
C	-3.42750700	-2.86488700	2.04051800
C	-4.44957100	0.24276100	0.30551700
C	-3.37149900	0.89527300	0.94328800
C	-3.49640400	1.41491800	2.23428100
C	-4.70362500	1.29508500	2.92666900
C	-5.78462700	0.65755100	2.31785000
C	-5.65538300	0.14284900	1.02548200
C	-3.41571700	0.86431500	-2.51227900
C	-2.70684100	0.55878200	-3.69105900
C	-2.19153400	1.55995100	-4.51450000
C	-2.38298600	2.90227300	-4.18384000
C	-3.08893900	3.23327200	-3.02719700
C	-3.59352700	2.22654900	-2.20247900
C	-5.77438100	-1.20248600	-2.23974100
C	-6.30017600	-2.41647900	-1.44111300
C	-6.87309000	-0.12474600	-2.36824800
C	-5.41573000	-1.69546700	-3.66096500
H	-0.39016600	-0.89749200	0.60623000
H	-1.28274000	-1.00256600	-1.57563400
H	-2.15097100	-3.66940300	-2.75916900
H	-1.34677300	-2.34239400	-3.60504200
H	-1.79831700	-3.47857200	0.10266500
H	0.81680400	-4.15805500	-4.08309900
H	2.89800600	-4.95137000	-2.97714400
H	3.20158900	-4.68411900	-0.53691400
H	1.41530600	-3.65660800	0.84508600
H	1.01543400	-0.09785900	2.03437900
H	1.74819800	-1.69244800	2.28747000
H	2.12779600	-1.24213600	4.63960800
H	2.37751400	0.37366200	3.96526000
H	0.02540300	0.99104300	4.44790100
H	0.49085600	0.10238900	5.90293500
H	-0.53997800	-1.92539800	5.14043800
H	-1.67625200	-0.75129300	4.44151600
H	-2.01343600	-3.29461800	4.69949900
H	-0.93674900	-4.28693900	3.69794200
H	-3.37539300	-5.26749200	4.43585200

H	-2.84704900	-5.49965000	2.76057900
H	-4.61546800	-3.22754400	3.82582300
H	-5.00411500	-4.31758700	2.48950200
H	-3.44521600	-3.24985600	1.01890900
H	-3.83037400	-1.85145100	2.01647000
H	-2.41564000	1.00485900	0.43684700
H	-2.65879200	1.93154000	2.69581900
H	-4.80309500	1.70680800	3.92720700
H	-6.73171400	0.56726700	2.84278600
H	-6.51742600	-0.34013600	0.57913400
H	-2.55574900	-0.47733500	-3.97908600
H	-1.64251700	1.29309000	-5.41303200
H	-1.98382500	3.68420200	-4.82338700
H	-3.24377600	4.27578500	-2.76361600
H	-4.12844000	2.50861000	-1.30043200
H	-6.61707700	-2.15628900	-0.42659000
H	-5.53572200	-3.19574400	-1.36108300
H	-7.16983700	-2.85400900	-1.95000700
H	-7.74841200	-0.53943600	-2.88571500
H	-6.52553500	0.73458300	-2.95197800
H	-7.21535800	0.25243000	-1.40000300
H	-4.63648500	-2.46443300	-3.63871100
H	-5.07194200	-0.87910700	-4.30323600
H	-6.30191100	-2.13688700	-4.13621200
O	-0.09627800	0.78194700	0.18843600
C	0.70753800	1.58585300	-0.36666300
N	1.43370400	1.29292200	-1.44134900
C	0.72845100	2.98294700	0.22543300
C	2.92900100	0.24262100	-1.50082700
C	2.81177500	1.71698500	-1.65314800
C	1.14115700	4.11673600	-0.48239000
C	0.23142600	3.14529800	1.52336500
C	1.07095300	5.36872900	0.12620800
H	1.49214000	4.04766800	-1.50247000
C	0.18244700	4.41005400	2.09707000
H	-0.12602700	2.28162900	2.06439400
C	0.60179700	5.55179500	1.42174700
N	1.49642800	6.55713800	-0.64085200
N	-0.35055400	4.54955200	3.46360700
H	0.55587500	6.53271400	1.87352800
O	1.43683700	7.64678600	-0.07571300
O	1.87939000	6.37908500	-1.79504600
O	-0.77450500	3.53272700	4.02108200
O	-0.34528600	5.66778000	3.96835000
H	2.94578600	-0.16033200	-0.50014000
H	3.27028200	2.28710300	-0.84046900
S	5.55376000	0.01260800	-1.16701500
C	5.47030000	-1.15410100	0.12775800
C	5.80759100	-2.53001500	-0.03439600
C	5.06846200	-0.83406600	1.45518200
C	5.76749900	-3.46624600	0.99557700
C	5.02029000	-1.75099500	2.50320800
C	5.37099200	-3.07969500	2.27493300
H	6.05762300	-4.49109600	0.79078500
H	4.72992000	-1.41424600	3.49241300
H	5.35045600	-3.80133300	3.08544300
C	2.80383900	-0.69244700	-2.68111700
C	3.25183700	-0.04692800	-4.00163800
H	1.75742500	-1.00881700	-2.75139500
C	2.68534700	1.36923400	-4.17441000
H	2.94771700	-0.68712700	-4.83799000
H	4.34714700	-0.00276900	-4.01242000
C	3.14838000	2.28137400	-3.02946700
H	1.58874400	1.33651100	-4.19585700
H	3.01284600	1.79327700	-5.13058800
H	2.72044300	3.28624100	-3.13579400
H	4.23818100	2.39844800	-3.06936700
H	3.39604400	-1.58542600	-2.47400100
Cl	6.31902400	-3.12892000	-1.61074700
Cl	4.60599800	0.82924200	1.85535800

TS_{RR} conformation 3

Si	-4.08632300	-0.50609000	-1.48835600
O	-3.07695100	-1.86063300	-1.43517500
N	-0.80709700	-1.88795800	0.79892300
N	-0.22988900	-1.65530800	3.03284000
N	-2.01069800	-3.05311800	2.45884800
C	-1.67570500	-1.99999200	-1.55838200
C	-1.26905800	-2.86310700	-2.77670800
C	0.07449500	-3.41694100	-2.36511100
C	0.23115700	-3.32685400	-0.97580900
C	-1.03375300	-2.75125300	-0.35787900
C	1.09185700	-3.95555000	-3.15001100
C	2.26770200	-4.39164200	-2.53174200
C	2.42362000	-4.29185000	-1.14587300
C	1.39890800	-3.76147800	-0.35662900
C	-1.02146500	-2.19731000	2.08580800
C	1.10063500	-1.04779700	2.74880400
C	1.57569800	-0.58566400	4.12936000
C	0.26778800	-0.20024100	4.83611200
C	-0.69238800	-1.31387400	4.39999000
C	-1.87610900	-4.03784900	3.55153800
C	-3.01355500	-5.02022900	3.25922700
C	-4.12544400	-4.09001100	2.75110500
C	-3.37856700	-3.07608600	1.86973400
C	-4.42508500	0.09456600	0.28258900
C	-3.38718400	0.73648800	0.99318200
C	-3.56727400	1.17525700	2.30740700
C	-4.79141600	0.98092800	2.95163200
C	-5.83286000	0.34902400	2.27184700
C	-5.64864900	-0.08364800	0.95619900
C	-3.27266800	0.91788700	-2.42983700
C	-2.48250300	0.70565500	-3.57682000
C	-1.92927500	1.76885300	-4.29081300
C	-2.16373400	3.08214300	-3.88101900
C	-2.95201500	3.32187100	-2.75539600
C	-3.49398100	2.25305300	-2.03966300
C	-5.63482600	-1.15438900	-2.42299200
C	-6.19303000	-2.43785900	-1.76738700
C	-6.73263900	-0.07058700	-2.49927400
C	-5.21134600	-1.51324800	-3.86674200
H	-0.36083600	-0.97997900	0.57971300
H	-1.18749100	-1.01956600	-1.63001700
H	-2.01446500	-3.66029200	-2.90381800
H	-1.23861800	-2.29227500	-3.70940400
H	-1.69225300	-3.57101200	-0.06017800
H	0.98257500	-4.02203900	-4.22910800
H	3.07619500	-4.79549300	-3.13321200
H	3.35257300	-4.60732800	-0.68220900
H	1.52627900	-3.68075700	0.71940800
H	0.98879700	-0.20002700	2.06863300
H	1.76189300	-1.78168400	2.28148200
H	2.06532500	-1.41033200	4.65986100
H	2.29054300	0.23508000	4.05031200
H	-0.08896600	0.77373500	4.48547900
H	0.36127600	-0.14994700	5.92368400
H	-0.59368200	-2.17842200	5.06670400
H	-1.74229100	-1.01127200	4.37588300
H	-2.02618500	-3.58024600	4.53724700
H	-0.88040500	-4.48895100	3.53262500
H	-3.29847100	-5.59486700	4.14396400
H	-2.71325300	-5.72518500	2.47638200
H	-4.60371200	-3.58111700	3.59508400
H	-4.90492000	-4.61370100	2.19296100
H	-3.36546100	-3.39596300	0.82598200
H	-3.81463600	-2.07668400	1.90085500
H	-2.42051700	0.90267300	0.52444400
H	-2.76035000	1.68934700	2.82358900
H	-4.93503800	1.33055200	3.97028300
H	-6.79237700	0.20049600	2.75965200
H	-6.48209200	-0.56362100	0.45539400
H	-2.29354600	-0.30485200	-3.92627900
H	-1.31697900	1.57248200	-5.16627100
H	-1.73543700	3.91186500	-4.43588500
H	-3.14287200	4.34114100	-2.43137500
H	-4.09265500	2.46460500	-1.15863100
H	-6.55842900	-2.27449000	-0.74897200
H	-5.43179100	-3.22321400	-1.72614800
H	-7.03700900	-2.82205100	-2.35604000
H	-7.58222600	-0.43724000	-3.09073800

H	-6.36553800	0.84005900	-2.98515000
H	-7.11887100	0.21344100	-1.51578300
H	-4.42981300	-2.28014600	-3.88087500
H	-4.84422800	-0.64079900	-4.41549100
H	-6.07349900	-1.91070100	-4.41877100
O	-0.12241100	0.71802700	0.24016900
C	0.63695200	1.57202100	-0.30214200
N	1.38017500	1.33452800	-1.37918100
C	0.57988600	2.95918200	0.30869200
C	2.93028400	0.36870300	-1.43751500
C	2.73509200	1.83656700	-1.57133100
C	0.90840200	4.12427400	-0.39190400
C	0.09383600	3.07492700	1.61558600
C	0.76784800	5.36249300	0.23257000
H	1.24659800	4.08770900	-1.41806900
C	-0.02700300	4.32750700	2.20498300
H	-0.19966900	2.18507800	2.15260500
C	0.30817700	5.50100100	1.53708800
N	1.10347200	6.58385600	-0.52698000
N	-0.54819900	4.41754000	3.58030900
H	0.20698500	6.47196500	2.00121100
O	0.98331700	7.66145800	0.05141700
O	1.47807400	6.44316200	-1.68917700
O	-0.89990400	3.36998400	4.13070200
O	-0.60586100	5.52829300	4.09829300
H	2.95898300	-0.04795900	-0.44277900
H	3.15208700	2.42027600	-0.74606000
S	5.55983100	0.27379300	-1.06161600
C	5.49745700	-0.94841900	0.18211800
C	5.89186500	-2.30246000	-0.02832100
C	5.05365000	-0.70018900	1.51169900
C	5.86557900	-3.28207900	0.96093600
C	5.01860500	-1.66154100	2.51966900
C	5.42621600	-2.96504400	2.24538300
H	6.19975000	-4.28567000	0.72104200
H	4.69288500	-1.37797800	3.51453100
H	5.41637400	-3.72032300	3.02487200
C	2.87235000	-0.55465200	-2.63206300
C	3.30066100	0.13358600	-3.93721300
H	1.84662400	-0.92882500	-2.72101000
C	2.65789900	1.51828400	-4.09893000
H	3.04415100	-0.51060500	-4.78633400
H	4.39179000	0.23927500	-3.93147900
C	3.05395000	2.43887100	-2.93574400
H	1.56510000	1.42482400	-4.13528600
H	2.97329000	1.97326500	-5.04490400
H	2.56998000	3.41894100	-3.03265800
H	4.13557600	2.61907000	-2.96117800
H	3.51123000	-1.41603200	-2.42962800
Cl	4.51568500	0.92529900	1.96882800
Cl	6.46162600	-2.81450700	-1.61532900

TS_{RR} conformation 4

Si	-4.10534800	1.15057000	-0.86364300
O	-3.75110400	-0.43057500	-1.33472300
N	-1.56112300	-2.04712800	0.32883700
N	-0.70299600	-2.70616100	2.37686800
N	-2.96611800	-3.08243100	1.91506200
C	-2.56688300	-1.07630400	-1.75478900
C	-2.66345100	-1.60569500	-3.20595900
C	-1.71967800	-2.78406600	-3.20670500
C	-1.46538100	-3.20622100	-1.89555200
C	-2.25800800	-2.35162800	-0.91881100
C	-1.13242400	-3.44795400	-4.28199300
C	-0.29217900	-4.53668200	-4.03076200
C	-0.04135800	-4.95525800	-2.72040800
C	-0.63039500	-4.29031700	-1.64135200
C	-1.75137500	-2.60901500	1.53085200
C	0.71818800	-2.60922300	1.93245600
C	1.50386800	-2.70461100	3.24304300
C	0.57094800	-2.02152600	4.25352600
C	-0.80890800	-2.55393200	3.84793200
C	-3.15468500	-4.26806800	2.78167700
C	-4.66849600	-4.50697400	2.72367400
C	-5.22738700	-3.08271800	2.59020900
C	-4.26413500	-2.43444300	1.59082500
C	-4.05370900	1.26010500	1.03342200
C	-2.79732300	1.22534700	1.67711700
C	-2.68993300	1.28344100	3.06868400
C	-3.83850800	1.37119000	3.85887600
C	-5.09227500	1.40240900	3.24778600
C	-5.19363400	1.35057500	1.85522500
C	-2.83472300	2.38259000	-1.53098900
C	-2.21923900	2.23194400	-2.78881900
C	-1.32085000	3.17937500	-3.28191700
C	-1.02507300	4.31932100	-2.53238600
C	-1.63598000	4.50229500	-1.29077500
C	-2.52239600	3.54396300	-0.79720100
C	-5.83409100	1.46570700	-1.63840300
C	-6.83566400	0.35510400	-1.24996200
C	-6.38135500	2.84940100	-1.22512900
C	-5.68038400	1.44476500	-3.17740800
H	-0.79495800	-1.35459300	0.23903000
H	-1.70042300	-0.40806100	-1.67351400
H	-3.69876100	-1.92085800	-3.39460300
H	-2.41284600	-0.84515000	-3.95153800
H	-3.20161400	-2.85044100	-0.68961400
H	-1.31690500	-3.12146700	-5.30182200
H	0.17801100	-5.05669900	-4.85991200
H	0.62269800	-5.79486600	-2.53984200
H	-0.42741700	-4.61331500	-0.62379800
H	0.89406200	-1.64669000	1.44644100
H	0.95009000	-3.40735700	1.22355000
H	1.66228400	-3.75285600	3.52026900
H	2.48310900	-2.22953500	3.15832600
H	0.60903400	-0.93278000	4.13913900
H	0.80707300	-2.25820700	5.29388400
H	-0.98857600	-3.52494600	4.32479200
H	-1.63581200	-1.88448200	4.09829300
H	-2.85137100	-4.06765300	3.81438500
H	-2.55991500	-5.10787900	2.41073100
H	-5.03067300	-5.03809300	3.60711500
H	-4.92829100	-5.10114100	1.84072400
H	-5.18396800	-2.56288100	3.55357200
H	-6.26062700	-3.05395700	2.23656700
H	-4.58381800	-2.65596900	0.56791600
H	-4.17750400	-1.35213700	1.68786500
H	-1.88363500	1.15014200	1.09316200
H	-1.70786900	1.28714500	3.53509700
H	-3.75554100	1.42749500	4.94075300
H	-5.99214500	1.47849800	3.85199000
H	-6.18364100	1.38778700	1.41357900
H	-2.44041100	1.36259000	-3.40084200
H	-0.85217600	3.02741900	-4.24995500
H	-0.32007700	5.05527900	-2.90764200
H	-1.41857700	5.38987500	-0.70312300
H	-2.97099400	3.70081900	0.17950300
H	-7.04123000	0.32235800	-0.17556400
H	-6.46755300	-0.63160900	-1.54784000
H	-7.79553800	0.52064500	-1.75770900
H	-7.33975100	3.04073200	-1.72618000
H	-5.69720200	3.65536000	-1.51202100
H	-6.55502700	2.93209000	-0.14788900
H	-5.29739300	0.48254300	-3.53310900
H	-5.00837700	2.23129300	-3.53399300
H	-6.65776800	1.60586100	-3.65138400
O	0.07903000	0.14738000	0.32201100
C	0.96781800	0.80998300	-0.28741100
N	1.46238300	0.47505700	-1.47791500
C	1.39188700	2.08961800	0.39816600
C	2.67754800	-0.82807200	-1.76380100
C	2.86461500	0.64257800	-1.84887500
C	1.80736300	3.22634900	-0.30178100
C	1.26520600	2.15861100	1.78945900
C	2.09707200	4.39336900	0.40305900
H	1.87382500	3.22721100	-1.38104100
C	1.57799000	3.33682900	2.45605200
H	0.91156100	1.29833300	2.33909200
C	2.00390700	4.48025400	1.78768200

N	2.48726700	5.60010800	-0.35154100
N	1.42352000	3.38276900	3.92133100
H	2.23609700	5.39517500	2.31448900
O	2.80491200	6.59575200	0.29444500
O	2.46019700	5.53453300	-1.57982100
O	0.97195300	2.38021800	4.47915100
O	1.74863700	4.41718100	4.49700500
H	2.75302000	-1.30003900	-0.79640600
H	3.51961000	1.06455600	-1.08214600
S	5.24766100	-1.59153800	-1.78858000
C	5.50172700	-1.57225600	-0.06188300
C	5.01184100	-2.57463400	0.82160900
C	6.24264400	-0.55506000	0.60877700
C	5.25532600	-2.59822600	2.19316100
C	6.49409300	-0.55091600	1.97790800
C	6.00360100	-1.57968800	2.77962900
H	4.87268400	-3.42059300	2.78789900
H	7.07631900	0.25715300	2.40659100
H	6.20731300	-1.59060100	3.84558400
C	2.24639700	-1.65257200	-2.95396900
C	2.66925800	-1.02893200	-4.29420600
H	1.15685300	-1.75902400	-2.91987200
C	2.38353800	0.47919400	-4.34506700
H	2.15114600	-1.54596200	-5.11028600
H	3.74296300	-1.19421600	-4.44225200
C	3.14237400	1.21609700	-3.23194500
H	1.30631400	0.66011600	-4.23773400
H	2.68131400	0.88672800	-5.31801100
H	2.90505000	2.28742800	-3.24185000
H	4.22217100	1.12344900	-3.39577800
H	2.67413700	-2.65095900	-2.84297400
Cl	6.89997500	0.79935000	-0.30736700
Cl	4.03299200	-3.90937200	0.18500700

TS_{RR} conformation 5

Si	-4.08077300	-0.39902200	-1.35338800
O	-3.03233400	-1.67368500	-1.70151100
N	-0.69098200	-2.23264600	0.41298400
N	0.03372800	-2.45982800	2.60121700
N	-1.75825000	-3.76558700	1.85509900
C	-1.63130400	-1.76353300	-1.86412700
C	-1.23845200	-2.27095600	-3.27253500
C	0.08228500	-2.96309700	-3.03721900
C	0.24566100	-3.25409600	-1.67705700
C	-0.98241600	-2.80165000	-0.90209200
C	1.07046100	-3.32018400	-3.95280700
C	2.21967100	-3.96976200	-3.49298800
C	2.37871400	-4.25919500	-2.13427700
C	1.38704700	-3.90397100	-1.21582600
C	-0.81258900	-2.82036400	1.61147700
C	1.34044800	-1.78306800	2.35519600
C	1.88308000	-1.54310100	3.76629700
C	0.60706100	-1.29421200	4.58351200
C	-0.35951800	-2.34700100	4.02698000
C	-1.56591200	-4.90489700	2.78070400
C	-2.79262700	-5.78452000	2.51271300
C	-3.87949400	-4.74919900	2.18880000
C	-3.13729800	-3.74558000	1.30031200
C	-4.35325800	-0.28850200	0.52504300
C	-3.31214800	0.22119500	1.33115900
C	-3.44470300	0.31858800	2.71854400
C	-4.62260200	-0.09865100	3.34254100
C	-5.66495000	-0.61100600	2.56953800
C	-5.52955600	-0.69942000	1.18169500
C	-3.36636600	1.25832700	-1.91563400
C	-2.55613800	1.38111400	-3.06093300
C	-2.08157400	2.62114000	-3.49111200
C	-2.42142100	3.78064000	-2.79176100
C	-3.23826800	3.68846900	-1.66358200
C	-3.69713500	2.44378500	-1.23005400
C	-5.65319200	-0.84559100	-2.36265500
C	-6.13643700	-2.27768500	-2.04254800
C	-6.78440700	0.17329800	-2.10366500
C	-5.28841600	-0.79466500	-3.86468500
H	-0.27204800	-1.28486000	0.38660000
H	-1.14780600	-0.79578300	-1.68112700
H	-2.00618600	-2.97801500	-3.61488100
H	-1.18311400	-1.46560600	-4.01107700
H	-1.66821000	-3.64339000	-0.78796700
H	0.95646700	-3.08933800	-5.00840200
H	3.00157700	-4.24290700	-4.19498200
H	3.28209300	-4.75317700	-1.79033100
H	1.51633900	-4.12449600	-0.15944000
H	1.18289000	-0.83334600	1.83881900
H	1.98096700	-2.41719300	1.73695700
H	2.40371600	-2.43347300	4.13662900
H	2.58428600	-0.70681800	3.78360100
H	0.22226300	-0.28567700	4.39757500
H	0.75091900	-1.40516800	5.66101900
H	-0.21067200	-3.30105500	4.54654400
H	-1.41361000	-2.06819400	4.10513100
H	-1.56667900	-4.58073800	3.82640300
H	-0.61185300	-5.40052000	2.57963400
H	-3.03362000	-6.41878700	3.36908000
H	-2.61618700	-6.43377200	1.64818300
H	-4.22801600	-4.26096800	3.10551400
H	-4.74808200	-5.17574500	1.68179200
H	-3.15984800	-4.08241600	0.25951100
H	-3.54256700	-2.73432400	1.33579000
H	-2.37894500	0.54871900	0.88074400
H	-2.63831800	0.74622800	3.30913800
H	-4.73178000	-0.01222300	4.42010500
H	-6.58932600	-0.93038300	3.04302500
H	-6.36453300	-1.09117700	0.61092400
H	-2.28971200	0.49721700	-3.63270800
H	-1.44763600	2.68209900	-4.37101100
H	-2.04762200	4.74696400	-3.11726200
H	-3.51449900	4.58612500	-1.11735500
H	-4.31623700	2.39568300	-0.33877900
H	-6.44988300	-2.39907600	-1.00112600
H	-5.35044000	-3.01299200	-2.24069200
H	-6.99953000	-2.53311200	-2.67210500
H	-7.65183200	-0.05826800	-2.73606700
H	-6.46903200	1.19445600	-2.34401200
H	-7.12818800	0.17021600	-1.06475900
H	-4.49022600	-1.50241400	-4.11164300
H	-4.96569600	0.20400800	-4.17423400
H	-6.16474700	-1.06109200	-4.47041100
O	-0.09206400	0.44334900	0.47298200
C	0.51065900	1.41502100	-0.06758300
N	1.26297000	1.30685100	-1.16221700
C	0.24721700	2.76155600	0.56866500
C	2.95509300	0.68162000	-1.19489200
C	2.48258100	2.07535800	-1.38680100
C	0.23724100	3.95746300	-0.15530200
C	-0.09785200	2.78704200	1.92403200
C	-0.10150600	5.14455600	0.49185900
H	0.45278400	3.97357700	-1.21460800
C	-0.41708500	3.99333700	2.53509000
H	-0.12665000	1.86580400	2.48744400
C	-0.42420800	5.20034800	1.84322700
N	-0.15036800	6.39204400	-0.29480800
N	-0.78973700	3.98691300	3.96145300
H	-0.68229100	6.13241000	2.32604500
O	-0.39568900	7.43433600	0.30759900
O	0.05032800	6.30756800	-1.50589600
O	-0.85815600	2.89421500	4.52815000
O	-1.01483800	5.06853900	4.49672800
H	3.09805800	0.33622200	-0.18298500
H	2.77276500	2.76356500	-0.58866000
S	5.57797300	1.19051000	-0.80790400
C	5.87201100	-0.17685600	0.23506500
C	6.60604400	-1.32957000	-0.17285000
C	5.41711200	-0.25857500	1.58153100
C	6.87136300	-2.41550500	0.65670600
C	5.67036400	-1.33140000	2.43247000
C	6.40381300	-2.42127700	1.96934400
H	7.44784100	-3.24831900	0.26936900
H	5.30805700	-1.29949600	3.45423000

H	6.61673300	-3.25956400	2.62514200
C	3.10633700	-0.28232000	-2.34701200
C	3.38724900	0.42616800	-3.68114500
H	2.18645600	-0.87268500	-2.41972300
C	2.46973300	1.63886100	-3.89704100
H	3.27308100	-0.29225000	-4.50117400
H	4.43184400	0.75774000	-3.68294900
C	2.65934300	2.67292100	-2.77754600
H	1.42047000	1.31789100	-3.92418700
H	2.68589300	2.10849200	-4.86357300
H	1.97099000	3.51789800	-2.90611900
H	3.67580900	3.08159100	-2.82442200
H	3.91592400	-0.97575100	-2.10954700
Cl	4.47498900	1.07578000	2.27450300
Cl	7.24398900	-1.42880300	-1.81296700

TS_{RR} conformation 6

Si	-4.08079900	-0.39900100	-1.35336300
O	-3.03236300	-1.67366300	-1.70150400
N	-0.69099400	-2.23265700	0.41297600
N	0.03378300	-2.45991200	2.60118200
N	-1.75824100	-3.76561800	1.85508100
C	-1.63133400	-1.76351300	-1.86412200
C	-1.23848700	-2.27091500	-3.27253900
C	0.08224200	-2.96307500	-3.03723700
C	0.24561800	-3.25410000	-1.67708000
C	-0.98244900	-2.80164600	-0.90210200
C	1.07041200	-3.32016200	-3.95283300
C	2.21961300	-3.96976400	-3.49302800
C	2.37865400	-4.25922400	-2.13432200
C	1.38699400	-3.90400000	-1.21586300
C	-0.81257000	-2.82040500	1.61145800
C	1.34050200	-1.78315400	2.35514600
C	1.88317500	-1.54323300	3.76623900
C	0.60718100	-1.29437600	4.58350200
C	-0.35941200	-2.34714800	4.02696300
C	-1.56588500	-4.90497600	2.78062100
C	-2.79260600	-5.78458200	2.51260000
C	-3.87948300	-4.74923700	2.18879600
C	-3.13731900	-3.74553700	1.30037000
C	-4.35327000	-0.28849500	0.52507100
C	-3.31214500	0.22117800	1.33118400
C	-3.44468900	0.31855800	2.71857100
C	-4.62258900	-0.09867000	3.34257200
C	-5.66495100	-0.61100100	2.56957100
C	-5.52956900	-0.69940100	1.18172700
C	-3.36639100	1.25835000	-1.91560200
C	-2.55617200	1.38114300	-3.06090800
C	-2.08160900	2.62117100	-3.49108100
C	-2.42144800	3.78066700	-2.79171900
C	-3.23828600	3.68848900	-1.66353400
C	-3.69715200	2.44380300	-1.23001000
C	-5.65322500	-0.84556000	-2.36262200
C	-6.13647600	-2.27765200	-2.04251400
C	-6.78443200	0.17333400	-2.10362600
C	-5.28845600	-0.79463500	-3.86465500
H	-0.27205000	-1.28487400	0.38660300
H	-1.14783300	-0.79576700	-1.68110800
H	-2.00622800	-2.97795800	-3.61489800
H	-1.18313800	-1.46555100	-4.01106600
H	-1.66825100	-3.64338000	-0.78797500
H	0.95641800	-3.08929600	-5.00842400
H	3.00151300	-4.24290900	-4.19502900
H	3.28202500	-4.75322700	-1.79038600
H	1.51628500	-4.12454700	-0.15948100
H	1.18293600	-0.83341800	1.83879900
H	1.98099900	-2.41726700	1.73687200
H	2.40382600	-2.43361500	4.13652500
H	2.58437800	-0.70694800	3.78355000
H	0.22237300	-0.28583700	4.39761200
H	0.75107200	-1.40537000	5.66100200
H	-0.21054300	-3.30122400	4.54648000
H	-1.41350300	-2.06835100	4.10516300
H	-1.56663300	-4.58087500	3.82633800
H	-0.61183100	-5.40058900	2.57950500
H	-3.03357600	-6.41891100	3.36892700
H	-2.61618900	-6.43376800	1.64801700
H	-4.22798300	-4.26108300	3.10556100
H	-4.74808300	-5.17574400	1.68177800
H	-3.15993000	-4.08225600	0.25953300
H	-3.54257500	-2.73428000	1.33597900
H	-2.37894100	0.54869300	0.88076700
H	-2.63829200	0.74617700	3.30916400
H	-4.73175800	-0.01225300	4.42013900
H	-6.58932800	-0.93036900	3.04306200
H	-6.36455600	-1.09114000	0.61095700
H	-2.28975300	0.49725000	-3.63269100
H	-1.44767800	2.68213500	-4.37098500
H	-2.04764800	4.74699200	-3.11721500
H	-3.51451000	4.58614200	-1.11729800
H	-4.31624700	2.39569600	-0.33873200
H	-6.44991600	-2.39904400	-1.00109000
H	-5.35048500	-3.01296400	-2.24066500
H	-6.99957400	-2.53307400	-2.67206700
H	-7.65186300	-0.05822700	-2.73602300
H	-6.46905300	1.19449100	-2.34397500
H	-7.12820800	0.17025400	-1.06471800
H	-4.49027200	-1.50238800	-4.11161700
H	-4.96573100	0.20403600	-4.17420300
H	-6.16479200	-1.06105600	-4.47037600
O	-0.09205200	0.44332800	0.47305100
C	0.51064900	1.41500200	-0.06753700
N	1.26294400	1.30682300	-1.16218200
C	0.24719900	2.76154100	0.56869700
C	2.95507900	0.68162900	-1.19485900
C	2.48253500	2.07535200	-1.38680200
C	0.23720400	3.95744000	-0.15528300
C	-0.09785600	2.78704000	1.92406800
C	-0.10154800	5.14453700	0.49186700
H	0.45273500	3.97354400	-1.21459200
C	-0.41709400	3.99333800	2.53511500
H	-0.12663700	1.86580800	2.48749100
C	-0.42423700	5.20034100	1.84323800
N	-0.15043200	6.39201500	-0.29481400
N	-0.78973200	3.98692700	3.96148200
H	-0.68232400	6.13240600	2.32604800
O	-0.39575600	7.43431100	0.30758400
O	0.05025100	6.30752700	-1.50590400
O	-0.85813500	2.89423500	4.52819100
O	-1.01483600	5.06855800	4.49674700
H	3.09806800	0.33626500	-0.18294400
H	2.77271400	2.76358700	-0.58868400
S	5.57795600	1.19059700	-0.80790000
C	5.87206400	-0.17678100	0.23503400
C	6.60613600	-1.32945700	-0.17291800
C	5.41718800	-0.25854900	1.58150500
C	6.87150900	-2.41540100	0.65660800
C	5.67049500	-1.33138400	2.43241600
C	6.40397900	-2.42122200	1.96925200
H	7.44801300	-3.24818400	0.26924200
H	5.30820200	-1.29951800	3.45418100
H	6.61694000	-3.25951600	2.62502800
C	3.10633600	-0.28233800	-2.34695400
C	3.38721600	0.42612100	-3.68110900
H	2.18646900	-0.87272900	-2.41964100
C	2.46966600	1.63878300	-3.89702900
H	3.27306000	-0.29232200	-4.50111800
H	4.43180200	0.75772000	-3.68293000
C	2.65926300	2.67288000	-2.77756600
H	1.42041200	1.31778500	-3.92415400
H	2.68580200	2.10839200	-4.86357700
H	1.97088500	3.51783500	-2.90615400
H	3.67571700	3.08157600	-2.82446800
H	3.91594200	-0.97574300	-2.10948100
Cl	7.24406000	-1.42862500	-1.81304700
Cl	4.47502400	1.07575400	2.27452300

TS_{RR} conformation 7

Si	4.39536600	-1.44900300	-0.11719300
O	3.34843400	-1.57226700	1.20339800
N	0.28227800	-1.93900800	0.39482200
N	-1.01600900	-3.36296900	-0.90673200
N	0.39012200	-4.27344100	0.71728900
C	2.22583600	-0.75292200	1.49618800
C	2.35863600	-0.00218200	2.83899100
C	0.91744500	0.28370200	3.19180500
C	0.06577700	-0.59266900	2.50528200
C	0.89801600	-1.54561800	1.66505500
C	0.38667500	1.24999200	4.04310300
C	-1.00176200	1.32158400	4.20126300
C	-1.84634500	0.44111100	3.51791000
C	-1.31488100	-0.53065100	2.66291800
C	-0.11141000	-3.18017400	0.06472700
C	-1.79495600	-2.26356500	-1.52993700
C	-2.59819100	-2.96837300	-2.62770300
C	-1.69493700	-4.14061100	-3.03497400
C	-1.13361600	-4.61463000	-1.69106200
C	-0.46040300	-5.36931200	1.22635800
C	0.47695500	-6.08089800	2.20659800
C	1.83755200	-5.97686200	1.50039600
C	1.83641700	-4.55708000	0.90869700
C	3.48610800	-1.97793000	-1.70203000
C	2.50277800	-1.12036900	-2.24022100
C	1.78823500	-1.45827900	-3.39089900
C	2.03803700	-2.66833100	-4.04224600
C	3.00161900	-3.53747000	-3.52966000
C	3.71257900	-3.19252700	-2.37717700
C	4.96086700	0.33727300	-0.36263300
C	5.22664000	1.18210300	0.73304200
C	5.72234800	2.47469700	0.55549600
C	5.97054100	2.95501800	-0.73150700
C	5.72208900	2.13706000	-1.83444600
C	5.22174600	0.84707700	-1.64974800
C	5.88897600	-2.55241300	0.37857100
C	5.46346800	-3.98764600	0.75656000
C	6.92527600	-2.59553500	-0.76675400
C	6.56248700	-1.92381500	1.62160700
H	0.01089600	-1.15159800	-0.19644900
H	2.05238100	-0.01985100	0.69858000
H	2.82846500	-0.67391400	3.57152400
H	2.97689300	0.89388800	2.76281800
H	1.09105100	-2.45837500	2.23227700
H	1.03969800	1.94624500	4.56171900
H	-1.42894900	2.07609400	4.85566700
H	-2.92411000	0.50981700	3.62636600
H	-1.99015400	-1.19021200	2.12554200
H	-1.10186400	-1.53248300	-1.96187200
H	-2.44375900	-1.77670200	-0.79472700
H	-3.54638500	-3.32596600	-2.21601400
H	-2.83065200	-2.29207900	-3.45281500
H	-0.87714600	-3.79351800	-3.67571000
H	-2.22602800	-4.93984300	-3.55793300
H	-1.83747400	-5.29907400	-1.20394500
H	-0.16084100	-5.10588600	-1.76469200
H	-0.76866200	-6.06345700	0.43424300
H	-1.36147000	-4.96224600	1.69278400
H	0.16683200	-7.11114000	2.39771500
H	0.49791700	-5.54817200	3.16336400
H	1.90087700	-6.72299800	0.70054500
H	2.68548500	-6.13508000	2.17078000
H	2.30855000	-3.83993800	1.58260700
H	2.36000300	-4.49501000	-0.04919600
H	2.28568200	-0.16668500	-1.76690400
H	1.04766500	-0.76744500	-3.78420800
H	1.49721100	-2.92445300	-4.94927700
H	3.21163400	-4.47731900	-4.03288300
H	4.46525600	-3.88458200	-2.01439100
H	5.04713300	0.83066700	1.74431000
H	5.89910700	3.10931200	1.41845100
H	6.35399300	3.96154200	-0.87175400
H	5.91296100	2.50388000	-2.83907700
H	5.02605400	0.23204000	-2.52349200
H	4.98962700	-4.52588800	-0.07021100
H	4.76748000	-3.98488900	1.60112400
H	6.34452800	-4.57039900	1.05740600
H	7.81249500	-3.15867200	-0.44786100
H	7.25952400	-1.59139500	-1.04806400
H	6.53837400	-3.07972100	-1.66896600
H	5.87035900	-1.85710500	2.46727600
H	6.94708200	-0.92070900	1.41699600
H	7.41211000	-2.54470700	1.93582900
O	0.03030100	0.94774000	-0.61691800
C	-0.43373300	2.08983400	-0.83776800
N	-1.64865600	2.42659200	-1.34229600
C	0.41260900	3.30335100	-0.52606200
C	-2.99550000	1.72109900	-0.26940000
C	-2.56649400	1.31838800	-1.61674700
C	1.41332600	3.22841500	0.44688400
C	0.19606800	4.51483600	-1.19536500
C	2.17887400	4.35897600	0.72664900
H	1.57588800	2.30861000	0.99057000
C	1.00297800	5.61044800	-0.90327400
H	-0.59380300	4.59206400	-1.93005100
C	2.00884500	5.56425500	0.05488900
N	3.21003300	4.28972200	1.77262700
N	0.78646800	6.87636600	-1.63120400
H	2.62345600	6.42650000	0.27104400
O	4.02216400	5.21062700	1.83792800
O	3.20555500	3.31126400	2.52063900
O	-0.09373900	6.89564400	-2.48819600
O	1.50320900	7.83057600	-1.33377800
H	-2.45016800	1.32258700	0.57435700
H	-2.08469000	0.34552700	-1.67004300
S	-4.33158500	-0.60947700	0.56522700
C	-6.07895000	-0.55525200	0.54599000
C	-6.87476700	-1.06321800	-0.51715700
C	-6.84942900	-0.00137100	1.60660500
C	-8.26648400	-1.03642800	-0.53144400
C	-8.24057400	0.03839600	1.61736800
C	-8.95762900	-0.48239100	0.54284600
H	-8.79757400	-1.44743500	-1.38265100
H	-8.75225600	0.47716200	2.46656500
H	-10.04244000	-0.45533900	0.54219500
C	-3.53025700	1.58162200	-2.76726800
C	-4.36206900	2.85771400	-2.56814000
C	-5.06351200	2.84654900	-1.20280700
H	-5.10338900	2.93795200	-3.37132000
H	-3.71011800	3.73584300	-2.64477200
C	-4.05717200	2.76050500	-0.04253100
H	-4.19998400	0.71592500	-2.83923700
H	-2.95734700	1.63456500	-3.70122400
H	-4.56298200	2.52748300	0.89804800
H	-3.55687700	3.72778800	0.09537900
H	-5.73771400	1.98401700	-1.14879600
H	-5.68052200	3.74359600	-1.07999000
Cl	-6.10314300	-1.78324700	-1.93728700
Cl	-6.04547500	0.68951000	3.02095300

TS_{SS} conformation 1

Si	4.33202400	1.65465500	-0.03833900
O	3.80118900	0.75667400	1.29303100
N	2.13416600	-1.92081400	0.63298800
N	2.18032500	-3.89802000	-0.57119000
N	4.05923300	-3.28667700	0.67161400
C	2.46992400	0.38054500	1.61195400
C	1.95078600	1.03111900	2.91403400
C	0.89462300	0.05556500	3.37446200
C	1.09036500	-1.19540300	2.77648600
C	2.30779200	-1.14871000	1.86713000
C	-0.17312900	0.25501100	4.24763600
C	-1.03233800	-0.81309100	4.52200300
C	-0.82634100	-2.06449500	3.93188800
C	0.24190600	-2.26378100	3.05325600
C	2.79349100	-3.01961200	0.25186500
C	0.70699600	-3.92782000	-0.78550600
C	0.53037500	-5.00328900	-1.86360100
C	1.81611000	-4.87409800	-2.69257300

C	2.89004800	-4.66784500	-1.61912200
C	4.54007500	-4.64814800	0.98960400
C	5.83088300	-4.37787700	1.76878300
C	6.39167600	-3.13856800	1.05604300
C	5.14521000	-2.27793100	0.80424400
C	4.23721800	0.57243800	-1.59999000
C	2.96701900	0.16569800	-2.06079900
C	2.82380500	-0.66128400	-3.17636100
C	3.95131500	-1.10512400	-3.87059900
C	5.21980900	-0.71490600	-3.43964700
C	5.35577600	0.11220800	-2.32162500
C	3.21567100	3.15346300	-0.31150000
C	2.72558100	3.91246700	0.77020600
C	1.94493300	5.05125700	0.56902900
C	1.64029200	5.46665100	-0.72886600
C	2.12153800	4.73931300	-1.81824300
C	2.89552100	3.59635700	-1.60952000
C	6.10270000	2.19966000	0.47106600
C	7.00244800	0.99125500	0.81094800
C	6.75122100	3.04592800	-0.64723400
C	5.99687000	3.07643800	1.74145300
H	1.30900200	-1.63031400	0.08505700
H	1.78091500	0.63508700	0.79803500
H	2.77903800	1.09683500	3.63333500
H	1.56529900	2.04019600	2.75203900
H	3.18565900	-1.52863400	2.39529400
H	-0.34743900	1.22998100	4.69300900
H	-1.87936200	-0.66713600	5.18461100
H	-1.51241500	-2.87814900	4.14499400
H	0.39310900	-3.23324700	2.58560900
H	0.33494400	-2.95947900	-1.13299600
H	0.20347600	-4.16389700	0.15597900
H	0.47031600	-5.99932700	-1.41072100
H	-0.37834800	-4.84123900	-2.44599900
H	1.76343500	-3.99343700	-3.34140400
H	2.02293900	-5.74709600	-3.31642000
H	3.22629300	-5.63610600	-1.22893900
H	3.76256800	-4.11109200	-1.96936100
H	4.76694800	-5.22407600	0.08465600
H	3.78258200	-5.19357200	1.55896600
H	6.50856300	-5.23479900	1.74969700
H	5.60185500	-4.14762200	2.81494900
H	6.85517300	-3.42861200	0.10650100
H	7.14052300	-2.60261600	1.64344400
H	4.96677200	-1.59517000	1.63643500
H	5.20645700	-1.67820300	-0.10563300
H	2.06304200	0.48655700	-1.55149900
H	1.82805800	-0.94668900	-3.50415700
H	3.84248500	-1.73712700	-4.74784300
H	6.10425200	-1.04400900	-3.97828200
H	6.35627600	0.40352500	-2.02011500
H	2.95203700	3.61233600	1.78864800
H	1.56048500	5.60315400	1.42121100
H	1.02955000	6.35066700	-0.88662900
H	1.88975600	5.05754800	-2.83078400
H	3.24809400	3.03782600	-2.47182900
H	7.15236800	0.31785000	-0.03861000
H	6.58335500	0.40707900	1.63646100
H	7.99504800	1.34073500	1.12547600
H	7.72985600	3.41782500	-0.31599400
H	6.13811300	3.91739700	-0.89972800
H	6.91387000	2.47920700	-1.56923100
H	5.52993800	2.53406500	2.56976500
H	5.42098100	3.98900700	1.56275100
H	7.00100100	3.38081700	2.06589000
O	0.03754900	-0.60857100	-0.59056600
C	-1.14930200	-0.38079700	-0.94388400
N	-1.99432100	-1.32618300	-1.37979900
C	-1.55681500	1.07907400	-0.94519600
C	-3.44978200	-1.17188500	-1.27073100
C	-3.12157800	-2.24095300	-0.30654600
C	-1.21287100	1.87469800	0.15399900
C	-2.19491900	1.66785100	-2.04091300
C	-1.51688700	3.23194100	0.13843400
H	-0.72490600	1.44088200	1.01632100
C	-2.46419000	3.03554000	-2.02157600
H	-2.47265000	1.08649800	-2.91101100
C	-2.14092600	3.84679500	-0.94210300
N	-1.13935400	4.06136600	1.29511400
N	-3.10624600	3.65292500	-3.19816200
H	-2.36012700	4.90487700	-0.94500800
O	-1.37777900	5.26596200	1.23523100
O	-0.59260100	3.50436700	2.24686900
O	-3.35711200	2.92285300	-4.15493900
O	-3.34322600	4.85799400	-3.14854200
H	-3.78805200	-0.24619600	-0.80301700
H	-2.85182700	-1.95504300	0.69824600
S	-5.52537500	-2.35446100	1.03753900
C	-6.13871700	-0.72139800	1.09670900
C	-7.39467800	-0.34456800	0.53757200
C	-5.45679000	0.36577100	1.71065600
C	-7.91265200	0.94590100	0.59309700
C	-5.95059600	1.66576500	1.77694800
C	-7.19017400	1.96189900	1.21576800
H	-8.87967300	1.14704400	0.14553500
H	-5.36555100	2.43324200	2.27192700
H	-7.58862100	2.97019100	1.26348500
C	-3.09759900	-3.69240400	-0.70729700
C	-3.37952600	-3.90447000	-2.20335000
C	-4.56393800	-3.03820900	-2.65025000
H	-3.58891200	-4.96505500	-2.38401500
H	-2.48962400	-3.64179300	-2.78965300
C	-4.25228500	-1.53502100	-2.52822300
H	-3.86501200	-4.20054600	-0.11534900
H	-2.13857800	-4.13571800	-0.41396600
H	-5.19025600	-0.97220600	-2.51851600
H	-3.68087300	-1.19496400	-3.40100400
H	-5.42792100	-3.27049800	-2.01804400
H	-4.84312300	-3.27099100	-3.68395400
Cl	-8.38736600	-1.54947100	-0.28200000
Cl	-3.86969100	0.10208800	2.45816300

TS_{SS} conformation 2

Si	-4.49036600	0.93222300	-0.65435900
O	-3.51192400	0.00744900	-1.67829600
N	-1.51296300	-2.04188900	-0.20352700
N	-1.37356100	-3.76986800	1.33156200
N	-3.02916400	-3.84673200	-0.31221000
C	-2.09534300	-0.07984100	-1.67560400
C	-1.44903400	0.46453700	-2.96896200
C	-0.13311900	-0.27480600	-3.01368600
C	-0.19668000	-1.43044100	-2.22515500
C	-1.56874600	-1.54308600	-1.58136900
C	1.04538300	0.05194900	-3.68303900
C	2.15071400	-0.79545500	-3.56236300
C	2.07634500	-1.95942600	-2.78957800
C	0.89663600	-2.28470900	-2.11454200
C	-1.97533500	-3.20652400	0.26290800
C	-0.02073700	-3.37448100	1.81125800
C	0.16693000	-4.22296200	3.07328200
C	-1.26229900	-4.34807100	3.62091900
C	-2.09310200	-4.56692200	2.35176600
C	-3.10569200	-5.31454100	-0.46308600
C	-4.19000400	-5.48540100	-1.53111300
C	-5.17487000	-4.35988400	-1.18168600
C	-4.26222400	-3.17986100	-0.81174400
C	-4.51749600	0.14477800	1.07770200
C	-3.32835600	0.14211000	1.83837000
C	-3.26779300	-0.45454000	3.09906900
C	-4.39994300	-1.06539300	3.64229400
C	-5.58999000	-1.07467500	2.91375400
C	-5.64320000	-0.47715900	1.65167600
C	-3.79757900	2.67987600	-0.47403100
C	-3.24740300	3.36879900	-1.57364100
C	-2.78541400	4.68026800	-1.45741300
C	-2.87090100	5.34228000	-0.23096200
C	-3.42126200	4.68718800	0.87141000
C	-3.87424500	3.37226100	0.74989700
C	-6.18325400	0.95067000	-1.56235300

C	-6.69765100	-0.47912700	-1.83882100
C	-7.22858600	1.74365000	-0.74612200
C	-6.00072800	1.65611600	-2.92687900
H	-0.89520500	-1.48007900	0.40290600
H	-1.66922200	0.45876100	-0.82103500
H	-2.08860600	0.20295500	-3.82355800
H	-1.33539100	1.55050800	-2.95530600
H	-2.21128100	-2.20539600	-2.16671600
H	1.11023100	0.96229700	-4.27193700
H	3.08555500	-0.54604200	-4.05448300
H	2.94840400	-2.59800800	-2.69834000
H	0.84732200	-3.18161800	-1.50253600
H	0.02078400	-2.30648000	2.04452900
H	0.71941600	-3.57524300	1.03239900
H	0.56396800	-5.21214300	2.81928800
H	0.85869500	-3.75172300	3.77392900
H	-1.56528000	-3.41556000	4.10885200
H	-1.38527000	-5.16421100	4.33706200
H	-2.09779500	-5.62928700	2.08000000
H	-3.12735600	-4.22469900	2.43720100
H	-3.41852700	-5.80752800	0.46571800
H	-2.13031400	-5.71608500	-0.75051600
H	-4.64059300	-6.48048800	-1.50380900
H	-3.76635200	-5.32985400	-2.52918200
H	-5.78841100	-4.65240500	-0.32233100
H	-5.85026400	-4.10599400	-2.00173300
H	-4.06009200	-2.54808500	-1.67765000
H	-4.68036300	-2.54135800	-0.03075800
H	-2.42341300	0.60579700	1.45593800
H	-2.33559400	-0.42943400	3.65665400
H	-4.35955200	-1.51781800	4.62945100
H	-6.48102000	-1.53673200	3.33000600
H	-6.58702000	-0.49524600	1.11721600
H	-3.17548800	2.87664700	-2.53864000
H	-2.34505000	5.17882800	-2.31540700
H	-2.50801900	6.36164800	-0.13763700
H	-3.49223700	5.19691100	1.82818700
H	-4.28565000	2.87700900	1.62464900
H	-6.87828300	-1.05326600	-0.92454300
H	-5.98782600	-1.04030600	-2.45481000
H	-7.64881000	-0.43662800	-2.38636800
H	-8.17361400	1.80114000	-1.30241800
H	-6.89724400	2.77034000	-0.55797100
H	-7.44908300	1.28593700	0.22323800
H	-5.26221400	1.14513900	-3.55284400
H	-5.68688600	2.69753400	-2.81004300
H	-6.95385100	1.65972400	-3.47223800
O	-0.00692300	-0.08729900	1.04846600
C	1.05897400	0.44159000	1.46050600
N	2.00183800	-0.20532600	2.15787200
C	1.18395700	1.93343600	1.21277500
C	3.40134800	0.22728100	2.15821500
C	3.44566900	-1.07875100	1.46551500
C	0.83840400	2.44244800	-0.04420500
C	1.56410400	2.81956600	2.22574200
C	0.88714100	3.81569200	-0.26416800
H	0.54598900	1.77614600	-0.84469700
C	1.57882700	4.18888000	1.96788800
H	1.83432900	2.46437500	3.21185500
C	1.24817000	4.72067600	0.72836400
N	0.51644400	4.34110100	-1.58927700
N	1.94948500	5.11585600	3.05534500
H	1.26766200	5.78577900	0.54660600
O	0.47238800	5.56152100	-1.72726800
O	0.25747500	3.52799000	-2.47657900
O	2.21811300	4.62575600	4.15025200
O	1.96040800	6.31729800	2.79736000
H	3.63566300	1.07126200	1.50805500
H	3.27492200	-1.09784900	0.39914300
S	6.02346500	-0.75248800	0.56809100
C	6.00636100	-0.88294500	-1.17149300
C	6.24381900	0.22394000	-2.03772400
C	5.79119200	-2.10183700	-1.87373500
C	6.29192000	0.12738000	-3.42573200
C	5.83921400	-2.22736100	-3.25961300
C	6.09321500	-1.10495400	-4.04642200
H	6.49056900	1.01825700	-4.01121200
H	5.68580300	-3.20106900	-3.71217100
H	6.14444600	-1.19155500	-5.12716100
C	3.62345700	-2.37062300	2.21776000
C	3.69178900	-2.16858900	3.73902500
C	4.61404300	-0.99045700	4.07846700
H	4.05728500	-3.08887900	4.20866500
H	2.68729400	-1.97387400	4.13606000
C	4.06286700	0.34378600	3.54010900
H	4.55859400	-2.80613000	1.85476800
H	2.82611300	-3.06993200	1.94134800
H	4.87442900	1.07468500	3.47763600
H	3.31742700	0.74744200	4.23635500
H	5.59950100	-1.17817700	3.63654800
H	4.76129700	-0.91433100	5.16152000
Cl	6.50323900	1.82987600	-1.35986500
Cl	5.43307600	-3.58567800	-0.97463900

TS_{SS} conformation 3

Si	4.33202500	1.65465400	-0.03833800
O	3.80118900	0.75667300	1.29303100
N	2.13416500	-1.92081400	0.63298800
N	2.18032400	-3.89802100	-0.57119000
N	4.05923200	-3.28667800	0.67161500
C	2.46992400	0.38054400	1.61195400
C	1.95078500	1.03111900	2.91403400
C	0.89462300	0.05556500	3.37446100
C	1.09036400	-1.19540300	2.77648500
C	2.30779200	-1.14871000	1.86713000
C	-0.17313000	0.25501200	4.24763500
C	-1.03234000	-0.81309000	4.52200200
C	-0.82634300	-2.06449400	3.93188700
C	0.24190400	-2.26378000	3.05325500
C	2.79349000	-3.01961300	0.25186500
C	0.70699500	-3.92782000	-0.78550600
C	0.53037400	-5.00328800	-1.86360100
C	1.81611000	-4.87409800	-2.69257300
C	2.89004700	-4.66784600	-1.61912100
C	4.54007300	-4.64815000	0.98960600
C	5.83088200	-4.37787900	1.76878300
C	6.39167400	-3.13857000	1.05604300
C	5.14520900	-2.27793300	0.80424500
C	4.23721900	0.57243800	-1.59998900
C	2.96701900	0.16569700	-2.06079900
C	2.82380600	-0.66128400	-3.17636100
C	3.95131600	-1.10512400	-3.87059900
C	5.21981000	-0.71490700	-3.43964600
C	5.35577700	0.11220600	-2.32162400
C	3.21567300	3.15346300	-0.31149900
C	2.72558200	3.91246600	0.77020600
C	1.94493500	5.05125600	0.56903000
C	1.64029400	5.46665100	-0.72886500
C	2.12154000	4.73931300	-1.81824300
C	2.89552300	3.59635700	-1.60951900
C	6.10270100	2.19965800	0.47106700
C	7.00244900	0.99125300	0.81095000
C	6.75122300	3.04592600	-0.64723300
C	5.99687100	3.07643700	1.74145400
H	1.30900200	-1.63031400	0.08505600
H	1.78091500	0.63508700	0.79803500
H	2.77903700	1.09683400	3.63333500
H	1.56529900	2.04019600	2.75203900
H	3.18565800	-1.52863400	2.39529400
H	-0.34744000	1.22998200	4.69300800
H	-1.87936400	-0.66713500	5.18460900
H	-1.51241800	-2.87814700	4.14499200
H	0.39310700	-3.23324700	2.58560800
H	0.33494400	-2.95947800	-1.13299700
H	0.20347400	-4.16389700	0.15597800
H	0.47031400	-5.99932600	-1.41072200
H	-0.37834900	-4.84123800	-2.44600000
H	1.76343600	-3.99343700	-3.34140300
H	2.02293800	-5.74709600	-3.31642000

H	3.22629100	-5.63610700	-1.22893800
H	3.76256700	-4.11109300	-1.96936000
H	4.76694500	-5.22407800	0.08465800
H	3.78258000	-5.19357300	1.55896800
H	6.50856200	-5.23480100	1.74969600
H	5.60185500	-4.14762400	2.81495000
H	6.85517000	-3.42861400	0.10650000
H	7.14052200	-2.60261900	1.64344400
H	4.96677200	-1.59517300	1.63643700
H	5.20645600	-1.67820300	-0.10563100
H	2.06304300	0.48655700	-1.55149900
H	1.82805900	-0.94668800	-3.50415800
H	3.84248600	-1.73712700	-4.74784300
H	6.10425300	-1.04401000	-3.97828100
H	6.35627700	0.40352300	-2.02011400
H	2.95203900	3.61233500	1.78864900
H	1.56048700	5.60315400	1.42121100
H	1.02955200	6.35066700	-0.88662900
H	1.88975900	5.05754900	-2.83078300
H	3.24809600	3.03782500	-2.47182800
H	7.15236800	0.31784800	-0.03860800
H	6.58335500	0.40707700	1.63646300
H	7.99504800	1.34073200	1.12547800
H	7.72985700	3.41782300	-0.31599200
H	6.13811500	3.91739500	-0.89972700
H	6.91387200	2.47920500	-1.56922900
H	5.52993900	2.53406300	2.56976600
H	5.42098200	3.98900500	1.56275200
H	7.00100200	3.38081400	2.06589100
O	0.03754900	-0.60857000	-0.59056700
C	-1.14930200	-0.38079600	-0.94388500
N	-1.99432100	-1.32618200	-1.37980000
C	-1.55681400	1.07907500	-0.94519600
C	-3.44978200	-1.17188300	-1.27073200
C	-3.12157800	-2.24095200	-0.30654700
C	-1.21287000	1.87469900	0.15399900
C	-2.19491700	1.66785200	-2.04091300
C	-1.51688600	3.23194200	0.13843400
H	-0.72490500	1.44088200	1.01632100
C	-2.46418800	3.03554100	-2.02157700
H	-2.47264900	1.08650000	-2.91101200
C	-2.14092400	3.84679600	-0.94210300
N	-1.13935300	4.06136600	1.29511400
N	-3.10624400	3.65292600	-3.19816200
H	-2.36012500	4.90487800	-0.94500800
O	-1.37777800	5.26596200	1.23523100
O	-0.59260000	3.50436700	2.24687000
O	-3.35710900	2.92285500	-4.15493900
O	-3.34322400	4.85799500	-3.14854200
H	-3.78805200	-0.24619500	-0.80301700
H	-2.85182700	-1.95504300	0.69824500
S	-5.52537500	-2.35446100	1.03753700
C	-6.13871900	-0.72139900	1.09670900
C	-7.39468000	-0.34456800	0.53757300
C	-5.45679100	0.36577100	1.71065600
C	-7.91265500	0.94590100	0.59310000
C	-5.95059800	1.66576500	1.77694900
C	-7.19017600	1.96189800	1.21577100
H	-8.87967600	1.14704400	0.14553900
H	-5.36555200	2.43324100	2.27192800
H	-7.58862400	2.97019000	1.26348800
C	-3.09760000	-3.69240200	-0.70729900
C	-3.37952600	-3.90446800	-2.20335300
C	-4.56393900	-3.03820600	-2.65025200
H	-3.58891300	-4.96505200	-2.38401800
H	-2.48962400	-3.64179100	-2.78965500
C	-4.25228500	-1.53501800	-2.52822400
H	-3.86501300	-4.20054500	-0.11535200
H	-2.13857900	-4.13571800	-0.41396800
H	-5.19025600	-0.97220300	-2.51851600
H	-3.68087300	-1.19496100	-3.40100500
H	-5.42792200	-3.27049600	-2.01804700
H	-4.84312400	-3.27098800	-3.68395600
Cl	-8.38736800	-1.54947100	-0.28199700
Cl	-3.86969000	0.10208800	2.45816000

TS_{SS} conformation 4

Si	-4.87866300	-0.18548600	-0.21286400
O	-3.81765000	-0.81058300	-1.37445500
N	-1.08154100	-1.99758300	-0.20217700
N	-0.28435600	-3.53777600	1.33468600
N	-1.95854600	-4.19113100	-0.15060000
C	-2.47423400	-0.41893300	-1.60551400
C	-2.24763700	0.19392600	-3.00476400
C	-0.76233100	0.00337300	-3.19695600
C	-0.29174400	-1.01750100	-2.36043600
C	-1.45067500	-1.59431000	-1.56036100
C	0.12265400	0.69819800	-4.01981600
C	1.47896800	0.36077900	-3.99174600
C	1.94807900	-0.66119200	-3.15904600
C	1.05675700	-1.36373300	-2.34077900
C	-1.11769900	-3.22956300	0.31889400
C	0.92934800	-2.74434800	1.66956000
C	1.45303400	-3.41878000	2.94338900
C	0.17259800	-3.93203300	3.61816200
C	-0.64361700	-4.46155400	2.43476000
C	-1.57324500	-5.61366400	-0.26830000
C	-2.64340400	-6.17571600	-1.20809900
C	-3.89801300	-5.40261000	-0.77540000
C	-3.37827600	-3.97588000	-0.54029600
C	-4.40469700	-0.86200000	1.50051100
C	-3.19009400	-0.43532500	2.07903700
C	-2.76103700	-0.91693300	3.31702700
C	-3.53894700	-1.83985300	4.01943400
C	-4.74575900	-2.27750300	3.47208300
C	-5.16854300	-1.79254000	2.23149700
C	-4.74081500	1.69795100	-0.13348200
C	-4.59656000	2.47638300	-1.29940700
C	-4.54194200	3.86976000	-1.24632000
C	-4.64089200	4.52384700	-0.01677200
C	-4.79775800	3.77805300	1.15211600
C	-4.84315200	2.38418700	1.09225600
C	-6.60687000	-0.72476100	-0.85202700
C	-6.69432700	-2.25368700	-1.05310800
C	-7.71284600	-0.25316100	0.11833600
C	-6.85107000	-0.05618000	-2.22581300
H	-0.62803500	-1.24662300	0.34293600
H	-2.14447600	0.30580500	-0.85071800
H	-2.83200100	-0.37677400	-3.74037500
H	-2.56089700	1.23796500	-3.06359400
H	-1.86569800	-2.46420400	-2.07608100
H	-0.23307300	1.50659500	-4.65180900
H	2.18424800	0.90788500	-4.60986400
H	3.00983900	-0.88358400	-3.11938000
H	1.42489300	-2.15108700	-1.68845200
H	0.67971700	-1.69539800	1.85193000
H	1.63393300	-2.78418900	0.83484600
H	2.11295900	-4.25721000	2.69430000
H	2.01666000	-2.71965700	3.56413800
H	-0.36234300	-3.10622000	4.09884300
H	0.35570800	-4.70496200	4.36871900
H	-0.34003200	-5.48768300	2.19486500
H	-1.72323700	-4.44629900	2.60201800
H	-1.61881200	-6.13278400	0.69683800
H	-0.55356700	-5.69814600	-0.65323700
H	-2.74599800	-7.25934000	-1.11204400
H	-2.39161800	-5.94805100	-2.24957600
H	-4.29562400	-5.82328600	0.15497400
H	-4.69744500	-5.42381500	-1.51944900
H	-3.46612500	-3.37144700	-1.44405200
H	-3.90453600	-3.44917100	0.25787800
H	-2.55295000	0.28234700	1.57047200
H	-1.82268600	-0.55810900	3.73050300
H	-3.21542300	-2.20435000	4.99075500
H	-5.36534700	-2.98693700	4.01386900
H	-6.11677600	-2.14622600	1.84057200
H	-4.52336400	1.99168900	-2.26794200
H	-4.40556900	4.44221300	-2.15869800
H	-4.59489500	5.60809200	0.02728300

H	-4.87833400	4.28033100	2.11205900
H	-4.95073900	1.82368300	2.01620000
H	-6.56454600	-2.81536700	-0.12271200
H	-5.94094600	-2.60263100	-1.76647400
H	-7.67991800	-2.52210500	-1.45685400
H	-8.70128900	-0.50308500	-0.28942900
H	-7.68421100	0.83184900	0.26425500
H	-7.63970400	-0.72071800	1.10509400
H	-6.08748600	-0.33993800	-2.95714600
H	-6.86483300	1.03524500	-2.15321200
H	-7.82534100	-0.37101600	-2.62281000
O	-0.14240500	0.35570200	0.97126200
C	0.83049600	1.15452200	1.04066400
N	2.04467000	0.84807700	1.50565000
C	0.52198200	2.59840600	0.67681100
C	3.25057000	1.49644300	0.98420000
C	3.45816500	0.08052800	0.58780400
C	-0.20717200	2.88466300	-0.48268700
C	0.88366900	3.64713000	1.52867200
C	-0.55286800	4.20345200	-0.76650000
H	-0.49397300	2.09415700	-1.16311600
C	0.50177400	4.95012800	1.21527300
H	1.44195800	3.46185700	2.43695100
C	-0.21907200	5.26294400	0.07065000
N	-1.32501900	4.49547900	-1.98602400
N	0.86623900	6.04301900	2.13833800
H	-0.50872400	6.27924900	-0.15556400
O	-1.73003500	5.64519900	-2.14392800
O	-1.53153300	3.56866700	-2.76942200
O	1.48869300	5.74202000	3.15462200
O	0.52175300	7.18245200	1.83229500
H	3.07802200	2.16643000	0.13821000
H	2.98955500	-0.27211100	-0.31618000
S	5.30971300	0.48339600	-1.34929600
C	6.55976100	-0.69262200	-1.03671800
C	6.38528200	-2.09833300	-1.17248400
C	7.87385400	-0.33301900	-0.61477200
C	7.38472200	-3.03984000	-0.93791200
C	8.89057900	-1.25287200	-0.37839100
C	8.64898700	-2.61608300	-0.53952700
H	7.16720700	-4.09328900	-1.07440400
H	9.86578200	-0.89506900	-0.06748100
H	9.43786400	-3.33866800	-0.35713300
C	4.13890900	-0.89041900	1.51469000
C	4.51069500	-0.26960800	2.86964800
C	5.17339300	1.09643900	2.65803200
H	5.18902900	-0.94741000	3.40003100
H	3.61093300	-0.15649700	3.48681200
C	4.20470600	2.11020100	2.02154700
H	5.04812900	-1.23892900	1.01502800
H	3.51105900	-1.77769700	1.64282700
H	4.77953700	2.90487500	1.53701400
H	3.59413200	2.58418300	2.79936100
H	6.03975300	0.96960300	1.99936900
H	5.54941600	1.49562100	3.60652900
Cl	8.28452800	1.36301700	-0.37369700
Cl	4.81919400	-2.75454200	-1.68787200

TS_{SS} conformation 5

Si	-4.87866000	-0.18550300	-0.21286600
O	-3.81764200	-0.81059400	-1.37445400
N	-1.08152600	-1.99757800	-0.20218100
N	-0.28433200	-3.53777200	1.33467600
N	-1.95852100	-4.19112900	-0.15061000
C	-2.47422900	-0.41893300	-1.60551400
C	-2.24763900	0.19392900	-3.00476400
C	-0.76233000	0.00339000	-3.19695600
C	-0.29173400	-1.01748000	-2.36043700
C	-1.45066100	-1.59430200	-1.56036500
C	0.12264900	0.69822600	-4.01981300
C	1.47896600	0.36082100	-3.99174200
C	1.94808600	-0.66114600	-3.15904200
C	1.05677100	-1.36369800	-2.34077800
C	-1.11767700	-3.22955900	0.31888600
C	0.92937100	-2.74434100	1.66955100
C	1.45305300	-3.41876600	2.94338600
C	0.17261700	-3.93202500	3.61815400
C	-0.64358800	-4.46155500	2.43474800
C	-1.57321600	-5.61366100	-0.26831200
C	-2.64339300	-6.17572300	-1.20808600
C	-3.89799400	-5.40261500	-0.77536800
C	-3.37825200	-3.97588000	-0.54030700
C	-4.40469700	-0.86201800	1.50050900
C	-3.19009500	-0.43534400	2.07903700
C	-2.76103900	-0.91695500	3.31702700
C	-3.53894900	-1.83987700	4.01943100
C	-4.74576200	-2.27752400	3.47207800
C	-5.16854400	-1.79255900	2.23149200
C	-4.74082100	1.69793500	-0.13348000
C	-4.59657200	2.47637100	-1.29940300
C	-4.54196100	3.86974800	-1.24631200
C	-4.64091200	4.52383100	-0.01676200
C	-4.79777200	3.77803200	1.15212400
C	-4.84315900	2.38416600	1.09226000
C	-6.60686300	-0.72478500	-0.85203600
C	-6.69431300	-2.25371100	-1.05311600
C	-7.71284500	-0.25318900	0.11832000
C	-6.85105800	-0.05620600	-2.22582400
H	-0.62802300	-1.24661700	0.34293400
H	-2.14447600	0.30580700	-0.85071700
H	-2.83199700	-0.37677600	-3.74037600
H	-2.56090800	1.23796500	-3.06359300
H	-1.86567600	-2.46419800	-2.07608700
H	-0.23308600	1.50662100	-4.65180500
H	2.18424100	0.90793500	-4.60985800
H	3.00984900	-0.88352800	-3.11937500
H	1.42491400	-2.15104900	-1.68845200
H	0.67973800	-1.69539000	1.85191400
H	1.63395900	-2.78418800	0.83484100
H	2.11298500	-4.25719200	2.69430500
H	2.01666900	-2.71963700	3.56413700
H	-0.36233300	-3.10621400	4.09882900
H	0.35572700	-4.70495200	4.36871400
H	-0.33999000	-5.48768000	2.19485400
H	-1.72320900	-4.44631200	2.60200100
H	-1.61876100	-6.13277700	0.69682800
H	-0.55354600	-5.69814100	-0.65327100
H	-2.74598200	-7.25934700	-1.11202000
H	-2.39163000	-5.94806600	-2.24957000
H	-4.29557600	-5.82327400	0.15502600
H	-4.69744600	-5.42383500	-1.51939400
H	-3.46610200	-3.37147700	-1.44408300
H	-3.90450600	-3.44914300	0.25785200
H	-2.55295000	0.28233000	1.57047600
H	-1.82268800	-0.55813200	3.73050400
H	-3.21542700	-2.20437600	4.99075100
H	-5.36535000	-2.98695900	4.01386100
H	-6.11677600	-2.14624400	1.84056600
H	-4.52337500	1.99168000	-2.26794000
H	-4.40559400	4.44220400	-2.15868900
H	-4.59492000	5.60807600	0.02729600
H	-4.87834800	4.28030700	2.11206900
H	-4.95074100	1.82366000	2.01620300
H	-6.56452400	-2.81539100	-0.12272200
H	-5.94093300	-2.60265200	-1.76648600
H	-7.67990400	-2.52213500	-1.45685800
H	-8.70128500	-0.50311000	-0.28945500
H	-7.68421100	0.83182000	0.26424600
H	-7.63971200	-0.72075200	1.10507600
H	-6.08746700	-0.33995800	-2.95715200
H	-6.86483200	1.03521900	-2.15322300
H	-7.82532400	-0.37105100	-2.62282700
O	-0.14239800	0.35570700	0.97128400
C	0.83049900	1.15453300	1.04067700
N	2.04467600	0.84809800	1.50565800
C	0.52197400	2.59841400	0.67681900
C	3.25057100	1.49646700	0.98419800
C	3.45817300	0.08054900	0.58781700
C	-0.20718600	2.88466400	-0.48267600

C	0.88365900	3.64714300	1.52867600
C	-0.55288900	4.20345100	-0.76649200
H	-0.49398600	2.09415500	-1.16310200
C	0.50175800	4.95013700	1.21527400
H	1.44195300	3.46187500	2.43695200
C	-0.21909500	5.26294700	0.07065300
N	-1.32504500	4.49547100	-1.98601500
N	0.86622200	6.04303400	2.13833300
H	-0.50875200	6.27924900	-0.15556300
O	-1.73006800	5.64518900	-2.14391900
O	-1.53155400	3.56865700	-2.76941100
O	1.48867800	5.74204000	3.15461700
O	0.52173200	7.18246500	1.83228700
H	3.07801500	2.16644300	0.13820000
H	2.98956300	-0.27210400	-0.31616200
S	5.30972100	0.48340700	-1.34928100
C	6.55975200	-0.69263200	-1.03671700
C	6.38524300	-2.09834100	-1.17246600
C	7.87386000	-0.33305000	-0.61480000
C	7.38467000	-3.03986500	-0.93790400
C	8.89057300	-1.25292000	-0.37843100
C	8.64895100	-2.61612800	-0.53954900
H	7.16713200	-4.09331100	-1.07438200
H	9.86578800	-0.89513400	-0.06754400
H	9.43781700	-3.33872700	-0.35716400
C	4.13892300	-0.89038500	1.51471200
C	4.51072500	-0.26955300	2.86965600
C	5.17341300	1.09649500	2.65801100
H	5.18906900	-0.94734400	3.40004000
H	3.61097100	-0.15643800	3.48683100
C	4.20470600	2.11024200	2.02153500
H	5.04813700	-1.23890700	1.01504600
H	3.51107100	-1.77765900	1.64287100
H	4.77952000	2.90492500	1.53699700
H	3.59413200	2.58421500	2.79935600
H	6.03975900	0.96965500	1.99933000
H	5.54945400	1.49569000	3.60649600
Cl	4.81913200	-2.75452500	-1.68781500
Cl	8.28457200	1.36298100	-0.37375100

TS_{SS} conformation 6

Si	4.33202700	1.65465300	-0.03834200
O	3.80119200	0.75667300	1.29302800
N	2.13416700	-1.92081400	0.63298800
N	2.18032200	-3.89802400	-0.57118500
N	4.05923200	-3.28668000	0.67161700
C	2.46992700	0.38054500	1.61195200
C	1.95079000	1.03112100	2.91403200
C	0.89462600	0.05556800	3.37446000
C	1.09036600	-1.19540000	2.77648500
C	2.30779400	-1.14870900	1.86712900
C	-0.17312600	0.25501600	4.24763400
C	-1.03233700	-0.81308400	4.52200200
C	-0.82634100	-2.06448900	3.93188800
C	0.24190600	-2.26377700	3.05325600
C	2.79348900	-3.01961500	0.25186700
C	0.70699300	-3.92782000	-0.78550100
C	0.53037000	-5.00329200	-1.86359300
C	1.81610600	-4.87410800	-2.69256500
C	2.89004300	-4.66785500	-1.61911300
C	4.54007200	-4.64815000	0.98961200
C	5.83088300	-4.37787700	1.76878600
C	6.39167500	-3.13857200	1.05604100
C	5.14520900	-2.27793400	0.80424200
C	4.23721600	0.57243700	-1.59999300
C	2.96701600	0.16569800	-2.06080200
C	2.82380000	-0.66128300	-3.17636300
C	3.95130800	-1.10512500	-3.87060200
C	5.21980400	-0.71490900	-3.43965200
C	5.35577300	0.11220400	-2.32162900
C	3.21567500	3.15346300	-0.31150200
C	2.72558600	3.91246700	0.77020400
C	1.94493900	5.05125700	0.56902900
C	1.64029700	5.46665200	-0.72886600
C	2.12154100	4.73931400	-1.81824400
C	2.89552400	3.59635700	-1.60952100
C	6.10270400	2.19965600	0.47106000
C	7.00245100	0.99125100	0.81094100
C	6.75122400	3.04592300	-0.64724100
C	5.99687600	3.07643500	1.74144700
H	1.30900300	-1.63031400	0.08505600
H	1.78091700	0.63508800	0.79803300
H	2.77904200	1.09683600	3.63333200
H	1.56530400	2.04019800	2.75203700
H	3.18566000	-1.52863300	2.39529300
H	-0.34743500	1.22998700	4.69300600
H	-1.87936000	-0.66712800	5.18460900
H	-1.51241600	-2.87814200	4.14499400
H	0.39310800	-3.23324400	2.58561000
H	0.33494400	-2.95947900	-1.13299500
H	0.20347100	-4.16389200	0.15598400
H	0.47030600	-5.99932800	-1.41070900
H	-0.37835300	-4.84124100	-2.44599300
H	1.76343400	-3.99345000	-3.34139800
H	2.02293200	-5.74710900	-3.31640800
H	3.22628500	-5.63611500	-1.22892600
H	3.76256500	-4.11110500	-1.96935300
H	4.76694100	-5.22408300	0.08466600
H	3.78258000	-5.19357100	1.55897800
H	6.50856200	-5.23480000	1.74970100
H	5.60185800	-4.14761900	2.81495200
H	6.85516900	-3.42861900	0.10649800
H	7.14052400	-2.60261800	1.64343700
H	4.96677400	-1.59517100	1.63643200
H	5.20645500	-1.67820800	-0.10563600
H	2.06304000	0.48655900	-1.55150000
H	1.82805200	-0.94668600	-3.50415800
H	3.84247700	-1.73712700	-4.74784700
H	6.10424500	-1.04401300	-3.97828800
H	6.35627400	0.40351900	-2.02012100
H	2.95204400	3.61233600	1.78864600
H	1.56049200	5.60315500	1.42121100
H	1.02955500	6.35066800	-0.88662900
H	1.88975800	5.05754900	-2.83078400
H	3.24809500	3.03782500	-2.47183100
H	7.15236900	0.31784500	-0.03861700
H	6.58335800	0.40707500	1.63645500
H	7.99505100	1.34072900	1.12546800
H	7.72986000	3.41781900	-0.31600200
H	6.13811700	3.91739300	-0.89973400
H	6.91387100	2.47920300	-1.56923800
H	5.52994500	2.53406200	2.56976000
H	5.42098700	3.98900400	1.56274500
H	7.00100800	3.38081300	2.06588200
O	0.03754800	-0.60857000	-0.59056400
C	-1.14930200	-0.38079500	-0.94388200
N	-1.99432200	-1.32618000	-1.37979900
C	-1.55681400	1.07907600	-0.94519200
C	-3.44978200	-1.17188200	-1.27073100
C	-3.12158000	-2.24095200	-0.30654800
C	-1.21286900	1.87469900	0.15400300
C	-2.19491800	1.66785400	-2.04090800
C	-1.51688400	3.23194200	0.13843900
H	-0.72490400	1.44088200	1.01632500
C	-2.46418800	3.03554300	-2.02157100
H	-2.47265100	1.08650200	-2.91100700
C	-2.14092300	3.84679700	-0.94209700
N	-1.13935000	4.06136600	1.29512000
N	-3.10624500	3.65292900	-3.19815600
H	-2.36012300	4.90487900	-0.94500100
O	-1.37777400	5.26596200	1.23523700
O	-0.59259600	3.50436600	2.24687400
O	-3.35711100	2.92285900	-4.15493300
O	-3.34322500	4.85799800	-3.14853400
H	-3.78805300	-0.24619400	-0.80301600
H	-2.85183000	-1.95504500	0.69824500
S	-5.52537800	-2.35446200	1.03753400
C	-6.13872000	-0.72139900	1.09670600
C	-7.39468100	-0.34456700	0.53757000

C	-5.45679300	0.36576900	1.71065600
C	-7.91265400	0.94590200	0.59309700
C	-5.95059800	1.66576300	1.77695000
C	-7.19017600	1.96189800	1.21577000
H	-8.87967500	1.14704600	0.14553600
H	-5.36555300	2.43323800	2.27193000
H	-7.58862300	2.97019000	1.26348800
C	-3.09760100	-3.69240200	-0.70730200
C	-3.37952600	-3.90446500	-2.20335600
C	-4.56393800	-3.03820300	-2.65025500
H	-3.58891200	-4.96505000	-2.38402300
H	-2.48962300	-3.64178700	-2.78965700
C	-4.25228500	-1.53501500	-2.52822500
H	-3.86501500	-4.20054500	-0.11535700
H	-2.13858100	-4.13571800	-0.41397000
H	-5.19025600	-0.97220100	-2.51851700
H	-3.68087200	-1.19495600	-3.40100500
H	-5.42792200	-3.27049400	-2.01805200
H	-4.84312100	-3.27098300	-3.68396100
Cl	-8.38736900	-1.54946800	-0.28200400
Cl	-3.86969400	0.10208400	2.45816200

TS_{SS} conformation 7

Si	-2.79079400	-1.69226500	2.27819000
O	-2.02906600	-2.28425100	0.89085600
N	0.30790100	-1.75452100	-1.48191600
N	2.25881900	-1.93112200	-2.74805600
N	1.93615000	-3.30779800	-0.87106200
C	-1.97701400	-1.71100000	-0.41031100
C	-3.33344000	-1.78418300	-1.16908300
C	-2.99854800	-2.35433200	-2.52248800
C	-1.67619700	-2.79892900	-2.57516700
C	-0.94640900	-2.50775600	-1.27409800
C	-3.83764900	-2.50891800	-3.62805200
C	-3.34392900	-3.13385800	-4.77387500
C	-2.02776600	-3.60900800	-4.81426700
C	-1.18668000	-3.44353300	-3.71257200
C	1.51280500	-2.33430500	-1.70631900
C	1.69996600	-1.14255600	-3.88450900
C	2.90224400	-0.97043300	-4.81730600
C	4.08676500	-0.89950400	-3.84307200
C	3.74490800	-1.96079800	-2.79386000
C	2.83737200	-4.41799000	-1.23529200
C	2.68477400	-5.37920500	-0.05192400
C	2.53945800	-4.41652300	1.13645500
C	1.64100600	-3.29810700	0.59008600
C	-1.77298300	-0.26004300	2.96493900
C	-0.39557000	-0.16958900	2.69029900
C	0.40015400	0.82000800	3.27007900
C	-0.17261100	1.75187400	4.13828600
C	-1.53784400	1.68878300	4.42190100
C	-2.32580500	0.69286300	3.84267000
C	-4.53145700	-1.04360700	1.89292800
C	-5.69127600	-1.83898300	1.96408200
C	-6.94531400	-1.33919600	1.60944600
C	-7.07404400	-0.02341000	1.16491800
C	-5.94348600	0.79077500	1.08793200
C	-4.69393300	0.28585600	1.45161500
C	-2.73405900	-3.19592500	3.47361000
C	-1.26250000	-3.45316400	3.87343700
C	-3.54332800	-2.88700700	4.75169100
C	-3.27177400	-4.48012600	2.80426700
H	0.18777000	-0.79797700	-1.82770400
H	-1.63631500	-0.66997600	-0.34753600
H	-4.00933200	-2.45282700	-0.62520700
H	-3.83534100	-0.81467900	-1.23138300
H	-0.70473400	-3.43445700	-0.75038200
H	-4.85984200	-2.14285700	-3.59720900
H	-3.98685900	-3.25705600	-5.64046700
H	-1.65995400	-4.10690400	-5.70666700
H	-0.16614200	-3.81747700	-3.74696000
H	1.33648800	-0.17379900	-3.53003300
H	0.86166700	-1.67808100	-4.33486200
H	3.00222100	-1.83852200	-5.47920900
H	2.80108500	-0.08053500	-5.44318000
H	4.13668600	0.08267500	-3.36317900
H	5.05229600	-1.09325600	-4.31635100
H	4.09182700	-2.94758700	-3.12121200
H	4.14695300	-1.72534900	-1.80503300
H	3.87755900	-4.08376200	-1.31184600
H	2.53935100	-4.84548500	-2.19732500
H	3.53908200	-6.05482200	0.03715700
H	1.78025100	-5.98648000	-0.16987400
H	3.51528400	-4.00490300	1.41326900
H	2.10727100	-4.88753600	2.02244300
H	0.58504800	-3.50848000	0.77974500
H	1.89431500	-2.31689000	0.99999200
H	0.06633400	-0.88796900	2.01891800
H	1.46323300	0.84933500	3.05365500
H	0.44441400	2.52044300	4.59536400
H	-1.98887300	2.41247200	5.09522000
H	-3.38774600	0.66417000	4.07296500
H	-5.62577100	-2.86834700	2.30025000
H	-7.82055300	-1.97918500	1.67809600
H	-8.04685200	0.36661100	0.88049100
H	-6.03795700	1.81550400	0.74072900
H	-3.82973300	0.94248200	1.39663400
H	-0.81515600	-2.59258800	4.37882100
H	-0.64274300	-3.69047800	3.00201900
H	-1.20739800	-4.30886800	4.55982900
H	-3.47233300	-3.72647700	5.45619800
H	-4.60476900	-2.72113900	4.54246700
H	-3.16178600	-1.99798300	5.26608600
H	-2.73031600	-4.70659800	1.88094000
H	-4.33591200	-4.41942200	2.55702500
H	-3.15024900	-5.33448800	3.48410700
O	-0.08045200	1.02503100	-2.07434500
C	-0.05055800	2.19800900	-1.62522500
N	1.02642200	2.93662700	-1.28599600
C	-1.36759200	2.91811100	-1.46147800
C	2.32760200	2.26057700	-1.42675900
C	2.11262900	2.00358100	0.00519300
C	-2.53761200	2.28363200	-1.88968000
C	-1.44694700	4.19133900	-0.88528800
C	-3.76384000	2.92012600	-1.71566400
H	-2.47839100	1.30651300	-2.35010200
C	-2.69334600	4.79253100	-0.73527300
H	-0.54647400	4.69632000	-0.56312700
C	-3.87569900	4.18052900	-1.13856600
N	-4.99399800	2.23438400	-2.14960400
N	-2.77346800	6.13318700	-0.12150100
H	-4.83357800	4.66450000	-1.01085500
O	-6.06799100	2.78853800	-1.91965500
O	-4.87393000	1.14660000	-2.71260600
O	-1.72148200	6.65883200	0.23413700
O	-3.88921500	6.63728100	-0.00497700
H	2.28556600	1.36039600	-2.03920100
S	3.76717600	-0.16728400	0.40371000
C	5.26781400	0.29133600	1.18235300
C	5.43091900	0.34178100	2.59414600
C	6.44424700	0.64558100	0.46618200
C	6.61499700	0.71537800	3.22513300
C	7.63912300	1.02264400	1.07286200
C	7.72622200	1.06274900	2.46209900
H	6.65753200	0.72855600	4.30834400
H	8.49148400	1.27963500	0.45420600
H	8.65244300	1.35712600	2.94467800
C	2.50568200	3.00343800	1.05262800
C	3.13148200	4.27859200	0.46553000
C	4.13529200	3.92411600	-0.63806200
H	3.62380200	4.83856300	1.26794000
H	2.34229300	4.91915300	0.05798800
C	3.46278300	3.21269900	-1.82834000
H	3.22569100	2.50422500	1.71197800
H	4.21935400	2.64652000	-2.38061100
H	3.03554600	3.94799200	-2.51934600
H	4.90761900	3.27046200	-0.21574500
H	4.64832600	4.82463800	-0.99306900
H	1.63322000	3.23113200	1.67639500

H	1.47005800	1.17867400	0.27547700	Cl	4.09593600	-0.10765200	3.65750700
Cl	6.45579500	0.60602400	-1.30077400				

TS structures for Mechanism 2: Ar = C_6H_5

7 conformations for both (*R*,*R*) and (*S*,*S*) transition state were located by removal of Cl from the corresponding TS structures of Ar = 2,6-$Cl_2C_6H_3$

Table 12: CPCM/RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Relative Energy (kcal/mol)	Conformation	Electronic energy (hartree)	Relative Energy (kcal/mol)
TS_{RR} conformation 1	-3524.11187518	8.4	TS_{SS} conformation 1	-3524.11818433	4.5
TS_{RR} conformation 2	-3524.11332647	7.5	TS_{SS} conformation 2	-3524.11818413	4.5
TS_{RR} conformation 3	-3524.11187513	8.4	TS_{SS} conformation 3	-3524.11437397	6.8
TS_{RR} conformation 4	-3524.11187504	8.4	TS_{SS} conformation 4	-3524.11284319	7.8
TS_{RR} conformation 5	-3524.11332623	7.5	TS_{SS} conformation 5	-3524.11818438	4.5
TS_{RR} conformation 6	-3524.11332621	7.5	TS_{SS} conformation 6	-3524.11433202	6.9
TS_{RR} conformation 7	-3524.12530926	0.0	TS_{SS} conformation 7	-3524.12528354	0.0

Table 13: RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)	Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)
TS_{RR} conformation 7	-3524.09752201	0	TS_{SS} conformation 7	-3524.10236991	3.0

Table 14: Correction to zero-point energy, thermal correction to electronic energy, enthalpy and Gibbs derived from RB3LYP/6-31G(d,p) for (R,R) TS structures

Conformation	Zero-point correction	Thermal correction to Energy	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
1	1.072540	1.136929	1.137873	0.964218
2	1.072122	1.136606	1.137550	0.963536
3	1.072540	1.136929	1.137873	0.964218
4	1.072540	1.136929	1.137873	0.964218
5	1.072122	1.136606	1.137550	0.963541
6	1.072122	1.136606	1.137550	0.963541
7	1.073167	1.137532	1.138476	0.964826

Table 15: Correction to zero-point energy, thermal correction to electronic energy, enthalpy and Gibbs derived from RB3LYP/6-31G(d,p) for (S,S) TS structures

Conformation	Zero-point correction	Thermal correction to Energy	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy
1	1.072565	1.137028	1.137972	0.964553
2	1.072565	1.137028	1.137972	0.964553
3	1.072405	1.136922	1.137867	0.963536
4	1.072272	1.136898	1.137843	0.962936

5	1.072565	1.137028	1.137972	0.964552
6	1.072337	1.136872	1.137816	0.964714
7	1.072572	1.137077	1.138021	0.963635

TS_{RR} conformation 1

Si	-3.97434900	0.73362300	-0.96583800
O	-3.34056400	-0.77216400	-1.39057800
N	-0.88830100	-1.87487300	0.34303100
N	0.05357400	-2.27639100	2.42297600
N	-2.09780000	-3.07775000	1.97150500
C	-2.04609800	-1.19274300	-1.77659000
C	-2.02542900	-1.78282200	-3.20730300
C	-0.89534200	-2.78281100	-3.15825200
C	-0.57634200	-3.09627900	-1.83097000
C	-1.51204200	-2.35452900	-0.88955700
C	-0.20594900	-3.38995400	-4.20620800
C	0.80113500	-4.31333500	-3.91142400
C	1.11737400	-4.62224100	-2.58488500
C	0.42765500	-4.01282100	-1.53263500
C	-0.98361900	-2.40891700	1.57049800
C	1.44198500	-1.94873800	1.98486200
C	2.21425000	-1.85484000	3.30314400
C	1.16435800	-1.31911900	4.28635000
C	-0.09511600	-2.09805900	3.88813400
C	-2.07496000	-4.24050300	2.88745800
C	-3.51600000	-4.76130600	2.82998000
C	-4.32897200	-3.47315300	2.63545700
C	-3.48969800	-2.69421500	1.61727000
C	-3.84799100	0.97072700	0.91522600
C	-2.58173600	1.22061600	1.48830400
C	-2.42585200	1.37503000	2.86827700
C	-3.53174500	1.27857600	3.71609200
C	-4.79340700	1.03058500	3.17542200
C	-4.94461100	0.88232900	1.79461900
C	-3.01047700	2.13613500	-1.78750200
C	-2.50192100	2.02104500	-3.09610400
C	-1.84235500	3.07999900	-3.72020100
C	-1.68344500	4.29420000	-3.05097500
C	-2.18682500	4.43932700	-1.75810700
C	-2.83698900	3.37239800	-1.13571000
C	-5.77244300	0.64509700	-1.63986500
C	-6.50078900	-0.61802900	-1.12782100
C	-6.56957200	1.91344300	-1.26383800
C	-5.70627900	0.55490400	-3.18220200
H	-0.24035400	-1.08142800	0.20850300
H	-1.32526000	-0.36794700	-1.71117100
H	-2.98857500	-2.27681100	-3.39410300
H	-1.89607100	-1.01673200	-3.97757300
H	-2.34917000	-3.00646900	-0.63367000
H	-0.44155700	-3.14623000	-5.23860500
H	1.34949900	-4.78883200	-4.71905500
H	1.90804900	-5.33471100	-2.37063800
H	0.68641100	-4.24739100	-0.50382500
H	1.44966900	-0.99043600	1.46061800
H	1.82698300	-2.72183500	1.31560300
H	2.56481300	-2.84646200	3.60522000
H	3.09402400	-1.21649100	3.20496600
H	1.01061500	-0.24372500	4.14714200
H	1.42584800	-1.48560700	5.33436800
H	-0.10627000	-3.06992400	4.39535400
H	-1.03002700	-1.57692400	4.10947500
H	-1.83225600	-3.94355500	3.91265400
H	-1.32759800	-4.96836000	2.55872900
H	-3.78375700	-5.31576100	3.73260400
H	-3.64870100	-5.42825500	1.97101500
H	-4.39850600	-2.91792500	3.57748400
H	-5.34401300	-3.65182300	2.27298300
H	-3.75188500	-3.00814300	0.60257500
H	-3.60818500	-1.61214400	1.67300000
H	-1.69891300	1.29739100	0.85818100
H	-1.44588600	1.59397000	3.28395200
H	-3.41091100	1.40924300	4.78792000
H	-5.66239200	0.96315200	3.82429700
H	-5.94049300	0.69986500	1.40615900
H	-2.62362800	1.09144900	-3.64417500
H	-1.45271100	2.95746800	-4.72673500
H	-1.17096900	5.12100200	-3.53428900
H	-2.06974400	5.38202700	-1.23089200
H	-3.20725200	3.50507400	-0.12328800
H	-6.63285600	-0.62507600	-0.04153700
H	-5.95548000	-1.52643900	-1.40229100
H	-7.50194500	-0.68120300	-1.57532800
H	-7.57185400	1.87469800	-1.71099900
H	-6.08142800	2.82088600	-1.63577600
H	-6.69870600	2.02839100	-0.18337500
H	-5.14752100	-0.32698200	-3.51256000
H	-5.24007400	1.43995800	-3.62519400
H	-6.72126300	0.47531800	-3.59395800
O	0.41308100	0.56274000	0.05171400
C	1.39108600	1.23193700	-0.38710600
N	2.04264200	0.95638600	-1.51832500
C	1.76728800	2.44937600	0.43029900
C	3.17748700	-0.40916200	-1.73760600
C	3.49575100	1.03837100	-1.65103700
C	2.39247200	3.57618600	-0.11491200
C	1.40884700	2.46559000	1.78298200
C	2.65480600	4.67561000	0.70001000
H	2.65569800	3.62023700	-1.16296300
C	1.70007000	3.57688200	2.56530400
H	0.89883200	1.61333100	2.20777200
C	2.32673600	4.70753700	2.05088700
N	3.29871000	5.86426100	0.10574300
N	1.32372000	3.56178300	3.99003000
H	2.54198100	5.57059300	2.66488700
O	3.52535500	6.81649100	0.84906900
O	3.56413900	5.82491500	-1.09383600
O	0.75946700	2.55344500	4.42422800
O	1.59325400	4.55175300	4.66296100
H	3.06712700	-0.96834600	-0.82187000
H	4.04484800	1.32971000	-0.75207700
S	5.64877600	-1.39431000	-1.30592600
C	5.22580400	-2.54338900	-0.03776900
C	4.34723700	-3.63023400	-0.26522000
C	5.77410800	-2.43475300	1.26307800
C	4.04721200	-4.55217200	0.73919100
H	3.92718800	-3.76065400	-1.25819500
C	5.48384600	-3.36350700	2.25996400
H	6.45381300	-1.61272600	1.46657100
C	4.61434900	-4.43204700	2.01172600
H	3.38793700	-5.39001400	0.51752200
H	5.94422400	-3.25656800	3.23987400
H	4.40245400	-5.16557700	2.78499800
C	2.88892100	-1.08348300	-3.05940900
C	3.58570600	-0.39388800	-4.24208500
H	1.80381200	-1.08975500	-3.21176400
C	3.42484100	1.13206300	-4.19665500

H	3.18556200	-0.79376600	-5.18123000
H	4.65246700	-0.64582700	-4.21271900
C	4.03725700	1.70335400	-2.91004300
H	2.36177600	1.39917000	-4.24824700
H	3.91233800	1.59077000	-5.06453100
H	3.88255700	2.78831600	-2.85252900
H	5.12153400	1.53865900	-2.91445400
H	3.21347300	-2.12257000	-2.98671300

TS_{RR} conformation 2

Si	-3.74355900	-0.18118000	-1.49569000
O	-2.79009900	-1.56435900	-1.65641700
N	-0.52811600	-1.97558100	0.55331000
N	0.10114900	-2.00562400	2.78476300
N	-1.71372600	-3.30767500	2.09856900
C	-1.39477200	-1.74751800	-1.79179200
C	-1.02042700	-2.45837500	-3.11399900
C	0.28191900	-3.14381700	-2.77638200
C	0.43053100	-3.24948300	-1.38726200
C	-0.79989500	-2.67994600	-0.69907900
C	1.26691600	-3.64474400	-3.62488200
C	2.40087000	-4.24419200	-3.06821500
C	2.55006000	-4.33944400	-1.68128600
C	1.55826400	-3.84402600	-0.83003700
C	-0.71927900	-2.42944800	1.79970000
C	1.43641500	-1.39266100	2.53364700
C	1.93041400	-1.04015300	3.93999600
C	0.63378000	-0.69878000	4.68913200
C	-0.33952700	-1.76960700	4.18100200
C	-1.57791700	-4.38818800	3.10012300
C	-2.79978400	-5.27023900	2.82293100
C	-3.86363200	-4.24122700	2.41413200
C	-3.08285500	-3.27270600	1.51689500
C	-4.05426900	0.16304700	0.34777500
C	-3.00506300	0.69717900	1.12734800
C	-3.16768300	0.95123300	2.49179000
C	-4.38351800	0.67019200	3.11929600
C	-5.43467500	0.13738200	2.37284300
C	-5.26920400	-0.10714500	1.00726900
C	-2.87610300	1.33320600	-2.22352000
C	-2.07172800	1.25066500	-3.37707300
C	-1.47508100	2.38136600	-3.93536200
C	-1.68014200	3.63545300	-3.35852000
C	-2.48324200	3.74823000	-2.22333200
C	-3.06800600	2.61111500	-1.66336500
C	-5.32413600	-0.61742100	-2.49772600
C	-5.91717500	-1.97159200	-2.04820900
C	-6.38133300	0.50103100	-2.37170300
C	-4.93233200	-0.74895500	-3.98809000
H	-0.05208800	-1.06514200	0.43487900
H	-0.86238600	-0.78987500	-1.73104000
H	-1.80858700	-3.18512400	-3.35453500
H	-0.94502600	-1.76742500	-3.95896500
H	-1.51008600	-3.48639700	-0.50669100
H	1.16336500	-3.56148400	-4.70345400
H	3.18161200	-4.62626900	-3.71916500
H	3.44919300	-4.77413900	-1.25761700
H	1.68537300	-3.91307400	0.24667600
H	1.32489700	-0.49274700	1.92392200
H	2.08801700	-2.09378100	2.00655900
H	2.42187000	-1.90389600	4.40121200
H	2.64892400	-0.21816100	3.92052900
H	0.28120000	0.30133900	4.41571700
H	0.73934100	-0.73057600	5.77629100
H	-0.23623600	-2.68333400	4.77803300
H	-1.38739200	-1.45946000	4.19634800
H	-1.62593600	-4.00193300	4.12430500
H	-0.62079600	-4.90196300	2.97468400
H	-3.08017600	-5.86550800	3.69526300
H	-2.59386200	-5.95682300	1.99451700
H	-4.24537600	-3.71829600	3.29791800
H	-4.71487100	-4.68187800	1.89003900
H	-3.09380800	-3.62399000	0.48154900
H	-3.47043900	-2.25344500	1.52716200
H	-2.04376900	0.92172100	0.67184300
H	-2.35455600	1.39317800	3.06197400
H	-4.51354200	0.87791200	4.17781900
H	-6.38801100	-0.07735300	2.84796700
H	-6.11146000	-0.51070300	0.45603700
H	-1.90546100	0.28956700	-3.85439100
H	-0.85119300	2.28359700	-4.81914400
H	-1.21818300	4.51793300	-3.79173700
H	-2.65238800	4.72126700	-1.77057300
H	-3.67682200	2.72276100	-0.77086800
H	-6.25784300	-1.96590700	-1.00831100
H	-5.18430200	-2.77763600	-2.15217200
H	-6.78522600	-2.22713500	-2.67102500
H	-7.25154400	0.27045500	-3.00070000
H	-5.98598900	1.46733000	-2.70333400
H	-6.74318500	0.62782400	-1.34692800
H	-4.18242800	-1.53197400	-4.14234000
H	-4.53617400	0.18712500	-4.39290600
H	-5.81584500	-1.01769100	-4.58240500
O	0.23643900	0.66011900	0.25163700
C	1.05413900	1.52787200	-0.16995300
N	1.89906900	1.32829700	-1.18222600
C	0.98158300	2.87355200	0.51726100
C	3.37757100	0.33191600	-1.08394900
C	3.27860300	1.80905800	-1.19236200
C	1.35464500	4.07391800	-0.09725700
C	0.44494100	2.91617600	1.80906900
C	1.19915600	5.27391200	0.59413700
H	1.73833100	4.09233500	-1.10830800
C	0.31693600	4.13210900	2.46915200
H	0.12297500	1.99966300	2.28117700
C	0.68803300	5.33954400	1.88599500
N	1.57848100	6.53406000	-0.07542800
N	-0.24333500	4.14296500	3.83226100
H	0.57832400	6.28201800	2.40363600
O	1.44380500	7.57665100	0.56129200
O	2.00140100	6.45889400	-1.22728300
O	-0.57717100	3.06118800	4.32403700
O	-0.34554600	5.22623100	4.39942900
H	3.30810100	-0.11491100	-0.10462700
H	3.60525100	2.35360500	-0.30215600
S	5.94435200	0.13011100	-0.23008900
C	5.74498600	-1.52432100	0.34086700
C	6.16190900	-2.63252700	-0.43407700
C	5.15576000	-1.81488200	1.59522000
C	5.99846300	-3.94243000	0.01481800
H	6.63526400	-2.44100000	-1.39239200
C	4.98860600	-3.12642900	2.04054700
H	4.86132200	-0.98198600	2.22832700
C	5.40394100	-4.20517900	1.25337800
H	6.34858500	-4.76668100	-0.60323300
H	4.55237500	-3.30899500	3.02137400
H	5.28934300	-5.22599200	1.60733900
C	3.48090200	-0.55726500	-2.29852400
C	4.10419700	0.15758000	-3.50781400
H	2.47602000	-0.91623900	-2.54776700
C	3.51376700	1.55935900	-3.71591500
H	3.96075300	-0.45623600	-4.40475100
H	5.18387000	0.24395300	-3.33946000
C	3.77220100	2.44234300	-2.48659600
H	2.43367100	1.49108800	-3.89849600
H	3.95865300	2.03096600	-4.59970400
H	3.31452400	3.43190100	-2.61286400
H	4.85075000	2.60416300	-2.37264400
H	4.07160400	-1.43513100	-2.02586800

TS_{RR} conformation 3

Si	-3.97435300	0.73362400	-0.96583600
O	-3.34056800	-0.77216500	-1.39057100
N	-0.88830100	-1.87487200	0.34303400
N	0.05357100	-2.27638800	2.42298100
N	-2.09780400	-3.07774400	1.97150800
C	-2.04610200	-1.19274300	-1.77658600
C	-2.02543500	-1.78282300	-3.20729900

C	-0.89534600	-2.78281000	-3.15824900
C	-0.57634300	-3.09627600	-1.83096800
C	-1.51204300	-2.35452900	-0.88955400
C	-0.20595500	-3.38995200	-4.20620600
C	0.80113200	-4.31333100	-3.91142400
C	1.11737400	-4.62223600	-2.58488600
C	0.42765600	-4.01281700	-1.53263400
C	-0.98362100	-2.40891300	1.57050100
C	1.44198200	-1.94873700	1.98486900
C	2.21424600	-1.85483700	3.30315200
C	1.16435200	-1.31911400	4.28635500
C	-0.09512200	-2.09805500	3.88813900
C	-2.07496600	-4.24049800	2.88746000
C	-3.51600600	-4.76130000	2.82997700
C	-4.32897700	-3.47314700	2.63545700
C	-3.48970100	-2.69420500	1.61727400
C	-3.84798900	0.97073500	0.91522600
C	-2.58173200	1.22062400	1.48830000
C	-2.42584400	1.37504300	2.86827200
C	-3.53173500	1.27859500	3.71609000
C	-4.79339900	1.03060400	3.17542500
C	-4.94460700	0.88234300	1.79462300
C	-3.01048400	2.13613200	-1.78751000
C	-2.50193800	2.02103800	-3.09611500
C	-1.84237300	3.07998900	-3.72021800
C	-1.68345500	4.29419200	-3.05099600
C	-2.18682600	4.43932300	-1.75812500
C	-2.83698900	3.37239600	-1.13572100
C	-5.77245000	0.64509200	-1.63985600
C	-6.50079000	-0.61803300	-1.12780300
C	-6.56957800	1.91343800	-1.26383300
C	-5.70629100	0.55489100	-3.18219300
H	-0.24035300	-1.08142700	0.20850500
H	-1.32526500	-0.36794600	-1.71116900
H	-2.98858100	-2.27681500	-3.39409600
H	-1.89608100	-1.01673300	-3.97756900
H	-2.34916900	-3.00647100	-0.63366500
H	-0.44156500	-3.14622900	-5.23860300
H	1.34949500	-4.78882700	-4.71905600
H	1.90805000	-5.33470500	-2.37064000
H	0.68641400	-4.24738600	-0.50382500
H	1.44966800	-0.99043600	1.46062300
H	1.82698000	-2.72183500	1.31561200
H	2.56480800	-2.84645900	3.60523000
H	3.09401900	-1.21648800	3.20497400
H	1.01061000	-0.24372000	4.14714600
H	1.42584100	-1.48560200	5.33437400
H	-0.10627800	-3.06991900	4.39536000
H	-1.03003300	-1.57691900	4.10947800
H	-1.83226500	-3.94355100	3.91265700
H	-1.32760300	-4.96835400	2.55873200
H	-3.78376500	-5.31575800	3.73259900
H	-3.64870600	-5.42824600	1.97101000
H	-4.39851300	-2.91792100	3.57748600
H	-5.34401700	-3.65181500	2.27298100
H	-3.75188800	-3.00812700	0.60257700
H	-3.60818700	-1.61213400	1.67301000
H	-1.69891100	1.29739400	0.85817500
H	-1.44587600	1.59398200	3.28394300
H	-3.41089800	1.40926500	4.78791800
H	-5.66238200	0.96317600	3.82430300
H	-5.94049100	0.69988000	1.40616700
H	-2.62365100	1.09144100	-3.64418300
H	-1.45273600	2.95745500	-4.72675500
H	-1.17098000	5.12099100	-3.53431500
H	-2.06973900	5.38202300	-1.23091300
H	-3.20724500	3.50507600	-0.12329700
H	-6.63285300	-0.62507500	-0.04151800
H	-5.95548000	-1.52644300	-1.40227100
H	-7.50194800	-0.68121100	-1.57530500
H	-7.57186300	1.87468900	-1.71099100
H	-6.08143800	2.82088000	-1.63577800
H	-6.69870900	2.02839200	-0.18337000
H	-5.14753200	-0.32699500	-3.51254900
H	-5.24009000	1.43994400	-3.62519100
H	-6.72127600	0.47530000	-3.59394500
O	0.41308700	0.56274000	0.05171600
C	1.39109300	1.23193500	-0.38710500
N	2.04264900	0.95638100	-1.51832400
C	1.76729500	2.44937500	0.43029700
C	3.17749200	-0.40916900	-1.73760400
C	3.49575800	1.03836400	-1.65103500
C	2.39248100	3.57618300	-0.11491500
C	1.40885300	2.46559200	1.78298000
C	2.65481500	4.67560800	0.70000300
H	2.65570800	3.62023200	-1.16296600
C	1.70007600	3.57688700	2.56529900
H	0.89883800	1.61333400	2.20777200
C	2.32674300	4.70753900	2.05088000
N	3.29872000	5.86425800	0.10573500
N	1.32372400	3.56179100	3.99002500
H	2.54198900	5.57059700	2.66487900
O	3.52536600	6.81649000	0.84905800
O	3.56415100	5.82490900	-1.09384400
O	0.75947000	2.55345500	4.42422500
O	1.59325900	4.55176200	4.66295400
H	3.06713200	-0.96835200	-0.82186800
H	4.04485500	1.32970200	-0.75207500
S	5.64877900	-1.39432100	-1.30592700
C	5.22580500	-2.54339700	-0.03776700
C	4.34723800	-3.63024200	-0.26521800
C	5.77410500	-2.43475700	1.26308000
C	4.04721000	-4.55217700	0.73919600
H	3.92719100	-3.76066500	-1.25819300
C	5.48384000	-3.36350800	2.25996900
H	6.45380900	-1.61273000	1.46657300
C	4.61434300	-4.43204800	2.01173200
H	3.38793500	-5.39002000	0.51752800
H	5.94421500	-3.25656600	3.23988000
H	4.40244600	-5.16557600	2.78500600
C	2.88892400	-1.08349000	-3.05940700
C	3.58571000	-0.39389700	-4.24208300
H	1.80381500	-1.08975900	-3.21176200
C	3.42484800	1.13205500	-4.19665400
H	3.18556500	-0.79377400	-5.18122800
H	4.65247100	-0.64583800	-4.21271700
C	4.03726600	1.70334500	-2.91004200
H	2.36178400	1.39916400	-4.24824600
H	3.91234600	1.59076000	-5.06453000
H	3.88256800	2.78830800	-2.85252900
H	5.12154200	1.53864800	-2.91445300
H	3.21347300	-2.12257700	-2.98671100

TS_{RR} conformation 4

Si	-3.97435800	0.73361900	-0.96583000
O	-3.34056900	-0.77216800	-1.39056600
N	-0.88829600	-1.87487000	0.34303200
N	0.05357800	-2.27638900	2.42297800
N	-2.09779500	-3.07774800	1.97150600
C	-2.04610300	-1.19274200	-1.77658400
C	-2.02543800	-1.78281900	-3.20729800
C	-0.89534600	-2.78280400	-3.15825200
C	-0.57634000	-3.09627100	-1.83097100
C	-1.51203900	-2.35452700	-0.88955500
C	-0.20595500	-3.38994400	-4.20621100
C	0.80113300	-4.31332100	-3.91143100
C	1.11737800	-4.62222700	-2.58489400
C	0.42766200	-4.01281100	-1.53264100
C	-0.98361400	-2.40891400	1.57049900
C	1.44198900	-1.94873200	1.98486500
C	2.21425400	-1.85484000	3.30314800
C	1.16436100	-1.31912400	4.28635600
C	-0.09511300	-2.09806400	3.88813700
C	-2.07495300	-4.24050600	2.88745000
C	-3.51599000	-4.76131700	2.82995900
C	-4.32896800	-3.47316600	2.63545200
C	-3.48969400	-2.69420600	1.61728000
C	-3.84799100	0.97073200	0.91523200
C	-2.58173300	1.22062100	1.48830400

C	-2.42584300	1.37504200	2.86827400
C	-3.53173200	1.27859600	3.71609500
C	-4.79339800	1.03060500	3.17543200
C	-4.94460800	0.88234200	1.79463000
C	-3.01049700	2.13613100	-1.78750600
C	-2.50195300	2.02104000	-3.09611200
C	-1.84239400	3.07999400	-3.72021600
C	-1.68348000	4.29419700	-3.05099400
C	-2.18684900	4.43932500	-1.75812100
C	-2.83700600	3.37239600	-1.13571700
C	-5.77245600	0.64507900	-1.63984500
C	-6.50079200	-0.61804700	-1.12778900
C	-6.56958900	1.91342400	-1.26382400
C	-5.70630100	0.55487600	-3.18218300
H	-0.24034900	-1.08142500	0.20850300
H	-1.32526700	-0.36794300	-1.71116800
H	-2.98858200	-2.27681300	-3.39409400
H	-1.89608600	-1.01672900	-3.97756800
H	-2.34916300	-3.00647100	-0.63366500
H	-0.44156800	-3.14622000	-5.23860600
H	1.34949600	-4.78881600	-4.71906500
H	1.90805700	-5.33469500	-2.37065100
H	0.68642300	-4.24738100	-0.50383200
H	1.44967100	-0.99042700	1.46062700
H	1.82698700	-2.72182500	1.31560200
H	2.56481700	-2.84646400	3.60521900
H	3.09402700	-1.21649000	3.20497300
H	1.01061700	-0.24373000	4.14715300
H	1.42585100	-1.48561700	5.33437300
H	-0.10626700	-3.06993100	4.39535200
H	-1.03002400	-1.57693000	4.10947900
H	-1.83225800	-3.94356400	3.91265100
H	-1.32758500	-4.96835600	2.55872100
H	-3.78374800	-5.31578700	3.73257400
H	-3.64868400	-5.42825400	1.97098500
H	-4.39850900	-2.91795200	3.57748700
H	-5.34400600	-3.65183600	2.27297100
H	-3.75188200	-3.00811100	0.60257800
H	-3.60818200	-1.61213600	1.67303300
H	-1.69891300	1.29739000	0.85817600
H	-1.44587400	1.59398100	3.28394400
H	-3.41089300	1.40926800	4.78792200
H	-5.66238000	0.96317800	3.82431100
H	-5.94049200	0.69987800	1.40617600
H	-2.62366300	1.09144300	-3.64418000
H	-1.45275900	2.95746300	-4.72675400
H	-1.17101000	5.12099900	-3.53431400
H	-2.06976500	5.38202600	-1.23091000
H	-3.20726100	3.50507300	-0.12329200
H	-6.63285200	-0.62508700	-0.04150300
H	-5.95547900	-1.52645500	-1.40225700
H	-7.50195000	-0.68123000	-1.57528900
H	-7.57187400	1.87467000	-1.71097900
H	-6.08145300	2.82086700	-1.63577100
H	-6.69871900	2.02838000	-0.18336100
H	-5.14753900	-0.32700900	-3.51253800
H	-5.24010400	1.43993000	-3.62518400
H	-6.72128600	0.47528000	-3.59393200
O	0.41308700	0.56274200	0.05171100
C	1.39109300	1.23193800	-0.38710900
N	2.04265000	0.95638600	-1.51832700
C	1.76729400	2.44937700	0.43029600
C	3.17749500	-0.40916300	-1.73760700
C	3.49575900	1.03837000	-1.65103600
C	2.39247800	3.57618700	-0.11491600
C	1.40885400	2.46559200	1.78297800
C	2.65481100	4.67561100	0.70000400
H	2.65570300	3.62023700	-1.16296700
C	1.70007600	3.57688600	2.56529900
H	0.89883900	1.61333300	2.20776900
C	2.32674100	4.70754000	2.05088100
N	3.29871400	5.86426300	0.10573700
N	1.32372600	3.56178800	3.99002600
H	2.54198600	5.57059700	2.66488100
O	3.52536000	6.81649400	0.84906100
O	3.56414500	5.82491500	-1.09384300
O	0.75947500	2.55344900	4.42422500
O	1.59326000	4.55175800	4.66295600
H	3.06713400	-0.96834700	-0.82187100
H	4.04485500	1.32970800	-0.75207600
S	5.64878300	-1.39431200	-1.30592500
C	5.22580700	-2.54339200	-0.03776800
C	4.34723800	-3.63023500	-0.26522200
C	5.77410900	-2.43475800	1.26307900
C	4.04721000	-4.55217200	0.73918900
H	3.92719000	-3.76065300	-1.25819700
C	5.48384300	-3.36351200	2.25996400
H	6.45381500	-1.61273200	1.46657400
C	4.61434400	-4.43204900	2.01172500
H	3.38793300	-5.39001300	0.51751800
H	5.94422000	-3.25657400	3.23987500
H	4.40244700	-5.16557900	2.78499500
C	2.88892900	-1.08348300	-3.05941000
C	3.58571700	-0.39388900	-4.24208500
H	1.80382000	-1.08975400	-3.21176700
C	3.42485200	1.13206300	-4.19665500
H	3.18557300	-0.79376600	-5.18123000
H	4.65247800	-0.64582800	-4.21271800
C	4.03726800	1.70335300	-2.91004200
H	2.36178800	1.39917000	-4.24824800
H	3.91235100	1.59076900	-5.06453000
H	3.88256900	2.78831500	-2.85252800
H	5.12154400	1.53865700	-2.91445100
H	3.21348000	-2.12257000	-2.98671400

TS_{RR} conformation 5

Si	-3.74357900	-0.18128800	-1.49586400
O	-2.79016200	-1.56452700	-1.65635100
N	-0.52829100	-1.97544000	0.55357000
N	0.10102500	-2.00529900	2.78501100
N	-1.71394500	-3.30730300	2.09898500
C	-1.39483100	-1.74773700	-1.79161500
C	-1.02041900	-2.45881100	-3.11368800
C	0.28192700	-3.14416600	-2.77589200
C	0.43045200	-3.24962300	-1.38674800
C	-0.80002200	-2.67999500	-0.69872500
C	1.26700300	-3.64517800	-3.62425200
C	2.40095200	-4.24448500	-3.06742000
C	2.55006000	-4.33952500	-1.68046600
C	1.55817400	-3.84403900	-0.82936100
C	-0.71945500	-2.42916200	1.80001200
C	1.43634200	-1.39249200	2.53379900
C	1.93043300	-1.03993200	3.94010400
C	0.63386300	-0.69839700	4.68927800
C	-0.33956900	-1.76915900	4.18125300
C	-1.57816700	-4.38772900	3.10062900
C	-2.79996600	-5.26985200	2.82338600
C	-3.86385100	-4.24089700	2.41453600
C	-3.08309300	-3.27229800	1.51735300
C	-4.05436400	0.16320700	0.34753800
C	-3.00514900	0.69733800	1.12710000
C	-3.16781300	0.95156900	2.49150400
C	-4.38370700	0.67071900	3.11898300
C	-5.43487500	0.13791700	2.37253900
C	-5.26935700	-0.10679200	1.00700400
C	-2.87602400	1.33295700	-2.22386800
C	-2.07168300	1.25024500	-3.37743400
C	-1.47498900	2.38085200	-3.93586200
C	-1.67996000	3.63501300	-3.35915000
C	-2.48301600	3.74795900	-2.22394800
C	-3.06783000	2.61093800	-1.66384200
C	-5.32412800	-0.61761300	-2.49790800
C	-5.91723400	-1.97169500	-2.04821400
C	-6.38128300	0.50090300	-2.37209600
C	-4.93226800	-0.74938400	-3.98823500
H	-0.05219000	-1.06506000	0.43501800
H	-0.86242200	-0.79009800	-1.73098900
H	-1.80855600	-3.18561600	-3.35413200
H	-0.94499700	-1.76800200	-3.95876600

H	-1.51022300	-3.48641600	-0.50624000
H	1.16352000	-3.56208600	-4.70284300
H	3.18176000	-4.62661100	-3.71826200
H	3.44920000	-4.77408000	-1.25666300
H	1.68520800	-3.91293300	0.24737000
H	1.32490400	-0.49262600	1.92399000
H	2.08783600	-2.09372900	2.00674000
H	2.42183500	-1.90368800	4.40135500
H	2.64901300	-0.21800300	3.92055400
H	0.28136000	0.30174000	4.41582700
H	0.73947400	-0.73014200	5.77643400
H	-0.23634400	-2.68286400	4.77833000
H	-1.38740400	-1.45891200	4.19662500
H	-1.62630100	-4.00140200	4.12478100
H	-0.62100700	-4.90146000	2.97531200
H	-3.08036800	-5.86513500	3.69570500
H	-2.59396300	-5.95642400	1.99498100
H	-4.24568000	-3.71800900	3.29831000
H	-4.71503200	-4.68159200	1.89038900
H	-3.09406800	-3.62347400	0.48197300
H	-3.47068300	-2.25304000	1.52773000
H	-2.04381000	0.92174300	0.67162100
H	-2.35467200	1.39350100	3.06167800
H	-4.51376400	0.87857700	4.17747400
H	-6.38825600	-0.07667000	2.84764000
H	-6.11162100	-0.51033700	0.45577600
H	-1.90548200	0.28908700	-3.85465500
H	-0.85113100	2.28295200	-4.81965200
H	-1.21796400	4.51742000	-3.79247600
H	-2.65209000	4.72105300	-1.77128600
H	-3.67661000	2.72271600	-0.77133800
H	-6.25790300	-1.96586300	-1.00831800
H	-5.18439500	-2.77778300	-2.15207100
H	-6.78529400	-2.22728200	-2.67100000
H	-7.25147200	0.27028000	-3.00110500
H	-5.98588000	1.46713900	-2.70384100
H	-6.74317900	0.62785700	-1.34735700
H	-4.18237200	-1.53244000	-4.14233900
H	-4.53608000	0.18662700	-4.39318100
H	-5.81576100	-1.01819800	-4.58254400
O	0.23642100	0.66019000	0.25166300
C	1.05413400	1.52791100	-0.16996700
N	1.89905000	1.32827800	-1.18224000
C	0.98161500	2.87361600	0.51720400
C	3.37753200	0.33184900	-1.08389300
C	3.27860100	1.80898700	-1.19239000
C	1.35474600	4.07395200	-0.09733400
C	0.44495100	2.91629800	1.80900100
C	1.19930500	5.27396800	0.59403000
H	1.73845200	4.09232700	-1.10837900
C	0.31699100	4.13225200	2.46905400
H	0.12293800	1.99980900	2.28112600
C	0.68816200	5.33965500	1.88587800
N	1.57871100	6.53408100	-0.07555500
N	-0.24330600	4.14316500	3.83215100
H	0.57848900	6.28214600	2.40349700
O	1.44405800	7.57669500	0.56113300
O	2.00167000	6.45886600	-1.22739100
O	-0.57718400	3.06141300	4.32395500
O	-0.34550000	5.22645200	4.39928400
H	3.30800600	-0.11492100	-0.10454900
H	3.60526300	2.35357300	-0.30221300
S	5.94428200	0.13012100	-0.22990500
C	5.74506800	-1.52443200	0.34075600
C	6.16219500	-2.63245000	-0.43434700
C	5.15572700	-1.81528600	1.59498400
C	5.99879600	-3.94245500	0.01426900
H	6.63564900	-2.44069500	-1.39256800
C	4.98860300	-3.12693100	2.04002600
H	4.86114900	-0.98253400	2.22821300
C	5.40412400	-4.20549500	1.25269600
H	6.34906200	-4.76655600	-0.60390000
H	4.55223700	-3.30971500	3.02075400
H	5.28955200	-5.22638700	1.60643700
C	3.48085700	-0.55740000	-2.29842100
C	4.10419600	0.15736400	-3.50773500
H	2.47596400	-0.91634700	-2.54765900
C	3.51379500	1.55914100	-3.71593000
H	3.96076900	-0.45650300	-4.40464000
H	5.18386600	0.24373300	-3.33935700
C	3.77222600	2.44218900	-2.48665600
H	2.43370100	1.49088000	-3.89852800
H	3.95870600	2.03068900	-4.59973700
H	3.31456700	3.43174700	-2.61298300
H	4.85077800	2.60399100	-2.37269800
H	4.07152000	-1.43528300	-2.02572500

TS_{RR} conformation 6

Si	-3.74360700	-0.18135000	-1.49582500
O	-2.79015900	-1.56456500	-1.65632700
N	-0.52823500	-1.97544300	0.55355100
N	0.10111800	-2.00529400	2.78498300
N	-1.71384200	-3.30732700	2.09898500
C	-1.39482600	-1.74774200	-1.79161500
C	-1.02041900	-2.45879400	-3.11370100
C	0.28194200	-3.14413300	-2.77593100
C	0.43049100	-3.24960200	-1.38679100
C	-0.79997900	-2.67999700	-0.69874100
C	1.26701000	-3.64512600	-3.62431100
C	2.40097400	-4.24442700	-3.06750300
C	2.55010400	-4.33948000	-1.68055300
C	1.55822700	-3.84401200	-0.82942700
C	-0.71937000	-2.42917100	1.79999600
C	1.43642100	-1.39246400	2.53375100
C	1.93052100	-1.03987900	3.94004700
C	0.63395200	-0.69837300	4.68923700
C	-0.33946000	-1.76916300	4.18123100
C	-1.57803500	-4.38775300	3.10062500
C	-2.79983400	-5.26988400	2.82340900
C	-3.86373300	-4.24093700	2.41457800
C	-3.08300100	-3.27233800	1.51737600
C	-4.05437400	0.16313500	0.34758200
C	-3.00516100	0.69729100	1.12713000
C	-3.16781400	0.95151600	2.49153700
C	-4.38369100	0.67063300	3.11903200
C	-5.43485600	0.13780600	2.37260200
C	-5.26935100	-0.10689600	1.00706400
C	-2.87609900	1.33291800	-2.22383700
C	-2.07176900	1.25022800	-3.37741300
C	-1.47510400	2.38085000	-3.93584300
C	-1.68009700	3.63500400	-3.35912400
C	-2.48314400	3.74792900	-2.22391400
C	-3.06792700	2.61089400	-1.66380600
C	-5.32415900	-0.61771000	-2.49784900
C	-5.91722800	-1.97180700	-2.04815000
C	-6.38133800	0.50078100	-2.37202200
C	-4.93231400	-0.74947100	-3.98818100
H	-0.05215700	-1.06505100	0.43499300
H	-0.86243900	-0.79009000	-1.73098700
H	-1.80854600	-3.18560800	-3.35414500
H	-0.94501700	-1.76797200	-3.95877100
H	-1.51016400	-3.48643000	-0.50624700
H	1.16350900	-3.56202400	-4.70290000
H	3.18177600	-4.62654000	-3.71836200
H	3.44925400	-4.77403400	-1.25676900
H	1.68527900	-3.91291500	0.24730100
H	1.32495800	-0.49260500	1.92393500
H	2.08792500	-2.09369300	2.00669300
H	2.42195200	-1.90361800	4.40129800
H	2.64907800	-0.21793200	3.92048100
H	0.28141900	0.30175300	4.41578500
H	0.73957800	-0.73010900	5.77639100
H	-0.23619900	-2.68286400	4.77830900
H	-1.38730300	-1.45894500	4.19662000
H	-1.62614700	-4.00142600	4.12477800
H	-0.62087400	-4.90147800	2.97528500
H	-3.08021400	-5.86516600	3.69573700
H	-2.59384300	-5.95645800	1.99500300
H	-4.24554700	-3.71804800	3.29835800

H	-4.71492300	-4.68164100	1.89045100
H	-3.09399000	-3.62352100	0.48199800
H	-3.47060000	-2.25308300	1.52775200
H	-2.04383500	0.92172200	0.67163700
H	-2.35467600	1.39346700	3.06170000
H	-4.51374000	0.87848600	4.17752500
H	-6.38822500	-0.07680700	2.84771500
H	-6.11161300	-0.51046200	0.45584700
H	-1.90555100	0.28907500	-3.85463800
H	-0.85125400	2.28296500	-4.81963900
H	-1.21812400	4.51742200	-3.79245300
H	-2.65223400	4.72101800	-1.77124800
H	-3.67670200	2.72265600	-0.77129600
H	-6.25788900	-1.96598200	-1.00825000
H	-5.18437300	-2.77787800	-2.15201200
H	-6.78528800	-2.22741300	-2.67092700
H	-7.25153000	0.27013700	-3.00102000
H	-5.98596200	1.46702600	-2.70377300
H	-6.74322300	0.62772600	-1.34727800
H	-4.18240400	-1.53251100	-4.14229400
H	-4.53615200	0.18654900	-4.39313100
H	-5.81581000	-1.01830300	-4.58248000
O	0.23639900	0.66020300	0.25162900
C	1.05410800	1.52793300	-0.16999200
N	1.89903500	1.32830800	-1.18225800
C	0.98157100	2.87363700	0.51717900
C	3.37752800	0.33189700	-1.08389400
C	3.27858100	1.80903300	-1.19239400
C	1.35468800	4.07397600	-0.09735800
C	0.44490700	2.91631100	1.80897600
C	1.19923100	5.27399100	0.59400500
H	1.73839500	4.09235600	-1.10840300
C	0.31693200	4.13226300	2.46902900
H	0.12290600	1.99981800	2.28110100
C	0.68808700	5.33967200	1.88585300
N	1.57862100	6.53410900	-0.07558000
N	-0.24336300	4.14317000	3.83212700
H	0.57840200	6.28216100	2.40347100
O	1.44395300	7.57672100	0.56110800
O	2.00158300	6.45889900	-1.22741500
O	-0.57721800	3.06141200	4.32393500
O	-0.34557600	5.22645600	4.39925700
H	3.30799900	-0.11487300	-0.10455000
H	3.60522700	2.35362400	-0.30221300
S	5.94426800	0.13019500	-0.22987100
C	5.74507700	-1.52436800	0.34077200
C	6.16223100	-2.63237000	-0.43433800
C	5.15572900	-1.81524400	1.59499100
C	5.99885400	-3.94238300	0.01426400
H	6.63568800	-2.44059700	-1.39255300
C	4.98862800	-3.12689700	2.04002100
H	4.86112900	-0.98250500	2.22822600
C	5.40417800	-4.20544600	1.25268500
H	6.34914100	-4.76647100	-0.60390900
H	4.55225700	-3.30969900	3.02074300
H	5.28962300	-5.22634300	1.60641600
C	3.48087800	-0.55735200	-2.29842000
C	4.10422500	0.15741800	-3.50772600
H	2.47599200	-0.91631100	-2.54767100
C	3.51380800	1.55918700	-3.71593100
H	3.96081800	-0.45645200	-4.40463200
H	5.18389200	0.24380100	-3.33933300
C	3.77221300	2.44224000	-2.48665400
H	2.43371800	1.49091200	-3.89854200
H	3.95872500	2.03074000	-4.59973300
H	3.31454100	3.43179200	-2.61298800
H	4.85076000	2.60405900	-2.37268400
H	4.07154700	-1.43522800	-2.02571500

TS_{RR} conformation 7

Si	4.00133200	-1.44185200	-0.33488500
O	3.06345000	-1.54213000	1.06683100
N	-0.04291800	-1.94693400	0.47811800
N	-1.43740200	-3.37829100	-0.70583100
N	0.07445100	-4.27678900	0.83039800
C	1.95661000	-0.72948600	1.42901700
C	2.17592100	0.03661400	2.75163100
C	0.76023300	0.31102600	3.20332900
C	-0.12891200	-0.57991200	2.58652500
C	0.65272300	-1.53298500	1.69902400
C	0.28126900	1.27931700	4.08239800
C	-1.09308400	1.33869000	4.33822600
C	-1.97397900	0.44328600	3.72385300
C	-1.49576400	-0.53125900	2.84095800
C	-0.46715900	-3.19120500	0.19740500
C	-2.24597900	-2.27714900	-1.28539100
C	-3.16089800	-2.99270900	-2.28293700
C	-2.31955600	-4.19116300	-2.74430900
C	-1.63940700	-4.64361900	-1.44832400
C	-0.74104800	-5.36246600	1.41154500
C	0.25344300	-6.04736000	2.35374300
C	1.57021500	-5.96187900	1.56603200
C	1.52968100	-4.56264700	0.92667300
C	2.97110600	-1.99683600	-1.83485300
C	1.95534800	-1.14186200	-2.31349400
C	1.15183700	-1.49788300	-3.39824800
C	1.34137100	-2.72406800	-4.03967400
C	2.33532500	-3.59086200	-3.58428400
C	3.13630400	-3.22739200	-2.49838600
C	4.54459600	0.33912500	-0.65856100
C	4.87282400	1.21241100	0.39676300
C	5.35018600	2.50198400	0.15632600
C	5.51800200	2.94898000	-1.15529000
C	5.20627400	2.10209100	-2.21980300
C	4.72346700	0.81617700	-1.97208700
C	5.53257800	-2.53255000	0.06432700
C	5.14464800	-3.96161500	0.50163500
C	6.47498600	-2.59438000	-1.15845500
C	6.29547500	-1.87551500	1.23862800
H	-0.35191600	-1.17158400	-0.10851500
H	1.71990400	-0.00672300	0.63821500
H	2.70376300	-0.62290500	3.45517900
H	2.77770900	0.93813400	2.62416600
H	0.89473000	-2.43719700	2.26107000
H	0.96216900	1.98593800	4.54865200
H	-1.48060600	2.09481500	5.01512600
H	-3.04198300	0.50254200	3.90774200
H	-2.20014100	-1.20348000	2.35859100
H	-1.57810500	-1.57902800	-1.80409400
H	-2.81744100	-1.75552400	-0.50539900
H	-4.06971600	-3.32625100	-1.77112900
H	-3.46062900	-2.33436400	-3.10118400
H	-1.56254600	-3.87257100	-3.46913300
H	-2.90961200	-4.99354000	-3.19426200
H	-2.30226800	-5.30923800	-0.88413500
H	-0.68321200	-5.14922000	-1.60172900
H	-1.08867000	-6.07673200	0.65423300
H	-1.61700400	-4.94764900	1.91725200
H	-0.04241100	-7.07258000	2.58940200
H	0.32864300	-5.48985800	3.29351800
H	1.59097800	-6.73469500	0.78969300
H	2.45629100	-6.09533800	2.19094600
H	2.05184900	-3.82449100	1.53786200
H	1.98350700	-4.53783700	-0.06804400
H	1.78181100	-0.17722000	-1.84423900
H	0.38821100	-0.80907400	-3.74876500
H	0.72965000	-2.99472400	-4.89607200
H	2.49885900	-4.54296900	-4.08171500
H	3.91070100	-3.91738200	-2.17981800
H	4.75561200	0.88628200	1.42550500
H	5.57556300	3.15853000	0.99110700
H	5.88804300	3.95245400	-1.34504100
H	5.33379100	2.44356800	-3.24325000
H	4.47696700	0.17874000	-2.81649600
H	4.60442000	-4.51497600	-0.27289600
H	4.52228200	-3.94557300	1.40167100
H	6.04962700	-4.53785600	0.73702100
H	7.38572600	-3.15201100	-0.90271500
H	6.78384000	-1.59452300	-1.48121100

H	6.01782000	-3.09318600	-2.01900600
H	5.66778400	-1.79327400	2.13181600
H	6.65682200	-0.87508700	0.98446200
H	7.17010800	-2.48550200	1.50155700
O	-0.33129800	1.00739400	-0.54343300
C	-0.85821100	2.13233200	-0.68768800
N	-2.12006300	2.42200700	-1.11283600
C	-0.05837300	3.37339600	-0.36929000
C	-3.34685000	1.67581000	-0.00338600
C	-2.99467200	1.27744600	-1.37257800
C	1.06016100	3.28926400	0.46510700
C	-0.42744000	4.61806300	-0.89668400
C	1.78979900	4.44241000	0.74679600
H	1.34619600	2.34044900	0.89561400
C	0.34323900	5.73955900	-0.60549300
H	-1.30348600	4.69899800	-1.52552600
C	1.46616200	5.68439800	0.21229300
N	2.95086100	4.35715100	1.64472300
N	-0.04019300	7.04297600	-1.18269100
H	2.05370400	6.56595600	0.42628800
O	3.73698500	5.30234100	1.65596600
O	3.07256500	3.34166100	2.33134000
O	-1.02309300	7.07140400	-1.91936300
O	0.65070200	8.01741400	-0.88941700
H	-2.75986300	1.26682000	0.80599000
H	-2.47245200	0.32893900	-1.45905300
S	-4.59399500	-0.71839900	1.01080700
C	-6.31672500	-0.89093900	0.64186200
C	-6.77580500	-1.38947500	-0.59711500
C	-7.29941300	-0.53177400	1.59027600
C	-8.13642600	-1.52159100	-0.87106900
H	-6.04440200	-1.67391800	-1.34874700
C	-8.65903500	-0.66653600	1.31543800
H	-6.97454000	-0.14873700	2.55298900
C	-9.09156900	-1.16204300	0.08264300
H	-8.45312400	-1.90910900	-1.83703500
H	-9.38750000	-0.38146800	2.07114200
H	-10.15166600	-1.26530100	-0.13066800
C	-4.02929500	1.50966900	-2.46533100
C	-4.90679700	2.74424000	-2.20788700
C	-5.52443100	2.69354800	-0.80343700
H	-5.69765000	2.79205400	-2.96515600
H	-4.30244600	3.65239400	-2.31909200
C	-4.44937900	2.65510200	0.29615900
H	-4.66407700	0.61548800	-2.50609100
H	-3.51505600	1.59202500	-3.43087900
H	-4.89105700	2.37380900	1.25556800
H	-4.00040600	3.64870100	0.42353300
H	-6.14936900	1.79792700	-0.71411700
H	-6.17757300	3.55825700	-0.64110900

TS_{SS} conformation 1

Si	3.54146500	2.06348400	-0.04703100
O	3.12175700	1.08791100	1.26784700
N	1.85091500	-1.79233600	0.60676800
N	2.14192500	-3.74469300	-0.60277800
N	3.94022200	-2.89438300	0.61816800
C	1.86232300	0.52727600	1.59869500
C	1.27826800	1.08842300	2.91559000
C	0.40038400	-0.03925500	3.40215200
C	0.75974300	-1.24332300	2.78389000
C	1.93115900	-1.01040900	1.84348700
C	-0.64464400	-0.01065100	4.32384600
C	-1.31881700	-1.19850200	4.62164300
C	-0.95418600	-2.40010200	4.00499700
C	0.09327600	-2.42915300	3.08016100
C	2.64541200	-2.79441800	0.21450700
C	0.68192900	-3.96921900	-0.79270400
C	0.63105300	-5.06597800	-1.86122100
C	1.86962100	-4.76552700	-2.71781600
C	2.92810600	-4.40990200	-1.66765700
C	4.59946100	-4.18312000	0.92095500
C	5.85003600	-3.75096400	1.69239900
C	6.23770800	-2.44568500	0.98239200
C	4.88752900	-1.75362700	0.74527600
C	3.66324400	0.98597300	-1.60966900
C	2.48947400	0.36781500	-2.09136800
C	2.51038700	-0.46903500	-3.20853900
C	3.70913100	-0.71030400	-3.88324200
C	4.88401500	-0.10843000	-3.43103000
C	4.85654400	0.72662200	-2.31096300
C	2.22103000	3.37721700	-0.35639500
C	1.59357800	4.05323800	0.70931100
C	0.65866400	5.06391800	0.48330500
C	0.33187800	5.43037500	-0.82388700
C	0.94489100	4.78296100	-1.89743900
C	1.87403300	3.76746000	-1.66429300
C	5.19541200	2.85981500	0.51836300
C	6.24450800	1.78748800	0.88699600
C	5.75593000	3.79617100	-0.57573300
C	4.92344200	3.70719400	1.78335300
H	0.99426800	-1.60969300	0.06046100
H	1.13458300	0.68820100	0.79447600
H	2.10384400	1.28429500	3.61371100
H	0.73489700	2.02448300	2.76643600
H	2.86793600	-1.25542100	2.34954700
H	-0.94161400	0.92264200	4.79324400
H	-2.14387600	-1.18732700	5.32698300
H	-1.49877200	-3.31017700	4.23604000
H	0.37017200	-3.36187600	2.59564300
H	0.18252400	-3.06075500	-1.14162400
H	0.22830100	-4.26106800	0.15830700
H	0.71755300	-6.05823900	-1.40426900
H	-0.30344600	-5.03259100	-2.42424100
H	1.68170100	-3.90311000	-3.36603400
H	2.18086700	-5.60408800	-3.34555800
H	3.40282200	-5.32221000	-1.28740300
H	3.70703000	-3.73805800	-2.03650000
H	4.89317900	-4.71706600	0.00923000
H	3.92494800	-4.82772800	1.49105900
H	6.63361300	-4.51185500	1.66229500
H	5.60177400	-3.55792600	2.74167000
H	6.72550700	-2.66878100	0.02700500
H	6.91608100	-1.81950000	1.56620800
H	4.63035300	-1.10226300	1.58230300
H	4.86401000	-1.14870500	-0.16271400
H	1.53503400	0.52859100	-1.59796800
H	1.58411200	-0.91970700	-3.55430000
H	3.72560200	-1.35001100	-4.76150400
H	5.82095000	-0.27937200	-3.95409400
H	5.78671600	1.18409100	-1.99105900
H	1.83397300	3.78839100	1.73442400
H	0.17408400	5.55310500	1.32273400
H	-0.39883900	6.21394300	-1.00140300
H	0.69521400	5.06340600	-2.91687400
H	2.32807500	3.26698300	-2.51474200
H	6.51397800	1.14506300	0.04249700
H	5.88444000	1.14546600	1.69739400
H	7.16820200	2.27000900	1.23404900
H	6.66802700	4.28971000	-0.21483200
H	5.04036200	4.58276200	-0.83730000
H	6.01615200	3.26755100	-1.49798600
H	4.51147000	3.10198400	2.59712300
H	4.22861100	4.52805700	1.58288900
H	5.86184300	4.15167600	2.14078900
O	-0.37276900	-0.77958800	-0.68321900
C	-1.58628900	-0.70093500	-1.00908100
N	-2.33064100	-1.75713800	-1.38097200
C	-2.18357700	0.68769500	-1.01514000
C	-3.79164200	-1.75737200	-1.20106800
C	-3.25549900	-2.71204500	-0.21387500
C	-1.95853200	1.51787600	0.08812000
C	-2.92055900	1.17303200	-2.09889500
C	-2.48034100	2.80719900	0.09034400
H	-1.40472800	1.15886700	0.94432500
C	-3.40152100	2.48073000	-2.06605300
H	-3.11666900	0.55760100	-2.96775700
C	-3.20427500	3.32262500	-0.97842900
N	-2.24290000	3.66932200	1.25777200

N	-4.14701800	2.99518800	-3.22877300
H	-3.59510900	4.32984000	-0.96602500
O	-2.66723800	4.82233100	1.21398500
O	-1.61779800	3.19282000	2.20636800
O	-4.29939000	2.23759600	-4.18600800
O	-4.56376100	4.15055100	-3.17147900
H	-4.21367100	-0.85587600	-0.75788100
H	-2.98431800	-2.34301200	0.76337300
S	-5.54693800	-2.80099700	1.38852000
C	-5.55657300	-1.05777500	1.65825900
C	-6.53839500	-0.22128900	1.07461100
C	-4.57365500	-0.41992500	2.45262300
C	-6.53862700	1.15721900	1.27799000
H	-7.30939700	-0.68135900	0.46346300
C	-4.57423400	0.96105300	2.65252700
H	-3.81624400	-1.03406900	2.93164900
C	-5.55608900	1.76502100	2.06732600
H	-7.31562900	1.76443900	0.81840200
H	-3.80155000	1.41197000	3.27189100
H	-5.56414700	2.83916200	2.23168900
C	-3.10972700	-4.18043300	-0.51643200
C	-3.48483700	-4.53216800	-1.96412100
C	-4.78279500	-3.82043700	-2.36719500
H	-3.59579700	-5.61887100	-2.05512200
H	-2.67631100	-4.22994100	-2.64254700
C	-4.60839100	-2.29169200	-2.38414100
H	-3.77160500	-4.70661700	0.17748300
H	-2.08959700	-4.50654400	-0.28041200
H	-5.59227800	-1.81336800	-2.37191600
H	-4.10908500	-1.97932500	-3.30989100
H	-5.56584600	-4.07703700	-1.64461100
H	-5.12146800	-4.16258000	-3.35173100

TS_{SS} conformation 2

Si	3.54146100	2.06349000	-0.04703000
O	3.12175400	1.08791400	1.26784600
N	1.85091700	-1.79233500	0.60676700
N	2.14192900	-3.74469400	-0.60277500
N	3.94022600	-2.89438000	0.61816900
C	1.86232000	0.52727700	1.59869400
C	1.27826300	1.08842400	2.91558700
C	0.40038100	-0.03925600	3.40214900
C	0.75974300	-1.24332300	2.78388900
C	1.93115900	-1.01040800	1.84348600
C	-0.64464900	-0.01065300	4.32384000
C	-1.31882000	-1.19850600	4.62163800
C	-0.95418500	-2.40010600	4.00499300
C	0.09327800	-2.42915500	3.08015900
C	2.64541500	-2.79441700	0.21450800
C	0.68193300	-3.96922300	-0.79270100
C	0.63105900	-5.06598400	-1.86121500
C	1.86962600	-4.76553400	-2.71781100
C	2.92811000	-4.40990500	-1.66765200
C	4.59946500	-4.18311600	0.92095900
C	5.85003700	-3.75095600	1.69240600
C	6.23771000	-2.44567800	0.98239700
C	4.88753200	-1.75362200	0.74527300
C	3.66324600	0.98598000	-1.60966900
C	2.48947900	0.36781800	-2.09137000
C	2.51039600	-0.46903200	-3.20854200
C	3.70914200	-0.71029800	-3.88324100
C	4.88402400	-0.10842100	-3.43102700
C	4.85654800	0.72663100	-2.31096100
C	2.22102200	3.37721900	-0.35639700
C	1.59356700	4.05323800	0.70930900
C	0.65864900	5.06391500	0.48330200
C	0.33186400	5.43037000	-0.82389100
C	0.94488000	4.78295800	-1.89744200
C	1.87402600	3.76746000	-1.66429500
C	5.19540500	2.85982500	0.51836700
C	6.24450300	1.78750000	0.88700200
C	5.75592300	3.79618200	-0.57572700
C	4.92343100	3.70720300	1.78335700
H	0.99427000	-1.60969400	0.06045900
H	1.13458100	0.68820100	0.79447300
H	2.10383700	1.28429800	3.61371000
H	0.73489000	2.02448300	2.76643200
H	2.86793700	-1.25541800	2.34954600
H	-0.94162300	0.92263900	4.79323700
H	-2.14388000	-1.18733200	5.32697600
H	-1.49876900	-3.31018200	4.23603600
H	0.37017800	-3.36187800	2.59564200
H	0.18252700	-3.06076000	-1.14162200
H	0.22830600	-4.26107000	0.15831200
H	0.71755900	-6.05824400	-1.40426100
H	-0.30344100	-5.03259900	-2.42423500
H	1.68170500	-3.90311800	-3.36603100
H	2.18087300	-5.60409600	-3.34555100
H	3.40282800	-5.32221200	-1.28739600
H	3.70703500	-3.73806200	-2.03649600
H	4.89318800	-4.71706100	0.00923500
H	3.92495200	-4.82772400	1.49106100
H	6.63361500	-4.51184600	1.66230700
H	5.60177100	-3.55791600	2.74167600
H	6.72551400	-2.66877700	0.02701300
H	6.91608000	-1.81949100	1.56621500
H	4.63035200	-1.10225400	1.58229600
H	4.86401500	-1.14870600	-0.16272100
H	1.53503700	0.52859200	-1.59797200
H	1.58412300	-0.91970700	-3.55430300
H	3.72561700	-1.35000500	-4.76150400
H	5.82096100	-0.27936000	-3.95408900
H	5.78671900	1.18410300	-1.99105400
H	1.83396100	3.78839300	1.73442300
H	0.17406700	5.55310000	1.32273000
H	-0.39885600	6.21393500	-1.00140800
H	0.69520300	5.06340200	-2.91687700
H	2.32807000	3.26698400	-2.51474300
H	6.51397500	1.14507500	0.04250400
H	5.88443300	1.14547700	1.69740000
H	7.16819500	2.27002200	1.23405700
H	6.66801800	4.28972500	-0.21482400
H	5.04035400	4.58277000	-0.83729800
H	6.01615200	3.26756200	-1.49797900
H	4.51145700	3.10199200	2.59712500
H	4.22859900	4.52806500	1.58289100
H	5.86183000	4.15168600	2.14079600
O	-0.37276700	-0.77959700	-0.68323100
C	-1.58628800	-0.70094300	-1.00909000
N	-2.33064000	-1.75714500	-1.38098000
C	-2.18357500	0.68768800	-1.01514600
C	-3.79164200	-1.75737700	-1.20107500
C	-3.25549900	-2.71204700	-0.21387800
C	-1.95853400	1.51786500	0.08811900
C	-2.92055300	1.17302900	-2.09890100
C	-2.48034400	2.80718800	0.09034600
H	-1.40473300	1.15885300	0.94432400
C	-3.40151700	2.48072600	-2.06605600
H	-3.11666000	0.55760100	-2.96776600
C	-3.20427500	3.32261700	-0.97842800
N	-2.24290800	3.66930600	1.25777800
N	-4.14700900	2.99518900	-3.22877600
H	-3.59511000	4.32983100	-0.96602100
O	-2.66725300	4.82231300	1.21399600
O	-1.61780300	3.19280300	2.20637100
O	-4.29937500	2.23760000	-4.18601600
O	-4.56375500	4.15055000	-3.17147900
H	-4.21367000	-0.85587900	-0.75789100
H	-2.98431600	-2.34301000	0.76336700
S	-5.54693600	-2.80098900	1.38852200
C	-5.55656800	-1.05776700	1.65826000
C	-6.53838700	-0.22127900	1.07460900
C	-4.57365300	-0.41991800	2.45262700
C	-6.53861900	1.15722800	1.27798700
H	-7.30938900	-0.68134900	0.46345900
C	-4.57423000	0.96106100	2.65253100
H	-3.81624300	-1.03406200	2.93165600
C	-5.55608300	1.76502900	2.06732700
H	-7.31561900	1.76444800	0.81839700
H	-3.80154800	1.41197700	3.27189700

H	-5.56414000	2.83917000	2.23168900
C	-3.10972900	-4.18043600	-0.51643000
C	-3.48484000	-4.53217600	-1.96411800
C	-4.78279800	-3.82044500	-2.36719300
H	-3.59580200	-5.61888000	-2.05511300
H	-2.67631400	-4.22995300	-2.64254500
C	-4.60839200	-2.29170000	-2.38414600
H	-3.77160600	-4.70661600	0.17748800
H	-2.08959800	-4.50654700	-0.28041000
H	-5.59227800	-1.81337500	-2.37192200
H	-4.10908600	-1.97933800	-3.30989700
H	-5.56584800	-4.07704100	-1.64460700
H	-5.12147200	-4.16259200	-3.35172700

TS_{SS} conformation 3

Si	-4.33239300	0.03530800	-0.29933700
O	-3.31745100	-0.71043500	-1.42951100
N	-0.71746100	-2.09790100	-0.15306200
N	-0.00793200	-3.60852000	1.45112500
N	-1.75432300	-4.21241300	0.02539600
C	-1.93572300	-0.46187800	-1.63752200
C	-1.61907900	0.08827900	-3.04617300
C	-0.17314300	-0.30754900	-3.23218100
C	0.16097300	-1.35439900	-2.36395700
C	-1.05204700	-1.74049800	-1.53388800
C	0.79021000	0.22553500	-4.08687900
C	2.08328300	-0.30574600	-4.06503500
C	2.41139500	-1.35862300	-3.20417000
C	1.44461400	-1.89196500	-2.34676800
C	-0.83468900	-3.29522300	0.43153400
C	1.25754300	-2.87702700	1.73079200
C	1.77360900	-3.54149400	3.01160300
C	0.48110200	-3.94080900	3.73884900
C	-0.40289200	-4.45727700	2.59858700
C	-1.48360700	-5.66515600	-0.02302300
C	-2.60915700	-6.18872800	-0.91966800
C	-3.79144000	-5.29513700	-0.51647900
C	-3.15549600	-3.90457400	-0.36939200
C	-3.91172500	-0.59829200	1.44464100
C	-2.67160800	-0.23554400	2.01223700
C	-2.28223100	-0.69198100	3.27273000
C	-3.12688000	-1.52479100	4.00975700
C	-4.36043900	-1.89750400	3.47422500
C	-4.74307700	-1.43788000	2.21114500
C	-4.06635300	1.90521100	-0.30503200
C	-3.85429400	2.61090200	-1.50628200
C	-3.71019400	3.99873600	-1.52288600
C	-3.78256100	4.72040700	-0.32979800
C	-4.00281000	4.04768900	0.87278500
C	-4.13924400	2.65839000	0.88291600
C	-6.09318200	-0.40776400	-0.92326700
C	-6.28688600	-1.93386000	-1.06412100
C	-7.16528800	0.17802900	0.02277700
C	-6.29003100	0.21954700	-2.32402400
H	-0.19004800	-1.36020500	0.33871600
H	-1.54718600	0.24463200	-0.89467100
H	-2.27224900	-0.40847800	-3.77720600
H	-1.78630000	1.16475400	-3.12286100
H	-1.57007900	-2.58426100	-1.99578700
H	0.54590800	1.05461500	-4.74468700
H	2.84788000	0.11270300	-4.71238500
H	3.42596000	-1.74421200	-3.18289000
H	1.70332000	-2.70192000	-1.66980900
H	1.07452600	-1.81001400	1.88708200
H	1.93596100	-2.97848000	0.87987300
H	2.36597300	-4.43215000	2.77424700
H	2.40309900	-2.86250700	3.58967900
H	0.01747300	-3.06293900	4.20126900
H	0.63264100	-4.69591600	4.51410600
H	-0.18000400	-5.51136800	2.39499300
H	-1.47403300	-4.35744800	2.79021100
H	-1.55427600	-6.12917400	0.96827300
H	-0.47987300	-5.85034700	-0.41490600
H	-2.79629700	-7.25389600	-0.76372500
H	-2.35590200	-6.03773600	-1.97463300
H	-4.20519900	-5.63013700	0.44118200
H	-4.60224000	-5.29335400	-1.24839100
H	-3.20260300	-3.35141700	-1.30875700
H	-3.62955900	-3.29009200	0.39811900
H	-1.98330200	0.41085300	1.47529900
H	-1.32239800	-0.38401400	3.67801400
H	-2.83375500	-1.86836100	4.99815700
H	-5.03177800	-2.53553900	4.04248700
H	-5.71359000	-1.73789200	1.83025800
H	-3.79909300	2.07196500	-2.44711500
H	-3.52436600	4.51385200	-2.46027200
H	-3.66621300	5.80016400	-0.34030600
H	-4.06262100	4.60318200	1.80452500
H	-4.29617800	2.15491100	1.83252300
H	-6.20386200	-2.46664600	-0.11141800
H	-5.55507200	-2.36259400	-1.75617700
H	-7.28626500	-2.14844400	-1.46608100
H	-8.16812400	-0.02179300	-0.37740300
H	-7.06375600	1.26383100	0.12295300
H	-7.12478800	-0.25093500	1.02887800
H	-5.54997400	-0.14869100	-3.04175200
H	-6.22499000	1.31116500	-2.29684100
H	-7.28506500	-0.04069900	-2.70881000
O	0.43021900	0.25534000	0.77092400
C	1.37861800	1.04776200	1.01375800
N	2.52417200	0.68867200	1.61408800
C	1.12844700	2.50151100	0.67021000
C	3.78688100	1.40034300	1.38725400
C	3.96316000	0.06591600	0.78060500
C	0.48359400	2.80861700	-0.53381000
C	1.45970200	3.53988800	1.54786600
C	0.19447000	4.13480400	-0.83924600
H	0.22268600	2.02416300	-1.23112000
C	1.13194900	4.85176200	1.21175500
H	1.95303800	3.34418700	2.49129200
C	0.49970500	5.18503200	0.02057400
N	-0.47912400	4.44350000	-2.11160700
N	1.45843700	5.93369700	2.16149300
H	0.25540400	6.20910800	-0.22298100
O	-0.82249000	5.60737500	-2.30765300
O	-0.67117500	3.51648800	-2.89880500
O	1.99544600	5.61528300	3.22049700
O	1.16852600	7.08227700	1.83402300
H	3.74648700	2.21131300	0.65819100
H	3.68538000	-0.06294800	-0.25491300
S	6.20294700	0.83958700	-0.75140000
C	6.64472600	-0.73198500	-1.40982500
C	6.22282000	-1.14197600	-2.69839800
C	7.43534100	-1.65222500	-0.68112000
C	6.55592300	-2.39248100	-3.21425000
H	5.64217000	-0.44222500	-3.29277000
C	7.76199600	-2.90698200	-1.19732000
H	7.81186400	-1.35173900	0.29258600
C	7.32225400	-3.29258800	-2.46507700
H	6.22340700	-2.66586300	-4.21382300
H	8.37536600	-3.58448200	-0.60686900
H	7.58329300	-4.26661300	-2.86941700
C	4.54510900	-1.08982000	1.54438200
C	4.84471300	-0.74692200	3.01206200
C	5.52454900	0.62444300	3.11335100
H	5.48462700	-1.52636600	3.44118200
H	3.91150300	-0.73746100	3.59097300
C	4.59024100	1.75490100	2.64663000
H	5.46797300	-1.37639100	1.02918500
H	3.87704400	-1.95535000	1.46899900
H	5.17942900	2.65508000	2.44678200
H	3.87915500	2.00622900	3.44363200
H	6.41758900	0.62252100	2.47850700
H	5.85015000	0.82012000	4.14128300

TS_{SS} conformation 4

Si	-4.49543700	0.14232500	-0.16617000
O	-3.52866700	-0.53320800	-1.37975500

N	-0.90557900	-2.05039000	-0.33856800
N	-0.22679700	-3.70193300	1.13464800
N	-2.00714500	-4.14163900	-0.30809700
C	-2.15578200	-0.27691700	-1.62699600
C	-1.89132000	0.38744100	-2.99610500
C	-0.44575400	0.03117000	-3.24831700
C	-0.07934800	-1.08493900	-2.48533500
C	-1.27171500	-1.56059500	-1.66933200
C	0.49469300	0.66274300	-4.06094800
C	1.80096400	0.16648200	-4.09637200
C	2.16452700	-0.95293200	-3.33928200
C	1.21695400	-1.59140000	-2.53215900
C	-1.05667400	-3.28496300	0.15398500
C	1.07269200	-3.04262800	1.43582100
C	1.58165700	-3.80693500	2.66231200
C	0.28498000	-4.19371300	3.38867500
C	-0.63877300	-4.60239600	2.23595900
C	-1.78312300	-5.59742600	-0.44845300
C	-2.95745900	-6.04078500	-1.32611300
C	-4.09220900	-5.12663300	-0.84185700
C	-3.40028300	-3.76738300	-0.67143800
C	-4.04107200	-0.64261600	1.50619600
C	-2.77517500	-0.35867000	2.06261900
C	-2.36216100	-0.92757800	3.26857000
C	-3.20723200	-1.79763100	3.96083400
C	-4.46516500	-2.09477700	3.43491900
C	-4.87181500	-1.52286800	2.22642700
C	-4.18681700	2.00035800	-0.01968700
C	-3.99653600	2.80730200	-1.15917400
C	-3.81271700	4.18661000	-1.05552000
C	-3.82541700	4.79815000	0.19955000
C	-4.02601200	4.02455500	1.34353600
C	-4.19978300	2.64388200	1.23317600
C	-6.28282900	-0.21173700	-0.77303900
C	-6.51580200	-1.71752100	-1.02690100
C	-7.31508900	0.32059100	0.24594000
C	-6.50028700	0.52864000	-2.11404600
H	-0.35438500	-1.36854500	0.20732500
H	-1.72994900	0.36205000	-0.84364200
H	-2.55987300	-0.06125700	-3.74434400
H	-2.07527800	1.46371900	-2.98301900
H	-1.80016800	-2.35656000	-2.19970500
H	0.22285600	1.54428100	-4.63433000
H	2.55384200	0.66389500	-4.69980500
H	3.19796300	-1.28704600	-3.34332500
H	1.50133300	-2.45304400	-1.93353100
H	0.93879800	-1.98080300	1.66106900
H	1.73044200	-3.12017500	0.56675100
H	2.12894000	-4.70652600	2.35933100
H	2.25124400	-3.19282500	3.26754600
H	-0.13303300	-3.32621700	3.90994100
H	0.41506600	-5.00009800	4.11465400
H	-0.46359400	-5.65096100	1.96663900
H	-1.70116100	-4.47020400	2.45492000
H	-1.82945000	-6.11340000	0.51765700
H	-0.80114800	-5.78864500	-0.88966600
H	-3.17586800	-7.10511300	-1.21038900
H	-2.73706400	-5.85117100	-2.38223500
H	-4.47891700	-5.48324600	0.11942200
H	-4.93063800	-5.06867300	-1.53962500
H	-3.44032100	-3.19444200	-1.59957900
H	-3.83471600	-3.15045000	0.11633900
H	-2.08434100	0.31337500	1.56139300
H	-1.38311200	-0.67664100	3.66699200
H	-2.89489400	-2.22906400	4.90807000
H	-5.13655200	-2.76137600	3.96934200
H	-5.86052100	-1.76736600	1.85274900
H	-3.98846300	2.35590300	-2.14638000
H	-3.64032700	4.77934800	-1.94849300
H	-3.67735000	5.87086600	0.28250400
H	-4.03951400	4.49405900	2.32315000
H	-4.33841400	2.05950200	2.13811000
H	-6.41777700	-2.32481200	-0.12131600
H	-5.81310000	-2.10507600	-1.77139700
H	-7.53063200	-1.87951000	-1.41448000
H	-8.33296500	0.17034900	-0.13762200
H	-7.18806700	1.39351000	0.42466100
H	-7.25425000	-0.18422800	1.21498600
H	-5.78990500	0.19974100	-2.87931800
H	-6.40475300	1.61268200	-2.00298100
H	-7.51186600	0.32457300	-2.48937500
O	0.32315900	0.16152500	0.82947700
C	1.36466600	0.86388600	0.93691000
N	2.56112800	0.40196100	1.32338200
C	1.18418800	2.35189600	0.70133000
C	3.80988600	1.00114300	0.83540200
C	3.79110300	-0.35659200	0.24622100
C	0.43489800	2.78736900	-0.39745800
C	1.69189300	3.29949100	1.59681300
C	0.21467200	4.14937600	-0.58125300
H	0.03921100	2.07647100	-1.10986500
C	1.42950800	4.65173300	1.38612400
H	2.27347400	2.99989900	2.45903900
C	0.69226200	5.11156200	0.30255700
N	-0.57095800	4.59523700	-1.74393100
N	1.94613700	5.63861200	2.35489800
H	0.49919000	6.16466500	0.15566200
O	-0.88281100	5.78296500	-1.80059400
O	-0.88089400	3.75074100	-2.58450400
O	2.57512600	5.20963200	3.31998200
O	1.71147800	6.82499200	2.13567000
H	3.68672800	1.80127100	0.10381600
H	3.27456100	-0.50450800	-0.68762100
S	5.57829500	0.09258600	-1.86443800
C	7.00302500	-0.83750800	-1.40693800
C	7.06118100	-2.24179000	-1.56578900
C	8.14309900	-0.21225900	-0.84808300
C	8.18722700	-2.97442300	-1.18777400
H	6.20934700	-2.74690400	-2.01280900
C	9.26687700	-0.94576100	-0.47494300
H	8.13003800	0.86669200	-0.72510800
C	9.29963400	-2.33468400	-0.63825000
H	8.19685100	-4.05298400	-1.33059500
H	10.12684000	-0.42955700	-0.05391200
H	10.17747500	-2.90444900	-0.34676200
C	4.43228700	-1.52343000	0.94366700
C	4.94027800	-1.17466900	2.35050900
C	5.74086300	0.13248900	2.30974500
H	5.56667200	-1.99428200	2.71979200
H	4.09238700	-1.07133700	3.03959200
C	4.86403400	1.33152600	1.90205300
H	5.27770400	-1.84425300	0.32420200
H	3.73680300	-2.36967300	0.97221100
H	5.50148600	2.13544300	1.52144400
H	4.33987600	1.72805600	2.78031600
H	6.55714700	0.01664100	1.58762100
H	6.20261900	0.33297000	3.28312400

TS_{SS} conformation 5

Si	3.54146700	2.06348200	-0.04703600
O	3.12175800	1.08791300	1.26784500
N	1.85091100	-1.79233100	0.60677000
N	2.14192600	-3.74468900	-0.60277300
N	3.94021800	-2.89438000	0.61818300
C	1.86232100	0.52728300	1.59869300
C	1.27826700	1.08843400	2.91558600
C	0.40037400	-0.03923900	3.40214400
C	0.75972800	-1.24330900	2.78388500
C	1.93115100	-1.01040200	1.84348800
C	-0.64466000	-0.01062700	4.32383100
C	-1.31884300	-1.19847400	4.62162400
C	-0.95421700	-2.40007700	4.00498000
C	0.09325100	-2.42913500	3.08015100
C	2.64541000	-2.79441400	0.21451500
C	0.68193100	-3.96921400	-0.79270600
C	0.63106000	-5.06597400	-1.86122200
C	1.86963100	-4.76552400	-2.71781100
C	2.92811200	-4.40990000	-1.66764700
C	4.59945200	-4.18311900	0.92097400

C	5.85002100	-3.75096500	1.69242900
C	6.23770200	-2.44568600	0.98242700
C	4.88752700	-1.75362600	0.74529400
C	3.66324600	0.98596500	-1.60967100
C	2.48947500	0.36780900	-2.09137000
C	2.51038800	-0.46904500	-3.20853900
C	3.70913300	-0.71032000	-3.88323600
C	4.88401900	-0.10845000	-3.43102400
C	4.85654700	0.72660600	-2.31096000
C	2.22103200	3.37721400	-0.35640600
C	1.59357900	4.05323900	0.70929700
C	0.65866300	5.06391600	0.48328600
C	0.33187800	5.43036600	-0.82390800
C	0.94489200	4.78294900	-1.89745700
C	1.87403500	3.76745000	-1.66430500
C	5.19541400	2.85981300	0.51835600
C	6.24450800	1.78748500	0.88699500
C	5.75593500	3.79616200	-0.57574300
C	4.92344500	3.70719800	1.78334200
H	0.99426800	-1.60968800	0.06045800
H	1.13458300	0.68820900	0.79447300
H	2.10384200	1.28429900	3.61371100
H	0.73490200	2.02449800	2.76643100
H	2.86792400	-1.25541700	2.34955400
H	-0.94162800	0.92266800	4.79322700
H	-2.14390700	-1.18729300	5.32695800
H	-1.49881000	-3.31014800	4.23601900
H	0.37014400	-3.36186000	2.59563500
H	0.18252900	-3.06075000	-1.14162800
H	0.22829800	-4.26106200	0.15830300
H	0.71755600	-6.05823500	-1.40426900
H	-0.30343700	-5.03258600	-2.42424600
H	1.68171600	-3.90310700	-3.36603000
H	2.18088000	-5.60408600	-3.34555100
H	3.40282600	-5.32220800	-1.28739000
H	3.70703900	-3.73805700	-2.03648600
H	4.89317800	-4.71706400	0.00925100
H	3.92493400	-4.82772600	1.49107100
H	6.63359700	-4.51185800	1.66233200
H	5.60175000	-3.55792800	2.74169800
H	6.72551300	-2.66878300	0.02704600
H	6.91606900	-1.81950200	1.56625100
H	4.63034400	-1.10225700	1.58231500
H	4.86401800	-1.14870900	-0.16269900
H	1.53503500	0.52859000	-1.59797300
H	1.58411200	-0.91971500	-3.55429900
H	3.72560400	-1.35003000	-4.76149700
H	5.82095400	-0.27939700	-3.95408400
H	5.78672000	1.18407300	-1.99105500
H	1.83397400	3.78839800	1.73441100
H	0.17408300	5.55310600	1.32271200
H	-0.39884100	6.21393300	-1.00142800
H	0.69521500	5.06338900	-2.91689300
H	2.32807800	3.26697000	-2.51475200
H	6.51397600	1.14505400	0.04250000
H	5.88443700	1.14546900	1.69739700
H	7.16820300	2.27000500	1.23404500
H	6.66803200	4.28970300	-0.21484300
H	5.04036900	4.58275200	-0.83731700
H	6.01616100	3.26753700	-1.49799300
H	4.51146800	3.10199200	2.59711300
H	4.22861600	4.52806200	1.58287300
H	5.86184600	4.15167800	2.14077800
O	-0.37276600	-0.77958800	-0.68323100
C	-1.58628700	-0.70093500	-1.00908900
N	-2.33063900	-1.75713700	-1.38098100
C	-2.18357600	0.68769500	-1.01514200
C	-3.79164000	-1.75737200	-1.20107200
C	-3.25549400	-2.71204900	-0.21388300
C	-1.95852900	1.51787200	0.08812100
C	-2.92056100	1.17303600	-2.09889300
C	-2.48033900	2.80719500	0.09035100
H	-1.40472300	1.15886000	0.94432300
C	-3.40152400	2.48073300	-2.06604600
H	-3.11667300	0.55760800	-2.96775700
C	-3.20427600	3.32262500	-0.97841900
N	-2.24289600	3.66931400	1.25778200
N	-4.14702500	2.99519500	-3.22876100
H	-3.59511000	4.32983900	-0.96601000
O	-2.66723500	4.82232300	1.21399900
O	-1.61779300	3.19280800	2.20637500
O	-4.29939800	2.23760600	-4.18599900
O	-4.56376900	4.15055700	-3.17146200
H	-4.21366800	-0.85587800	-0.75788000
H	-2.98430900	-2.34301700	0.76336500
S	-5.54691800	-2.80100500	1.38853000
C	-5.55655700	-1.05778100	1.65826400
C	-6.53838500	-0.22130100	1.07461900
C	-4.57363700	-0.41992600	2.45262000
C	-6.53862100	1.15720800	1.27799300
H	-7.30938900	-0.68137600	0.46347700
C	-4.57421900	0.96105300	2.65252000
H	-3.81622000	-1.03406600	2.93164400
C	-5.55608000	1.76501500	2.06732200
H	-7.31562800	1.76442300	0.81840700
H	-3.80153200	1.41197500	3.27187600
H	-5.56414000	2.83915700	2.23168100
C	-3.10972400	-4.18043500	-0.51644400
C	-3.48484200	-4.53216700	-1.96413300
C	-4.78280200	-3.82043300	-2.36719800
H	-3.59580500	-5.61887000	-2.05513500
H	-2.67632000	-4.22993900	-2.64256200
C	-4.60839200	-2.29168800	-2.38414400
H	-3.77159900	-4.70662000	0.17747300
H	-2.08959300	-4.50654800	-0.28043100
H	-5.59227700	-1.81336000	-2.37192000
H	-4.10908500	-1.97932400	-3.30989500
H	-5.56584800	-4.07703000	-1.64460800
H	-5.12148300	-4.16257400	-3.35173200

TS_{SS} conformation 6

Si	-4.20397000	0.62498600	-0.46881800
O	-3.23836000	-0.28211300	-1.51933700
N	-0.96769300	-2.06794400	-0.10540800
N	-0.61049600	-3.66775400	1.53071600
N	-2.35192400	-3.97768400	0.00873500
C	-1.82454000	-0.25641700	-1.64009600
C	-1.33976500	0.24018300	-3.02049900
C	0.03355900	-0.37867300	-3.12438700
C	0.14384000	-1.46970600	-2.25355800
C	-1.16263800	-1.66059800	-1.50038600
C	1.11984800	-0.00033700	-3.91193200
C	2.30869800	-0.72943200	-3.82036300
C	2.41320900	-1.82656800	-2.95810400
C	1.32322400	-2.20473000	-2.16886600
C	-1.31571900	-3.22463600	0.46732200
C	0.73788300	-3.14984000	1.88739700
C	1.05604800	-3.87018500	3.20262300
C	-0.32718200	-4.03455800	3.84852500
C	-1.21292300	-4.41675300	2.65776700
C	-2.32783400	-5.45548500	-0.02650300
C	-3.48659800	-5.78984200	-0.97072800
C	-4.51544700	-4.70288800	-0.62658900
C	-3.65787000	-3.43995300	-0.45863200
C	-4.00799800	-0.04319100	1.30224100
C	-2.76060900	0.10986100	1.94421800
C	-2.53276600	-0.38988600	3.22754400
C	-3.55125300	-1.05629000	3.91241300
C	-4.79620100	-1.21826700	3.30316800
C	-5.01684200	-0.71661200	2.01771500
C	-3.65316600	2.43182000	-0.45173400
C	-3.23517600	3.08502700	-1.62818700
C	-2.87792000	4.43389800	-1.62760200
C	-2.93911700	5.16991600	-0.44276900
C	-3.36047300	4.55065800	0.73468800
C	-3.70785500	3.19862000	0.72859100
C	-5.96182500	0.45009500	-1.22316000
C	-6.38841300	-1.02850900	-1.35464300
C	-6.99444700	1.22542800	-0.37500900

C	-5.94096600	1.06192900	-2.64352600
H	-0.35204600	-1.42643000	0.41758400
H	-1.37529200	0.37698700	-0.86590600
H	-2.01821600	-0.14475700	-3.79478400
H	-1.33029900	1.32976300	-3.09443000
H	-1.78141700	-2.41109700	-1.99833600
H	1.04918100	0.86061400	-4.57054000
H	3.17431900	-0.44014600	-4.40688500
H	3.35127700	-2.36905600	-2.89658100
H	1.40677300	-3.04967800	-1.48995100
H	0.72280500	-2.06524700	2.02786600
H	1.44251200	-3.37317000	1.08218700
H	1.50244200	-4.85176000	3.00793600
H	1.75460600	-3.29699700	3.81489500
H	-0.66449700	-3.08294200	4.27272900
H	-0.35345500	-4.78989400	4.63774400
H	-1.16004400	-5.49714200	2.47726600
H	-2.26135300	-4.13449900	2.78049200
H	-2.51660100	-5.89264000	0.96141100
H	-1.35402700	-5.80939100	-0.37551800
H	-3.85953900	-6.80558500	-0.81866400
H	-3.16510700	-5.69718200	-2.01374900
H	-5.02205100	-4.94902300	0.31332500
H	-5.28122700	-4.57223700	-1.39449700
H	-3.56285900	-2.90220000	-1.40319000
H	-4.05478600	-2.74068700	0.27941300
H	-1.94175500	0.62256600	1.44767700
H	-1.56083700	-0.24581600	3.69124100
H	-3.38137200	-1.43308400	4.91744400
H	-5.60009000	-1.72447100	3.83062500
H	-5.99927500	-0.85162100	1.57760500
H	-3.18413100	2.53486800	-2.56249600
H	-2.53503400	4.90446000	-2.54385800
H	-2.65701400	6.21868700	-0.43988300
H	-3.41180300	5.11749500	1.66008100
H	-4.01746400	2.73415400	1.66053700
H	-6.44922900	-1.54239900	-0.39012200
H	-5.69333200	-1.58531000	-1.99122300
H	-7.38224100	-1.09136400	-1.81809300
H	-7.98253500	1.17858000	-0.85167700
H	-6.72591400	2.28286700	-0.28152700
H	-7.10173700	0.82168400	0.63664700
H	-5.21543600	0.55822900	-3.29005200
H	-5.69931500	2.12863300	-2.62589700
H	-6.93087300	0.95684700	-3.10741000
O	0.49238300	0.06612600	0.90156900
C	1.53685500	0.69647600	1.21252100
N	2.56919800	0.16162100	1.88272300
C	1.54028700	2.17250000	0.87081400
C	3.93906000	0.66604400	1.74612500
C	3.95794800	-0.68863900	1.15776000
C	1.03029100	2.57844300	-0.36816300
C	1.96886300	3.14417700	1.78167800
C	0.96626100	3.93466200	-0.67236600
H	0.69783200	1.84474800	-1.09026300
C	1.86747400	4.49207400	1.44361000
H	2.36359200	2.87114300	2.75179700
C	1.37104000	4.92241500	0.21972800
N	0.42594100	4.34896200	-1.97806900
N	2.29353900	5.50752000	2.42655500
H	1.30015600	5.97272900	-0.02430500
O	0.27378800	5.55259100	-2.17649600
O	0.14525600	3.46618500	-2.78884300
O	2.70652300	5.10648500	3.51283900
O	2.20437300	6.68824200	2.09721200
H	4.08015900	1.46179200	1.01376200
H	3.73185900	-0.79532400	0.10722100
S	6.42326000	-0.33161600	-0.10846100
C	6.24440400	-1.24212700	-1.60898000
C	6.18350500	-0.58777100	-2.86190400
C	6.17747100	-2.65515200	-1.62830100
C	6.07269100	-1.30054100	-4.05443600
H	6.24019100	0.49646100	-2.87855400
C	6.05433400	-3.36696300	-2.82161100
H	6.24885600	-3.19133800	-0.68600800
C	6.00047300	-2.69801800	-4.04832500
H	6.04943400	-0.76139700	-4.99950900
H	6.01572800	-4.45420000	-2.79494900
H	5.91842700	-3.25261900	-4.97887700
C	4.27807000	-1.90932800	1.98127600
C	4.48324000	-1.58898300	3.46979500
C	5.37349200	-0.34920400	3.62606200
H	4.94011300	-2.45372100	3.96461800
H	3.51413800	-1.41060400	3.95359700
C	4.69699800	0.91228400	3.05883200
H	5.20190800	-2.31882900	1.56397700
H	3.49835800	-2.66654900	1.84070800
H	5.45199100	1.68589100	2.88810700
H	3.98544500	1.31518700	3.79032100
H	6.31309000	-0.52482700	3.08992000
H	5.62763300	-0.18483900	4.67919400

TS_{SS} conformation 7

Si	4.00133200	-1.44185200	-0.33488500
O	3.06345000	-1.54213000	1.06683100
N	-0.04291800	-1.94693400	0.47811800
N	-1.43740200	-3.37829100	-0.70583100
N	0.07445100	-4.27678900	0.83039800
C	1.95661000	-0.72948600	1.42901700
C	2.17592100	0.03661400	2.75163100
C	0.76023300	0.31102600	3.20332900
C	-0.12891200	-0.57991200	2.58652500
C	0.65272300	-1.53298500	1.69902400
C	0.28126900	1.27931700	4.08239800
C	-1.09308400	1.33869000	4.33822600
C	-1.97397900	0.44328600	3.72385300
C	-1.49576400	-0.53125900	2.84095800
C	-0.46715900	-3.19120500	0.19740500
C	-2.24597900	-2.27714900	-1.28539100
C	-3.16089800	-2.99270900	-2.28293700
C	-2.31955600	-4.19116300	-2.74430900
C	-1.63940700	-4.64361900	-1.44832400
C	-0.74104800	-5.36246600	1.41154500
C	0.25344300	-6.04736000	2.35374300
C	1.57021500	-5.96187900	1.56603200
C	1.52968100	-4.56264700	0.92667300
C	2.97110600	-1.99683600	-1.83485300
C	1.95534800	-1.14186200	-2.31349400
C	1.15183700	-1.49788300	-3.39824800
C	1.34137100	-2.72406800	-4.03967400
C	2.33532500	-3.59086200	-3.58428400
C	3.13630400	-3.22739200	-2.49838600
C	4.54459600	0.33912500	-0.65856100
C	4.87282400	1.21241100	0.39676300
C	5.35018600	2.50198400	0.15632600
C	5.51800200	2.94898000	-1.15529000
C	5.20627400	2.10209100	-2.21980300
C	4.72346700	0.81617700	-1.97208700
C	5.53257800	-2.53255000	0.06432700
C	5.14464800	-3.96161500	0.50163500
C	6.47498600	-2.59438000	-1.15845500
C	6.29547500	-1.87551500	1.23862800
H	-0.35191600	-1.17158400	-0.10851500
H	1.71990400	-0.00672300	0.63821500
H	2.70376300	-0.62290500	3.45517900
H	2.77770900	0.93813400	2.62416600
H	0.89473000	-2.43719700	2.26107000
H	0.96216900	1.98593800	4.54865200
H	-1.48060600	2.09481500	5.01512600
H	-3.04198300	0.50254200	3.90774200
H	-2.20014100	-1.20348000	2.35859100
H	-1.57810500	-1.57902800	-1.80409400
H	-2.81744100	-1.75552400	-0.50539900
H	-4.06971600	-3.32625100	-1.77112900
H	-3.46062900	-2.33436400	-3.10118400
H	-1.56254600	-3.87257100	-3.46913300
H	-2.90961200	-4.99354000	-3.19426200
H	-2.30226800	-5.30923800	-0.88413500
H	-0.68321200	-5.14922000	-1.60172900

H	-1.08867000	-6.07673200	0.65423300
H	-1.61700400	-4.94764900	1.91725200
H	-0.04241100	-7.07258000	2.58940200
H	0.32864300	-5.48985800	3.29351800
H	1.59097800	-6.73469500	0.78969300
H	2.45629100	-6.09533800	2.19094600
H	2.05184900	-3.82449100	1.53786200
H	1.98350700	-4.53783700	-0.06804400
H	1.78181100	-0.17722000	-1.84423900
H	0.38821100	-0.80907400	-3.74876500
H	0.72965000	-2.99472400	-4.89607200
H	2.49885900	-4.54296900	-4.08171500
H	3.91070100	-3.91738200	-2.17981800
H	4.75561200	0.88628200	1.42550500
H	5.57556300	3.15853000	0.99110700
H	5.88804300	3.95245400	-1.34504100
H	5.33379100	2.44356800	-3.24325000
H	4.47696700	0.17874000	-2.81649600
H	4.60442000	-4.51497600	-0.27289600
H	4.52228200	-3.94557300	1.40167100
H	6.04962700	-4.53785600	0.73702100
H	7.38572600	-3.15201100	-0.90271500
H	6.78384000	-1.59452300	-1.48121100
H	6.01782000	-3.09318600	-2.01900600
H	5.66778400	-1.79327400	2.13181600
H	6.65682200	-0.87508700	0.98446200
H	7.17010800	-2.48550200	1.50155700
O	-0.33129800	1.00739400	-0.54343300
C	-0.85821100	2.13233200	-0.68768800
N	-2.12006300	2.42200700	-1.11283600
C	-0.05837300	3.37339600	-0.36929000
C	-3.34685000	1.67581000	-0.00338600
C	-2.99467200	1.27744600	-1.37257800
C	1.06016100	3.28926400	0.46510700
C	-0.42744000	4.61806300	-0.89668400
C	1.78979900	4.44241000	0.74679600
H	1.34619600	2.34044900	0.89561400
C	0.34323900	5.73955900	-0.60549300
H	-1.30348600	4.69899800	-1.52552600
C	1.46616200	5.68439800	0.21229300
N	2.95086100	4.35715100	1.64472300
N	-0.04019300	7.04297600	-1.18269100
H	2.05370400	6.56595600	0.42628800
O	3.73698500	5.30234100	1.65596600
O	3.07256500	3.34166100	2.33134000
O	-1.02309300	7.07140400	-1.91936300
O	0.65070200	8.01741400	-0.88941700
H	-2.75986300	1.26682000	0.80599000
H	-2.47245200	0.32893900	-1.45905300
S	-4.59399500	-0.71839900	1.01080700
C	-6.31672500	-0.89093900	0.64186200
C	-6.77580500	-1.38947500	-0.59711500
C	-7.29941300	-0.53177400	1.59027600
C	-8.13642600	-1.52159100	-0.87106900
H	-6.04440200	-1.67391800	-1.34874700
C	-8.65903500	-0.66653600	1.31543800
H	-6.97454000	-0.14873700	2.55298900
C	-9.09156900	-1.16204300	0.08264300
H	-8.45312400	-1.90910900	-1.83703500
H	-9.38750000	-0.38146800	2.07114200
H	-10.15166600	-1.26530100	-0.13066800
C	-4.02929500	1.50966900	-2.46533100
C	-4.90679700	2.74424000	-2.20788700
C	-5.52443100	2.69354800	-0.80343700
H	-5.69765000	2.79205400	-2.96515600
H	-4.30244600	3.65239400	-2.31909200
C	-4.44937900	2.65510200	0.29615900
H	-4.66407700	0.61548800	-2.50609100
H	-3.51505600	1.59202500	-3.43087900
H	-4.89105700	2.37380900	1.25556800
H	-4.00040600	3.64870100	0.42353300
H	-6.14936900	1.79792700	-0.71411700
H	-6.17757300	3.55825700	-0.64110900

TS structures for Mechanism 2: Ar = 4-BrC_6H_4

The Ar=4-BrC_6H_4 is derived from the lowest energy conformational of the TS structures of Ar=4-C_6H_5.

Table 16: CPCM/RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)	Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)
TS_{RR} conformation 7	-6097.69861169	0.0	TS_{SS} conformation 7	-6097.69748872	0.7

Table 17: RM06-2x/6-311+G(2df,2p)//RB3LYP/6-31G(d,p) single point calculation results

Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)	Conformation	Electronic energy (hartree)	Energy relative to RR (kcal/mol)

TS_{RR} conformation 7	-6097.67169836	0.0	TS_{SS} conformation 7	-6097.67474461	1.9

Table 18: Correction to zero-point energy, thermal correction to electronic energy, enthalpy and Gibbs derived from RB3LYP/6-31G(d,p) for TS structures

Correction	TS_{RR} conformation 7	TS_{ss} conformation 7
Zero-point correction	1.062827	1.062129
Thermal correction to Energy	1.128814	1.128300
Thermal correction to Enthalpy	1.129759	1.129244
Thermal correction to Gibbs Free Energy	0.949813	0.949107

TS_{RR} conformation 7 (derived from TS_{SS} conformation 7 of $Ar=C_6H_5$)

Si	4.56647900	-1.74579500	-0.34722200
O	3.62660600	-1.76499200	1.05667300
N	0.49248600	-1.88876700	0.48239700
N	-1.01898500	-3.19510200	-0.70474500
N	0.41672400	-4.22197100	0.82375900
C	2.59922500	-0.85992000	1.43090100
C	2.89200700	-0.13094100	2.76064700
C	1.50862800	0.25882800	3.22752200
C	0.54112600	-0.54146400	2.60492600
C	1.23076500	-1.54822500	1.70085400
C	1.12166600	1.25040800	4.12602300
C	-0.24044600	1.42521700	4.39407500
C	-1.20028400	0.62011700	3.77279400
C	-0.81443200	-0.37799300	2.87148800
C	-0.03472000	-3.09182100	0.19693700
C	-1.72562200	-2.02889900	-1.28900000
C	-2.69870000	-2.66326200	-2.28707800
C	-1.96762200	-3.93446600	-2.74152100
C	-1.33060900	-4.44040400	-1.44348100
C	-0.48330000	-5.23296800	1.41556300
C	0.46128400	-6.00704700	2.33971500
C	1.76747600	-6.03686800	1.53072700
C	1.84230800	-4.63664400	0.89690100
C	3.49348100	-2.23454900	-1.84049100
C	2.53670300	-1.31311300	-2.31786100
C	1.70768500	-1.61542300	-3.39967700
C	1.81139400	-2.85264900	-4.03956400
C	2.74500400	-3.78447700	-3.58509500
C	3.57214800	-3.47453900	-2.50222800
C	5.24030300	-0.01436000	-0.68768400
C	5.64538700	0.83683800	0.35889000
C	6.22874700	2.07943900	0.10560100
C	6.42723200	2.49996700	-1.21057900
C	6.03873300	1.67440000	-2.26661600
C	5.45092100	0.43562700	-2.00589500
C	6.01034100	-2.94752200	0.05885000
C	5.51001900	-4.34029900	0.49975900
C	6.94855400	-3.08574200	-1.16085600
C	6.81938300	-2.34902600	1.23367900
H	0.24491900	-1.08291800	-0.09312200
H	2.42742700	-0.11142300	0.64718600
H	3.36686800	-0.84147200	3.45204200
H	3.56718700	0.71791200	2.63919300
H	1.39771200	-2.47539400	2.25261900
H	1.86452300	1.88694100	4.59850300
H	-0.55578300	2.20072500	5.08628200
H	-2.25765400	0.76876700	3.96785100
H	-1.57666900	-0.98114600	2.38630700
H	-0.99696800	-1.39366400	-1.80684600
H	-2.24826800	-1.45741400	-0.51106100
H	-3.63541300	-2.91234000	-1.77736900
H	-2.93532800	-1.98377300	-3.10875300
H	-1.18515100	-3.68820800	-3.46723200
H	-2.62708600	-4.68243500	-3.18866800
H	-2.04840500	-5.04431700	-0.87697300
H	-0.42174700	-5.02721100	-1.59403300
H	-0.90633200	-5.91081200	0.66299300
H	-1.31048400	-4.74381200	1.93685100
H	0.07870800	-7.00237000	2.57864000
H	0.60199100	-5.46120600	3.27874400
H	1.70710500	-6.80528900	0.75210900
H	2.64773400	-6.25161800	2.14106400
H	2.43677200	-3.95109200	1.50321400
H	2.28176900	-4.64764400	-0.10452800
H	2.43076700	-0.33784300	-1.85001200
H	0.99307500	-0.87610300	-3.75087400
H	1.18100700	-3.08177900	-4.89449500
H	2.84196500	-4.74625200	-4.08128300
H	4.29902400	-4.21477700	-2.18460900
H	5.50622800	0.52973100	1.39060400
H	6.51501400	2.72054000	0.93377300
H	6.88062400	3.46660900	-1.41038200
H	6.18907500	1.99591200	-3.29340200
H	5.14740100	-0.18599700	-2.84340900
H	4.93524700	-4.85544300	-0.27631300
H	4.88365500	-4.27102900	1.39460700
H	6.36590400	-4.98302900	0.74595100
H	7.80698600	-3.72076100	-0.90450400
H	7.34384400	-2.11492900	-1.47787400
H	6.45415200	-3.53940600	-2.02574600
H	6.19665600	-2.21132400	2.12347000

H	7.26378700	-1.38325100	0.97672500
H	7.63939000	-3.02797500	1.50325700
O	0.43058500	1.04915400	-0.51430000
C	0.01316000	2.21928000	-0.66252800
N	-1.21726300	2.62851400	-1.07684500
C	0.93365400	3.37948400	-0.36242800
C	-2.51115600	1.98479900	0.04934600
C	-2.20068200	1.57375300	-1.32671100
C	2.03656100	3.19915300	0.47731400
C	0.69016200	4.64563000	-0.91107000
C	2.87519300	4.27976400	0.74370800
H	2.22668100	2.23443600	0.92538400
C	1.56697400	5.69040000	-0.63553800
H	-0.17333700	4.80257900	-1.54288600
C	2.67681800	5.53835200	0.18747500
N	4.02084600	4.09588300	1.64665300
N	1.31567300	7.01580600	-1.23537400
H	3.34775600	6.36128000	0.38929900
O	4.89095000	4.96435800	1.65197400
O	4.04645100	3.07987400	2.34262100
O	0.33869100	7.13028300	-1.97145700
O	2.10236100	7.92010600	-0.95983800
H	-1.94980800	1.52753700	0.85127600
H	-1.77297200	0.58010500	-1.42508400

TS_{SS} conformation 7 (derived from TS_{SS} conformation 7 of Ar=C_6H_5)

Si	-2.51830200	-1.24919800	2.82082000
O	-2.19982300	-2.02828700	1.35416900
N	-0.50730600	-2.05501800	-1.51312000
N	1.19024800	-2.62398400	-3.00546100
N	0.96957700	-3.78045800	-0.97460400
C	-2.45390700	-1.58149200	0.02871000
C	-3.96368000	-1.54463700	-0.33603700
C	-4.03837200	-2.12627900	-1.72347500
C	-2.83455700	-2.73863400	-2.07936200
C	-1.78965000	-2.56327200	-0.98877800
C	-5.12614100	-2.15004800	-2.59809500
C	-5.00140200	-2.81766300	-3.81757200
C	-3.80678500	-3.46293900	-4.15735200
C	-2.71531600	-3.42551600	-3.28779100
C	0.55835000	-2.82392700	-1.83475900
C	0.58065000	-1.86948300	-4.13699800
C	1.66451000	-1.92121000	-5.21846000
C	2.96711200	-1.92727400	-4.40535300
C	2.64330000	-2.84935100	-3.22639400
C	1.63839400	-5.03976300	-1.35349300
C	1.55015200	-5.86705100	-0.06719600
C	1.74556400	-4.80045300	1.02140700
C	0.94167200	-3.59824600	0.50522600
C	-1.16186300	0.02102400	3.14775700
C	0.08337700	-0.07494500	2.50043400
C	1.12932200	0.80041700	2.79772200
C	0.94873600	1.80026700	3.75519500
C	-0.27950000	1.92047200	4.40844700
C	-1.32035700	1.04107700	4.10640600
C	-4.17510900	-0.32868200	2.76788500
C	-5.40525800	-0.91758300	3.11824700
C	-6.61039900	-0.22439000	2.99613400
C	-6.61946800	1.08324500	2.51032900
C	-5.41540300	1.69526600	2.16018900
C	-4.21296400	0.99846900	2.29280900
C	-2.42516400	-2.67327900	4.10948100
C	-0.95878600	-3.15119900	4.22118100
C	-2.87995700	-2.16033900	5.49355100
C	-3.28550200	-3.88555000	3.68966700
H	-0.55679300	-1.12601700	-1.94185300
H	-2.01100900	-0.58942500	-0.12623200
H	-4.51366400	-2.17339200	0.37387900
H	-4.39208200	-0.54172700	-0.26822600
H	-1.59675500	-3.51213900	-0.48371000
H	-6.05280400	-1.64839700	-2.33569200
H	-5.83957500	-2.84001400	-4.50782400
S	-3.94358700	-0.28721100	1.03692200
C	-5.67763600	-0.31463500	0.70217600
C	-6.20172400	-0.75707400	-0.53241200
C	-6.61185600	0.10618900	1.67431300
C	-7.57182200	-0.78335900	-0.78624000
H	-5.51435800	-1.08711600	-1.30587600
C	-7.98419200	0.08377400	1.43580500
H	-6.24357800	0.45062500	2.63555000
C	-8.45698200	-0.36236100	0.20339500
H	-7.94898700	-1.12841700	-1.74329900
H	-8.68070200	0.41008800	2.20084800
C	-3.21653900	1.91228700	-2.41059300
C	-3.97053600	3.22218300	-2.13666700
C	-4.58273600	3.21752200	-0.72912500
H	-4.75686200	3.35341200	-2.88862400
H	-3.28247900	4.06920700	-2.24225000
C	-3.50886800	3.06716300	0.36139800
H	-3.93382300	1.08312000	-2.45768800
H	-2.70133000	1.95494800	-3.37807100
H	-3.96618700	2.83218800	1.32602800
H	-2.96087300	4.01017900	0.48536800
H	-5.29160300	2.38593200	-0.64369700
H	-5.14865900	4.13935400	-0.55471400
Br	-10.34686900	-0.39824500	-0.13506000
H	-3.72799500	-3.99130600	-5.10296000
H	-1.78968300	-3.93027200	-3.55298900
H	0.36887000	-0.83799300	-3.84058500
H	-0.36171500	-2.33450700	-4.43417300
H	1.57716000	-2.84344700	-5.80422100
H	1.58655400	-1.07695000	-5.90765100
H	3.19430000	-0.92434500	-4.02961900
H	3.83087000	-2.28107600	-4.97371300
H	2.82755800	-3.89552900	-3.49688800
H	3.19302500	-2.58640500	-2.31758500
H	2.68880500	-4.87528800	-1.61710000
H	1.13266600	-5.49228800	-2.21157700
H	2.30238900	-6.65924800	-0.03882800
H	0.56163900	-6.33189200	0.01940400
H	2.80406700	-4.53201900	1.10005900
H	1.40466700	-5.12401000	2.00769100
H	-0.08291600	-3.60630400	0.88422600
H	1.41017800	-2.64160800	0.75198400
H	0.24528100	-0.84583400	1.75316500
H	2.07545200	0.68912000	2.27678800
H	1.76069400	2.48219900	3.99209200
H	-0.42748000	2.69927100	5.15146000
H	-2.27188700	1.15882900	4.61888200
H	-5.43439900	-1.93579000	3.49174000
H	-7.54207900	-0.70747800	3.27692000
H	-7.55601900	1.62264600	2.40482600
H	-5.41603100	2.71372600	1.78274100
H	-3.28695800	1.50022900	2.02565600
H	-0.28209300	-2.34646900	4.52232500
H	-0.59378500	-3.55999300	3.27290400
H	-0.88463100	-3.94891000	4.97264800
H	-2.79035100	-2.96051000	6.24028600
H	-3.92233900	-1.82604300	5.49223700
H	-2.26176700	-1.32409400	5.83846600
H	-3.00010600	-4.25475700	2.70011300
H	-4.35587100	-3.65995900	3.66308700
H	-3.15005400	-4.70626700	4.40720000
O	-0.75855100	0.68356100	-2.33948600
C	-0.51265600	1.88158200	-2.05713500
N	0.68873800	2.50317900	-2.03661200
C	-1.67693000	2.77727900	-1.71377600
C	1.85003100	1.64367900	-2.31568900
C	1.87206600	1.64194700	-0.84605500
C	-2.97133200	2.24949900	-1.76503200
C	-1.49267700	4.11150700	-1.33155100
C	-4.05140200	3.05323000	-1.40958700
H	-3.12127700	1.22441200	-2.07686000
C	-2.60208300	4.88091000	-0.99390700
H	-0.49736400	4.53363200	-1.30114500
C	-3.89935800	4.37916600	-1.01858900

N	-5.40978100	2.48125800	-1.43543500
N	-2.40291500	6.28686400	-0.58872400
H	-4.74682900	4.99304800	-0.74824300
O	-6.33432800	3.18889300	-1.03980200
O	-5.53594400	1.32819000	-1.84705400
O	-1.25163700	6.71552000	-0.57246200
O	-3.40331400	6.93812100	-0.29279900
H	1.58918400	0.68100200	-2.75198300
S	3.32131500	-0.72250400	-0.34672500
C	4.91920200	-0.24522600	0.23288400
C	5.17388000	-0.02319100	1.60377700
C	5.99969600	-0.05345500	-0.65668600
C	6.42988300	0.37046800	2.06439100
H	4.37267400	-0.18028500	2.31928600
C	7.25951700	0.33874600	-0.21009600
H	5.83977000	-0.22443000	-1.71676100
C	7.46628200	0.55087300	1.15206300
H	6.60133100	0.53241700	3.12331600
H	8.07425400	0.47839900	-0.91269100
C	2.60429700	2.68983600	-0.06335900
C	3.25173700	3.76382400	-0.95179200
C	3.96328700	3.11125800	-2.14278400
H	3.96173100	4.34412600	-0.35303000
H	2.48352800	4.45795500	-1.30964200
C	2.97742700	2.36782600	-3.06451000
H	3.38546500	2.16797400	0.50431500
H	3.52581300	1.63956100	-3.67247800
H	2.50371800	3.07071100	-3.75899800
H	4.70952200	2.40427500	-1.75948200
H	4.51007100	3.86298400	-2.72268400
H	1.92885200	3.12986600	0.67958700
H	1.22594600	0.94679700	-0.33312700
Br	9.19655800	1.09544200	1.77489100