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**Bromenium-Catalysed Tandem Ring Opening/Cyclisation of
Vinylcyclopropanes and Vinylcyclobutanes: A Metal-Free [3+2+1]/[4+2+1]
Cascade for the Synthesis of Chiral Amidines and Computational
Investigation**

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Experimental Details

All reactions were carried out in oven-dried apparatus using dry solvents under anhydrous conditions, unless otherwise noted. Reaction mixtures were stirred magnetically unless otherwise stated. Commercial grade solvents were distilled and dried according to literature procedures ("Purification of laboratory chemicals", 3rd Ed., D. D. Perrin, W. L. F. Armarego, Pergamon Press, Oxford, 1988). Analytical TLC was performed on commercial plates coated with silica gel GF₂₅₄ (0.25 mm). Silica gel (230 - 400 mesh) was used for column chromatography. NMR spectra were recorded on 300 or 400 MHz instruments and chemical shifts are cited with respect to SiMe₄ as internal (¹H and ¹³C). The following abbreviations explain the multiplicity s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad and dd = doublet of a doublet. IR spectra were recorded on a FT-IR spectrometer. High-resolution mass spectra (HR-MS) were recorded on a Micromass Q-TOF mass spectrometer.

Scheme 1. Synthesis of diversely functionalized VCPs; Reagents and conditions: (a) LiAlH_4 , THF, 0 °C, 2 h (b) NaH, MeI, DMF, 0 °C rt, 1 h (c) NaH, BnBr, DMF, 0 °C to rt, 1 h.

General procedure for the reduction of cyclopropyl esters with LiAlH_4 : To a vigorously stirred suspension of LiAlH_4 (10 mmol, 1 equiv) in THF (15 mL) at 0 °C, a solution of cyclopropyl ester (10 mmol, 1 equiv) in THF (10 mL) was added drop-wise. The reaction mixture was stirred at rt for additional 1 h followed by quenching with EtOAc. The mixture was diluted with DCM (20 mL) and stirred and washed with 20% citric acid (20 mL X 2). The solvent was evaporated *in vacuo* and the resultant oil was further purified by column chromatography using silica to afford the desired cyclopropyl methanol.

General procedure for the protection of alcohol as (benzyl/methyl) ether: To a stirred solution of cyclopropyl methanol (10 mmol, 1 equiv) in dry THF (15 mL) at 0 °C, a suspension of 60% NaH in mineral oil (10 mmol, 1 equiv) was added slowly. The reaction mixture was stirred at 0 °C for additional 10 min followed by a drop wise addition of the respective alkyl halide (10 mmol, 1 equiv). The reaction mixture was allowed to warm to rt and quenched with water at 0 °C. The mixture was diluted with ether (40 mL) and stirred and

washed with water (20 mL X 2). The solvent was evaporated *in vacuo* and the resultant oil was further purified by column chromatography using silica to afford the desired VCP ether.

Scheme 2. Synthesis of VCP and its reactivity with chloramine-T; Reagents : (a) OsO₄, NMMO, ^tBuOH/H₂O, 18 h, reflux; (b) NaIO₄/Silica gel, CH₂Cl₂, 30 min, rt; (c) 4% w/v Aq. NaOH (4 mL/mmol), 10 min, rt; (d) CeCl₃.7H₂O (10 mol%), NaBH₄, MeOH, -15 °C ; (e) BnBr, DMF, 0 °C, 1 h.

General procedure for Luche's reduction: To a stirred solution of unsaturated ketone (4 mmol, 1 equiv) in MeOH (20 mL), solid CeCl₃.7H₂O was added (20 mol%) at -15 °C The mixture was stirred for additional 30 min followed by slow addition of NaBH₄ (4 mmol, 1 equiv). The reaction mixture was warmed to room temperature and the progress of the reaction was monitored by TLC. The mixture was diluted with DCM (60 mL) and stirred and washed with 20% citric acid (20 mL X 2). The organic layer was dried over Na₂SO₄ and the solvent was evaporated *in vacuo* resulting in an oily crude product. The crude product was further purified by column chromatography using silica to afford the desired VCP. **(S)-1-**

((1S,5R)-6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)ethanol 3ob: To a stirred solution of ketone **3oa** (0.22 g, 1.46 mmol, 1 equiv) in MeOH (6 mL), solid CeCl₃.7H₂O was added (0.084g, 0.30 mmol, 20 mol%) at -15

°C The mixture was stirred for additional 30 min followed by slow addition of NaBH₄ (0.055g, 1.46 mmol, 1 equiv). The reaction mixture was warmed to room temperature and the

progress of the reaction was monitored by TLC. The mixture was diluted with DCM (20 mL) and stirred and washed with 20% citric acid (10 mL). The organic layer was dried over Na₂SO₄ and the solvent was evaporated *in vacuo* resulting in an oily crude product. The crude product was further purified by column chromatography using silica to afford **3ob**. *R_f* = 0.30 (hexanes/EtOAc, 3 : 1); Yield: 0.20 g, 90%; IR (neat) $\bar{\nu}$: 3416, 2945, 2918, 1522, 1090, 738, 667 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 5.28 (s, 1H), 4.28 (dd, *J* = 5.7 Hz, 12.0 Hz, 1H), 2.35 (dd, *J* = 7.8 Hz, 18.0 Hz, 1H), 2.13 (s, 1H), 2.02–1.96 (m, 1H), 1.65–1.60 (m, 1H), 1.29–1.17 (m, 5H), 0.98 (s, 3H), 0.73 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 148.2, 122.5, 67.1, 36.7, 31.5, 29.1, 27.3, 21.8, 19.2, 13.0; HR - MS *m/z*: calcd for C₁₀H₁₆NNaO[M+Na⁺]: 175.1099; found: 175.1090.

General procedure for the synthesis of cyclic *N*-sulfonylamidines

To the stirred solution of the olefin (1 equiv) in the respective nitriles (~ 2M concentration) was added chloramine-T (1.1 equiv) and phenyltrimethylammonium bromide dibromide (**PTAB**) (10 mol%). The mixture was allowed to stir for 5- 18 h at room temperature (25 °C) and the reaction was monitored by TLC. When the reaction was found to be complete, the solvent was removed under reduced pressure. The solid residue was directly purified by flash column chromatography on silica gel. **Compound 4aa**: *R_f* = 0.25 (hexanes/EtOAc, 7 : 3); Yield: 82%; m. p. 163°C; [α]_D²⁵ = +93.0 (CHCl₃, *c* = 1); IR (neat) $\bar{\nu}$: 2945, 1643, 1336, 1159, 1091, 813 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 5.93-5.91 (m, 1H), 4.63 (t, *J* = 5.1 Hz, 1H), 2.36 (s, 3H), 2.33 (s, 1H), 1.99-1.86 (m, 4H), 1.80-1.66 (m, 2H), 1.70 (s, 3H), 1.24 (s, 3H), 1.13-1.00 (m, 1H), 1.09 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): 148.3, 143.7, 140.0, 138.9, 129.6, 129.5, 126.9, 126.2, 120.7, 52.8, 52.1, 42.6, 29.8, 28.7, 25.6, 24.7, 23.4, 21.4, 19.5; HR - MS *m/z*: calcd for C₁₉H₂₇N₂O₂S[M+H⁺]:

347.1793; found: 347.1806. CHN Analysis for $C_{19}H_{26}N_2O_2S$: C, 65.86; H, 7.56; N, 8.08; Found: C, 65.90; H, 7.47; N, 8.32.

Procedure for Cbz-deprotection in 4acB: To compound **4acB** (0.089 g, 0.27 mmol), 40% KOH in methanol solution (3 mL) was added and heated to reflux for 12 h. The solvent was removed in vacuo and the mixture was extracted in Et₂O (10 mL) and 1N HCl (10 mL) to remove the benzyl alcohol side-product by discarding the ether layer. The aqueous layer was basified with 10% NaOH followed by extraction with ether. The organic layer was separated and dried over Na₂SO₄ and the solvent was removed in vacuo to obtain the amidine **7a** (0.035 g, 68%). The crude product was found to be pure enough for characterization and processing.

Procedure for Boc-deprotection in 4aaA: To a solution **4aaA** (0.120 g, 0.29 mmol) in dry CH₂Cl₂ (1.7 mL) at 0 °C, trifluoroacetic acid (0.3 mL) was added. The starting material was completely converted to the desired amidinium trifluoroacetate in 2 h. The solvent was removed in vacuo. The crude amidine **7b** was found to be pure enough for further processing.

¹H and ¹³C Spectral Data

Compound 4aa: R_f = 0.25 (hexanes/EtOAc, 7 : 3); Yield: 82%; m. p.

163°C; $[\alpha]_D^{25} = +93.0$ (CHCl₃, c = 1); IR (neat) $\bar{\nu}$: 2945, 1643, 1336,

1159, 1091, 813 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.73 (d, J = 8.4

Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 5.93-5.91 (m, 1H), 4.63 (t, J = 5.1 Hz, 1H), 2.36 (s, 3H),

2.33 (s, 1H), 1.99-1.86 (m, 4H), 1.80-1.66 (m, 2H), 1.70 (s, 3H), 1.24 (s, 3H), 1.13-1.00 (m,

1H), 1.09 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): 148.3, 143.7, 140.0, 138.9, 129.6, 129.5,

126.9, 126.2, 120.7, 52.8, 52.1, 42.6, 29.8, 28.7, 25.6, 24.7, 23.4, 21.4, 19.5; HR - MS m/z :

calcd for C₁₉H₂₇N₂O₂S[M+H⁺]: 347.1793; found: 347.1806. CHN Analysis for C₁₉H₂₆N₂O₂S:

C, 65.86; H, 7.56; N, 8.08; Found: C, 65.90; H, 7.47; N, 8.32.

HPLC Chromatogram for Compound 4aa

Column Details : Chiralpak AD-H; 150 mm x 40mm

Solvent System : n-Heptane/Isopropyl alcohol 80:20 isocratic flow

Injection volume : 2 μ L in Isopropyl alcohol

Flow Rate : 1.0 mL/min, 5.2 MPa, 298 K

Detector Wavelength : 220 nm

Compound 4ab: R_f = 0.40 (hexanes/EtOAc, 8 : 2); Yield: 74%; $[\alpha]_D^{25}$ =

+80.0 (CHCl₃, c = 2.1) IR (neat) $\bar{\nu}$: 2964, 2930, 2873, 1645, 1339, 1156, 968, 680 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.80 (d, J = 8.4

Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 5.97 (br, 1H), 4.70 (t, J = 5.7 Hz, 1H), 2.50-2.40 (m, 1H), 2.43 (s, 3H), 2.26-2.16 (m, 1H), 2.04-1.71 (m, 5H), 1.78 (s, 3H), 1.43-1.14 (m, 3H), 1.27 (s, 3H), 1.10 (s, 3H), 0.62 (t, J = 7.2 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃): 151.9, 143.6, 139.8, 138.9, 129.5, 127.1, 120.9, 52.8, 51.9, 42.9, 39.3, 29.9, 29.0, 25.5, 23.5, 21.8, 21.5, 19.4, 13.5; HR - MS m/z : calcd for C₂₁H₃₁N₂O₂S[M+H⁺]: 375.2106; found: 375.2115.

Compound 4ac: R_f = 0.50 (hexanes/EtOAc, 7 : 3); Yield: 87%;

$[\alpha]_D^{25}$ = +90.5 (CHCl₃, c = 1); IR (neat) $\bar{\nu}$: 2927, 1652, 1340, 1149, 1093, 813 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.82 (d, J = 8.4 Hz,

2H), 7.29 (d, J = 8.4 Hz, 2H), 5.94–5.93 (m, 1H), 4.66 (dd, J = 5.1 Hz, 5.1 Hz, 1H), 2.42 (s, 3H), 1.99–1.90 (m, 2H), 1.81–1.68 (m, 3H), 1.74 (s, 3H), 1.19 (s, 3H), 1.16–1.03 (m, 1H), 1.01 (s, 3H), 0.88–0.81 (m, 1H), 0.77–0.60 (m, 2H), 0.44–0.35 (m, 1H); ¹³C NMR (75 MHz, CDCl₃): 151.6, 143.4, 139.4, 129.4, 129.4, 127.1, 121.2, 52.4, 52.3, 43.0, 29.9, 29.2, 25.5, 23.4, 21.4, 19.5, 15.7, 9.6, 9.5; HR - MS m/z : calcd for C₂₁H₂₉N₂O₂S[M+H⁺]: 373.1950; found: 373.1961.

Compound 4ad: R_f = 0.60 (hexanes/EtOAc, 8 : 2); Yield: 25%;

$[\alpha]_D^{25}$ = +66.0 (CHCl₃, c = 1.2); IR (neat) $\bar{\nu}$: 2972, 2932, 1656, 1636, 1522, 1504, 1352, 1163, 992, 674 cm⁻¹; ¹H NMR (300 MHz, CDCl₃):

δ 7.44 (d, J = 8.1 Hz, 2H), 7.19 (d, J = 8.1 Hz, 2H), 6.11 (br, 1H), 4.79 (t, J = 6 Hz, 1H), 2.40 (s, 3H), 2.25 - 1.94 (m, 2H), 1.85 (s, 5H), 1.78-1.70 (m, 1H), 1.61 (s, 1H), 1.35 (s, 3H), 1.27 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): 144.6, 140.9, 136.3, 130.2, 129.2, 127.2, 119.5, 55.4, 52.3, 42.9, 29.9, 28.5, 25.8, 23.6, 21.4, 19.2; ¹⁹F NMR (300 MHz, CDCl₃): -243.95 (d, J

= 30 Hz), -257.5 – -257.7(t, J = 24 Hz), -265.3 (t, J = 27 Hz) HR - MS m/z : calcd for $C_{24}H_{24}F_5N_2O_2S[M+H]^+$: 499.1479; found: 499.1476.

Compound 4ae: R_f = 0.40 (hexanes/EtOAc, 8 : 2); Yield: 62%; $[\alpha]_D^{25}$ =

+92.3 ($CHCl_3$, c = 0.87); IR (neat) $\bar{\nu}$: 2985, 2916, 2832, 1652, 1466,

1118 cm^{-1} ; ^1H NMR (300 MHz, $CDCl_3$): δ 7.26-7.03 (m, 9H), 6.07 (d, J

= 3.9 Hz, 1H), 4.84 (t, J = 5.4 Hz, 1H), 2.35 (s, 3H), 2.07-1.84 (m, 5H), 1.83 (s, 3H), 1.35 (s, 3H), 1.27-1.11 (m, 1H), 1.20 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): 151.3, 143.4, 139.6, 137.3, 137.0, 128.9, 128.8, 128.7, 127.7, 127.3, 120.4, 54.2, 51.5, 43.6, 29.9, 29.2, 25.1, 23.6, 21.4, 19.8; HR - MS m/z : calcd for $C_{24}H_{29}N_2O_2S[M+H]^+$: 409.1950; found: 409.1944.

Compound 4ba: R_f = 0.60 (hexanes/EtOAc, 8 : 2); Yield: 82%; $[\alpha]_D^{25}$ =

-120.8 ($CHCl_3$, c = 1); IR (neat) $\bar{\nu}$: 2945, 1643, 1336, 1159, 1091, 813

cm^{-1} ; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 6.9 Hz, 2H), 7.31 (d, J

= 6.9 Hz, 2H), 6.15 (dd, J = 4.2 Hz, 12 Hz, 1H), 5.96 (dd, J = 3.6 Hz, 8 Hz, 1H), 4.64 (dd, J = 4.4 Hz, 4.4 Hz, 1H), 2.43 (s, 3H), 2.38 (dd, J = 4.8 Hz, 9.6 Hz, 1H), 2.07 (s, 3H), 1.98-1.94 (m, 1H), 1.57 (d, J = 8.4 Hz, 1H), 1.38 (ddd, J = 3.6 Hz, 10.1 Hz, 21.2 Hz, 1H), 1.27 (s, 3H), 1.16 (s, 3H), 1.01 (d, J = 5.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.7, 143.9, 138.7, 137.5, 129.6, 127.1, 125.0, 53.0, 51.3, 38.2, 28.5, 28.5, 26.3, 26.2, 24.8, 21.5, 19.7. HR - MS m/z : calcd for $C_{19}H_{27}N_2O_2S[M+H]^+$: 347.1793; found: 347.1794

Compound 4ca: R_f = 0.60 (hexanes/EtOAc, 8 : 2); Yield: 73%; $[\alpha]_D^{25}$ =

-55.0 ($CHCl_3$, c = 1); IR (neat) $\bar{\nu}$: 2945, 1643, 1336, 1159, 1091, 813

cm^{-1} ; ^1H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 4.8 Hz, 2H), 7.21 (d, J

= 4.8 Hz, 2H), 6.23-6.20 (m, 1H), 5.85 (d, J = 8 Hz, 1H), 4.67 (dd, J = 4.4 Hz, 1H), 2.43 (s, 3H), 2.15-2.10 (m, 1H), 2.09 (s, 3H), 1.89-1.84 (m, 2H), 1.30 (s, 3H), 1.12 (s, 3H), 1.03 (d, J

= 5.6 Hz, 3H), 0.7 (dd, J = 6 Hz, 12 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): 148.6, 143.9, 138.8, 138.5, 129.7, 127.1, 125.4, 52.9, 51.4, 43.5, 30.9, 28.8, 28.3, 25.5, 24.9, 21.5, 21.0; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 347.1793; found: 347.1794.

Compound 4da: R_f = 0.60 (hexanes/EtOAc, 1 : 1); Yield: 84%;

$[\alpha]_{\text{D}}^{25}$ = +117.3 (CHCl_3 , c = 1); IR (neat) $\bar{\nu}$: 3338, 2966, 2929, 2873, 1637, 1340, 1153, 1088, 680; ^1H -NMR (400 MHz; CDCl_3): δ 7.75

(d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 6.10 (dd, J = 1.6 Hz, 3.2 Hz, 1H), 4.64 (dd, J = 5.2 Hz, 5.2 Hz, 1H), 4.02 (s, 1H), 2.51 (ddd, J = 4.8 Hz, 10.4 Hz, 14.8 Hz, 1H), 2.34 (s, 3H), 2.27 – 2.13 (m, 2H), 1.90 (s, 3H), 1.87 (m, 1H), 1.42–1.29 (m, 4H), 1.27 (s, 3H), 1.05 (s, 3H), 0.66 (t, J = 7.2 Hz, 3H); ^{13}C -NMR (100 MHz; CDCl_3): δ 152.8, 144.0, 139.0, 138.4, 129.6, 127.1, 124.5, 66.8, 60.4, 52.5, 51.4, 39.4, 37.0, 28.9, 28.8, 25.5, 21.8, 21.4, 21.0, 14.1, 13.5; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{31}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 391.2055; found: 391.2054.

Compound 4db: R_f = 0.50 (hexanes/EtOAc, 7 : 3); Yield: 80%;

$[\alpha]_{\text{D}}^{25}$ = +111.5 (CHCl_3 , c = 1); IR (neat) $\bar{\nu}$: 3376, 2967, 2927, 1643, 1336, 1157, 1089, 765, 682; ^1H -NMR (400 MHz; CDCl_3): δ

7.73 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 5.99 (dd, J = 0.8 Hz, 4 Hz, 1H), 4.72 (dd, J = 6.0 Hz, 6.0 Hz, 1H), 4.03 (s, 1H), 2.85–2.78 (m, 1H), 2.43 (s, 3H), 2.17 (ddd, J = 3.0 Hz, 6.4 Hz, 13.2 Hz, 1H), 1.95 (s, 1H), 1.88 (s, 3H), 1.86 (m, 1H), 1.34 (dt, 6.4 Hz, 13.2 Hz, 1H), 1.27 (s, 3H), 1.12 (s, 3H), 1.01 (d, J = 6.4 Hz, 3H), 0.86 (d, J = 6.4 Hz, 3H); ^{13}C -NMR (100 MHz; CDCl_3): δ 156.7, 143.6, 139.1, 138.8, 129.6, 126.6, 124.4, 66.9, 52.2, 51.3, 37.2, 34.2, 29.0, 28.6, 25.4, 22.5, 21.4, 21.0, 20.2, 19.1; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{31}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 391.2055; found: 391.2055.

Compound 4dc: R_f = 0.7 (hexanes/EtOAc, 7 : 3); Yield: 83%;

$[\alpha]_D^{25}$ = +103.4 (CHCl_3 , c = 1); IR (neat) $\bar{\nu}$: 3392, 2957, 2925,

1624, 1156, 1037, 768; $^1\text{H-NMR}$ (300 MHz; CDCl_3): δ 7.78 (d, J

= 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 6.06 (d, J = 4.8 Hz, 1H), 5.24 (s, 1H), 4.61 (dd, J = 5.7 Hz, 5.7 Hz, 1H), 4.02 (s, 1H), 2.11 (ddd, J = 3 Hz, 6 Hz, 13.2 Hz, 1H), 1.86 (s, 3H), 1.82–1.71 (m, 2H), 1.34–1.21 (m, 2H), 1.18 (s, 3H), 0.97 (s, 3H), 0.85–0.62 (m, 3H), 0.48–0.40 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz; CDCl_3): δ 152.5, 143.7, 138.7, 138.6, 129.5, 127.1, 126.3, 124.7, 67.0, 52.1, 51.7, 37.0, 29.0, 28.8, 25.4, 21.5, 21.0, 15.6, 9.9, 9.8; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{29}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 389.1899; found: 389.1892.

Compound 4dd: R_f = 0.50 (hexanes/EtOAc, 7 : 3); Yield: 74%;

$[\alpha]_D^{25}$ = +65.2 (CHCl_3 , c = 1); IR (neat) $\bar{\nu}$: 3395, 2924, 1626, 1156,

1025, 767; $^1\text{H-NMR}$ (400 MHz; CDCl_3): δ 7.24–7.21 (m, 3H),

7.13 (d, J = 6.8 Hz, 2H), 7.09–7.06 (m, 4H), 6.17 (dd, J = 0.8 Hz, 4.4 Hz, 1H), 4.79 (dd, J = 5.2 Hz, 5.2 Hz, 1H), 3.94 (s, 1H), 2.36 (s, 3H), 2.27 (ddd, J = 2.8 Hz, 6.4 Hz, 13.6 Hz, 1H), 1.91 (s, 3H), 1.87 (dt, J = 2.4 Hz, 14.4 Hz, 1H), 1.39 (dd, J = 3.6 Hz, 14.4 Hz, 1H), 1.33 (s, 3H), 1.17 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz; CDCl_3): δ 152.2, 143.7, 136.8, 129.1, 128.6, 128.2, 127.7, 127.4, 123.9, 66.7, 50.0, 51.1, 37.6, 29.2, 29.0, 26.8, 25.2, 21.4, 21.2, 21.0, 14.1; HR - MS m/z : calcd for $\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 425.1899; found: 425.1891.

Compound 4ea: R_f = 0.50 (hexanes/EtOAc, 8 : 2); Yield: 87%;

$[\alpha]_D^{25}$ = +109.1 (CHCl_3 , c = 1.1); IR (neat) $\bar{\nu}$: 2967, 2928, 2877,

1542, 1270, 1141, 1089, 711; $^1\text{H-NMR}$ (400 MHz; CDCl_3): δ 7.75

(d, J = 7.9 Hz, 2H), 7.26–7.22 (m, 3H), 5.99 (d, J = 9.7 Hz, 1H), 5.88 (dd, J = 9.5, 3.7 Hz, 1H), 3.14–3.09 (m, 1H), 2.75 (t, J = 7.9 Hz, 2H), 2.40–2.25 (m, 8H), 2.04 (s, 3H), 1.69 (dd, J = 15.5, 7.6 Hz, 2H), 1.35–1.22 (m, 8H), 1.01 (t, J = 7.2 Hz, 3H). $^{13}\text{C-NMR}$ (100 MHz;

CDCl₃): δ 201.1, 167.0, 141.8, 140.9, 138.2, 132.6, 131.3, 129.9, 129.6, 129.02, 128.97, 127.1, 125.9, 58.4, 40.0, 36.9, 29.8, 25.3, 24.22, 24.12, 21.3, 21.0, 20.2, 13.7; HR - MS m/z : calcd for C₂₃H₃₃N₂O₃S[M+Na⁺]: 439.2031; found: 439.2034.

Compound 4eb: R_f = 0.70 (hexanes/EtOAc, 8 : 2); Yield: 85%;

$[\alpha]_D^{25}$ = +146.3 (CHCl₃, c = 1); IR (neat) $\bar{\nu}$: 2968, 2925, 1706,

1361, 1088, 677; ¹H-NMR (400 MHz; CDCl₃): δ 7.79 (d, J = 8.2

Hz, 2H), 7.30 (d, J = 8.1 Hz, 2H), 6.17 (d, J = 3.9 Hz, 1H), 4.60 (t, J = 5.2 Hz, 1H), 3.13 (d, J = 6.5 Hz, 1H), 2.42 (s, 3H), 2.21 (s, 3H), 1.91 (d, J = 13.9 Hz, 1H), 1.81 (ddt, J = 16.3, 7.8, 3.9 Hz, 1H), 1.75 (s, 3H), 1.64 (s, 1H), 1.39 (td, J = 13.6, 6.8 Hz, 1H), 1.13 (s, 3H), 0.85 (s, 3H), 0.79 (dd, J = 4.2, 2.6 Hz, 2H), 0.68 (dd, J = 12.3, 6.6 Hz, 1H), 0.50 (td, J = 8.4, 3.4 Hz, 1H). ¹³C-NMR (100 MHz; CDCl₃): δ 208.73, 152.07, 143.71, 138.35, 135.37, 129.45, 127.16, 125.24, 52.63, 52.00, 51.74, 38.83, 29.27, 29.06, 25.23, 23.03, 22.64, 21.45, 15.56, 10.01, 9.90; HR - MS m/z : calcd for C₂₃H₃₁N₂O₃S[M+H⁺]: 415.2055; found: 415.2052.

Compound 4ec: R_f = 0.50 (hexanes/EtOAc, 8 : 2); Yield: 80%;

$[\alpha]_D^{25}$ = +129.0 (CHCl₃, c = 1); IR (neat) $\bar{\nu}$: 2968, 2926, 2857, 1715,

1340, 1157, 1088, 768; ¹H-NMR (400 MHz; CDCl₃): δ 7.25 (dt, J

= 23.1, 8.4 Hz, 5H), 7.13 (dd, J = 12.5, 7.8 Hz, 4H), 6.27 (d, J = 3.7 Hz, 1H), 4.80 (t, J = 5.2 Hz, 1H), 3.18 (d, J = 6.3 Hz, 1H), 2.38 (s, 3H), 2.24 (s, 3H), 2.02-1.91 (m, 2H), 1.83 (s, 3H), 1.64-1.46 (m, 3H), 1.31 (s, 3H), 1.07 (s, 3H). ¹³C NMR (100 MHz; CDCl₃): δ 208.6, 151.6, 143.8, 137.2, 136.7, 135.6, 129.13, 129.11, 128.6, 127.9, 127.5, 124.5, 53.9, 52.7, 51.1, 39.6, 29.4, 29.1, 25.0, 23.2, 23.0, 21.4; HR - MS m/z : calcd for C₂₆H₃₁N₂O₃S[M+H⁺]: 451.2055; found: 451.2053

Compound 4fa: $R_f = 0.30$ (hexanes/EtOAc, 8 : 2); Yield: 80%;

$[\alpha]_D^{25} = +52.8$ (CHCl₃, $c = 1$); IR (neat) $\bar{\nu}$: 2968, 2926, 2857, 1715,

1340, 1157, 1088, 768; ¹H-NMR (400 MHz; CDCl₃): δ 7.77 (d, $J =$

8.0 Hz, 2H), 7.32 (d, $J = 8.0$ Hz, 2H), 6.09 (s, 1H), 4.63 (s, 1H), 4.13 (dd, $J = 9.1, 4.9$ Hz, 1H), 2.60 (ddd, $J = 14.4, 9.4, 5.3$ Hz, 1H), 2.43 (s, 3H), 2.31-2.21 (m, 2H), 2.00 (dd, $J = 26.4, 11.9$ Hz, 3H), 1.84 (s, 3H), 1.38 (dt, $J = 16.0, 8.0$ Hz, 2H), 1.27-1.13 (m, 8H), 0.97 (s, 3H), 0.71 (t, $J = 7.3$ Hz, 3H); ¹³C-NMR (100 MHz; CDCl₃): δ 151.68, 143.85, 138.40, 138.35, 129.64, 127.09, 126.04, 67.19, 53.10, 51.86, 44.57, 39.87, 39.55, 28.85, 26.09, 22.06, 21.75, 21.49, 20.57, 20.28, 13.57; HR - MS m/z : calcd for C₂₃H₃₅N₂O₃S[M+H⁺]: 419.2368; found: 419.2364.

Compound 4fb: $R_f = 0.50$ (hexanes/EtOAc, 8 : 2); Yield: 76%;

$[\alpha]_D^{25} = +52.3$ (CHCl₃, $c = 1$); IR (neat) $\bar{\nu}$: 3410, 2961, 2925, 2863,

1600, 1157, 1088, 1025, 767; ¹H-NMR (400 MHz; CDCl₃): δ 7.76

(d, $J = 8.3$ Hz, 2H), 7.31 (d, $J = 8.1$ Hz, 2H), 6.00 (dd, $J = 2.6, 0.6$ Hz, 1H), 4.70 (t, $J = 4.6$ Hz, 1H), 4.12 (qd, $J = 6.2, 4.7$ Hz, 1H), 2.89 (dt, $J = 13.3, 6.6$ Hz, 1H), 2.43 (s, 3H), 2.31 (ddd, $J = 12.5, 7.1, 3.5$ Hz, 1H), 1.99 (dd, $J = 11.3, 2.9$ Hz, 2H), 1.81 (s, 3H), 1.68 (s, 3H), 1.27 (s, 3H), 1.04 (s, 3H), 1.03 (d, $J = 5.6$ Hz, 3H), 0.91 (d, $J = 6.7$ Hz, 3H); ¹³C-NMR (100 MHz; CDCl₃): δ 155.71, 143.59, 139.15, 138.11, 129.62, 126.82, 126.46, 125.96, 67.28, 52.86, 51.78, 44.68, 40.20, 34.26, 29.10, 25.88, 22.57, 22.07, 21.53, 20.56, 20.12, 19.28; HR - MS m/z : calcd for C₂₃H₃₅N₂O₃S[M+H⁺]: 419.2368; found: 419.2368.

Compound 4fc: $R_f = 0.50$ (hexanes/EtOAc, 8 : 2); Yield: 80%;

$[\alpha]_D^{25} = +56.2$ (CHCl₃, $c = 1$); IR (neat) $\bar{\nu}$: 3423, 2960, 2925, 1604,

1156, 1047, 771; ¹H-NMR (400 MHz; CDCl₃): δ 7.81 (d, $J = 8.2$

Hz, 2H), 7.30 (d, $J = 8.0$ Hz, 2H), 6.11 (dd, $J = 2.6, 0.8$ Hz, 1H), 4.63 (t, $J = 4.6$ Hz, 1H),

4.15-4.11 (m, 1H), 2.42 (s, 3H), 2.25 (ddd, $J = 12.1, 6.8, 3.4$ Hz, 1H), 1.97 (dd, $J = 11.5, 2.9$ Hz, 2H), 1.82 (s, 3H), 1.25 (d, $J = 6.4$ Hz, 3H), 1.19 (s, 3H), 1.10 (dt, $J = 13.1, 6.7$ Hz, 1H), 0.90 (s, 3H), 0.80 (d, $J = 4.8$ Hz, 2H), 0.67 (ddd, $J = 11.3, 8.5, 2.6$ Hz, 1H), 0.49 (td, $J = 7.9, 3.2$ Hz, 1H). ^{13}C -NMR (100 MHz; CDCl_3): δ 151.36, 143.63, 138.80, 138.08, 129.50, 127.14, 126.41, 67.23, 52.63, 52.19, 44.63, 39.87, 28.96, 26.04, 22.03, 21.52, 20.50, 20.25, 15.70, 9.92, 9.66; HR - MS m/z : calcd for $\text{C}_{23}\text{H}_{33}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 417.2212; found: 417.2214.

Compound 4fd: $R_f = 0.50$ (hexanes/EtOAc, 8 : 2); Yield: 72%;

$[\alpha]_{\text{D}}^{25} = +69.2$ (CHCl_3 , $c = 1$); IR (neat) $\bar{\nu}$: 3410, 2961, 2925, 2863, 1600, 1157, 1088, 1025, 767; ^1H -NMR (400 MHz; CDCl_3): δ 7.30-

7.10 (m, 9H), 6.20 (s, 1H), 4.81 (s, 1H), 4.15 (dd, $J = 6.1, 3.1$ Hz, 1H), 2.47-2.33 (m, 5H), 2.07-1.96 (m, 2H), 1.88 (d, $J = 19.4$ Hz, 3H), 1.36 (s, 3H), 1.26 (d, $J = 6.3$ Hz, 3H), 1.19 (dd, $J = 18.2, 5.8$ Hz, 2H), 1.11 (s, 3H). ^{13}C -NMR (100 MHz; CDCl_3): δ 151.11, 143.71, 138.46, 137.29, 137.09, 129.16, 128.95, 128.71, 127.84, 127.51, 127.38, 126.23, 125.43, 67.25, 54.60, 51.60, 44.76, 40.68, 29.11, 25.77, 22.25, 21.51, 20.67, 20.61; HR - MS m/z : calcd for $\text{C}_{26}\text{H}_{33}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 453.2212; found: 453.2213.

Compound 5a: $R_f = 0.20$ (hexanes/EtOAc, 9 : 1); Yield: 35%; IR

(neat) $\bar{\nu}$: 3296, 2967, 2921, 1632, 1435, 667 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): 7.84 (d, $J = 8.4$ Hz, 2H), 7.34 (d, $J = 8.4$ Hz, 2H), 5.70 (s, 1H), 4.79 (dd, $J = 6.6$ Hz, 6.6 Hz, 1H), 2.45 (s, 3H), 2.07-

2.02 (m, 3H), 1.84 (s, 3H), 1.79 (s, 3H), 1.73 (s, 3H), 1.61-1.45 (m, 1H), 1.34 (s, 3H), 1.21 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): 150.6, 143.8, 140.2, 139.0, 129.7, 126.7, 119.4, 53.6, 52.1, 46.1, 43.6, 30.0, 28.8, 25.4, 23.4, 22.1, 21.6, 18.9. ; HR - MS m/z : calcd for $\text{C}_{20}\text{H}_{31}\text{BrN}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 441.1211; found: 441.1217.

7-phenylbicyclo[4.1.0]hept-2-en-7-yl)methanol: To a vigorously stirred suspension of LiAlH_4 (0.38 g, 10 mmol, 1 equiv) in THF (15 mL) at 0 °C, a solution of cyclopropyl ester **3ga** (2.3 g, 10 mmol, 1 equiv) in THF (10 mL) was added drop wise. The reaction mixture was stirred at rt for additional 1 h followed by quenching with EtOAc. The mixture was diluted with DCM (20 mL) and washed with 20% citric acid. The solvent was evaporated *in vacuo* and the resultant oil was further purified by column chromatography using silica to give **3gb** as colorless oil. R_f = 0.50 (hexanes/EtOAc : 8:2); Yield: 1.86 g, 93%; IR (neat) $\bar{\nu}$: 3331, 2948, 2945, 830, 776 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.29-7.19 (m, 5H), 6.07-6.03 (m, 1H), 5.31 (ddd, J = 1.6, 8.4, 13.2 Hz, 1H), 3.55-3.53 (m, 1H), 3.35-3.31 (m, 1H), 1.96 (dd, J = 11.6, 18.4 Hz, 1H), 1.80-1.53 (m, 6H), 0.55-0.41 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): 138.1, 130.7, 128.0, 126.5, 126.0, 124.6, 72.8, 40.9, 22.6, 21.5, 19.4, 17.0; HR - MS m/z : calcd for $\text{C}_{14}\text{H}_{16}\text{O}$ [$\text{M}+\text{H}^+$]: 200.1201; found: 200.1193.

Compound 3g: To a solution of **3gb** (0.90 g, 5 mmol, 1 equiv) in dry DMF, (15 mL) cooled to -15 °C under inert atmosphere was added NaH (60% suspension in mineral oil) (0.24 g, 6 mmol, 1.2 equiv) at once and stirred vigorously until all the effervescence ceased. To this MeI (2.50 g, 0.93 mL, 1.1 equiv) was added drop wise and the mixture was allowed to stir at rt for 30 min. The reaction was quenched by the addition of water drop wise and the mixture was extracted with diethyl ether. The solution was concentrated *in vacuo* and was purified by column chromatography using silica gel to yield compound **3g** as colorless oil. R_f = 0.50 (hexanes); Yield: 1.50 g 98%; ^1H NMR (300 MHz, CDCl_3): δ 7.27-7.17 (m, 5H), 6.07-6.04 (m, 1H), 5.30 (ddd, J = 1.6, 8.4,

13.2 Hz, 1H), 3.38 (d, J = 6.4 Hz, 1H), 3.24 (d, J = 6.4 Hz, 1H), 3.21 (s, 3H), 1.96 (dd, J = 8.8, 14.0 Hz, 1H), 1.72-1.62 (m, 1H), 1.60-1.50 (m, 2H), 0.52-0.42 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): 138.8, 130.7, 127.6, 126.1, 126.0, 124.6, 82.6, 58.8, 38.6, 24.5, 21.5, 19.4, 17.0; HR - MS m/z : calcd for $\text{C}_{15}\text{H}_{19}\text{O}$ [$\text{M}+\text{H}^+$]: 214.1358; found: 214.1362.

Bicyclo[3.1.0]hex-2-en-6-yl methanol: R_f = 0.50 (hexanes); Yield: 95%;

^1H -NMR (400 MHz; CDCl_3): δ 5.91 – 5.89 (m, 1H), 5.42 (dd, J = 2.4 Hz, 2.4 Hz, 1H), 3.53–3.49 (m, 1H), 3.42–3.37 (m, 1H), 2.58 (dd, J = 6.4 Hz, 17.6 Hz, 1H), 2.34 (d, J = 17.6 Hz, 1H), 2.24 (s, 1H), 1.79–1.78 (m, 1H), 1.51–1.47 (m, 1H), 0.57–0.54 (m, 1H). ^{13}C -NMR (100 MHz; CDCl_3): δ 133.1, 128.7, 66.0, 35.5, 31.7, 29.1, 24.4; HR - MS m/z : calcd for $\text{C}_{14}\text{H}_{16}\text{O}$ [$\text{M}+\text{Na}^+$]: 223.1099; found: 223.1093.

Compound 4ga: R_f = 0.30 (hexanes/EtOAc, 8 : 2); Yield: 72%; IR (neat)

$\bar{\nu}$: 2948, 2945, 1643, 1340, 1156, 1091, 830, 776 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.44 (d, J = 8.4 Hz, 2H), 7.36-7.26 (m, 5H), 7.18 (d, J = 8.4 Hz, 2H), 6.14 (dd, J = 1.5 Hz, 1H), 6.02 (dd, J = 1.5 Hz, 1H), 4.10 (m, 1H), 3.75 (d, J = 9.6 Hz, 1H), 3.47 (d, J = 9.2 Hz, 1H), 3.23 (s, 3H), 2.8-2.78 (m, 1H), 2.43-2.38 (m, 2H), 2.42 (s, 3H), 2.30 – 2.14 (m, 2H), 2.24 (s, 3H), 1.87-1.85 (m, 1H), 0.87 -0.85 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): 150.6, 143.8, 143.2, 138.3, 132.1, 129.7, 128.4, 127.2, 126.9, 126.4, 79.2, 61.7, 59.3, 51.8, 38.3, 25.1, 24.8, 21.5, 18.7; HR - MS m/z : calcd for $\text{C}_{24}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ [$\text{M}+\text{H}^+$]: 425.1899; found: 425.1903.

Compound 6a: R_f = 0.50 (hexanes/EtOAc, 7 : 3); Yield: 68%; IR

(neat) $\bar{\nu}$: 2942, 2940, 1341, 1056, 1090, 831, 776 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.80 (d, J = 8.0 Hz, 2H), 7.34–7.25 (m, 7H), 4.36 (s, 2H), 3.30–3.20 (m, 3H), 2.96–2.95 (m, 1H), 2.37 (s, 3H), 1.86–1.76 (m, 1H), 1.73–1.65 (m,

2H), 1.62–1.54 (m, 1H), 1.29–1.19 (m, 1H), 0.96–0.92 (m, 2H), 0.67–0.60 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): 144.0, 138.4, 135.7, 129.5, 128.3, 127.5, 127.4, 72.4, 72.0, 38.1, 22.1, 21.5, 20.1, 17.9, 11.6, 10.8; HR - MS m/z : calcd for $\text{C}_{22}\text{H}_{26}\text{NO}_3\text{S}$ $[\text{M}+\text{H}^+]$: 384.1633; found: 384.1634.

Compound 6b: $R_f = 0.50$ (hexanes/EtOAc, 7 : 3); Yield: 60%; IR

(neat) $\bar{\nu}$: 2952, 2947, 1346, 1053, 1092, 831, 770 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.82 (d, $J = 8.0$ Hz, 2H), 7.35–7.25 (m, 7 Hz), 4.43 (s, 2H) 3.44–3.37(m, 1H), 3.33–3.27 (m, 1H), 3.15–3.04 (m, 2H), 2.40 (s, 3H), 2.19–2.13 (m, 1H), 1.60–1.57 (m, 1H), 1.42–1.36 (m, 1H), 1.11–0.92 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): 143.4, 138.0, 137.3, 129.6, 129.5, 128.4, 127.6, 127.4, 72.7, 71.3, 47.7, 36.5, 24.9, 21.54, 18.0; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{24}\text{NO}_3\text{S}$ $[\text{M}+\text{H}^+]$: 370.1477; found: 370.1463.

Compound 4aaA: $R_f = 0.30$ (hexanes/EtOAc, 8 : 2); Yield: 86%; IR

(neat) $\bar{\nu}$: 2948, 2945, 1643, 1340, 1156, 1091, 830, 776 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3): δ 5.79 (s, 1H), 4.27 (s, 1H), 2.24 (s, 3H), 1.89-1.73 (m, 4H), 1.69 (s, 3H), 1.51 (s, 9H), 1.43 (s, 2H), 1.30-1.24 (m, 4H), 1.08-1.01 (m, 4H). ^{13}C -NMR (100 MHz; CDCl_3): δ 152.80, 152.38, 138.15, 120.62, 81.72, 53.76, 50.63, 42.94, 29.60, 28.94, 28.30, 25.70, 24.45, 23.67, 20.39; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}^+]$: 293.2229; found: 293.2225.

Compound 4abA: $R_f = 0.30$ (hexanes/EtOAc, 8 : 2); Yield: 85%; IR

(neat) $\bar{\nu}$: 2970, 2945, 1643, 1340, 1156, 1091, 830, 776 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3): δ 5.77 (s, 1H), 4.31 (dd, $J = 1$ Hz, 1Hz, 1H), 2.85–2.76 (m, 1H), 2.47–2.38 (m, 1H), 1.93–1.71 (m, 4H), 1.79 (s, 3H), 1.51 (s, 9H), 1.33 (s, 3H), 1.10 (s, 3H), 1.08 (t, $J = 7.3$ Hz, 3H); ^{13}C -NMR (100 MHz; CDCl_3): δ 152.80, 152.38,

138.15, 120.62, 81.72, 53.76, 50.63, 42.94, 29.60, 28.94, 28.30, 25.70, 24.45, 23.67, 20.39;
 HR - MS m/z: calcd for C₁₉H₂₇N₂O₂[M+H⁺]: 293.2229; found: 293.2225.

Compound 4acA: : *R_f* = 0.30 (hexanes/EtOAc, 9 : 1); Yield: 74%;

IR (neat) $\bar{\nu}$: 2975, 2929, 1705, 1634, 1323, 1159, 891, 773 cm⁻¹; ¹H-

NMR (400 MHz; CDCl₃): δ 5.81 (s, 1H), 4.28 (s, 1H), 1.88-1.82 (m,

2H), 1.75-1.72 (m, 2H), 1.72 (s, 3H), 1.52 (s, 9H), 1.52 (m, 1H), 1.25 (s, 3H), 1.03 (s, 3H),
 0.98-0.91 (m, 3H), 0.89-0.86 (m, 2H), 0.84-0.79 (m, 1H); ¹³C-NMR (100 MHz; CDCl₃): δ
 156.4, 153.3, 137.7, 120.8, 81.2, 53.6, 50.6, 43.5, 29.6, 29.3, 28.3, 24.1, 23.6, 20.2, 17.0, 9.9,
 8.0 ; HR - MS m/z: calcd for C₁₉H₃₁N₂O₂ [M+H⁺]: 319.2386; found: 319.2386.

Compound 4aaB: *R_f* = 0.30 (hexanes/EtOAc, 8 : 2); Yield: 73%; IR

(neat) $\bar{\nu}$: 2975, 2914, 1753, 1574, 1307, 1238, 1001, 830, 776 cm⁻¹;

¹H-NMR (300 MHz; CDCl₃): δ 7.40-7.30 (m, 5H), 5.83 (s, 1H),

5.27 (d, *J* = 12.6 Hz, 1H), 5.21 (d, *J* = 12.6 Hz, 1H), 4.36 (s, 1H), 1.90-1.83 (m, 2H), 1.78-
 1.71 (m, 2H), 1.71 (s, 3H), 1.25 (s, 3H), 1.02 (s, 3H), 1.00-0.93 (m, 2H), 0.90-0.58 (m, 3H);
¹³C-NMR (100 MHz; CDCl₃): δ 156.1, 154.6, 138.2, 136.5, 129.0, 128.7, 128.4, 120.9, 68.2,
 54.2, 51.5, 43.6, 30.1, 29.8, 24.7, 24.2, 20.7, 17.4, 10.4, 9.4; HR - MS m/z: calcd for
 C₂₂H₂₉N₂O₂ [M+H⁺]: 353.2229; found: 353.2238.

Compound 4abB: *R_f* = 0.30 (hexanes/EtOAc, 8 : 2); Yield: 69%; IR

(neat) $\bar{\nu}$: 2975, 2914, 1750, 1544, 1313, 1238, 1004, 833, 779 cm⁻¹;

¹H-NMR (300 MHz; CDCl₃): δ 7.37-7.26 (m, 5H), 5.77 (s, 1H), 5.27

(d, *J* = 12.3 Hz, 1H), 5.17 (d, *J* = 12.3 Hz, 1H), 4.39 (s, 1H), 2.83 (ddd, *J* = 6.9 Hz, 8.7 Hz,
 15.3 Hz, 1H), 2.37-2.27 (m, 1H), 1.89-1.76 (m, 3H), 1.70 (s, 3H), 1.56-1.38 (m, 2H), 1.32
 (s, 3H), 1.19-1.01 (m, 1H), 1.07 (s, 3H). ¹³C-NMR (100 MHz; CDCl₃): 156.4, 154.9, 138.9,

138.6, 129.5, 127.1, 120.9, 68.1, 52.8, 51.9, 42.9, 29.9, 29.1, 25.2, 23.5, 21.8, 21.5, 19.4, 13.5; HR - MS m/z : calcd for $C_{22}H_{31}N_2O_2$ $[M+H]^+$: 355.2386; found: 355.2382.

Compound 4acB: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 69%;

$[\alpha]_D^{25}$ = +57.5 ($CHCl_3$, c = 1); IR (neat) $\bar{\nu}$: 2975, 2914, 1750, 1544, 1313, 1238, 1004, 833, 779 cm^{-1} ; ^1H -NMR (400 MHz; $CDCl_3$): δ

7.49-7.47 (m, 2H), 7.35-7.26 (m, 3H), 7.20-7.13 (m, 3H), 6.75 (d, J = 7.1 Hz, 2H), 5.99 (s, 1H), 4.97 (d, J = 12.4 Hz, 1H), 4.89 (d, J = 12.4 Hz, 1H), 4.53 (d, J = 0.4 Hz, 1H), 1.95-1.80 (m, 4H), 1.76 (s, 3H), 1.44 (s, 3H), 1.19 (s, 3H), 1.04 (qd, J = 12.6, 5.9 Hz, 1H). ^{13}C -NMR (101 MHz; $CDCl_3$): δ 154.07, 153.04, 138.91, 138.87, 135.25, 129.15, 128.17, 128.12, 127.76, 127.52, 126.54, 119.71, 67.74, 55.58, 51.25, 43.85, 29.61, 29.26, 23.75, 23.64, 20.59.

Compound 3j: ^1H -NMR (400 MHz; $CDCl_3$): δ 7.36-7.23 (m, 8H), 5.68

(d, J = 1.4 Hz, 1H), 4.62 (d, J = 11.9 Hz, 1H), 4.49 (d, J = 11.9 Hz, 1H), 3.53 (t, J = 4.5 Hz, 1H), 2.17 (dq, J = 11.1, 4.1 Hz, 1H), 1.77-1.70 (m,

4H), 1.07 (s, 4H), 0.88 (td, J = 8.5, 4.2 Hz, 1H), 0.82 (s, 3H). ^{13}C -NMR (100 MHz; $CDCl_3$): δ 139.16, 138.24, 134.51, 128.38, 128.24, 127.78, 127.76, 127.61, 127.36, 124.63, 73.31, 72.09, 70.35, 27.80, 24.39, 23.28, 22.66, 21.59, 17.83, 15.18; HR - MS m/z : calcd for $C_{19}H_{27}N_2O_2S$ $[M+H]^+$: 256.1568; found: 256.1565.

Compound 4jaA: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 82%;

$[\alpha]_D^{25}$ = +107.2 ($CHCl_3$, c = 1); IR (neat) $\bar{\nu}$: 2975, 2934, 1702, 1634, 1302, 1152, 776; ^1H -NMR (400 MHz; $CDCl_3$): δ 7.35-7.29

(m, 5H), 5.97 (d, J = 2.9 Hz, 1H), 4.62 (d, J = 11.7 Hz, 1H), 4.49 (d, J = 11.7 Hz, 1H), 3.69 (s, 1H), 2.25-2.18 (m, 4H), 2.08 (d, J = 14.2 Hz, 1H), 1.79 (d, J = 20.4 Hz, 4H), 1.46-1.41 (m, 10H), 1.29 (s, 3H), 1.19-1.11 (m, 4H). ^{13}C -NMR (100 MHz; $CDCl_3$): δ 153.25, 152.73,

138.57, 136.37, 128.47, 128.06, 127.79, 125.04, 82.04, 74.40, 71.89, 53.55, 50.57, 37.18, 28.83, 28.35, 25.72, 24.65, 24.49, 21.56; HR - MS m/z : calcd for $C_{19}H_{27}N_2O_2S[M+H]^+$: 399.2648; found: 399.2648.

Compound 8a: R_f = 0.30 (hexanes/EtOAc, 8 : 2); Yield: 43%; IR

(neat) $\bar{\nu}$: 3588, 3476, 2982, 2946, 1756, 1575, 1331, 1181, 831 cm^{-1} ; ^1H -NMR (400 MHz; $CDCl_3$): δ 7.40–7.36 (m, 10H), 5.83–

5.82 (m, 1H), 5.25 (dd, J = 12Hz, 17.2 Hz, 2H), 5.11 (s, 2H), 4.70 (m, 2H), 4.41–4.39 (m, 1H), 2.30 (s, 3H), 1.93–1.74 (m, 4H), 1.71 (s, 3H), 1.34 (s, 3H), 1.10 (s, 3H), 1.11–1.10 (m, 1H). ^{13}C -NMR (101 MHz; $CDCl_3$): δ 157.4, 154.2, 152.3, 139.2, 136.7, 136.2, 129.1, 129.0, 128.8, 128.7, 128.6, 120.7, 68.4, 67.3, 54.4, 51.4, 43.1, 30.1, 29.4, 26.0, 25.0, 24.2, 20.8; HR - MS m/z : calcd for $C_{28}H_{35}N_3O_4[M+Na]^+$: 500.2525; found: 500.2520. Traces of cyclized product was also found; HR - MS m/z : calcd for $C_{20}H_{26}N_2O_2[M+Na]^+$: 349.1892; found: 349.1887.

Compound 8b: R_f = 0.30 (hexanes/EtOAc, 8 : 2); Yield: 45%;

$[\alpha]_D^{25}$ = +81.2 ($CHCl_3$, c = 2.0); IR (neat) $\bar{\nu}$: 3576, 3480, 2967, 2942, 1761, 1570, 1335, 1187, 778 cm^{-1} ; ^1H -NMR (400 MHz; $CDCl_3$): δ 7.37–7.35 (m, 10H), 5.97 (d, J = 3.2 Hz, 1H), 5.27–

5.19 (m, 2H), 4.62 (d, J = 11.7 Hz, 1H), 4.49 (d, J = 11.7 Hz, 1H), 4.43 (s, 1H), 3.69 (s, 1H), 2.28 (s, 3H), 2.23 (ddd, J = 13.1, 7.7, 2.9 Hz, 1H), 2.10 (d, J = 14.3 Hz, 1H), 1.76 (s, 3H), 1.30 (s, 3H), 1.21–1.14 (m, 1H), 1.11 (s, 3H); ^{13}C -NMR (100 MHz; $CDCl_3$): δ 156.76, 153.59, 152.51, 138.47, 136.85, 136.21, 135.59, 128.76, 128.72, 128.68, 128.65, 128.55, 128.52, 128.50, 128.43, 128.39, 128.36, 128.22, 128.18, 128.13, 128.09, 127.99, 127.77, 124.50, 74.26, 71.88, 68.02, 66.91, 53.64, 50.79, 36.81, 28.78, 25.50, 24.58, 24.47, 21.50; HR - MS m/z : calcd for $C_{35}H_{41}N_3O_5[M+Na]^+$: 606.2944; found: 606.2971.

Compound 7a: Yield: 63%; IR (neat) $\bar{\nu}$: 3347, 2927, 1620, 1332, 1273,

772 cm^{-1} ; ^1H NMR (400 MHz, Benzene- d_6): δ 7.90 – 7.89 (m, 2H), 7.24 (s, 1H), 7.21 – 7.20 (m, 3H), 5.84 (s, 1H), 4.09 (m, 1H), 1.86 (s, 3H),

1.72 (s, 3H), 1.61-1.58 (m, 1H), 1.32 – 1.30 (m, 2H), 1.22 (s, 6H); ^{13}C NMR (100 MHz, Benzene d_6): 149.8, 137.6, 129.2, 127.9, 127.6, 126.5, 51.2, 39.1, 30.8, 27.5, 23.3, 19.4; HR - MS m/z : calcd for $\text{C}_{17}\text{H}_{22}\text{N}_2[\text{M}+\text{H}^+]$: 255.1861; found: 255.1862.

Compound 7b: Yield: 76%; IR (neat) $\bar{\nu}$: 3352, 2922, 1621, 1325, 1274,

769, 699 cm^{-1} ; ^1H NMR (400 MHz, Benzene- D_6): δ 6.99, 6.88 (s, 1H), 5.82 (d, $J = 3.6$ Hz, 1H), 3.93 (s, 1H), 2.00 (s, 3H), 1.88 (d, $J = 4.0$ Hz,

2H), 1.73 (s, 3H), 1.59 (s, 1H), 1.22 (s, 3H), 1.20 (s, 3H), 1.10–1.01 (m, 1H); ^{13}C NMR (100 MHz, Benzene d_6): 152.1, 136.1, 122.5, 50.7, 47.4, 38.5, 30.6, 30.5, 26.4, 23.1, 20.6, 19.1; HR - MS m/z : calcd for $\text{C}_{12}\text{H}_{21}\text{N}_2[\text{M}+\text{H}^+]$: 193.1705; found: 193.1706.

Compound 4ka: $R_f = 0.70$ (hexanes/EtOAc, 7 : 3); Yield: 92%;

$[\alpha]_D^{25} = 79.3$ (CHCl_3 , $c = 1.01$); IR (neat) $\bar{\nu}$: 2964, 2930, 2873,

1649, 1343, 1156, 970, 681 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3):

δ 7.76 (d, $J = 8.3$ Hz, 2H), 7.31 (m, $J = 7.1$ Hz, 7H), 5.86 (s, 1H), 4.95 (d, $J = 8.7$ Hz, 1H), 4.46 (d, $J = 11.7$ Hz, 1H), 4.33 (d, $J = 11.6$ Hz, 1H), 4.09 (q, $J = 6.3$ Hz, 1H), 2.81 (dd, $J_1 = 18.0$, $J_2 = 9.0$ Hz, 1H), 2.42 (s, 3H), 2.37 (d, $J = 8.6$ Hz, 1H), 2.30 (d, $J = 8.2$ Hz, 1H), 2.27 (s, 3H), 1.26 (d, $J = 9.0$ Hz, 3H), 1.26 (s, 3H), 0.95 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): 150.6, 150.2, 144.2, 138.2, 137.3, 129.7, 128.4, 127.7, 127.5, 127.2, 72.7, 70.2, 62.9, 52.1, 49.3, 32.0, 29.6, 25.8, 25.7, 21.5, 19.6. HR - MS m/z : calcd for $\text{C}_{26}\text{H}_{33}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 453.2212; found: 453.2211.

Compound 4kb: $R_f = 0.70$ (hexanes/EtOAc, 7 : 3); Yield: 91%;

$[\alpha]_D^{25} = 47.9$ (CHCl₃, $c = 1.11$); IR (neat) $\bar{\nu}$: 2979, 2925, 2890,

1647, 1332, 1153, 679 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ 7.81

(d, $J = 7.9$ Hz, 2H), 7.35-7.26 (m, 7H), 5.79 (s, 1H), 4.98 (d, $J = 8.8$ Hz, 1H), 4.49 (d, $J = 11.7$ Hz, 1H), 4.34 (d, $J = 11.7$ Hz, 1H), 4.09 (q, $J = 6.4$ Hz, 1H), 2.80 (dd, $J = 16.0, 8.0$ Hz, 1H), 2.42 (s, 3H), 2.26 (dd, $J = 17.8, 8.2$ Hz, 2H), 2.13-2.08 (m, 1H), 1.26 (d, $J = 6.5$ Hz, 3H), 1.18 (s, 3H), 0.88 (s, 3H), 0.75-0.70 (m, 2H), 0.59-0.53 (m, 1H). ¹³C NMR (100 MHz, CDCl₃): 154.2, 149.9, 143.8, 138.3, 137.7, 129.6, 128.3, 127.8, 127.6, 127.5, 127.3, 127.2, 72.8, 70.1, 63.1, 51.7, 49.5, 31.9, 29.9, 25.4, 21.5, 19.8, 15.9, 10.0, 9.0; HR - MS m/z : calcd for C₂₈H₃₄N₂O₃S[M+H⁺]: 479.2368; found: 479.2361.

Compound 4kc: $R_f = 0.70$ (hexanes/EtOAc, 7 : 3); Yield: 81%;

$[\alpha]_D^{25} = 13.5$ (CHCl₃, $c = 1.00$); IR (neat) $\bar{\nu}$: 2967, 2936, 2874,

1626, 1348, 1167, 681 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ 7.42

(d, $J = 8.0$ Hz, 2H), 7.35-7.20 (m, 12H), 5.83 (s, 1H), 5.28 (d, $J = 9.0$ Hz, 2H), 4.45 (d, $J = 11.8$ Hz, 1H), 4.32 (d, $J = 11.8$ Hz, 1H), 4.10 (q, $J = 6.3$ Hz, 1H), 3.02 (dd, $J_1 = 17.0, J_2 = 8.5$ Hz, 1H), 2.42 (s, 1H), 2.28 (dd, $J = 16.9, 8.4$ Hz, 1H), 1.38 (s, 3H), 1.26 (d, $J = 6.4$ Hz, 3H), 1.18 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): 153.8, 150.9, 143.9, 138.2, 137.9, 136.8, 129.4, 129.3, 128.4, 128.3, 127.8, 127.7, 127.4, 126.0, 73.1, 70.3, 62.8, 53.9, 50.4, 32.4, 25.1, 21.5, 20.1; HR - MS m/z : calcd for HR - MS m/z : calcd for C₃₁H₃₅N₂O₃S[M+H⁺]: 515.2368; found: 515.2365.

Compound 4kaA : $R_f = 0.40$ (hexanes/EtOAc, 7 : 3); Yield: 81%;

$[\alpha]_D^{25} = +48.4$ (CHCl₃, $c = 1.18$); IR (neat) $\bar{\nu}$: 2972, 2925, 2871,

1725, 1648, 1162, 667 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ 7.37–

7.26 (m, 10H), 5.81 (s, 1H), 5.27 (d, $J = 12$ Hz, 1H), 5.23 (d, $J = 12$ Hz, 1H), 4.92 (d, $J = 4.8$

Hz, 1H), 4.50 (d, $J=12$ Hz, 1H), 4.33 (d, $J=12$ Hz, 1H), 4.08 (dd, $J=6.4$ Hz, 12.8 Hz, 1H), 2.83 (dd, $J=8.8$ Hz, 17.6 Hz, 1H), 2.34–2.18 (m, 2H), 1.91–1.78 (m, 2H), 1.26 (s, 3H), 1.13 (s, 3H), 0.86–0.79 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3): 153.5, 149.6, 138.4, 135.9, 128.5, 128.3, 128.2, 127.9, 127.6, 127.5, 127.1, 73.1, 70.2, 67.8, 62.1, 52.9, 48.5, 32.2, 29.7, 24.8, 19.9, 16.5; HR - MS m/z : calcd for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}^+]$: 459.2648; found: 459.2653.

Compound 4kbB: $R_f=0.70$ (hexanes/EtOAc, 7 : 3); Yield:

83%; $[\alpha]_{\text{D}}^{25}=+53.5$ (CHCl_3 , $c=1.00$); IR (neat) $\bar{\nu}$: 2967, 2936, 2874, 1626, 1348, 1167, 681 cm^{-1} ; ^1H -NMR (400 MHz;

CDCl_3): δ 7.37–7.26 (m, 10H), 5.81 (s, 1H), 5.27 (d, $J=12$ Hz, 1H), 5.23 (d, $J=12$ Hz, 1H), 4.92 (d, $J=4.8$ Hz, 1H), 4.50 (d, $J=12$ Hz, 1H), 4.33 (d, $J=12$ Hz, 1H), 4.08 (dd, $J=6.4$ Hz, 12.8 Hz, 1H), 2.83 (dd, $J=8.8$ Hz, 17.6 Hz, 1H), 2.34–2.18 (m, 2H), 1.91–1.78 (m, 2H), 1.26 (s, 3H), 1.13 (s, 3H), 0.86–0.79 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3): 153.5, 149.6, 138.4, 135.9, 128.5, 128.3, 128.2, 127.9, 127.6, 127.5, 127.1, 73.1, 70.2, 67.8, 62.1, 52.9, 48.5, 32.2, 29.7, 24.8, 19.9, 16.5; HR - MS m/z : calcd for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}^+]$: 459.2648; found: 459.2653.

Compound 4la: $R_f=0.40$ (hexanes/EtOAc, 8 : 2); Yield: 45%; $[\alpha]_{\text{D}}^{25}=$

$+44.4$ (CHCl_3 , $c=1$); IR (neat) $\bar{\nu}$: 2973, 2929, 1660, 1343, 1162, 669 cm^{-1} ;

^1H NMR (300 MHz, CDCl_3): δ 7.88 (d, $J=8.4$ Hz, 2H), 7.34 (d, $J=8.4$

Hz, 2H), 5.54 (t, $J=1.2$ Hz, 1H), 4.09 (d, $J=1.8$ Hz, 1H), 2.61–2.54 (m, 1H), 2.45 (s, 3H), 2.39–2.31 (m, 1H), 1.80–1.71 (m, 2H), 1.45 (s, 3H), 1.40 (s, 3H), 1.11 (d, $J=1.85$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): 147.0, 143.8, 137.2, 129.6, 128.5, 127.6, 59.9, 54.2, 34.9, 33.0, 29.7, 26.6, 26.4, 25.3, 21.51, 21.0; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}^+]$: 347.1793; found: 347.1802.

HPLC Chromatogram for Compound 33aa

Column Details : Chiralpak AD-3; 150 mm x 40mm

Solvent System : n-Heptane/Isopropyl alcohol 80:20 isocratic flow

Injection volume : 2 μ L in Isopropyl alcohol

Flow Rate : 1.0 mL/min, 5.2 MPa, 298 K

Detector Wavelength : 220 nm

Figure 1: HPLC Chromatogram for racemic mixture of **14a**

Figure 2. HPLC Chromatogram for **14a** resulting from (+)-pinene

From the chromatogram the enantiomeric ratio was found to be 65:35

Compound 4lb: $R_f = 0.45$ (hexanes/EtOAc, 9 : 1); Yield: 43%; $[\alpha]_D^{25} = +32.6$ (CHCl_3 , $c = 1$); IR (neat) $\bar{\nu}$: 2976, 2927, 1658, 1342, 1162, 669 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.85(d, $J = 7.8$ Hz, 2H), 7.34 (d, $J = 7.8$ Hz, 2H), 5.41 (t, $J = 1.7$ Hz, 1H), 4.06 (s, 1H), 2.68 – 2.56 (m, 2H), 2.45 (s, 3H), 2.09 – 1.86 (m, 2H), 1.82 – 1.64 (m, 2H), 1.45 (s, 3H), 1.13 (s, 3H), 1.00 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): 149.8, 143.6, 137.7, 129.6, 128.9, 127.5, 59.6, 54.1, 35.0, 33.0, 31.9, 29.7, 26.5, 25.5, 21.5, 21.0, 11.6; HR - MS m/z : calcd for $\text{C}_{20}\text{H}_{29}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 361.1950; found: 361.1945.

Compound 4lc: $R_f = 0.6$ (hexanes/EtOAc, 8 : 2); Yield: 35%; $[\alpha]_D^{25} = +46.1$ (CHCl_3 , $c = 0.83$); IR (neat) $\bar{\nu}$: 2977, 2925, 1653, 1340, 1163, 669 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.86 (d, $J = 8.1$ Hz, 2H), 7.34 (d, $J = 8.1$ Hz, 2H), 5.40 (s, 1H), 4.07 (s, 1H), 2.60-2.22 (m,

5H), 2.45 (s, 3H), 2.07-1.87 (m, 2H), 1.80-1.69 (m, 1H), 1.62 (s, 3H), 1.44 (s, 3H), 1.37 (s, 3H), 1.14 (s, 3H), 0.84 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): 143.6, 137.7, 129.6, 129.2, 128.8, 127.6, 127.5, 125.4, 59.7, 54.2, 40.5, 35.0, 33.0, 29.7, 26.6, 26.1, 25.5, 21.1, 20.1, 13.5; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{31}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 375.2106; found: 375.2101.

Compound 4ld: $R_f = 0.50$ (hexanes/EtOAc, 8 : 2); Yield: 37%; $[\alpha]_D^{25} = +13.4$ (CHCl_3 , $c = 1$); IR (neat) $\bar{\nu}$: 2973, 2929, 1660, 1343, 1162, 669 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.31-7.26 (m, 4H), 7.22-7.14 (m, 5H), 5.48 (s, 1H), 4.43 (s, 1H), 2.73 (d, $J = 13.5$ Hz, 1H), 2.47 (s, 1H), 2.41 (s, 3H), 2.18 – 2.10 (m, 1H), 1.98-1.95 (m, 3H), 1.88 (td, $J = 14.1$ Hz, 4.2 Hz, 1H), 1.58 (s, 3H), 1.52 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): 143.6, 137.4, 129.6, 129.4, 129.3, 129.0, 128.6, 128.3, 127.8, 127.6, 127.0, 61.2, 55.5, 40.0, 36.5, 35.2, 33.1, 29.9, 26.5, 25.9, 22.0, 21.5; HR - MS m/z : calcd for $\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 409.1950; found: 409.1940. CHN Analysis found for $\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_2\text{S}$: C, 70.55; H, 6.91; N, 6.86. Found: C, 70.16; H, 6.99; N, 6.87.

Compound 4le: $R_f = 0.60$ (hexanes/EtOAc, 9 : 1); Yield: 48%; $[\alpha]_D^{25} = +36.5$ (CHCl_3 , $c = 0.54$); IR (neat) $\bar{\nu}$: 2973, 1664, 1342, 1162, 669 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.90 (d, $J = 8.4$ Hz, 2H), 7.33 (d, $J = 8.4$ Hz, 2H), 5.41 (s, 1H), 4.13 (s, 1H), 2.58-2.50 (m, 1H), 2.44 (s, 3H), 2.28-2.23 (m, 1H), 2.06-1.95 (m, 1H), 1.75-1.67 (m, 2H), 1.48-1.40 (m, 1H), 1.33 (s, 3H), 1.30 (s, 3H), 1.23 (s, 3H), 1.08-0.86 (m, 2H), 0.8-0.66 (m, 2H), 0.52-0.44 (m, 1H); ^{13}C NMR (75 MHz, CDCl_3): 149.3, 143.5, 138.2, 129.5, 129.4, 127.5, 127.2, 58.9, 54.3, 35.0, 33.1, 29.9, 26.6, 25.6, 21.5, 20.9, 17.6, 10.9, 9.9, 9.2; HR - MS m/z : calcd for $\text{C}_{21}\text{H}_{29}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 373.1950; found: 373.1947.

Compound 9: $R_f = 0.45$ (hexanes/EtOAc, 9 : 1); $[\alpha]_D^{25} = -50.1$ (CHCl_3 , $c =$

1); IR (neat) $\bar{\nu}$: 3276, 2918, 2360, 1435, 1328, 1160, 665 cm^{-1} ; ^1H NMR

(300 MHz, CDCl_3): δ 7.77 (d, $J = 7.8$ Hz, 2H), 7.30 (d, $J = 8.1$ Hz, 2H),

5.53 (s, 1H), 4.69 (s, 1H), 4.62 (s, 1H), 4.45(d, $J = 9.9$ Hz, 1H) 3.86 (br,

1H), 2.43 (s, 3H), 2.17 – 1.84 (m, 6H), 1.65 (s, 3H), 1.52 (s, 3H) 1.39-1.31(m, 1H); ^{13}C NMR

(100 MHz, CDCl_3): 148.4, 143.2, 138.4, 132.9, 129.6, 127.0, 125.8, 109.5, 54.3, 40.1, 36.5,

30.3, 21.5, 20.8, 19.9; HR - MS m/z : calcd for $\text{C}_{17}\text{H}_{23}\text{NNaO}_2\text{S}[\text{M}+\text{Na}^+]$: 328.1347; found:

328.1337. CHN Analysis found for $\text{C}_{17}\text{H}_{23}\text{NO}_2\text{S}$: C, 66.85; H, 7.59; N, 4.59; Found: C,

66.67; H, 7.49; N, 5.10.

Compound 4ma: $R_f = 0.30$ (hexanes/EtOAc, 7 : 3); Yield: 48%;

$[\alpha]_D^{25} = +10.5$ (CHCl_3 , $c = 0.96$); IR (neat) $\bar{\nu}$: 2974, 2927, 1662,

1342, 1162, 1095, 670 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.9 (d,

$J = 8.1$ Hz, 2H), 7.35 (d, $J = 8.1$ Hz, 2H), 5.79 (t, $J = 3.6$ Hz, 1H), 4.52 (s, 1H), 3.20 (dd, $J =$

10.8 Hz, 8.7 Hz, 2H), 2.98 (s, 3H), 2.63 (d, $J = 13.8$ Hz, 1H), 2.45 (s, 3H), 2.45-2.41 (m, 1H)

2.21-2.12 (m, 1H), 2.03 (s, 3H), 1.88-1.83(m, 1H), 1.75 (td, $J = 13.8$ Hz, 3.3 Hz, 1H), 1.46 (s,

3H), 1.43 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): 172.3, 143.7, 137.5, 130.4, 129.6, 127.7,

73.5, 60.1, 57.6, 49.8, 35.1, 33.0, 29.6, 26.5, 25.3, 21.5; HR - MS m/z : calcd for

$\text{C}_{20}\text{H}_{29}\text{N}_2\text{O}_3\text{S}[\text{M}+\text{H}^+]$: 377.1899; found: 377.1894.

Compound 4na: $R_f = 0.30$ (hexanes/EtOAc, 7 : 3); Yield: 42%;

$[\alpha]_D^{25} = +51.4$ (CHCl_3 , $c = 2.9$); IR (neat) $\bar{\nu}$: 2974, 2929, 2870, 1659,

1598, 1343, 1162, 1093, 670 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ

7.82(d, $J = 8.7$ Hz, 2H), 7.38-7.24 (m, 7H), 5.56-5.53 (m, 1H), 4.39 (d, $J = 12$ Hz, 1H), 4.34

(d, $J = 12$ Hz, 1H), 4.19 (s, 1H), 3.19 (t, $J = 6.6$ Hz, 2H), 2.58-2.53 (m, 1H), 2.42-2.36 (m,

2H), 2.38 (s, 3H), 2.09 (s, 3H), 1.85-1.68 (m, 2H), 1.53-1.45 (m, 1H), 1.45 (s, 3H), 1.40 (s,

3H); ^{13}C NMR (75 MHz, CDCl_3): 147.2, 143.9, 138.2, 137.0, 130.0, 129.6, 128.9, 127.6, 127.6, 127.4, 126.3, 72.7, 68.6, 60.0, 52.5, 35.0, 33.8, 32.9, 29.5, 26.6, 26.5, 25.3, 21.4; HR - MS m/z : calcd for $\text{C}_{27}\text{H}_{35}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}^+]$: 467.2368; found: 467.2366.

Compound 4nb: R_f = 0.30 (hexanes/EtOAc, 6 : 4); Yield: 57%;

IR (neat) $\bar{\nu}$: 3281, 2973, 2929, 2858, 1715, 1705, 1525, 1318, 1204, 1065, 737 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.85(d, J

= 8.4 Hz, 2H), 7.38-7.21 (m, 7H), 5.51 (m, 1H), 4.42 (d, J = 12 Hz, 1H), 4.34 (d, J = 12 Hz, 1H), 4.21 (s, 1H), 3.25 (dd, J = 7.2 Hz, 7.2 Hz, 2H), 2.54-2.36 (m, 4H), 2.39 (s, 3H), 2.05 (dd, J = 6.9 Hz, 19.2 Hz, 1H), 1.96-1.68 (m, 1H), 1.75-1.67 (m, 4H), 1.41 (ddd, J = 4.8 Hz, 8.4 Hz, 12.6 Hz, 1H), 1.33 (s, 3H), 1.30 (s, 3H), 0.98-0.89 (m, 1H), 0.79-0.63 (m, 2H), 0.49-0.40 (m, 1H); ^{13}C NMR (75 MHz, CDCl_3): 149.4, 143.6, 130.8, 129.6, 128.5, 128.3, 127.6, 127.4, 127.1, 121.6, 72.7, 68.7, 58.9, 52.6, 35.2, 34.0, 33.1, 30.5, 29.8, 26.6, 25.6, 21.5, 17.8, 9.8, 9.5.

Compound 4laA: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 52%; $[\alpha]_D^{25}$ =

+32.6 (CHCl_3 , c = 0.91); IR (neat) $\bar{\nu}$: 2978, 2925, 1720, 1343, 1162, 1098, 776 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3): δ 5.52 (s, 1H), 4.50 (s, 1H), 2.32

(m, 2H), 2.12-2.06 (m, 2H), 2.02 (s, 3H), 1.71-1.64 (m, 5H), 1.48 (s, 9H), 1.47 (s, 3H), 1.43 (s, 3H), 1.11 (s, 3H). ^{13}C -NMR (100 MHz; CDCl_3): δ 152.75, 129.56, 126.74, 81.10, 59.54, 34.51, 33.12, 28.74, 28.46, 28.06, 26.75, 24.57, 21.67; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}^+]$: 293.2229; found: 293.2235.

Compound 4laB: R_f = 0.30 (hexanes/EtOAc, 6 : 4); Yield: 48%; IR (neat)

$\bar{\nu}$: 3281, 2973, 2929, 2858, 1715, 1705, 1525, 1318, 1204, 1065, 737 cm^{-1} ;

^1H NMR (300 MHz, CDCl_3): δ 7.36-7.33 (m, 5H), 5.56-5.54 (m, 1H), 5.21

(s, 2H), 4.58 (s, 1H), 2.40-2.28 (m, 2H), 2.15-2.06 (m, 1H), 2.02 (s, 3H), 1.72-1.68 (m, 5H), 1.43 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 153.5, 151.2, 136.0, 129.1, 128.5, 128.1, 128.0, 127.0, 67.6, 59.6, 50.6, 34.4, 33.0, 28.7, 26.6, 24.7, 21.6; HR - MS m/z : calcd for $\text{C}_{20}\text{H}_{27}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}^+]$: 327.2072; found: 327.2064.

(S)-1-((1S,5R)-6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)ethanol: R_f =

0.30 (hexanes/EtOAc, 3 : 1); Yield: 90%; IR (neat) $\bar{\nu}$: 3416, 2945, 2918, 1522, 1090, 738, 667 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 5.28 (s, 1H),

4.28 (dd, J = 5.7 Hz, 12.0 Hz, 1H), 2.35 (dd, J = 7.8 Hz, 18.0 Hz, 1H), 2.13 (s, 1H), 2.02–1.96 (m, 1H), 1.65–1.60 (m, 1H), 1.29–1.17 (m, 5H), 0.98 (s, 3H), 0.73 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 148.2, 122.5, 67.1, 36.7, 31.5, 29.1, 27.3, 21.8, 19.2, 13.0; HR - MS m/z : calcd for $\text{C}_{10}\text{H}_{16}\text{NNaO}[\text{M}+\text{Na}^+]$: 175.1099; found: 175.1090.

Compound 3o: R_f = 0.40 (hexanes); Yield: 98%; ^1H NMR (400 MHz, CDCl_3): δ 7.35–7.22 (m, 5H), 5.41 (s, 1H), 4.57 (d, J = 12.0 Hz), 4.40 (d, J = 12.0, 1H), 4.06 (dd, J = 5.8 Hz, 11.6 Hz, 1H), 2.44 (dd, J = 7.6 Hz,

18.0 Hz, 1H), 2.27–2.10 (m, 1H), 1.68–1.66 (m, 1H), 1.35–1.24 (m, 9H), 1.09 (s, 3H), 0.98 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 140.3, 133.1, 122.3, 121.5, 118.5, 67.8, 63.3, 30.9, 25.9, 23.6, 20.4, 17.6, 13.5, 7.3; HR - MS m/z : calcd for $\text{C}_{17}\text{H}_{23}\text{NaO}[\text{M}+\text{H}^+]$: 243.1749; found: 249.1757.

Compound 4oa: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 90%; $[\alpha]_D^{25}$ =

+103.6 (CHCl_3 , c = 1); IR (neat) $\bar{\nu}$: 2974, 2929, 2870, 1659, 1598, 1343, 1162, 1093, 670 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3): δ 7.71 (d, J = 8.2

Hz, 1H), 7.41 (d, J = 7.3 Hz, 1H), 7.35 (t, J = 7.3 Hz, 1H), 7.27 (d, J = 6.8 Hz, 1H), 5.92 (s, 1H), 5.14 (d, J = 9.0 Hz, 1H), 4.56 (d, J = 11.0 Hz, 1H), 4.49 (d, J = 11.0 Hz, 1H), 4.39 (q, J

= 5.9 Hz, 1H), 2.83 (q, J = 8.5 Hz, 1H), 2.41 (s, 1H), 2.41-2.37 (m, 1H), 2.34 (s, 1H), 2.21 (ddd, J = 17.3, 8.3, 2.8 Hz, 1H), 1.38 (d, J = 6.3 Hz, 1H), 1.20 (s, 1H), 0.73 (s, 1H); ^{13}C -NMR (100 MHz; CDCl_3): δ 152.01, 147.05, 144.09, 139.23, 137.39, 131.58, 129.70, 128.26, 128.02, 127.45, 127.37, 71.13, 70.46, 63.59, 52.66, 50.86, 33.20, 30.01, 26.63, 25.24, 21.55, 18.90; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 453.2212; found: 453.2211.

Compound 4ob: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 87%;

$[\alpha]_{\text{D}}^{25}$ = +105.8 (CHCl_3 , c = 1); ^1H -NMR (300 MHz; CDCl_3): δ 7.78

(d, J = 8.4 Hz, 2H), 7.43–7.29 (m, 5H), 7.26 (d, J = 8.4 Hz, 2H), 5.89

(s, 1H), 5.17 (dd, J = 1.5 Hz, 9.0 Hz, 1H), 4.60 (d, J = 7.8 Hz, 1H),

4.49 (d, J = 7.8 Hz, 1H), 4.40 (dd, J = 7.2 Hz, 12.6 Hz, 1H), 2.79 (dd, J = 8.1 Hz, 17.1 Hz,

1H), 2.40 (s, 3H), 2.34–2.10 (m, 3H), 1.41 (d, J = 6.3 Hz, 3H), 1.11 (s, 3H), 0.90–0.67 (m,

5H), 0.64 (s, 3H); ^{13}C -NMR (100 MHz; CDCl_3): δ 158.0, 149.0, 144.0, 139.5, 138.0, 132.0,

129.0, 128.9, 128.6, 128.3, 127.9, 72.0, 71.5, 63.5, 53.5, 52.0, 34.5, 31.0, 23.5, 21.5, 19.5,

18.0, 15.0; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 479.2368; found: 479.2155.

Compound 4oc: R_f = 0.30 (hexanes/EtOAc, 7 : 3); Yield: 73%; $[\alpha]_{\text{D}}^{25}$ =

+98.0 (CHCl_3 , c = 1); ^1H -NMR (300 MHz; CDCl_3): δ 7.48 (d, J = 7.8

Hz, 2H), 7.41–7.24 (m, 10H), 7.07 (d, J = 7.8 Hz, 2H), 5.92 (s, 1H), 5.45

(dd, J = 3 Hz, 9.6 Hz, 1H), 4.63 (d, J = 11.1 Hz, 1H), 4.57 (d, J = 11.1 Hz,

1H), 4.55 – 4.51 (m, 1H), 2.97 (dd, J = 8.4 Hz, 17.1 Hz, 1H), 2.47 – 2.36 (m, 2H), 2.36 (s,

3H), 2.24 (dd, J = 2.1 Hz, 8.1 Hz, 1H), 1.50 (d, J = 6.6 Hz, 3H), 1.33 (s, 3H), 1.04 (s,

3H); ^{13}C -NMR (100 MHz; CDCl_3): δ 154.6, 146.3, 143.9, 139.2, 138.2, 136.4, 131.8, 129.7,

129.0, 128.8, 128.5, 128.3, 127.9, 127.8, 127.4, 127.1, 70.4, 69.5, 63.1, 54.2, 51.4, 33.3, 30.4,

25.0, 21.5, 18.2; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 515.2368; found: 515.2355.

Compound 4oaA: $R_f = 0.30$ (hexanes/EtOAc, 7 : 3); Yield: 90%;

$[\alpha]_D^{25} = +92.6$ (CHCl₃, $c = 1.02$); IR (neat) $\bar{\nu}$: 2974, 2929, 2870, 1720,

1649, 1347, 1159, 1086, 877, 664 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ

7.34 (qd, $J = 7.4, 5.6$ Hz, 5H), 5.81 (s, 1H), 5.09 (dd, $J = 1.9, 9.8$ Hz,

1H), 4.54 (d, $J = 11.5$ Hz, 1H), 4.40 (d, $J = 11.4$ Hz, 1H), 4.19 (q, $J = 6.3$ Hz, 1H), 2.94 (q, J

$= 8.5$ Hz, 1H), 2.43 (dd, $J = 16.8, 7.5$ Hz, 1H), 2.28-2.24 (m, 1H), 2.19 (s, 3H), 1.47 (s, 9H),

1.42 (s, 3H), 1.35 (s, 3H), 1.33 (s, 3H), 1.14 (s, 3H); ¹³C-NMR (100 MHz; CDCl₃): δ 156.21,

152.29, 145.97, 138.93, 130.04, 128.30, 128.20, 127.63, 127.27, 81.57, 77.30, 76.98, 76.66,

72.37, 70.46, 61.57, 53.81, 49.96, 33.38, 29.51, 28.22, 25.37, 24.45, 20.86; HR - MS m/z :

calcd for C₂₄H₂₅N₂NaO₃[M+Na⁺]: 421.2467; found: 421.2467.

Compound 4obA: $R_f = 0.60$ (hexanes/EtOAc, 7 : 3); Yield: 85%;

$[\alpha]_D^{25} = +87.0$ (CHCl₃, $c = 1.08$); IR (neat) $\bar{\nu}$: 2971, 2938, 2845, 1727,

1643, 1346, 1283, 1082, 875, 660 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ

7.38 (d, $J = 7.6$ Hz, 2H), 7.34–7.30 (m, 3H), 5.81 (s, 1H), 5.10 (dd, $J =$

1.6, 9.6 Hz, 1H), 4.56 (d, $J = 10.8$ Hz, 1H), 4.45 (d, $J = 10.8$ Hz, 1H), 4.16 (dd, $J = 6.4$ Hz,

12.8 Hz, 1H), 2.91 (dd, $J = 8.8$ Hz, 13.2 Hz, 1H), 2.66–2.60 (m, 1H), 2.48-2.36 (m, 2H),

2.25–2.19 (m, 1H), 1.48 (s, 9H), 1.35 (d, $J = 6.0$ Hz, 3H), 1.33 (s, 3H), 1.14 (s, 3H), 1.04 (t, J

$= 7.6$ Hz, 3H); ¹³C-NMR (100 MHz; CDCl₃): δ 161.1, 152.5, 146.3, 139.0, 129.7, 128.2,

127.8, 127.3, 81.4, 71.9, 70.7, 61.8, 53.5, 50.1, 33.3, 31.3, 29.6, 28.2, 24.3, 20.0, 12.1; HR -

MS m/z : calcd for C₂₅H₃₆N₂O₃[M+H⁺]: 413.2804; found: 413.2809.

Compound 4ocA: $R_f = 0.60$ (hexanes/EtOAc, 7 : 3); Yield: 83%;

$[\alpha]_D^{25} = +114.4$ (CHCl₃, $c = 1.25$); IR (neat) $\bar{\nu}$: 2975, 2931, 2865, 1707,

1365, 1342, 1163, 698 cm⁻¹; ¹H-NMR (400 MHz; CDCl₃): δ 7.49–7.43

(m, 4H), 7.38–7.33 (m, 4H), 7.27–7.25 (m, 2H), 5.83 (s, 1H), 5.29 (dd, $J = 2.0, 9.6$ Hz, 1H), 4.67 (d, $J = 10.8$ Hz, 1H), 4.57 (d, $J = 10.8$ Hz, 1H), 4.37 (dd, $J = 6.4$ Hz, 12.8 Hz, 1H), 3.04 (dd, $J = 8.8$ Hz, 16.8 Hz, 1H), 2.47–2.40 (m, 1H), 2.29–2.22 (m, 1H), 1.53 (d, $J = 6.4$ Hz, 1H), 1.44 (s, 3H), 1.26 (s, 3H), 1.06 (s, 9H); ^{13}C -NMR (100 MHz; CDCl_3): δ 156.9, 152.8, 145.8, 139.0, 130.7, 129.1, 128.2, 128.0, 127.8, 127.3, 126.8, 81.0, 71.9, 71.0, 61.3, 54.8, 50.9, 33.3, 29.7, 27.5, 24.2, 19.1; HR - MS m/z : calcd for $\text{C}_{29}\text{H}_{37}\text{N}_2\text{O}_3[\text{M}+\text{H}^+]$: 461.2804; found: 461.2804.

Compound 4oaB: $R_f = 0.30$ (hexanes/EtOAc, 7 : 3); Yield: 80%;

$[\alpha]_{\text{D}}^{25} = +82.1$ (CHCl_3 , $c = 1$); IR (neat) $\bar{\nu}$: 2974, 2929, 2870, 1716, 1598, 1343, 1162, 1093, 670 cm^{-1} ; ^1H -NMR (400 MHz; CDCl_3): δ 7.37–7.30 (m, 10H), 5.80 (s, 1H), 5.23–5.11 (m, 3H), 4.48 (d, $J = 11.5$

Hz, 1H), 4.37 (d, $J = 11.5$ Hz, 1H), 4.14 (q, $J = 6.3$ Hz, 1H), 2.93 (q, $J = 8.5$ Hz, 1H), 2.43 (dd, $J = 17.1, 7.3$ Hz, 1H), 2.28–2.20 (m, 4H), 1.33 (s, 3H), 1.32 (d, $J = 6.6$ Hz, 3H), 1.29–1.23 (m, 1H), 1.11 (s, 3H). ^{13}C -NMR (100 MHz; CDCl_3): δ 153.25, 145.43, 138.96, 135.79, 131.16, 128.55, 128.35, 128.27, 127.56, 127.33, 72.27, 70.43, 67.95, 61.74, 53.99, 49.78, 33.43, 29.55, 25.27, 24.62, 20.19; HR - MS m/z : calcd for $\text{C}_{19}\text{H}_{27}\text{N}_2\text{O}_2\text{S}[\text{M}+\text{H}^+]$: 433.2491; found: 433.2493.

Compound 10: $R_f = 0.20$ (hexanes/EtOAc, 9 : 1); Yield: 23%;

$[\alpha]_{\text{D}}^{25} = +54.1$ (CHCl_3 , $c = 2.05$); IR (neat) $\bar{\nu}$: 3318, 2973, 2922, 1639, 1599, 1450 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.86 (d, $J =$

8.1 Hz, 2H), 7.38 (d, $J = 8.1$ Hz, 2H), 5.43 (s, 1H), 4.83 (dd, $J = 6.6$ Hz, 12.9 Hz, 1H), 3.92 (s, 1H), 2.64–2.58 (m, 1H), 2.46 (s, 3H), 2.36–2.31 (m, 1H), 2.09–2.04 (m, 1H), 1.87 (d, $J = 6.6$ Hz, 3H), 1.75 (dt, $J = 3.9$ Hz, 15.6 Hz, 1H), 1.49 (s, 3H), 1.33 (s, 3H), 1.22 (t, 3H); ^{13}C NMR (75 MHz, CDCl_3): 146.3, 144.2, 136.6, 129.9, 128.7, 127.9, 127.5, 60.7, 54.5, 47.8,

35.3, 32.6, 29.1, 26.5, 26.3, 24.9, 22.5, 21.6; HR - MS m/z : calcd for $C_{20}H_{31}BrN_2O_2S[M+H^+]$: 441.1211; found: 441.1179.

Compound 11: $R_f = 0.30$ (hexanes/EtOAc, 7 : 3); Yield: 54%; IR

(neat) $\bar{\nu}$: 3316, 2973, 2925, 2097, 1549, 1274, 1141, 1090, 738 cm^{-1} ;

^1H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, $J = 9$ Hz, 2H), 7.31 (d, $J = 9$

Hz, 2H), 5.50 (s, 1H), 4.46-4.42 (d, $J = 12$ Hz, 1H), 3.07(br, 1H), 3.07 (s, 3H) 2.43 (s, 3H),

1.89-1.55 (m, 9H), 0.99 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): 143.2, 138.4, 133.3, 129.5,

127.0, 125.8, 75.7, 55.0, 48.7, 41.6, 33.2, 26.4, 21.9, 21.8, 21.5, 19.7; HR - MS m/z : calcd for

$C_{18}H_{27}NNaO_3S[M+Na^+]$: 412.1783; found: 412.1782.

Compound 12: $R_f = 0.30$ (hexanes/EtOAc, 1 : 1); Yield: 59%; IR

(neat) $\bar{\nu}$: 3326, 3312, 2973, 2925, 1549, 1140, 1090, 738 cm^{-1} ; ^1H

NMR (400 MHz, $CDCl_3$): δ 7.73 (d, $J = 6.4$ Hz, 2H), 7.70 (d, $J =$

8.0 Hz, 2H), 7.29 (d, $J = 6.4$ Hz, 2H), 7.24 (d, $J = 6.4$ Hz, 2H), 5.45 (s, 1H), 5.42 – 5.41 (m,

1H), 4.53 (d, $J = 7.6$ Hz, 1H), 3.65 – 3.63 (m, 1H), 2.41 (s, 3H), 2.40 (s, 3H), 2.28 (s, 3H),

1.79 – 1.76 (m, 3H), 1.70 – 1.64 (m, 2H), 1.48 (s, 3H), 1.17 (s, 3H), 1.16 (s, 3H), 1.03 (dd, J

= 9.6, 18.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 164.0, 143.3, 142.1, 140.7, 138.1, 133.3,

129.6, 129.2, 127.0, 126.7, 125.3, 58.2, 54.8, 38.9, 33.4, 26.2, 23.6, 23.2, 21.9, 21.5, 21.4;

HR - MS m/z : calcd for $C_{18}H_{27}NNaO_3S[M+Na^+]$: 412.1783; found: 412.1782.

X-Ray Crystallography Data

Compound 4la: CCDC No. 748915

The structure was solved by direct methods (SIR92). Refinement was by full-matrix least-squares procedures on F^2 by using SHELXL-97. CCDC No. 748915. Crystal system: Orthorhombic, space group: $P 2_1 2_1 2_1$, cell parameters: $a = 7.320$, $b = 15.096$, $c = 16.520$ Å, $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00^\circ$, $V = 1825.5$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.26$ g cm⁻³, $F(000) = 743.9$, $\mu = 0.191$ mm⁻¹, $\lambda = 0.71073$ Å. Total number l.s. parameters = 222. $R1 = 0.043$ for $3208F_o > 4\sigma(F_o)$ and 0.09 for all 13144 data. $wR2 = 0.110$, GOF = 0.627, restrained GOF = 1.000 for all data.

Compound 4la: CCDC No. 849309

The structure was solved by direct methods (SIR92). Refinement was by full-matrix least-squares procedures on F^2 by using SHELXL-97. CCDC No. 849309. Crystal system: Monoclinic, space group: $P2_1/c$, cell parameters: $a = 15.100$, $b = 8.407$, $c = 15.402$ Å, $\alpha = 90.00^\circ$, $\beta = 110.02^\circ$, $\gamma = 90.00^\circ$, $V = 1837.21$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.25$ g cm⁻³, $F(000) = 743.9$, $\mu = 0.190$ mm⁻¹, $\lambda = 0.71073$ Å. Total number l.s. parameters = 222. $R1 = 0.050$ for $3386F_o > 4\sigma(F_o)$ and 0.09 for all 17625 data. $wR2 = 0.121$, GOF = 1.045, restrained GOF = 1.000 for all data.

Compound 4ld: CCDC No. 748919

The structure was solved by direct methods (SIR92). Refinement was by full-matrix least-squares procedures on F^2 by using SHELXL-97. CCDC No. 748919. Crystal system: Monoclinic, space group: $P2_1/c$, cell parameters: $a = 11.800$, $b = 8.641$, $c = 20.632$ Å, $\alpha = 90.00$, $\beta = 96.166$, $\gamma = 90.00^\circ$, $V = 2091.6$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.30$ g cm⁻³, $F(000) = 871.9$, $\mu = 0.178$ mm⁻¹, $\lambda = 0.71073$ Å. Total number l.s. parameters = 266. $R1 = 0.057$ for $3680F_o > 4\sigma(F_o)$ and 0.09 for all 14460 data. $wR2 = 0.121$, GOF = 1.078, restrained GOF = 1.000 for all data.

Compound 9: CCDC No. 748916

The structure was solved by direct methods (SIR92). Refinement was by full-matrix least-squares procedures on F^2 by using SHELXL-97. CCDC No. 748916. Crystal system: Orthorhombic, space group: $P2_12_12_1$, cell parameters: $a = 5.209$, $b = 17.961$, $c = 18.469$ Å, $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00^\circ$, $V = 1727.8$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.17$ g cm⁻³, $F(000) = 655.9$, $\mu = 0.19$ mm⁻¹, $\lambda = 0.71073$ Å. Total number l.s. parameters = 193. $R1 = 0.068$ for $3041F_o > 4\sigma(F_o)$ and 0.04 for all 12559 data. $wR2 = 0.140$, GOF = 1.238, restrained GOF = 1.000 for all data.

¹H, ¹³C, DEPT NMR Spectra

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VGE- 219- 1

$^1\text{H} - ^1\text{H}$ COSY CDCl_3 , 400 MHz

$^1\text{H} - ^{13}\text{C}$ COSY CDCl_3 , 400 MHz

NOESY CDCl₃, 400 MHz

VGE-2D

¹³C, CDCl₃, 100 MHz

DCB-58

VGf-29 (1)

DCB-46

^1H - ^1H COSY, 400 MHz

^1H - ^{13}C COSY, 400 MHz

NOESY, 400 MHz

Computational Details

References

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2. Gaussian 09, Revision A.1, 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.

Cartesian coordinates of Model Alkene

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.732099	-0.672886	-0.000005
2	1	0	-0.709158	-1.761874	0.000043
3	6	0	0.448799	-0.041089	-0.000017
4	6	0	1.741894	-0.820090	0.000002
5	1	0	2.349527	-0.573431	-0.879012
6	1	0	2.349655	-0.573201	0.878859
7	1	0	1.566432	-1.897797	0.000155
8	6	0	0.624913	1.456537	0.000000
9	1	0	-0.318094	2.002435	-0.000558
10	1	0	1.197840	1.775943	0.878623
11	1	0	1.198835	1.775856	-0.877999
12	6	0	-2.111694	-0.078788	-0.000003
13	1	0	-2.677639	-0.411296	-0.877896
14	1	0	-2.677337	-0.410574	0.878360
15	1	0	-2.110946	1.011826	-0.000440

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-196.465641
Sum of electronic and thermal Energies=	-196.458702
Sum of electronic and thermal Enthalpies=	-196.457758
Sum of electronic and thermal Free Energies=	-196.495570

Cartesian coordinates of 3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.805423	-0.994175	-0.750541
2	6	0	-1.744423	-0.284145	-0.108810
3	6	0	-3.134981	-0.812278	0.122331
4	6	0	-1.445907	1.081463	0.466860
5	6	0	-0.237049	1.802223	-0.166838
6	6	0	0.902318	0.908277	-0.631085
7	6	0	0.578807	-0.528196	-0.994829
8	6	0	1.557136	-0.207207	0.151419
9	6	0	3.028415	-0.438791	-0.156476
10	6	0	1.204537	-0.519554	1.594177
11	1	0	-1.059970	-1.982506	-1.126874
12	1	0	-3.885024	-0.163574	-0.346029
13	1	0	-3.375013	-0.844240	1.192303
14	1	0	-3.256348	-1.820106	-0.280990
15	1	0	-2.332764	1.718416	0.364807
16	1	0	-1.296032	0.979215	1.549592
17	1	0	0.133447	2.568704	0.522765
18	1	0	-0.589908	2.339480	-1.054447
19	1	0	1.577138	1.420116	-1.312584
20	1	0	1.043748	-0.937418	-1.887211
21	1	0	3.310080	-1.479811	0.035647
22	1	0	3.663168	0.198538	0.469902
23	1	0	3.261754	-0.215660	-1.201011
24	1	0	1.666416	-1.466005	1.894073
25	1	0	0.132934	-0.619046	1.757364
26	1	0	1.585797	0.258191	2.265447

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -390.535681
Sum of electronic and thermal Energies= -390.525222
Sum of electronic and thermal Enthalpies= -390.524278
Sum of electronic and thermal Free Energies= -390.570391

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.800879	-0.997540	-0.762882
2	6	0	-1.725434	-0.279952	-0.108443
3	6	0	-3.118833	-0.791308	0.133567
4	6	0	-1.405804	1.076499	0.471516
5	6	0	-0.224903	1.790109	-0.207553
6	6	0	0.912557	0.891165	-0.655199
7	6	0	0.589850	-0.545185	-0.999314
8	6	0	1.535763	-0.209570	0.155880
9	6	0	3.008726	-0.454054	-0.111268
10	6	0	1.142444	-0.481565	1.594773
11	1	0	-1.070340	-1.981799	-1.145288
12	1	0	-3.863346	-0.126365	-0.322358
13	1	0	-3.342382	-0.827016	1.207937
14	1	0	-3.256846	-1.795723	-0.277248
15	1	0	-2.295857	1.716357	0.404114
16	1	0	-1.212121	0.965720	1.548048
17	1	0	0.152670	2.580488	0.452721
18	1	0	-0.602526	2.291022	-1.107955

19	1	0	1.603084	1.390639	-1.333879
20	1	0	1.070134	-0.973576	-1.876884
21	1	0	3.274512	-1.497318	0.097057
22	1	0	3.629456	0.186661	0.527565
23	1	0	3.267354	-0.240295	-1.153892
24	1	0	1.724628	-1.325210	1.983125
25	1	0	0.087488	-0.742596	1.699344
26	1	0	1.353170	0.387417	2.231126

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-390.248006
Sum of electronic and thermal Energies=	-390.237621
Sum of electronic and thermal Enthalpies=	-390.236677
Sum of electronic and thermal Free Energies=	-390.282834

Cartesian coordinates of 3k (similar in skeleton)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.497978	-0.858599	-0.683422
2	6	0	-0.895812	-0.464406	-1.172867
3	6	0	0.477123	-0.749508	0.842811
4	6	0	-1.662509	-0.108973	0.091624
5	6	0	-0.898304	-0.288274	1.177614
6	1	0	-3.483040	0.541799	1.039608
7	6	0	1.125551	1.648144	-0.121969
8	6	0	1.381240	0.159680	0.006725
9	6	0	2.859809	-0.190960	0.044060
10	1	0	-3.123917	1.363565	-0.486670
11	6	0	-3.068434	0.402553	0.038746
12	1	0	0.991547	-1.694312	-1.167072
13	1	0	-1.380095	-1.292525	-1.706038
14	1	0	-0.873334	0.378808	-1.876528
15	1	0	0.961617	-1.485461	1.476972
16	1	0	-1.224717	-0.099998	2.195057
17	1	0	1.643830	2.194472	0.673361
18	1	0	0.066715	1.900553	-0.058803
19	1	0	1.506419	2.019536	-1.080055
20	1	0	3.357681	0.301764	0.886220
21	1	0	3.360836	0.132246	-0.875246
22	1	0	3.015806	-1.268304	0.147361
23	1	0	-3.719204	-0.290089	-0.508100

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -351.237831
Sum of electronic and thermal Energies= -351.228448
Sum of electronic and thermal Enthalpies= -351.227503
Sum of electronic and thermal Free Energies= -351.271111

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.505562	-0.834790	-0.714991
2	6	0	-0.883115	-0.416433	-1.187425
3	6	0	0.488651	-0.793469	0.808371
4	6	0	-1.648313	-0.122451	0.089894
5	6	0	-0.888714	-0.355055	1.168493
6	1	0	-3.463098	0.514480	1.057761
7	6	0	1.081417	1.643848	-0.057918
8	6	0	1.367566	0.160459	0.015158
9	6	0	2.848688	-0.160785	0.036159
10	1	0	-3.086605	1.383681	-0.442139
11	6	0	-3.048636	0.404195	0.051737
12	1	0	1.009671	-1.643779	-1.236848
13	1	0	-1.371494	-1.215425	-1.761510
14	1	0	-0.852912	0.466613	-1.843772
15	1	0	0.986863	-1.553334	1.406030
16	1	0	-1.216665	-0.210690	2.194892
17	1	0	1.577545	2.167760	0.767759
18	1	0	0.013683	1.870320	-0.002287
19	1	0	1.469559	2.055625	-0.997980
20	1	0	3.335934	0.304922	0.901202
21	1	0	3.339450	0.213012	-0.870951
22	1	0	3.022070	-1.241018	0.091782
23	1	0	-3.702642	-0.265278	-0.520809

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -350.979449
Sum of electronic and thermal Energies= -350.970225
Sum of electronic and thermal Enthalpies= -350.969281
Sum of electronic and thermal Free Energies= -351.012568

Cartesian coordinates of 3o (similar in skeleton)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.497978	-0.858599	-0.683422
2	6	0	-0.895812	-0.464406	-1.172867
3	6	0	0.477123	-0.749508	0.842811
4	6	0	-1.662509	-0.108973	0.091624
5	6	0	-0.898304	-0.288274	1.177614
6	1	0	-3.483040	0.541799	1.039608
7	6	0	1.125551	1.648144	-0.121969
8	6	0	1.381240	0.159680	0.006725
9	6	0	2.859809	-0.190960	0.044060
10	1	0	-3.123917	1.363565	-0.486670
11	6	0	-3.068434	0.402553	0.038746
12	1	0	0.991547	-1.694312	-1.167072
13	1	0	-1.380095	-1.292525	-1.706038
14	1	0	-0.873334	0.378808	-1.876528
15	1	0	0.961617	-1.485461	1.476972
16	1	0	-1.224717	-0.099998	2.195057
17	1	0	1.643830	2.194472	0.673361
18	1	0	0.066715	1.900553	-0.058803
19	1	0	1.506419	2.019536	-1.080055
20	1	0	3.357681	0.301764	0.886220
21	1	0	3.360836	0.132246	-0.875246
22	1	0	3.015806	-1.268304	0.147361
23	1	0	-3.719204	-0.290089	-0.508100

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -351.237831
Sum of electronic and thermal Energies= -351.228448
Sum of electronic and thermal Enthalpies= -351.227503
Sum of electronic and thermal Free Energies= -351.271111

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.592443	0.936135	-0.722592
2	6	0	-0.434142	1.863179	-0.072520
3	6	0	-0.034244	-0.449017	-0.786746
4	6	0	-1.599434	0.949613	0.237820
5	6	0	-2.300398	-1.485044	-0.012546
6	6	0	-1.386087	-0.309527	-0.166473
7	1	0	-3.258119	-1.193540	0.427783
8	1	0	-1.841696	-2.249255	0.627347
9	6	0	1.116448	-0.199586	1.591185
10	6	0	1.186921	-0.189643	0.080270
11	6	0	2.487342	-0.750750	-0.460444
12	1	0	1.176841	1.314433	-1.557166
13	1	0	-0.724702	2.673138	-0.753417
14	1	0	-0.038429	2.342146	0.834965
15	1	0	0.089101	-1.102874	-1.648721
16	1	0	-2.488530	1.284756	0.766746
17	1	0	-2.496636	-1.956843	-0.982939
18	1	0	1.294498	-1.211802	1.974039
19	1	0	0.148002	0.137877	1.968483
20	1	0	1.891114	0.456544	2.007437
21	1	0	2.624358	-1.791637	-0.143539

22	1	0	3.342571	-0.170064	-0.093368
23	1	0	2.508535	-0.725033	-1.555370

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -350.979879

Sum of electronic and thermal Energies= -350.970494

Sum of electronic and thermal Enthalpies= -350.969550

Sum of electronic and thermal Free Energies= -351.013258

Cartesian coordinates of compound 3l

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.864082	1.165654	-0.243184
2	6	0	-0.312207	0.607415	-1.585835
3	6	0	0.298476	1.811680	0.533056
4	6	0	-1.087581	-0.326368	0.206572
5	6	0	0.126630	-0.639981	-0.757598
6	6	0	1.445171	-0.287068	-0.084481
7	6	0	2.573087	-1.275686	-0.138569
8	6	0	-0.979812	-0.679214	1.690193
9	6	0	1.513328	0.908658	0.512104
10	6	0	-2.409839	-0.899340	-0.325602
11	1	0	-1.742548	1.817243	-0.272187
12	1	0	0.486039	1.171318	-2.071891
13	1	0	-1.095394	0.391830	-2.310897
14	1	0	0.000000	2.022304	1.568923
15	1	0	0.540984	2.786646	0.089607
16	1	0	0.148973	-1.617924	-1.245480
17	1	0	3.466161	-0.896774	0.363800
18	1	0	2.838147	-1.515776	-1.175281
19	1	0	2.287403	-2.221619	0.337393
20	1	0	-1.044580	-1.763920	1.829521
21	1	0	-1.811040	-0.231064	2.245824
22	1	0	-0.048295	-0.341839	2.143651
23	1	0	2.423474	1.244954	1.001802
24	1	0	-2.435495	-1.985660	-0.190258
25	1	0	-2.577465	-0.695009	-1.384015
26	1	0	-3.255385	-0.479205	0.229541

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -390.527401

Sum of electronic and thermal Energies= -390.517548

Sum of electronic and thermal Enthalpies= -390.516604

Sum of electronic and thermal Free Energies= -390.561094

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.873079	1.152071	-0.246027
2	6	0	-0.321967	0.597802	-1.583555
3	6	0	0.280619	1.811788	0.522977
4	6	0	-1.074384	-0.328807	0.207343
5	6	0	0.124055	-0.640434	-0.756647
6	6	0	1.439312	-0.278312	-0.091105
7	6	0	2.564131	-1.269021	-0.133810
8	6	0	-0.951874	-0.666078	1.688713
9	6	0	1.503653	0.921513	0.498020
10	6	0	-2.390970	-0.913119	-0.308870
11	1	0	-1.763303	1.792068	-0.272183
12	1	0	0.477180	1.167320	-2.067340
13	1	0	-1.105367	0.377909	-2.309849
14	1	0	-0.017852	2.012521	1.562768
15	1	0	0.510156	2.789768	0.076751
16	1	0	0.148486	-1.624389	-1.239805
17	1	0	3.460139	-0.882711	0.360987
18	1	0	2.821911	-1.525531	-1.169097
19	1	0	2.271331	-2.204089	0.361465
20	1	0	-1.003910	-1.752128	1.836591
21	1	0	-1.785739	-0.217679	2.243934
22	1	0	-0.018290	-0.312310	2.131194
23	1	0	2.415200	1.263324	0.986350
24	1	0	-2.406331	-2.000041	-0.163546
25	1	0	-2.564909	-0.717558	-1.369939
26	1	0	-3.235677	-0.490895	0.249485

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -390.241294
Sum of electronic and thermal Energies= -390.231464
Sum of electronic and thermal Enthalpies= -390.230519
Sum of electronic and thermal Free Energies= -390.275125

Cartesian coordinates of Model BrCl Complex (M)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.002660	-0.446202	-0.019862
2	6	0	-1.785619	0.738395	-0.650869
3	6	0	-2.048373	-1.734247	-0.800020
4	6	0	-1.875755	2.121061	-0.075334
5	6	0	-2.320837	-0.576893	1.444696
6	35	0	0.817347	0.037270	-0.094436
7	17	0	3.083001	-0.115918	0.174633
8	1	0	-1.635635	0.696623	-1.727340
9	1	0	-3.063460	-2.148094	-0.770464
10	1	0	-1.385853	-2.485761	-0.360894
11	1	0	-1.766268	-1.592282	-1.844089
12	1	0	-1.069389	2.751732	-0.457185
13	1	0	-1.831536	2.138573	1.013497
14	1	0	-2.819544	2.588647	-0.381277
15	1	0	-3.368552	-0.877270	1.567217
16	1	0	-2.166743	0.343834	2.004886
17	1	0	-1.711735	-1.362547	1.900501

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -3112.917757
Sum of electronic and thermal Energies= -3112.910962
Sum of electronic and thermal Enthalpies= -3112.910018
Sum of electronic and thermal Free Energies= -3112.949547

Cartesian coordinates of Intermediate Int-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.309277	.070373	1.830638
2	6	0	-.952427	1.457527	1.258164
3	6	0	-.475231	1.471609	-.172740
4	6	0	-.723336	.427103	-1.010873
5	6	0	-1.459219	-.791256	-.626902
6	6	0	-1.835888	-.950699	.832700
7	6	0	-2.936852	-.738342	-.177689
8	6	0	-3.759612	-1.970235	-.521130
9	6	0	-3.745269	.543636	-.260788

10	6	0	.128460	2.759419	-.661144
11	35	0	1.872611	-.108540	-.204284
12	17	0	3.982516	-.923176	.183884
13	1	0	-2.015598	.192838	2.658352
14	1	0	-.402336	-.359715	2.265788
15	1	0	-1.820628	2.126825	1.316438
16	1	0	-.192461	1.927041	1.891935
17	1	0	-.430740	.521103	-2.053105
18	1	0	-1.179820	-1.680671	-1.181844
19	1	0	-1.774837	-1.966823	1.211805
20	1	0	-4.160984	-1.902671	-1.537646
21	1	0	-4.607198	-2.070984	.165761
22	1	0	-3.166053	-2.885381	-.453650
23	1	0	-4.457616	.601663	.569363
24	1	0	-4.323552	.562197	-1.190030
25	1	0	-3.133554	1.443524	-.244397
26	1	0	.463332	2.685401	-1.697001
27	1	0	.980319	3.056346	-.042731
28	1	0	-.610520	3.567368	-.596518

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.894109
Sum of electronic and thermal Energies=	-3424.879444
Sum of electronic and thermal Enthalpies=	-3424.878500
Sum of electronic and thermal Free Energies=	-3424.936951

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.132958	-0.114876	1.751953
2	6	0	-0.800812	1.314583	1.288036
3	6	0	-0.422760	1.444142	-0.165810
4	6	0	-0.757161	0.499623	-1.077596
5	6	0	-1.506743	-0.729971	-0.756376
6	6	0	-1.753438	-1.023577	0.705851
7	6	0	-2.919832	-0.663266	-0.167760
8	6	0	-3.840026	-1.809080	-0.541155
9	6	0	-3.646991	0.659158	-0.019044
10	6	0	0.229260	2.737002	-0.569036
11	35	0	1.818961	-0.115860	-0.205186
12	17	0	3.844922	-0.928680	0.165920
13	1	0	-1.781212	-0.066421	2.635163
14	1	0	-0.201706	-0.592587	2.076347
15	1	0	-1.649964	1.986087	1.477998
16	1	0	0.026304	1.705625	1.894583
17	1	0	-0.486400	0.662718	-2.120488
18	1	0	-1.314024	-1.571527	-1.417803
19	1	0	-1.701740	-2.076801	0.977088
20	1	0	-4.328510	-1.620011	-1.504198
21	1	0	-4.622905	-1.933910	0.216911
22	1	0	-3.292922	-2.754546	-0.617791
23	1	0	-4.097035	0.744286	0.977969
24	1	0	-4.455683	0.723787	-0.755623
25	1	0	-2.996448	1.521477	-0.178277
26	1	0	0.560702	2.711807	-1.610994
27	1	0	1.098208	2.950099	0.063676
28	1	0	-0.475216	3.570149	-0.448081

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3422.194956
Sum of electronic and thermal Energies=	-3422.180575
Sum of electronic and thermal Enthalpies=	-3422.179631
Sum of electronic and thermal Free Energies=	-3422.237657

Cartesian coordinates of Int-2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.830566	-0.563104	0.965101
2	6	0	-1.265982	0.807020	1.335326
3	6	0	-1.502297	-0.799160	-0.511887
4	6	0	-2.954820	-0.663769	-0.040155
5	6	0	-0.664416	1.340698	0.046760
6	6	0	-0.784260	0.421482	-0.950112
7	35	0	1.806726	-0.062053	-0.171252
8	6	0	-3.735444	-1.967827	-0.013166
9	6	0	-3.811487	0.533896	-0.404088
10	6	0	-0.168989	2.745994	-0.070753
11	17	0	3.948216	-0.801145	0.176071
12	1	0	-1.722089	-1.369762	1.680186
13	1	0	-0.505494	0.735288	2.120153
14	1	0	-2.033416	1.495554	1.712018
15	1	0	-1.182634	-1.764999	-0.885758
16	1	0	-0.488068	0.602193	-1.976984
17	1	0	-4.185564	-2.174164	-0.989654
18	1	0	-4.543507	-1.918856	0.724430
19	1	0	-3.096640	-2.815541	0.247541
20	1	0	-4.307874	0.368943	-1.365705
21	1	0	-3.242928	1.461113	-0.484296
22	1	0	-4.591992	0.683726	0.349626
23	1	0	0.306223	2.930087	-1.035371
24	1	0	0.550721	2.976402	0.720296
25	1	0	-1.002259	3.449957	0.041964

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3385.596127
Sum of electronic and thermal Energies=	-3385.582601
Sum of electronic and thermal Enthalpies=	-3385.581657
Sum of electronic and thermal Free Energies=	-3385.637591

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.708837	-0.623523	0.884040
2	6	0	-1.113746	0.715752	1.304326
3	6	0	-1.514624	-0.752988	-0.624183
4	6	0	-2.907608	-0.633313	-0.024214
5	6	0	-0.608301	1.328646	0.012405
6	6	0	-0.820005	0.493651	-1.031832
7	35	0	1.757794	-0.072654	-0.168424
8	6	0	-3.713303	-1.917146	-0.024391
9	6	0	-3.757902	0.603796	-0.211590
10	6	0	-0.063809	2.720045	-0.035710
11	17	0	3.808742	-0.814499	0.188037
12	1	0	-1.553523	-1.485179	1.526926
13	1	0	-0.292862	0.595616	2.022094
14	1	0	-1.857251	1.374301	1.777388
15	1	0	-1.240367	-1.696064	-1.090012
16	1	0	-0.557864	0.727031	-2.060874
17	1	0	-4.239028	-2.045786	-0.977749
18	1	0	-4.461461	-1.902670	0.777160
19	1	0	-3.071532	-2.791212	0.129042
20	1	0	-4.359235	0.516477	-1.123919
21	1	0	-3.167002	1.519886	-0.291253
22	1	0	-4.446282	0.716355	0.634973
23	1	0	0.385127	2.938555	-1.008567
24	1	0	0.699327	2.861788	0.737985
25	1	0	-0.860630	3.450746	0.151918

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3382.925311
Sum of electronic and thermal Energies=	-3382.912014
Sum of electronic and thermal Enthalpies=	-3382.911070
Sum of electronic and thermal Free Energies=	-3382.966499

Cartesian coordinates of Int-3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.790684	-1.183519	0.264170
2	6	0	-1.096413	-0.710652	1.543948
3	6	0	-1.603527	-0.081158	-0.780643
4	6	0	-2.999764	-0.438654	-0.244696
5	6	0	-0.546450	0.651881	1.177795
6	6	0	-0.574084	2.314948	-0.766602
7	6	0	-0.847760	1.003129	-0.103788
8	35	0	1.873347	0.061009	0.111495
9	6	0	-3.874323	-1.201161	-1.226587
10	6	0	-3.783591	0.510410	0.641197
11	17	0	4.016892	-0.595865	-0.385348
12	1	0	-1.683396	-2.223237	-0.021637
13	1	0	-0.304895	-1.399456	1.851948
14	1	0	-1.789546	-0.635639	2.391227
15	1	0	-1.400112	-0.290523	-1.825362
16	1	0	-0.114201	1.328717	1.905942
17	1	0	0.042458	2.966311	-0.145829
18	1	0	-1.520068	2.825544	-0.980566
19	1	0	-0.066934	2.169503	-1.724824
20	1	0	-4.411524	-0.514374	-1.888574
21	1	0	-4.618338	-1.801658	-0.692472
22	1	0	-3.285588	-1.878082	-1.850735
23	1	0	-4.369969	1.205871	0.032227
24	1	0	-3.147360	1.101092	1.301122
25	1	0	-4.485273	-0.051008	1.267366

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3385.596275
Sum of electronic and thermal Energies=	-3385.582767
Sum of electronic and thermal Enthalpies=	-3385.581822
Sum of electronic and thermal Free Energies=	-3385.637787

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.704280	-1.119903	0.451458
2	6	0	-1.126726	-0.447314	1.695593
3	6	0	-1.463772	-0.183234	-0.724578
4	6	0	-2.875456	-0.480458	-0.242719
5	6	0	-0.603772	0.873190	1.177774
6	6	0	-0.466755	2.218148	-0.982092
7	6	0	-0.777745	1.010030	-0.157641
8	35	0	1.797004	0.059731	0.089555
9	6	0	-3.674891	-1.394097	-1.150473
10	6	0	-3.724110	0.566178	0.446246
11	17	0	3.851058	-0.653402	-0.316642
12	1	0	-1.568523	-2.190707	0.330524
13	1	0	-0.327253	-1.047592	2.146496
14	1	0	-1.887601	-0.292917	2.473579
15	1	0	-1.170366	-0.543639	-1.708298
16	1	0	-0.202513	1.650127	1.824031
17	1	0	0.119915	2.947107	-0.416842

18	1	0	-1.398362	2.692336	-1.315052
19	1	0	0.098875	1.939661	-1.877982
20	1	0	-4.166242	-0.820494	-1.945058
21	1	0	-4.451882	-1.919429	-0.582479
22	1	0	-3.034702	-2.147162	-1.621928
23	1	0	-4.292293	1.141415	-0.294279
24	1	0	-3.133576	1.271350	1.036702
25	1	0	-4.443578	0.081946	1.117675

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3382.925598
Sum of electronic and thermal Energies=	-3382.912444
Sum of electronic and thermal Enthalpies=	-3382.911500
Sum of electronic and thermal Free Energies=	-3382.966396

Cartesian coordinates of Int-4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.121118	-.735348	1.576612
2	6	0	2.031084	-1.319106	.480155
3	6	0	.478674	.552960	1.104596
4	6	0	2.972066	-.215783	-.130051
5	6	0	.780240	1.038635	-.127653
6	6	0	1.250178	-1.301918	-.862320
7	6	0	1.691809	.188346	-.984493
8	6	0	3.616487	.814678	.798166
9	6	0	4.077221	-.815839	-1.010989
10	6	0	.380017	2.394784	-.621283
11	35	0	-2.054746	.047136	.118539
12	1	0	1.695304	-.529702	2.489294
13	1	0	.357470	-1.467608	1.862075
14	1	0	2.498700	-2.253271	.802197
15	1	0	-.067227	1.158736	1.820514
16	1	0	.179033	-1.494347	-.826736
17	1	0	1.702253	-1.932307	-1.625302
18	1	0	1.852645	.613442	-1.977390
19	1	0	4.144088	1.577123	.215533
20	1	0	2.903299	1.326925	1.444211
21	1	0	4.357809	.326789	1.439766
22	1	0	4.843421	-1.282661	-.383347

23	1	0	3.717974	-1.573293	-1.708465
24	1	0	4.565943	-.030676	-1.596549
25	1	0	1.277046	3.004613	-.784930
26	1	0	-.270222	2.914798	.083719
27	1	0	-.134621	2.326221	-1.584852
28	17	0	-4.241186	-.467235	-.303238

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.883694
Sum of electronic and thermal Energies=	-3424.869607
Sum of electronic and thermal Enthalpies=	-3424.868663
Sum of electronic and thermal Free Energies=	-3424.925768

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.226404	-0.649579	1.680320
2	6	0	2.074205	-1.271394	0.559854
3	6	0	0.524268	0.594714	1.182076
4	6	0	2.915584	-0.185696	-0.185009
5	6	0	0.706925	0.997063	-0.093515
6	6	0	1.198933	-1.368922	-0.711728
7	6	0	1.578610	0.115555	-0.961573
8	6	0	3.578176	0.921280	0.627983
9	6	0	3.976404	-0.802136	-1.098850
10	6	0	0.227939	2.306701	-0.642292
11	35	0	-2.016719	0.025202	0.096982
12	1	0	1.858300	-0.380080	2.538882
13	1	0	0.497473	-1.382705	2.052352
14	1	0	2.604521	-2.167181	0.903203
15	1	0	-0.022579	1.213098	1.892447
16	1	0	0.138643	-1.590678	-0.573460
17	1	0	1.610866	-2.041538	-1.463990
18	1	0	1.653068	0.480708	-1.991836
19	1	0	4.000705	1.682214	-0.040215
20	1	0	2.893296	1.422358	1.315475
21	1	0	4.405051	0.505718	1.217211
22	1	0	4.795877	-1.213942	-0.497381
23	1	0	3.592867	-1.606668	-1.730856
24	1	0	4.400554	-0.034737	-1.757314
25	1	0	1.091999	2.936150	-0.893833
26	1	0	-0.398118	2.842360	0.076886
27	1	0	-0.346407	2.159596	-1.564226
28	17	0	-4.131509	-0.450133	-0.295372

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3422.185080
Sum of electronic and thermal Energies=	-3422.171330
Sum of electronic and thermal Enthalpies=	-3422.170386
Sum of electronic and thermal Free Energies=	-3422.226708

Cartesian coordinates of Intermediate Sol-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.234773	-0.040200	1.862231
2	6	0	-0.775161	1.325445	1.320845
3	6	0	-0.266143	1.345528	-0.095506
4	6	0	-0.596923	0.286479	-0.988285
5	6	0	-1.394958	-0.863748	-0.614868
6	6	0	-1.820768	-1.005179	0.839685
7	6	0	-2.888229	-0.685684	-0.161703
8	6	0	-3.782173	-1.843990	-0.574340
9	6	0	-3.605820	0.649112	-0.246330
10	6	0	0.165699	2.679964	-0.634518
11	35	0	1.623805	0.008489	-0.224521
12	17	0	4.144933	-1.003709	0.145855
13	1	0	-1.952934	0.126467	2.671325
14	1	0	-0.374365	-0.540111	2.316911
15	1	0	-1.602338	2.047124	1.341773
16	1	0	-0.016243	1.758979	1.979418
17	1	0	-0.361567	0.428289	-2.043722
18	1	0	-1.210770	-1.754174	-1.208796
19	1	0	-1.836090	-2.032582	1.198298
20	1	0	-4.142107	-1.714759	-1.599460
21	1	0	-4.655564	-1.889330	0.085336
22	1	0	-3.261784	-2.802203	-0.510481
23	1	0	-4.385815	0.693006	0.520986
24	1	0	-4.094983	0.749016	-1.219535
25	1	0	-2.965438	1.517615	-0.112808
26	1	0	0.590746	2.603583	-1.635643
27	1	0	0.884914	3.158818	0.032517
28	1	0	-0.717194	3.329823	-0.680705

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.910754
Sum of electronic and thermal Energies=	-3424.895935
Sum of electronic and thermal Enthalpies=	-3424.894991
Sum of electronic and thermal Free Energies=	-3424.953813

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.086390	-0.228991	1.829815
2	6	0	-0.708544	1.183553	1.375416
3	6	0	-0.209249	1.286663	-0.044398
4	6	0	-0.559985	0.263332	-1.006742

5	6	0	-1.387495	-0.885966	-0.682971
6	6	0	-1.753081	-1.094419	0.774846
7	6	0	-2.826037	-0.644386	-0.161007
8	6	0	-3.810576	-1.714327	-0.593099
9	6	0	-3.452146	0.740499	-0.125246
10	6	0	0.151689	2.662003	-0.533626
11	35	0	1.481941	0.049582	-0.249123
12	17	0	4.194618	-0.981543	0.123867
13	1	0	-1.739622	-0.151370	2.704879
14	1	0	-0.179568	-0.747733	2.158559
15	1	0	-1.568081	1.860648	1.442336
16	1	0	0.055466	1.603806	2.036814
17	1	0	-0.367312	0.485574	-2.054738
18	1	0	-1.262819	-1.742346	-1.338136
19	1	0	-1.818321	-2.140773	1.064594
20	1	0	-4.177085	-1.516291	-1.605719
21	1	0	-4.670272	-1.715047	0.086954
22	1	0	-3.359980	-2.710978	-0.574726
23	1	0	-3.935705	0.911331	0.843155
24	1	0	-4.221198	0.808478	-0.900585
25	1	0	-2.753973	1.559252	-0.306615
26	1	0	0.578966	2.638893	-1.537995
27	1	0	0.857949	3.135244	0.151932
28	1	0	-0.763993	3.264404	-0.555041

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -3422.208104
Sum of electronic and thermal Energies= -3422.193916
Sum of electronic and thermal Enthalpies= -3422.192972
Sum of electronic and thermal Free Energies= -3422.250175

Cartesian coordinates of Intermediate Sol-2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.745050	-0.625089	0.986022
2	6	0	-1.129791	0.717477	1.371761
3	6	0	-1.406364	-0.877360	-0.489843
4	6	0	-2.860213	-0.634646	-0.023908
5	6	0	-0.480966	1.238405	0.103848
6	6	0	-0.634405	0.286841	-0.935418
7	35	0	1.550360	0.018769	-0.181853
8	6	0	-3.722113	-1.885862	-0.047425

9	6	0	-3.629969	0.619105	-0.398563
10	6	0	-0.125293	2.674828	-0.073193
11	17	0	4.075099	-0.847111	0.155962
12	1	0	-1.685950	-1.441074	1.699685
13	1	0	-0.404093	0.630616	2.185481
14	1	0	-1.875228	1.450682	1.706489
15	1	0	-1.165438	-1.856658	-0.891033
16	1	0	-0.423322	0.516768	-1.978609
17	1	0	-4.145816	-2.048192	-1.043178
18	1	0	-4.551778	-1.780727	0.659278
19	1	0	-3.152244	-2.775518	0.230665
20	1	0	-4.089492	0.498646	-1.383972
21	1	0	-3.022916	1.525025	-0.432399
22	1	0	-4.433075	0.789471	0.325746
23	1	0	0.413629	2.857445	-1.003005
24	1	0	0.460051	3.042544	0.772497
25	1	0	-1.058607	3.252761	-0.093816

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3385.612030
Sum of electronic and thermal Energies=	-3385.598381
Sum of electronic and thermal Enthalpies=	-3385.597437
Sum of electronic and thermal Free Energies=	-3385.653505

Cartesian coordinates of Intermediate Sol-3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.246170	-0.739789	-0.863085
2	6	0	-1.001705	-1.313939	-0.166977
3	6	0	-2.024285	0.798370	-0.818741
4	6	0	-3.434077	-0.469451	-0.069567
5	6	0	-0.316785	-0.121741	0.532424
6	6	0	-0.459712	2.489051	0.212418
7	6	0	-0.960153	1.111822	-0.039845
8	35	0	1.665257	-0.123201	0.221599
9	6	0	-4.708679	-0.165726	-0.768878
10	6	0	-3.491223	-0.577726	1.407680
11	17	0	5.138474	-0.255165	-0.335880
12	1	0	-2.451618	-1.113067	-1.870180
13	1	0	-0.350861	-1.724523	-0.939655
14	1	0	-1.236530	-2.122798	0.527585
15	1	0	-2.610863	1.509843	-1.390842

16	1	0	-0.369755	-0.137065	1.626169
17	1	0	0.540606	2.620043	-0.209766
18	1	0	-0.366125	2.652803	1.292876
19	1	0	-1.127775	3.240922	-0.207839
20	1	0	-5.256757	0.651237	-0.293216
21	1	0	-5.329907	-1.068324	-0.656628
22	1	0	-4.579657	0.021560	-1.834507
23	1	0	-4.098423	0.215284	1.849421
24	1	0	-2.524333	-0.636710	1.900990
25	1	0	-4.019304	-1.524607	1.607013

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -3385.624250
Sum of electronic and thermal Energies= -3385.609904
Sum of electronic and thermal Enthalpies= -3385.608960
Sum of electronic and thermal Free Energies= -3385.668779

Cartesian coordinates of Intermediate Sol-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.923785	-0.803621	1.526418
2	6	0	1.902402	-1.369270	0.487386
3	6	0	0.233700	0.459043	0.995719
4	6	0	2.823266	-0.247845	-0.092844
5	6	0	0.712202	0.960548	-0.280534
6	6	0	1.177546	-1.432753	-0.877848
7	6	0	1.524784	0.066390	-1.090380
8	6	0	3.362324	0.846904	0.825742
9	6	0	3.976275	-0.778441	-0.947979
10	6	0	0.552556	2.381583	-0.664576
11	35	0	-1.690656	0.140922	0.217755
12	1	0	1.445541	-0.526394	2.448492
13	1	0	0.184485	-1.559657	1.801693
14	1	0	2.401396	-2.268748	0.859037
15	1	0	0.023084	1.227631	1.740381
16	1	0	0.119354	-1.689176	-0.878622
17	1	0	1.693539	-2.048284	-1.610898
18	1	0	1.747698	0.443207	-2.090795
19	1	0	3.824169	1.649238	0.242632
20	1	0	2.620248	1.297091	1.487947
21	1	0	4.142208	0.417819	1.462762
22	1	0	4.741676	-1.191119	-0.282139
23	1	0	3.682123	-1.564215	-1.643399

24	1	0	4.433834	0.032388	-1.521083
25	1	0	1.555697	2.832731	-0.678766
26	1	0	-0.078597	2.941449	0.024362
27	1	0	0.172974	2.465155	-1.687479
28	17	0	-4.509972	-0.463918	-0.387187

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.901723
Sum of electronic and thermal Energies=	-3424.887515
Sum of electronic and thermal Enthalpies=	-3424.886571
Sum of electronic and thermal Free Energies=	-3424.943991

Cartesian coordinates of Transition State TS-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.836958	-0.651684	1.815125
2	6	0	0.249413	-1.881555	1.092605
3	6	0	-0.449024	-1.587841	-0.221073
4	6	0	0.048383	-0.440960	-1.006099
5	6	0	0.948301	0.560352	-0.512884
6	6	0	1.425562	0.439116	0.926768
7	6	0	2.451088	0.280326	-0.154762
8	6	0	3.357325	1.476996	-0.401421
9	6	0	3.116575	-1.039444	-0.506102
10	6	0	-0.995981	-2.781467	-0.968339
11	35	0	-1.912662	-0.123622	0.039291
12	17	0	-1.201141	2.927197	-0.068214
13	1	0	1.578169	-0.995829	2.546528
14	1	0	0.031314	-0.177105	2.385502
15	1	0	1.039655	-2.608527	0.859441
16	1	0	-0.446281	-2.406695	1.756296
17	1	0	-0.267611	-0.392386	-2.046606
18	1	0	0.698750	1.566795	-0.869614
19	1	0	1.443876	1.406776	1.422938
20	1	0	3.685202	1.513539	-1.446944
21	1	0	4.253162	1.402076	0.228787
22	1	0	2.854154	2.419770	-0.168694
23	1	0	3.968281	-1.213344	0.163760
24	1	0	3.508492	-1.008113	-1.529522
25	1	0	2.455628	-1.904784	-0.433257
26	1	0	-1.541272	-2.482223	-1.867289
27	1	0	-1.666309	-3.364618	-0.330700
28	1	0	-0.164248	-3.433964	-1.269105

Level: B3LYP/6-311+G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3424.841795
 Sum of electronic and thermal Energies= -3424.828299
 Sum of electronic and thermal Enthalpies= -3424.827354
 Sum of electronic and thermal Free Energies= -3424.882298

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.681299	-0.243476	1.831792
2	6	0	0.195916	-1.599196	1.302032
3	6	0	-0.401153	-1.558358	-0.089409
4	6	0	0.027697	-0.478117	-0.998196
5	6	0	0.948947	0.572137	-0.636623
6	6	0	1.365179	0.653015	0.816267
7	6	0	2.390547	0.236044	-0.183749
8	6	0	3.398315	1.299949	-0.574927
9	6	0	2.956349	-1.170203	-0.283055
10	6	0	-0.813209	-2.882107	-0.676333
11	35	0	-1.879052	-0.176946	-0.115599
12	17	0	-1.176092	2.860444	0.018760
13	1	0	1.349695	-0.423713	2.681139
14	1	0	-0.175309	0.323194	2.213910
15	1	0	1.017378	-2.324925	1.269325
16	1	0	-0.554865	-2.020772	1.979318
17	1	0	-0.235967	-0.603013	-2.047927
18	1	0	0.787743	1.511602	-1.160321
19	1	0	1.429500	1.686419	1.150495
20	1	0	3.730924	1.160945	-1.609456
21	1	0	4.277350	1.234389	0.077619
22	1	0	2.974479	2.303313	-0.479169
23	1	0	3.550092	-1.405462	0.608422
24	1	0	3.620495	-1.238674	-1.151195
25	1	0	2.200524	-1.949511	-0.400744
26	1	0	-1.300270	-2.762091	-1.646917
27	1	0	-1.494684	-3.403242	0.000795
28	1	0	0.083977	-3.501043	-0.805025

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -3422.151110
 Sum of electronic and thermal Energies= -3422.137962
 Sum of electronic and thermal Enthalpies= -3422.137018
 Sum of electronic and thermal Free Energies= -3422.190963

Cartesian coordinates of Transition State TS-2a:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.820110	-0.416989	-1.005932
2	6	0	-1.344588	-1.740382	-0.408278
3	6	0	-0.900685	0.689241	-0.494838
4	6	0	-2.364170	0.643347	-0.067681
5	6	0	-0.199575	-1.382057	0.510638
6	6	0	0.101626	0.052013	0.404611
7	35	0	1.674536	-0.607337	-0.669658
8	6	0	-3.234052	1.711125	-0.715544
9	6	0	-2.787510	0.324908	1.357813
10	6	0	0.301252	-2.279826	1.586981
11	17	0	2.236778	2.319472	0.659414
12	1	0	-2.163304	-0.422410	-2.036026
13	1	0	-1.014027	-2.446257	-1.180052
14	1	0	-2.120400	-2.269719	0.166391
15	1	0	-0.557027	1.523590	-1.095745
16	1	0	0.602156	0.660053	1.172401
17	1	0	-3.182357	2.648764	-0.150475
18	1	0	-4.282483	1.389175	-0.743377
19	1	0	-2.918714	1.922046	-1.742764
20	1	0	-2.742751	1.229051	1.975245
21	1	0	-2.165372	-0.429063	1.850899
22	1	0	-3.821453	-0.041302	1.374884
23	1	0	1.221183	-1.902993	2.039058
24	1	0	0.463690	-3.297313	1.216493
25	1	0	-0.466259	-2.346141	2.374437

Level: B3LYP/6-311+G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3385.543494
Sum of electronic and thermal Energies= -3385.531046
Sum of electronic and thermal Enthalpies= -3385.530102
Sum of electronic and thermal Free Energies= -3385.583384

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.614817	-0.684470	-0.976547
2	6	0	-0.920210	-1.840250	-0.262035
3	6	0	-0.926556	0.616637	-0.561475
4	6	0	-2.359816	0.296147	-0.124671
5	6	0	0.168760	-1.184819	0.589353
6	6	0	0.106286	0.267217	0.402605
7	35	0	1.727100	-0.695983	-0.637476
8	6	0	-3.398089	1.146533	-0.828199
9	6	0	-2.712505	0.008881	1.321020
10	6	0	0.667190	-1.825925	1.850894
11	17	0	1.573950	2.873459	0.471933
12	1	0	-1.925850	-0.819909	-2.007566
13	1	0	-0.497461	-2.572200	-0.953771
14	1	0	-1.601571	-2.380166	0.408791
15	1	0	-0.756323	1.481598	-1.193774
16	1	0	0.648079	1.050338	0.973434
17	1	0	-3.497675	2.117327	-0.332609
18	1	0	-4.371706	0.643794	-0.803642

19	1	0	-3.130432	1.324707	-1.873839
20	1	0	-2.861887	0.950075	1.859157
21	1	0	-1.949514	-0.555135	1.864816
22	1	0	-3.646166	-0.563449	1.367650
23	1	0	1.444518	-1.220251	2.321324
24	1	0	1.054891	-2.827243	1.647750
25	1	0	-0.176024	-1.918581	2.545418

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3382.885210
Sum of electronic and thermal Energies=	-3382.873076
Sum of electronic and thermal Enthalpies=	-3382.872132
Sum of electronic and thermal Free Energies=	-3382.924345

Cartesian coordinates of Transition State TS-3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.755311	-0.468759	-1.024681
2	6	0	-1.332844	-1.785508	-0.361900
3	6	0	-1.016686	0.672641	-0.333364
4	6	0	-2.551722	0.520750	-0.213504
5	6	0	-0.275554	-1.384629	0.663679
6	6	0	0.426377	0.930215	1.795646
7	6	0	-0.202279	0.099156	0.748478
8	35	0	1.523832	-0.939213	-0.216901
9	6	0	-3.330615	1.563132	-1.001547
10	6	0	-3.220576	0.143099	1.098372
11	17	0	2.997261	1.627192	-0.299793
12	1	0	-1.869773	-0.455168	-2.104454
13	1	0	-0.929333	-2.492446	-1.091436
14	1	0	-2.170437	-2.287791	0.140032
15	1	0	-0.625336	1.545329	-0.848482
16	1	0	-0.106646	-1.991071	1.550126
17	1	0	0.822002	0.341514	2.627161
18	1	0	-0.286561	1.678384	2.160038
19	1	0	1.278704	1.479333	1.316713
20	1	0	-3.445863	2.487556	-0.423750
21	1	0	-4.333807	1.187226	-1.238013
22	1	0	-2.833718	1.814346	-1.944084
23	1	0	-3.356456	1.030814	1.726881
24	1	0	-2.660548	-0.590107	1.686297
25	1	0	-4.214530	-0.278322	0.903900

Level: B3LYP/6-311+G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3385.549555
Sum of electronic and thermal Energies=	-3385.537494

Sum of electronic and thermal Enthalpies= -3385.536549
Sum of electronic and thermal Free Energies= -3385.588523

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.507395	-0.474783	-1.105666
2	6	0	-1.051180	-1.847761	-0.615195
3	6	0	-0.832232	0.592419	-0.255725
4	6	0	-2.346320	0.340350	-0.171890
5	6	0	-0.058811	-1.539045	0.500782
6	6	0	0.442103	0.570989	1.983991
7	6	0	-0.057517	-0.090431	0.768841
8	35	0	1.709896	-1.008997	-0.258118
9	6	0	-3.168143	1.453104	-0.789218
10	6	0	-2.985690	-0.262587	1.063099
11	17	0	1.879624	2.496018	-0.250691
12	1	0	-1.607335	-0.309106	-2.173588
13	1	0	-0.588346	-2.436876	-1.409532
14	1	0	-1.878832	-2.439471	-0.205564
15	1	0	-0.444742	1.550121	-0.605727
16	1	0	0.105548	-2.240210	1.316049
17	1	0	0.949362	-0.113499	2.666249
18	1	0	-0.410743	1.056714	2.474826
19	1	0	1.115411	1.385297	1.635036
20	1	0	-3.312789	2.268030	-0.072662
21	1	0	-4.153777	1.072268	-1.081214
22	1	0	-2.679657	1.865955	-1.676086
23	1	0	-3.167771	0.517159	1.810519
24	1	0	-2.382198	-1.040522	1.542254
25	1	0	-3.952989	-0.706828	0.801223

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies= -3382.890345
Sum of electronic and thermal Energies= -3382.878289
Sum of electronic and thermal Enthalpies= -3382.877345
Sum of electronic and thermal Free Energies= -3382.929279

Cartesian coordinates of Transition State TS-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	4.499671	-0.218151	0.222557

2	35	0	1.944743	-0.185212	-0.127713
3	6	0	-0.201671	-0.138257	-0.558179
4	1	0	-0.146803	-0.282829	-1.638455
5	6	0	-0.675890	1.189913	-0.180551
6	6	0	-0.224699	2.356903	-1.020142
7	1	0	-0.489866	2.211479	-2.075546
8	1	0	0.867882	2.436695	-0.975532
9	1	0	-0.661653	3.300197	-0.679814
10	6	0	-1.470783	1.376111	0.915699
11	1	0	-1.725869	2.393673	1.206390
12	6	0	-1.962357	0.247359	1.793771
13	1	0	-2.865537	0.538869	2.338899
14	1	0	-1.223224	-0.026760	2.560065
15	6	0	-2.212445	-0.921257	0.839914
16	1	0	-2.535191	-1.851864	1.344775
17	6	0	-0.813292	-1.293271	0.211979
18	1	0	-0.864945	-2.191448	-0.410846
19	1	0	-0.187696	-1.551431	1.070765
20	6	0	-3.268232	-0.573491	-0.149853
21	6	0	-3.249472	-1.284764	-1.445525
22	1	0	-3.022168	-2.352944	-1.326166
23	1	0	-2.400792	-0.882750	-2.035963
24	1	0	-4.164694	-1.158522	-2.029033
25	6	0	-4.407860	0.354100	0.087077
26	1	0	-5.330730	-0.246794	0.178930
27	1	0	-4.573280	1.001845	-0.784381
28	1	0	-4.315653	0.973504	0.977263

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies= -3424.829192
Sum of electronic and thermal Energies= -3424.815288
Sum of electronic and thermal Enthalpies= -3424.814343
Sum of electronic and thermal Free Energies= -3424.870865

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	4.463572	-0.207088	0.220196
2	35	0	1.884382	-0.176039	-0.146303
3	6	0	-0.171973	-0.144900	-0.491601
4	1	0	-0.196996	-0.317004	-1.571996
5	6	0	-0.690092	1.191080	-0.152047
6	6	0	-0.257177	2.326110	-1.037362
7	1	0	-0.459564	2.095038	-2.090072
8	1	0	0.825078	2.472517	-0.946190
9	1	0	-0.764453	3.258825	-0.777970
10	6	0	-1.497056	1.401124	0.920170
11	1	0	-1.776184	2.422661	1.173494
12	6	0	-1.996523	0.287336	1.812193
13	1	0	-2.923758	0.571329	2.318903
14	1	0	-1.277331	0.042246	2.603909
15	6	0	-2.186776	-0.905170	0.882312
16	1	0	-2.541654	-1.828051	1.381334
17	6	0	-0.768083	-1.274780	0.321886
18	1	0	-0.769021	-2.207607	-0.249354
19	1	0	-0.164990	-1.459806	1.215281
20	6	0	-3.183852	-0.612275	-0.164409
21	6	0	-3.108538	-1.382856	-1.412609
22	1	0	-2.816924	-2.425616	-1.245408
23	1	0	-2.258255	-0.935060	-1.970428

24	1	0	-4.004586	-1.313911	-2.031477
25	6	0	-4.288932	0.367499	-0.054297
26	1	0	-5.230155	-0.205904	-0.010515
27	1	0	-4.352437	0.963595	-0.973478
28	1	0	-4.228854	1.029589	0.805815

Level: M06-2X/6-31+G*

Sum of electronic and zero-point Energies=	-3422.107526
Sum of electronic and thermal Energies=	-3422.093616
Sum of electronic and thermal Enthalpies=	-3422.092672
Sum of electronic and thermal Free Energies=	-3422.149350

Cartesian coordinates of Transition State Sol-TS-4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.325450	-0.383049	1.790906
2	6	0	1.228070	-1.630624	0.909337
3	6	0	0.386526	-1.468258	-0.334574
4	6	0	0.177533	-0.120983	-0.889015
5	6	0	0.733048	1.076589	-0.297552
6	6	0	1.429283	0.936170	1.045104
7	6	0	2.276042	1.188576	-0.156018
8	6	0	2.783104	2.609251	-0.315741
9	6	0	3.223738	0.167807	-0.764804
10	6	0	0.321318	-2.648724	-1.264048
11	35	0	-1.505830	-0.881186	0.197500
12	17	0	-3.398389	2.010274	-0.182482
13	1	0	2.188884	-0.493573	2.454625
14	1	0	0.439975	-0.332295	2.433275
15	1	0	2.218770	-1.948875	0.566199
16	1	0	0.824545	-2.470917	1.482477
17	1	0	-0.227086	-0.065299	-1.898280
18	1	0	0.215966	1.996151	-0.551795
19	1	0	1.299136	1.800032	1.693082
20	1	0	2.882570	2.866496	-1.375174
21	1	0	3.770985	2.695558	0.151202
22	1	0	2.115772	3.334421	0.158297
23	1	0	4.016104	-0.079840	-0.049692
24	1	0	3.695031	0.599992	-1.652481
25	1	0	2.751490	-0.761595	-1.084242
26	1	0	-0.373086	-2.481051	-2.089527
27	1	0	0.027805	-3.545594	-0.714905
28	1	0	1.325127	-2.807280	-1.674925

Level: M06-2x/6-31+G*

Sum of electronic and zero-point Energies=	-3422.202356
Sum of electronic and thermal Energies=	-3422.188846
Sum of electronic and thermal Enthalpies=	-3422.187902
Sum of electronic and thermal Free Energies=	-3422.244571

Cartesian coordinates of Intermediate Int-1b₁

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.260044	1.285017	-1.097611
2	6	0	-1.217578	1.481889	0.080220
3	6	0	-1.667402	0.167052	0.716592
4	6	0	-0.545745	-0.810758	0.842483
5	6	0	0.633455	-0.677000	0.229375
6	6	0	0.979767	0.414761	-0.757951
7	6	0	2.200676	1.222498	-0.319178
8	6	0	3.287607	1.280323	-1.101245
9	6	0	2.141830	1.959869	0.993645
10	6	0	-2.402888	0.381472	2.035250
11	35	0	-3.052380	-0.710852	-0.546543
12	17	0	4.667778	-1.715582	0.225208
13	1	0	0.060926	2.255776	-1.484942
14	1	0	-0.807824	0.791356	-1.904743
15	1	0	-0.729294	2.055497	0.876870
16	1	0	-2.089191	2.061528	-0.231154
17	1	0	-0.721545	-1.663950	1.491095
18	1	0	1.406994	-1.416594	0.419339
19	1	0	1.279463	-0.092645	-1.682417
20	1	0	4.155536	1.870328	-0.824228
21	1	0	3.323986	0.777969	-2.062726
22	1	0	4.079943	-0.612143	-0.141436
23	1	0	1.403204	2.767257	0.953142
24	1	0	3.107336	2.403992	1.241121
25	1	0	1.843819	1.295276	1.809680
26	1	0	-2.769612	-0.561474	2.443578
27	1	0	-3.250184	1.057357	1.907541
28	1	0	-1.710556	0.824444	2.760245

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.932082
Sum of electronic and thermal Energies=	-3424.917071
Sum of electronic and thermal Enthalpies=	-3424.916126
Sum of electronic and thermal Free Energies=	-3424.976951

Cartesian coordinates of Intermediate Sol-1b₁

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.972084	1.668647	-1.025869
2	6	0	-1.822175	1.310596	0.201437
3	6	0	-1.559346	-0.090481	0.746551
4	6	0	-0.121131	-0.490060	0.697011
5	6	0	0.826476	0.134829	-0.017784
6	6	0	0.532970	1.363526	-0.905185
7	6	0	1.428026	2.309378	-0.208027
8	6	0	2.864844	2.277284	-0.525115
9	6	0	0.961239	3.281874	0.788115
10	6	0	-2.201145	-0.337411	2.106015
11	35	0	-2.477218	-1.429079	-0.548099
12	17	0	5.054071	-2.463253	0.139969
13	1	0	-1.121456	2.721242	-1.284104
14	1	0	-1.331752	1.081800	-1.877184
15	1	0	-1.641749	2.004582	1.031435
16	1	0	-2.880875	1.419285	-0.048880
17	1	0	0.145430	-1.395041	1.237418
18	1	0	1.842536	-0.244772	-0.024264
19	1	0	0.960102	1.149101	-1.891718
20	1	0	3.474222	2.229732	0.384035
21	1	0	3.095799	3.258064	-0.974004
22	1	0	3.139183	1.502321	-1.241182
23	1	0	0.826799	4.217313	0.212815
24	1	0	1.715505	3.495999	1.548140
25	1	0	-0.002921	3.049281	1.233431
26	1	0	-2.066530	-1.372889	2.429029
27	1	0	-3.270259	-0.110272	2.079130
28	1	0	-1.726639	0.318223	2.847003

Level: B3LYP/6-311+G**

Geometry not converged even after 500 Cycles.

SCF Done: E(RB+HF-LYP) = -3422.59045622

Cartesian coordinates of Intermediate Int-2b₁

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.636596	0.257710	0.393315
2	6	0	0.661770	1.085862	0.600892
3	6	0	-0.469801	-0.231223	-1.032740
4	6	0	-1.917563	1.019142	0.685767
5	6	0	1.657864	0.572074	-0.454505
6	6	0	0.780887	-0.082792	-1.473291
7	35	0	2.795668	-0.936516	0.393300
8	6	0	-2.669968	0.705329	1.749130
9	6	0	-2.305701	2.130440	-0.256364
10	6	0	2.651061	1.597974	-0.975435
11	1	0	-0.610017	-0.616977	1.055588
12	1	0	1.045946	1.030064	1.618123
13	1	0	0.466308	2.139532	0.377124
14	1	0	-1.271731	-0.708750	-1.584032
15	1	0	1.163576	-0.421594	-2.428265
16	1	0	-3.569857	1.260634	1.992952
17	1	0	-2.387434	-0.092523	2.428305
18	1	0	-3.784212	-0.650173	0.262366
19	1	0	-3.225576	2.619895	0.066488
20	1	0	-2.456457	1.748997	-1.271331
21	1	0	-1.521839	2.891378	-0.322579
22	1	0	3.331080	1.157075	-1.705930
23	1	0	3.245023	2.021739	-0.163668
24	1	0	2.098499	2.409286	-1.462663
25	17	0	-4.522554	-1.431623	-0.473447

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3385.635310
Sum of electronic and thermal Energies=	-3385.621134
Sum of electronic and thermal Enthalpies=	-3385.620190
Sum of electronic and thermal Free Energies=	-3385.679745

Cartesian coordinates of Intermediate Int-3b₁

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.827587	0.707319	-0.653685
2	6	0	-0.035283	-0.561786	-0.238269
3	6	0	0.250420	1.778318	-0.617281
4	6	0	-2.011907	1.111256	0.221864
5	6	0	1.246620	-0.043932	0.432402
6	6	0	2.593272	2.212672	0.257820
7	6	0	1.381979	1.382261	-0.024954
8	35	0	2.843397	-1.178226	-0.053796
9	6	0	-2.917479	2.154678	-0.382458
10	6	0	-2.245104	0.611063	1.441449
11	1	0	-1.215253	0.592220	-1.673536
12	1	0	0.231322	-1.111959	-1.140622
13	1	0	-0.594299	-1.245850	0.398955
14	1	0	0.079629	2.784715	-0.982648
15	1	0	1.250794	-0.128389	1.519244
16	1	0	3.476695	1.797707	-0.235185
17	1	0	2.809997	2.231237	1.331809
18	1	0	2.454437	3.240433	-0.082214
19	1	0	-3.735175	2.417677	0.290163
20	1	0	-3.346978	1.794739	-1.323951
21	1	0	-2.363661	3.069431	-0.617782
22	1	0	-3.077989	0.965619	2.039665
23	1	0	-1.604324	-0.131157	1.902295
24	1	0	-3.590259	-0.873155	0.310462
25	17	0	-4.406084	-1.780967	-0.145596

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3385.634776
Sum of electronic and thermal Energies=	-3385.620490
Sum of electronic and thermal Enthalpies=	-3385.619546
Sum of electronic and thermal Free Energies=	-3385.680102

Cartesian coordinates of Intermediate Int-4b₁

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	3.627526	-1.628810	-1.354978
2	35	0	-2.759021	-1.168028	0.152568
3	6	0	-1.296166	0.214071	0.428752
4	1	0	-1.446901	0.467620	1.479005
5	6	0	-1.507156	1.417292	-0.447579
6	6	0	-2.874008	2.047685	-0.491665
7	1	0	-3.242276	2.249467	0.520398
8	1	0	-3.604241	1.388389	-0.966742
9	1	0	-2.847984	2.991479	-1.039205
10	6	0	-0.463242	1.947884	-1.098447
11	1	0	-0.629761	2.833096	-1.707278
12	6	0	0.967633	1.471633	-1.011433
13	1	0	1.613994	2.347477	-0.941027
14	1	0	1.242014	0.972796	-1.954247
15	6	0	1.166544	0.523510	0.153531
16	1	0	2.883280	-0.831783	-0.636677
17	6	0	0.043999	-0.490887	0.203377
18	1	0	0.186786	-1.258975	0.959708
19	1	0	-0.003507	-1.003786	-0.763819
20	6	0	2.173880	0.603387	1.049611
21	6	0	2.304203	-0.293619	2.259805
22	1	0	1.459384	-0.961791	2.413755
23	1	0	2.413013	0.319316	3.161445
24	1	0	3.210991	-0.905550	2.191103
25	6	0	3.294652	1.615602	0.966401
26	1	0	4.261454	1.115515	1.087139
27	1	0	3.213672	2.338469	1.786764
28	1	0	3.325842	2.169662	0.030299

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-3424.938160
Sum of electronic and thermal Energies=	-3424.922473
Sum of electronic and thermal Enthalpies=	-3424.921529
Sum of electronic and thermal Free Energies=	-3424.984003

Cartesian coordinates of Intermediate Int-1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.086479	-0.736576	-0.894655
2	6	0	-1.628758	-0.861330	0.554754
3	6	0	0.026337	-0.010407	-1.162114
4	6	0	-2.756246	-0.112292	0.012293
5	6	0	0.843768	0.739140	-0.165751
6	6	0	-0.678687	-0.314536	1.625923
7	6	0	0.191015	0.881353	1.208640
8	6	0	-3.878088	-0.876559	-0.605799
9	6	0	-2.970063	1.353539	0.143506
10	6	0	1.406222	2.050743	-0.702851
11	35	0	2.401089	-0.575792	-0.014638
12	1	0	-1.509417	-1.367303	-1.664177
13	1	0	-1.888601	-1.904247	0.741822
14	1	0	0.432810	-0.054574	-2.168647
15	1	0	-0.022786	-1.143226	1.901986
16	1	0	-1.250319	-0.060355	2.522246
17	1	0	-0.385892	1.809806	1.199039
18	1	0	0.967253	1.035474	1.959449
19	1	0	-4.234502	-0.418086	-1.530592
20	1	0	-3.651130	-1.929718	-0.765756
21	1	0	-4.712843	-0.822131	0.108957
22	1	0	-3.677392	1.477472	0.978410
23	1	0	-2.081630	1.924389	0.383339
24	1	0	-3.457072	1.770935	-0.739219
25	1	0	2.097332	2.491123	0.017049
26	1	0	0.587223	2.758823	-0.869792
27	1	0	1.934736	1.905886	-1.645447

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-2964.421510
Sum of electronic and thermal Energies=	-2964.408862
Sum of electronic and thermal Enthalpies=	-2964.407918
Sum of electronic and thermal Free Energies=	-2964.460918

Cartesian coordinates of Intermediate Int-2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.353902	-0.629150	-0.528795
2	6	0	0.281754	0.335137	-1.076428
3	6	0	1.044864	-0.716872	1.004577
4	6	0	2.680134	-0.123132	-0.205607
5	6	0	-0.694170	0.635293	0.092980
6	6	0	-0.048281	0.011663	1.287551
7	35	0	-2.359727	-0.500157	-0.122779
8	6	0	3.780246	-1.098563	-0.020243
9	6	0	3.014043	1.313580	-0.086647
10	6	0	-1.132209	2.085315	0.236976
11	1	0	1.370384	-1.620738	-0.983292
12	1	0	-0.227983	-0.114859	-1.925592
13	1	0	0.722444	1.266964	-1.434264
14	1	0	1.573966	-1.365777	1.687238
15	1	0	-0.507048	0.053095	2.268946
16	1	0	4.452209	-0.829856	0.797005
17	1	0	4.380481	-1.044469	-0.943690
18	1	0	3.435883	-2.127489	0.077876
19	1	0	3.709556	1.501752	0.733301
20	1	0	2.152995	1.970692	-0.009474
21	1	0	3.554584	1.574551	-1.011776
22	1	0	-1.815997	2.211845	1.076693
23	1	0	-1.635125	2.427192	-0.668799
24	1	0	-0.257599	2.722953	0.406922

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-2925.119032
Sum of electronic and thermal Energies=	-2925.107414
Sum of electronic and thermal Enthalpies=	-2925.106469
Sum of electronic and thermal Free Energies=	-2925.157585

Cartesian coordinates of Intermediate Int-3b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.498302	-0.678938	-0.849555
2	6	0	-0.242037	-1.354866	-0.280086
3	6	0	-1.202059	0.843289	-0.727401
4	6	0	-2.587689	-0.331581	0.048139
5	6	0	0.562465	-0.239207	0.425311
6	6	0	0.536778	2.390284	0.258267
7	6	0	-0.060170	1.060474	-0.018272
8	35	0	2.489117	-0.307843	-0.043412
9	6	0	-3.894478	0.088751	-0.536168
10	6	0	-2.550012	-0.518657	1.524746
11	1	0	-1.804687	-0.983495	-1.848645
12	1	0	0.333534	-1.761331	-1.110698
13	1	0	-0.474239	-2.184141	0.389115
14	1	0	-1.771872	1.611690	-1.229263
15	1	0	0.580560	-0.314330	1.513791
16	1	0	1.489014	2.496273	-0.270025
17	1	0	0.774127	2.477103	1.325152
18	1	0	-0.125568	3.204614	-0.032664
19	1	0	-4.338041	0.931089	-0.000931
20	1	0	-4.579312	-0.760918	-0.401313
21	1	0	-3.841967	0.303849	-1.602759
22	1	0	-3.027112	0.309455	2.051857
23	1	0	-1.560814	-0.701638	1.935263
24	1	0	-3.159688	-1.411015	1.730644

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-2925.129108
Sum of electronic and thermal Energies=	-2925.117395
Sum of electronic and thermal Enthalpies=	-2925.116451
Sum of electronic and thermal Free Energies=	-2925.167479

Cartesian coordinates of Intermediate Int-4b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.096633	-1.098257	1.170587
2	6	0	1.292607	-1.359633	0.250940
3	6	0	-0.638803	0.197404	0.732262
4	1	0	0.408139	-0.995857	2.212313
5	1	0	-0.580186	-1.951276	1.131472
6	6	0	2.250027	-0.157918	0.221386
7	6	0	0.082096	0.958398	-0.344808
8	6	0	0.804237	-1.270366	-1.210616
9	1	0	1.809388	-2.284237	0.528302
10	1	0	-0.871999	0.839765	1.577272
11	6	0	0.797380	0.246481	-1.284545
12	6	0	2.436748	0.736735	1.407049
13	6	0	3.476949	-0.246942	-0.639941
14	6	0	-0.012880	2.444359	-0.357621
15	1	0	-0.176676	-1.717705	-1.381251
16	1	0	1.501296	-1.703069	-1.924209
17	1	0	1.222710	0.775406	-2.131473
18	1	0	2.906796	1.682681	1.132787
19	1	0	1.540446	0.927258	1.991011
20	1	0	3.145038	0.215968	2.069425
21	1	0	4.245629	-0.732833	-0.020511
22	1	0	3.359732	-0.846195	-1.538883
23	1	0	3.865638	0.739057	-0.899630
24	1	0	0.562666	2.891376	-1.167693
25	1	0	0.312819	2.867116	0.599421
26	1	0	-1.062886	2.735639	-0.476322
27	35	0	-2.448529	-0.175562	-0.039148

Level: B3LYP/6-311+G**

Sum of electronic and zero-point Energies=	-2964.409462
Sum of electronic and thermal Energies=	-2964.397271
Sum of electronic and thermal Enthalpies=	-2964.396326
Sum of electronic and thermal Free Energies=	-2964.447753

Cartesian coordinates of Intermediate Int-1e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.027181	-1.497583	-0.003586
2	6	0	-2.904167	-1.066839	-1.202593
3	6	0	-0.529625	-0.977237	-0.020066
4	6	0	0.192496	-1.524987	1.236264
5	6	0	-3.521271	0.319604	-1.001311
6	6	0	-4.777551	1.819757	0.623864
7	6	0	-4.382087	0.396677	0.251059
8	6	0	-3.816157	-0.371129	1.390818
9	6	0	-2.747130	-1.172243	1.280877
10	7	0	-0.576865	0.487199	-0.036064
11	6	0	0.176399	-1.553459	-1.271150
12	6	0	0.499320	1.220806	-0.038045
13	6	0	0.258281	2.724520	-0.057088
14	7	0	1.778806	0.724070	-0.023206
15	6	0	4.359779	0.419407	-0.007683
16	6	0	4.960669	0.023196	-1.199532
17	6	0	5.959778	-0.952613	-1.180093
18	6	0	6.376124	-1.538285	0.020712
19	6	0	5.765603	-1.115753	1.211601
20	6	0	4.769122	-0.142684	1.203191
21	6	0	7.465925	-2.586437	0.043520
22	16	0	3.071154	1.690650	-0.023023
23	8	0	3.277715	2.453085	-1.284891
24	8	0	3.263806	2.464793	1.233891
25	35	0	-6.225245	-0.537417	-0.196758
26	1	0	-1.939196	-2.595822	-0.037898
27	1	0	-3.714199	-1.798311	-1.327938
28	1	0	-2.321699	-1.073341	-2.128252
29	1	0	1.258742	-1.303664	1.170910
30	1	0	0.056465	-2.612565	1.330167
31	1	0	-0.190495	-1.047604	2.144204
32	1	0	-2.692399	1.023135	-0.852065
33	1	0	-4.103878	0.632619	-1.874713
34	1	0	-3.866227	2.374645	0.882479
35	1	0	-5.452412	1.836173	1.485200
36	1	0	-5.269140	2.324832	-0.213091
37	1	0	-4.292897	-0.221190	2.358591
38	1	0	-2.372077	-1.643986	2.187170
39	1	0	1.232976	-1.281180	-1.245785
40	1	0	-0.249734	-1.144880	-2.193418
41	1	0	0.087520	-2.648764	-1.306483
42	1	0	0.734718	3.196615	0.809429
43	1	0	-0.815182	2.926643	-0.044712
44	1	0	0.711331	3.171321	-0.949324
45	1	0	4.644585	0.489145	-2.127188
46	1	0	6.425451	-1.262402	-2.114268

47	1	0	6.079414	-1.554387	2.157822
48	1	0	4.307794	0.195954	2.125310
49	1	0	8.372803	-2.217011	0.541612
50	1	0	7.748334	-2.890571	-0.970232
51	1	0	7.148784	-3.486454	0.585706

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3971.831730
Sum of electronic and thermal Energies= -3971.805751
Sum of electronic and thermal Enthalpies= -3971.804807
Sum of electronic and thermal Free Energies= -3971.888462

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.966005	-1.567649	-0.066387
2	6	0	-2.858923	-1.149740	-1.246884
3	6	0	-0.502867	-0.999072	-0.082399
4	6	0	0.242169	-1.554485	1.147930
5	6	0	-3.462842	0.238078	-1.053705
6	6	0	-4.535738	1.787684	0.615034
7	6	0	-4.282999	0.342515	0.221337
8	6	0	-3.716055	-0.447486	1.351340
9	6	0	-2.669058	-1.260219	1.226336
10	7	0	-0.608124	0.457662	-0.052194
11	6	0	0.207374	-1.499808	-1.352795
12	6	0	0.446934	1.201882	-0.030092
13	6	0	0.203290	2.698764	-0.009343
14	7	0	1.726138	0.718217	-0.026439
15	6	0	4.282817	0.444645	0.011365
16	6	0	4.970140	0.160541	-1.155838
17	6	0	5.965563	-0.813933	-1.141149
18	6	0	6.275819	-1.503335	0.027975
19	6	0	5.570704	-1.193419	1.195492
20	6	0	4.579264	-0.224450	1.193503
21	6	0	7.353819	-2.557563	0.051391
22	16	0	2.987516	1.688021	0.006725
23	8	0	3.187339	2.473276	-1.221285
24	8	0	3.142015	2.435853	1.264174
25	35	0	-6.143345	-0.458830	-0.144158
26	1	0	-1.848563	-2.659037	-0.109421
27	1	0	-3.671173	-1.879353	-1.342885
28	1	0	-2.294197	-1.173974	-2.179751
29	1	0	1.307106	-1.347430	1.058392
30	1	0	0.087049	-2.636376	1.236711
31	1	0	-0.117627	-1.069959	2.058066
32	1	0	-2.638229	0.947102	-0.941707
33	1	0	-4.076464	0.532150	-1.908335
34	1	0	-3.565464	2.233442	0.855676
35	1	0	-5.186257	1.854228	1.488468
36	1	0	-4.988903	2.340120	-0.209993
37	1	0	-4.183173	-0.294132	2.320554
38	1	0	-2.290681	-1.745103	2.121393
39	1	0	1.263308	-1.237040	-1.303735
40	1	0	-0.211305	-1.029756	-2.244619
41	1	0	0.106528	-2.587175	-1.447609
42	1	0	0.655120	3.135989	0.884253
43	1	0	-0.868015	2.890737	-0.021885

44	1	0	0.683401	3.166026	-0.872597
45	1	0	4.721267	0.713609	-2.053788
46	1	0	6.508053	-1.041570	-2.053421
47	1	0	5.807335	-1.721137	2.114675
48	1	0	4.033988	0.033293	2.094075
49	1	0	8.167995	-2.270276	0.722350
50	1	0	7.775438	-2.711917	-0.943121
51	1	0	6.958935	-3.513620	0.404824

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.395821
Sum of electronic and thermal Energies=	-3971.369734
Sum of electronic and thermal Enthalpies=	-3971.368790
Sum of electronic and thermal Free Energies=	-3971.455102

Cartesian coordinates of Intermediate Int-2e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.069579	-0.521319	0.203477
2	16	0	2.207110	-1.587531	-0.188933
3	8	0	2.505955	-2.642359	0.815147
4	8	0	1.918540	-2.042856	-1.564536
5	6	0	3.748949	-0.630761	-0.330344
6	6	0	3.832901	0.417125	-1.253975
7	6	0	5.009643	1.150549	-1.366162
8	6	0	6.126752	0.859130	-0.565388
9	6	0	6.025703	-0.193285	0.349270
10	6	0	4.847530	-0.936704	0.469295
11	6	0	0.831822	-0.036767	1.469503
12	6	0	7.398654	1.666251	-0.695671
13	6	0	-1.976962	-0.537411	-0.428503
14	6	0	-3.038620	-0.754198	-1.220175
15	6	0	-4.101614	0.257594	-0.999876
16	6	0	-3.410759	1.336999	-0.153690
17	6	0	-2.190595	0.635956	0.501034
18	7	0	-0.068531	0.853244	1.762729
19	6	0	-1.435974	2.783207	1.579052
20	6	0	-0.944887	1.537637	0.801874
21	6	0	-0.252077	2.024110	-0.491179
22	6	0	1.625986	-0.527068	2.675638
23	6	0	-4.872317	0.738771	-2.218924
24	35	0	-5.588494	-0.632604	0.212801
25	1	0	2.974190	0.646583	-1.877044

26	1	0	5.067224	1.964739	-2.087319
27	1	0	6.880705	-0.438585	0.977474
28	1	0	4.767195	-1.759874	1.171912
29	1	0	7.228096	2.728225	-0.474315
30	1	0	8.171968	1.305209	-0.008911
31	1	0	7.807979	1.615132	-1.713429
32	1	0	-1.055856	-1.111006	-0.419657
33	1	0	-3.151305	-1.568410	-1.930251
34	1	0	-3.055455	2.106879	-0.852854
35	1	0	-4.089057	1.817668	0.554092
36	1	0	-2.494658	0.233990	1.480443
37	1	0	-1.959960	2.478558	2.492070
38	1	0	-0.569547	3.381528	1.881655
39	1	0	-2.102681	3.417598	0.980995
40	1	0	0.075436	1.189566	-1.110752
41	1	0	-0.916193	2.677038	-1.075159
42	1	0	0.635644	2.610623	-0.224873
43	1	0	1.247615	-0.020586	3.565576
44	1	0	1.548521	-1.611710	2.784762
45	1	0	2.693461	-0.300702	2.557490
46	1	0	-5.641830	1.466651	-1.943566
47	1	0	-5.356021	-0.094367	-2.737755
48	1	0	-4.170034	1.218306	-2.914688

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3932.530233
Sum of electronic and thermal Energies=	-3932.505332
Sum of electronic and thermal Enthalpies=	-3932.504388
Sum of electronic and thermal Free Energies=	-3932.585532

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.030581	-0.731706	0.093459
2	16	0	2.227919	-1.689607	-0.314502
3	8	0	2.565941	-2.755857	0.638801
4	8	0	2.017950	-2.097256	-1.700917
5	6	0	3.685289	-0.622608	-0.343068
6	6	0	3.655540	0.536839	-1.114469
7	6	0	4.759981	1.373499	-1.133304
8	6	0	5.906119	1.070877	-0.389288
9	6	0	5.916328	-0.094216	0.371520
10	6	0	4.810627	-0.942769	0.398456
11	6	0	0.876235	-0.192662	1.346388
12	6	0	7.094219	1.999140	-0.417781
13	6	0	-2.040306	-0.722674	-0.186875
14	6	0	-3.107733	-0.968053	-0.947135
15	6	0	-4.072548	0.168227	-0.917921
16	6	0	-3.269187	1.301726	-0.274183
17	6	0	-2.142124	0.607987	0.515682
18	7	0	0.027439	0.733626	1.636457
19	6	0	-1.148106	2.761325	1.293476
20	6	0	-0.819357	1.404399	0.647765
21	6	0	-0.167136	1.680830	-0.720927
22	6	0	1.703384	-0.685415	2.520617
23	6	0	-4.745108	0.508530	-2.233184
24	35	0	-5.604614	-0.337727	0.358208
25	1	0	2.761095	0.769603	-1.681992

26	1	0	4.738795	2.280729	-1.730106
27	1	0	6.797602	-0.342731	0.955001
28	1	0	4.799966	-1.850091	0.991467
29	1	0	6.815232	3.000705	-0.080106
30	1	0	7.894152	1.635057	0.228783
31	1	0	7.494099	2.093828	-1.430981
32	1	0	-1.183542	-1.373051	-0.061368
33	1	0	-3.304802	-1.872481	-1.509978
34	1	0	-2.824640	1.873137	-1.097640
35	1	0	-3.887687	1.976443	0.317004
36	1	0	-2.474414	0.416609	1.545648
37	1	0	-1.612697	2.601687	2.269241
38	1	0	-0.217529	3.311846	1.450428
39	1	0	-1.812386	3.365353	0.667497
40	1	0	-0.127806	0.794925	-1.352101
41	1	0	-0.699960	2.484839	-1.240167
42	1	0	0.861405	2.012665	-0.554670
43	1	0	1.372133	-0.157421	3.411470
44	1	0	1.604536	-1.764482	2.636926
45	1	0	2.764608	-0.482955	2.346925
46	1	0	-5.418479	1.360236	-2.121649
47	1	0	-5.313577	-0.341212	-2.614076
48	1	0	-3.965306	0.762473	-2.957918

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3932.113846
Sum of electronic and thermal Energies=	-3932.088840
Sum of electronic and thermal Enthalpies=	-3932.087895
Sum of electronic and thermal Free Energies=	-3932.170789

Cartesian coordinates of Intermediate Int-3e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.007188	-0.346898	0.418989
2	16	0	2.115485	-1.510057	0.440606
3	8	0	2.413530	-2.124233	1.761275
4	8	0	1.793252	-2.436907	-0.664294
5	6	0	3.670466	-0.709300	-0.061648
6	6	0	4.767343	-0.691527	0.796678
7	6	0	5.952060	-0.062717	0.401355
8	6	0	6.061612	0.553405	-0.848729
9	6	0	4.947262	0.519374	-1.703747
10	6	0	3.763971	-0.103068	-1.319487
11	6	0	0.789162	0.573860	1.417930
12	6	0	7.337664	1.243551	-1.274633
13	6	0	-2.036379	-0.497959	-0.196299

14	6	0	-3.079200	-0.971290	-0.902873
15	6	0	-4.094858	0.097491	-1.083397
16	6	0	-3.403897	1.391246	-0.653436
17	6	0	-2.213464	0.938070	0.235692
18	6	0	-3.280341	-2.363102	-1.421225
19	7	0	-0.083931	1.534470	1.357327
20	6	0	-1.383766	3.305736	0.462434
21	6	0	-0.936413	1.846776	0.201334
22	6	0	-0.226457	1.802635	-1.170771
23	35	0	-5.742873	-0.281336	0.142898
24	6	0	1.571759	0.535279	2.726214
25	1	0	4.681263	-1.178606	1.762604
26	1	0	6.805422	-0.053273	1.077795
27	1	0	5.012117	0.988635	-2.684535
28	1	0	2.908119	-0.127698	-1.986751
29	1	0	8.123620	1.129558	-0.520094
30	1	0	7.721849	0.837697	-2.219771
31	1	0	7.182101	2.319604	-1.430345
32	1	0	-1.139666	-1.058039	0.049967
33	1	0	-4.602411	0.127584	-2.047657
34	1	0	-3.020191	1.867769	-1.565563
35	1	0	-4.081243	2.098697	-0.170654
36	1	0	-2.531028	0.939852	1.290407
37	1	0	-2.414410	-2.994249	-1.201120
38	1	0	-4.170726	-2.816938	-0.964849
39	1	0	-3.440667	-2.370671	-2.509100
40	1	0	-1.917149	3.373878	1.417445
41	1	0	-0.497398	3.945515	0.535381
42	1	0	-2.028955	3.698357	-0.334023
43	1	0	0.061864	0.787500	-1.442212
44	1	0	-0.862683	2.227219	-1.960042
45	1	0	0.687245	2.407376	-1.122774
46	1	0	1.210913	1.342406	3.366616
47	1	0	1.463688	-0.431699	3.223973
48	1	0	2.644904	0.672564	2.541769

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3932.534289

Sum of electronic and thermal Energies= -3932.509175

Sum of electronic and thermal Enthalpies= -3932.508231

Sum of electronic and thermal Free Energies= -3932.590388

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.964565	-0.653000	0.363650
2	16	0	2.140261	-1.698319	0.166852
3	8	0	2.512109	-2.501305	1.339879
4	8	0	1.877764	-2.431569	-1.069017
5	6	0	3.594370	-0.684691	-0.176332
6	6	0	4.728985	-0.772166	0.613043
7	6	0	5.829247	0.034570	0.324729
8	6	0	5.803960	0.925840	-0.743530
9	6	0	4.648115	0.995678	-1.529176
10	6	0	3.548845	0.199562	-1.251499
11	6	0	0.816770	0.140947	1.473338
12	6	0	6.983438	1.814698	-1.047960
13	6	0	-2.065048	-0.560637	-0.141335

14	6	0	-3.110163	-0.886775	-0.907450
15	6	0	-4.036391	0.275643	-1.028352
16	6	0	-3.236416	1.466435	-0.512677
17	6	0	-2.140565	0.850207	0.381831
18	6	0	-3.412915	-2.204615	-1.544805
19	7	0	-0.000049	1.135428	1.549237
20	6	0	-1.108912	3.087080	0.802054
21	6	0	-0.798684	1.627910	0.424622
22	6	0	-0.090598	1.633232	-0.943731
23	35	0	-5.685396	-0.042914	0.125748
24	6	0	1.610777	-0.123114	2.740838
25	1	0	4.733935	-1.472908	1.440056
26	1	0	6.720217	-0.031269	0.941740
27	1	0	4.616054	1.685025	-2.367700
28	1	0	2.648148	0.249223	-1.853509
29	1	0	7.855036	1.529387	-0.456488
30	1	0	7.255719	1.758165	-2.104857
31	1	0	6.752328	2.860032	-0.823809
32	1	0	-1.229295	-1.210821	0.091270
33	1	0	-4.498241	0.410995	-2.004215
34	1	0	-2.764381	1.930902	-1.385365
35	1	0	-3.850125	2.217416	-0.016644
36	1	0	-2.489437	0.812926	1.422974
37	1	0	-2.601884	-2.911581	-1.370047
38	1	0	-4.340069	-2.620364	-1.137150
39	1	0	-3.550890	-2.096415	-2.625515
40	1	0	-1.625387	3.116153	1.764504
41	1	0	-0.167532	3.630536	0.910700
42	1	0	-1.720133	3.589562	0.045990
43	1	0	-0.046322	0.641792	-1.390021
44	1	0	-0.591069	2.325704	-1.629320
45	1	0	0.936998	1.981114	-0.804654
46	1	0	1.276363	0.581767	3.498155
47	1	0	1.485535	-1.153741	3.071177
48	1	0	2.679616	0.018673	2.553149

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3932.115710
Sum of electronic and thermal Energies=	-3932.090626
Sum of electronic and thermal Enthalpies=	-3932.089682
Sum of electronic and thermal Free Energies=	-3932.173076

Cartesian coordinates of Intermediate Int-4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.274471	0.114562	0.537175
2	6	0	-2.742346	-0.833066	1.658900
3	6	0	-0.717289	0.045416	0.336810
4	6	0	-0.293743	1.059339	-0.752692
5	6	0	-4.219353	-1.103550	1.667701
6	6	0	-6.556613	-1.066201	0.758404
7	6	0	-5.076006	-0.798085	0.679592
8	6	0	-4.553188	-0.187177	-0.574945
9	6	0	-3.043950	-0.232868	-0.745529
10	35	0	-5.188923	1.789753	-0.638729
11	7	0	-0.426535	-1.338972	-0.045729
12	6	0	-0.026619	0.449616	1.662587
13	6	0	0.778920	-1.769821	-0.279368
14	6	0	0.874050	-3.241450	-0.659780
15	7	0	1.908008	-0.993329	-0.203538
16	6	0	4.346939	-0.103906	-0.142606
17	6	0	5.007361	0.022707	1.076750
18	6	0	5.763303	1.167036	1.339738
19	6	0	5.872930	2.194511	0.395669
20	6	0	5.212686	2.039500	-0.832695
21	6	0	4.458066	0.900865	-1.105631
22	6	0	6.665113	3.447443	0.694385
23	16	0	3.377687	-1.592170	-0.493597
24	8	0	3.844400	-2.611672	0.486701
25	8	0	3.641312	-1.911018	-1.923530
26	1	0	-2.535470	1.146002	0.815527
27	1	0	-2.457466	-0.437795	2.642888
28	1	0	-2.193675	-1.780877	1.543038
29	1	0	0.795620	1.105592	-0.803953
30	1	0	-0.687996	2.061555	-0.532046
31	1	0	-0.657379	0.757557	-1.740482
32	1	0	-4.615646	-1.601336	2.555174
33	1	0	-6.888813	-1.735340	-0.048661
34	1	0	-7.122162	-0.131841	0.649175
35	1	0	-6.829798	-1.526979	1.713661
36	1	0	-5.073589	-0.564640	-1.457619
37	1	0	-2.758966	0.419174	-1.574268
38	1	0	-2.768369	-1.257322	-1.033831
39	1	0	1.053268	0.496492	1.513061
40	1	0	-0.220646	-0.285363	2.450918
41	1	0	-0.385565	1.429756	2.009076
42	1	0	1.343046	-3.351316	-1.644412
43	1	0	-0.127552	-3.677079	-0.673473
44	1	0	1.507610	-3.779509	0.054100
45	1	0	4.928521	-0.782193	1.800239
46	1	0	6.278741	1.261953	2.294245
47	1	0	5.296223	2.821230	-1.586261
48	1	0	3.961791	0.774847	-2.062523
49	1	0	7.243363	3.777253	-0.177349
50	1	0	7.365451	3.290171	1.522270
51	1	0	6.008023	4.281779	0.977247

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3971.836251
Sum of electronic and thermal Energies= -3971.810174

Sum of electronic and thermal Enthalpies= -3971.809230
Sum of electronic and thermal Free Energies= -3971.893189

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.223681	0.124941	0.514163
2	6	0	-2.664528	-0.744556	1.696585
3	6	0	-0.685978	0.024170	0.282161
4	6	0	-0.282649	0.976746	-0.858090
5	6	0	-4.140567	-1.002735	1.750534
6	6	0	-6.486150	-0.993555	0.890296
7	6	0	-5.009654	-0.739184	0.773028
8	6	0	-4.514783	-0.197298	-0.527781
9	6	0	-3.014725	-0.292458	-0.724344
10	35	0	-5.117219	1.733751	-0.687951
11	7	0	-0.423386	-1.375779	-0.048516
12	6	0	0.031339	0.469426	1.570697
13	6	0	0.775927	-1.795265	-0.275462
14	6	0	0.913624	-3.270398	-0.599026
15	7	0	1.885664	-0.996083	-0.234446
16	6	0	4.291988	-0.096458	-0.147028
17	6	0	4.993626	-0.005094	1.043412
18	6	0	5.718011	1.151014	1.321944
19	6	0	5.743937	2.214233	0.422750
20	6	0	5.036029	2.093254	-0.776558
21	6	0	4.311985	0.945801	-1.065710
22	6	0	6.495631	3.482606	0.739892
23	16	0	3.341929	-1.576017	-0.508140
24	8	0	3.793778	-2.589469	0.459064
25	8	0	3.607103	-1.893268	-1.919701
26	1	0	-2.461563	1.173265	0.737072
27	1	0	-2.360418	-0.283424	2.641227
28	1	0	-2.127723	-1.699984	1.629234
29	1	0	0.802077	1.069006	-0.890985
30	1	0	-0.730717	1.965714	-0.707291
31	1	0	-0.611836	0.586557	-1.823271
32	1	0	-4.524959	-1.449007	2.666583
33	1	0	-6.827776	-1.685093	0.112968
34	1	0	-7.045795	-0.062055	0.764702
35	1	0	-6.733973	-1.420117	1.863399
36	1	0	-5.055183	-0.641745	-1.363522
37	1	0	-2.727773	0.291366	-1.599042
38	1	0	-2.771829	-1.340870	-0.934359
39	1	0	1.100321	0.559240	1.385382
40	1	0	-0.109695	-0.267640	2.364470
41	1	0	-0.362727	1.433978	1.912270
42	1	0	1.420719	-3.396186	-1.559233
43	1	0	-0.076034	-3.720811	-0.630642
44	1	0	1.532895	-3.759048	0.156443
45	1	0	4.968569	-0.845776	1.726521
46	1	0	6.271448	1.226405	2.252963
47	1	0	5.056805	2.911248	-1.490252
48	1	0	3.768853	0.837893	-1.997411
49	1	0	6.981409	3.886132	-0.151158
50	1	0	7.261344	3.309255	1.498103
51	1	0	5.816077	4.250486	1.121414

Level: M06-2X/6-311G**
Sum of electronic and zero-point Energies= -3971.398787
Sum of electronic and thermal Energies= -3971.372337
Sum of electronic and thermal Enthalpies= -3971.371393
Sum of electronic and thermal Free Energies= -3971.459645

Cartesian coordinates of Transition State A-1e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.795746	1.272012	-0.521859
2	6	0	-1.433359	0.325056	-1.681267
3	6	0	-1.410930	0.616162	0.761484
4	6	0	-1.291877	2.748094	-0.736588
5	6	0	-2.040398	-1.073866	-1.502835
6	6	0	-1.998068	-1.588798	-0.079024
7	6	0	-1.532853	-0.740860	0.940306
8	35	0	-4.663228	-1.579823	0.414573
9	7	0	0.911973	1.508142	0.465716
10	6	0	2.940512	-0.376357	0.545590
11	6	0	-1.445086	3.578962	0.556750
12	6	0	-2.188570	3.397751	-1.813176
13	7	0	0.077028	2.860786	-1.252572
14	6	0	1.073211	2.311733	-0.638536
15	6	0	4.311370	-0.315945	0.323901
16	6	0	4.953038	-1.368516	-0.329294
17	6	0	4.242173	-2.487135	-0.768197
18	6	0	2.861799	-2.529890	-0.528402
19	6	0	2.212809	-1.489043	0.124160
20	6	0	4.931740	-3.614554	-1.499605
21	16	0	2.090921	0.975667	1.424259
22	8	0	3.144155	1.974820	1.701817
23	8	0	1.441558	0.332417	2.576373
24	6	0	2.442014	2.567753	-1.241737
25	6	0	-1.910382	-3.076472	0.101871
26	1	0	-2.897899	1.335266	-0.470215
27	1	0	-0.344444	0.255864	-1.722637
28	1	0	-1.762837	0.739522	-2.635821
29	1	0	-1.199655	1.223857	1.626627
30	1	0	-1.501449	-1.795407	-2.131371
31	1	0	-3.078429	-1.096531	-1.837170
32	1	0	-1.342432	-1.158653	1.922332
33	1	0	-1.237970	4.628079	0.330410
34	1	0	-0.739905	3.257053	1.322376
35	1	0	-2.463429	3.510729	0.956132
36	1	0	-1.842325	4.417486	-1.995287

37	1	0	-3.237225	3.428670	-1.498532
38	1	0	-2.122362	2.859788	-2.761437
39	1	0	4.859089	0.552332	0.668790
40	1	0	6.024904	-1.317081	-0.497158
41	1	0	2.290371	-3.394346	-0.854249
42	1	0	1.146372	-1.530398	0.311052
43	1	0	6.015738	-3.567002	-1.371484
44	1	0	4.724410	-3.575253	-2.575017
45	1	0	4.591827	-4.590374	-1.140580
46	1	0	2.918003	1.628453	-1.540702
47	1	0	3.099477	3.043041	-0.511684
48	1	0	2.316550	3.206187	-2.114612
49	1	0	-2.131163	-3.369596	1.127204
50	1	0	-0.878279	-3.381304	-0.134013
51	1	0	-2.585771	-3.604179	-0.569960

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3971.817462
Sum of electronic and thermal Energies=	-3971.791121
Sum of electronic and thermal Enthalpies=	-3971.790177
Sum of electronic and thermal Free Energies=	-3971.876262

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.704476	1.123590	-0.542651
2	6	0	-1.144420	0.121146	-1.560453
3	6	0	-1.315373	0.675793	0.823216
4	6	0	-1.344324	2.603788	-0.881275
5	6	0	-1.560157	-1.322159	-1.258065
6	6	0	-1.726661	-1.620127	0.212206
7	6	0	-1.353874	-0.663117	1.157483
8	35	0	-4.372293	-1.495967	0.263891
9	7	0	0.775437	1.562522	0.524207
10	6	0	2.743136	-0.319830	0.561509
11	6	0	-1.642374	3.529184	0.309557
12	6	0	-2.222340	3.051697	-2.057284
13	7	0	0.040049	2.803312	-1.311949
14	6	0	0.998793	2.322706	-0.603988
15	6	0	4.108847	-0.273716	0.335416
16	6	0	4.715022	-1.296691	-0.391632
17	6	0	3.969559	-2.359548	-0.893903
18	6	0	2.592123	-2.385233	-0.649607
19	6	0	1.979016	-1.376091	0.075706
20	6	0	4.619541	-3.466843	-1.683648
21	16	0	1.920376	0.992580	1.483809
22	8	0	2.975363	1.957413	1.800825
23	8	0	1.246583	0.333130	2.596355
24	6	0	2.403673	2.594162	-1.095629
25	6	0	-1.708743	-3.070334	0.594426
26	1	0	-2.806701	1.044835	-0.549721
27	1	0	-0.055571	0.199045	-1.529346
28	1	0	-1.456687	0.387047	-2.571093
29	1	0	-1.289198	1.392811	1.630324
30	1	0	-0.780220	-2.008431	-1.620079
31	1	0	-2.480718	-1.599502	-1.770503
32	1	0	-1.227220	-0.953838	2.193023
33	1	0	-1.565869	4.566424	-0.023620

34	1	0	-0.919343	3.378942	1.111964
35	1	0	-2.653277	3.361360	0.695731
36	1	0	-1.957294	4.076324	-2.325137
37	1	0	-3.283861	3.009483	-1.795946
38	1	0	-2.048990	2.427910	-2.936004
39	1	0	4.675609	0.564362	0.724130
40	1	0	5.784597	-1.263965	-0.572649
41	1	0	1.997479	-3.209091	-1.033619
42	1	0	0.912419	-1.390005	0.274610
43	1	0	5.687423	-3.285065	-1.812709
44	1	0	4.167914	-3.556753	-2.674860
45	1	0	4.497575	-4.428993	-1.179283
46	1	0	2.912448	1.655209	-1.331629
47	1	0	2.989552	3.097958	-0.326331
48	1	0	2.331909	3.205537	-1.991985
49	1	0	-2.113801	-3.216701	1.594183
50	1	0	-0.660025	-3.402348	0.584170
51	1	0	-2.279715	-3.670415	-0.112286

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies= -3971.380321

Sum of electronic and thermal Energies= -3971.354744

Sum of electronic and thermal Enthalpies= -3971.353800

Sum of electronic and thermal Free Energies= -3971.436316

Cartesian coordinates of Transition State D-1e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.718756	2.172260	-0.373352
2	6	0	1.754403	1.173776	-1.499063
3	6	0	0.281464	2.605561	0.090789
4	6	0	2.629049	1.686393	0.761384
5	6	0	1.915103	-0.140430	-1.305871
6	6	0	1.952035	-0.646439	0.041084
7	6	0	1.942168	-2.101412	0.284288
8	7	0	-0.382554	-0.195957	0.297374
9	6	0	2.379205	0.232562	1.158305
10	7	0	-0.226459	1.928696	1.297001
11	6	0	-0.723686	2.508716	-1.066813

12	6	0	0.378455	4.079660	0.515089
13	6	0	-1.222114	0.244660	2.634722
14	6	0	-0.601682	0.705025	1.330613
15	6	0	-2.952460	-0.968838	-0.142142
16	6	0	-3.950432	-1.289434	0.763757
17	6	0	-5.251660	-0.851628	0.528424
18	6	0	-5.560981	-0.099289	-0.601467
19	6	0	-4.538297	0.201435	-1.506976
20	6	0	-3.240605	-0.230897	-1.286151
21	6	0	-6.964106	0.389340	-0.854998
22	16	0	-1.262483	-1.529020	0.126585
23	8	0	-0.845338	-2.146563	-1.130691
24	8	0	-1.319847	-2.393953	1.309478
25	1	0	2.168335	3.084704	-0.782027
26	1	0	1.637017	1.547907	-2.511908
27	1	0	3.663460	1.743549	0.410913
28	1	0	2.520014	2.330280	1.636195
29	1	0	1.915492	-0.855368	-2.118034
30	1	0	3.009001	-2.366091	0.193920
31	1	0	1.365661	-2.639296	-0.464746
32	1	0	1.594454	-2.340183	1.289525
33	1	0	1.679038	0.119684	1.988136
34	1	0	3.329635	-0.219114	1.474435
35	1	0	-1.703873	2.845467	-0.719748
36	1	0	-0.809634	1.481728	-1.417958
37	1	0	-0.411098	3.148917	-1.898415
38	1	0	-0.585011	4.402289	0.913887
39	1	0	0.652609	4.718711	-0.329611
40	1	0	1.123072	4.197679	1.306275
41	1	0	-1.155415	1.062122	3.348316
42	1	0	-0.718063	-0.649954	3.004756
43	1	0	-2.271369	-0.023204	2.487677
44	1	0	-3.696786	-1.886508	1.632270
45	1	0	-6.037374	-1.102449	1.233554
46	1	0	-4.769347	0.776853	-2.398097
47	1	0	-2.449433	-0.020233	-1.995917
48	1	0	-7.662505	-0.018020	-0.122687
49	1	0	-7.305562	0.097296	-1.850993
50	1	0	-7.011800	1.480090	-0.797409
51	35	0	5.258459	-0.865249	-0.427380

Level: B3lyp/6-311G**
E(RB+HF-LYP) = -3972.20720286
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.718756	2.172260	-0.373352
2	6	0	1.754403	1.173776	-1.499063
3	6	0	0.281464	2.605561	0.090789
4	6	0	2.629049	1.686393	0.761384
5	6	0	1.915103	-0.140430	-1.305871
6	6	0	1.952035	-0.646439	0.041084
7	6	0	1.942168	-2.101412	0.284288
8	7	0	-0.382554	-0.195957	0.297374
9	6	0	2.379205	0.232562	1.158305
10	7	0	-0.226459	1.928696	1.297001
11	6	0	-0.723686	2.508716	-1.066813
12	6	0	0.378455	4.079660	0.515089

13	6	0	-1.222114	0.244660	2.634722
14	6	0	-0.601682	0.705025	1.330613
15	6	0	-2.952460	-0.968838	-0.142142
16	6	0	-3.950432	-1.289434	0.763757
17	6	0	-5.251660	-0.851628	0.528424
18	6	0	-5.560981	-0.099289	-0.601467
19	6	0	-4.538297	0.201435	-1.506976
20	6	0	-3.240605	-0.230897	-1.286151
21	6	0	-6.964106	0.389340	-0.854998
22	16	0	-1.262483	-1.529020	0.126585
23	8	0	-0.845338	-2.146563	-1.130691
24	8	0	-1.319847	-2.393953	1.309478
25	1	0	2.168335	3.084704	-0.782027
26	1	0	1.637017	1.547907	-2.511908
27	1	0	3.663460	1.743549	0.410913
28	1	0	2.520014	2.330280	1.636195
29	1	0	1.915492	-0.855368	-2.118034
30	1	0	3.009001	-2.366091	0.193920
31	1	0	1.365661	-2.639296	-0.464746
32	1	0	1.594454	-2.340183	1.289525
33	1	0	1.679038	0.119684	1.988136
34	1	0	3.329635	-0.219114	1.474435
35	1	0	-1.703873	2.845467	-0.719748
36	1	0	-0.809634	1.481728	-1.417958
37	1	0	-0.411098	3.148917	-1.898415
38	1	0	-0.585011	4.402289	0.913887
39	1	0	0.652609	4.718711	-0.329611
40	1	0	1.123072	4.197679	1.306275
41	1	0	-1.155415	1.062122	3.348316
42	1	0	-0.718063	-0.649954	3.004756
43	1	0	-2.271369	-0.023204	2.487677
44	1	0	-3.696786	-1.886508	1.632270
45	1	0	-6.037374	-1.102449	1.233554
46	1	0	-4.769347	0.776853	-2.398097
47	1	0	-2.449433	-0.020233	-1.995917
48	1	0	-7.662505	-0.018020	-0.122687
49	1	0	-7.305562	0.097296	-1.850993
50	1	0	-7.011800	1.480090	-0.797409
51	35	0	5.258459	-0.865249	-0.427380

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.362348
Sum of electronic and thermal Energies=	-3971.336489
Sum of electronic and thermal Enthalpies=	-3971.335545
Sum of electronic and thermal Free Energies=	-3971.419376

Cartesian coordinates of Transition State A-2e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.665182	-1.030209	0.369169
2	6	0	1.608945	0.355351	1.052203
3	6	0	1.309202	-2.328011	1.198467
4	6	0	0.944706	-0.770771	-0.908253
5	6	0	1.399531	1.302877	-0.093554
6	6	0	1.328929	2.781234	0.080969
7	6	0	0.919455	0.592904	-1.182214
8	7	0	-1.036113	-1.645971	-0.097132
9	7	0	0.506895	-3.309336	0.460529
10	6	0	0.585489	-1.996833	2.524051
11	6	0	2.632063	-3.040951	1.539123
12	6	0	-1.395129	-4.060911	-0.775746
13	6	0	-0.606739	-2.962187	-0.091337
14	6	0	-2.577381	0.493096	-0.231423
15	6	0	-2.809607	0.683937	1.130336
16	6	0	-3.020224	1.967869	1.615251
17	6	0	-3.013614	3.077427	0.757074
18	6	0	-2.788608	2.859545	-0.602788
19	6	0	-2.570088	1.574290	-1.101223
20	6	0	-3.245680	4.467422	1.300215
21	16	0	-2.385882	-1.181332	-0.887701
22	8	0	-2.184382	-1.033805	-2.344786
23	8	0	-3.585381	-1.929151	-0.457434
24	1	0	2.714819	-1.130629	0.041305
25	1	0	2.492811	0.599991	1.638716
26	1	0	0.721355	0.426287	1.694769
27	1	0	0.791628	-1.533637	-1.655890
28	1	0	1.444185	3.297636	-0.872053
29	1	0	2.098997	3.136093	0.763670
30	1	0	0.338825	3.030176	0.492102
31	1	0	0.601722	1.028688	-2.118780
32	1	0	0.371607	-2.934342	3.044083
33	1	0	-0.357927	-1.484716	2.336566
34	1	0	1.207543	-1.377581	3.177546
35	1	0	2.430700	-3.930669	2.141514
36	1	0	3.128035	-3.363161	0.620070
37	1	0	3.312427	-2.382316	2.088747
38	1	0	-0.846424	-4.994638	-0.664163
39	1	0	-1.531750	-3.835205	-1.837831
40	1	0	-2.392502	-4.148644	-0.340715
41	1	0	-2.823364	-0.169676	1.796436
42	1	0	-3.195765	2.114578	2.676940
43	1	0	-2.780019	3.703639	-1.285324
44	1	0	-2.396692	1.398277	-2.155364
45	1	0	-2.480199	4.739765	2.033946
46	1	0	-4.215878	4.540704	1.802341
47	1	0	-3.223757	5.213734	0.503330
48	35	0	4.297937	1.472894	-0.609334

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3932.520839
Sum of electronic and thermal Energies=	-3932.495539
Sum of electronic and thermal Enthalpies=	-3932.494595
Sum of electronic and thermal Free Energies=	-3932.578407

Cartesian coordinates of Transition State A-3e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.168814	0.547079	-1.268381
2	6	0	2.519325	-0.882908	-1.015118
3	6	0	1.845138	1.064319	0.153888
4	6	0	2.039509	-1.315297	0.194958
5	6	0	-1.784379	1.195333	2.735176
6	6	0	2.146358	-2.705814	0.744660
7	6	0	1.503981	-0.198452	0.881518
8	7	0	-0.597175	0.036318	0.795376
9	7	0	-0.030109	2.197089	1.471473
10	6	0	0.053816	2.599437	-0.925149
11	6	0	0.897353	2.307379	0.336501
12	6	0	1.776650	3.537624	0.626615
13	6	0	-0.767663	1.152704	1.612022
14	6	0	-3.065486	-0.730157	-0.068129
15	6	0	-4.287083	-0.667664	0.590959
16	6	0	-5.426459	-0.269644	-0.109057
17	6	0	-5.361555	0.067718	-1.461928
18	6	0	-4.119615	-0.013821	-2.107646
19	6	0	-2.978285	-0.409992	-1.423372
20	6	0	-6.589432	0.519728	-2.215726
21	16	0	-1.577275	-1.274809	0.816156
22	8	0	-0.948701	-2.288149	-0.037305
23	8	0	-2.031072	-1.694718	2.155229
24	1	0	1.281355	0.582285	-1.912607
25	1	0	2.978575	1.089133	-1.755574
26	1	0	2.988483	-1.512253	-1.756218
27	1	0	2.824572	1.337328	0.577598
28	1	0	-1.652007	2.140304	3.259124
29	1	0	-1.668451	0.351532	3.415814
30	1	0	-2.803290	1.147421	2.339186
31	1	0	2.314135	-2.689878	1.825801
32	1	0	2.987518	-3.228049	0.283892
33	1	0	1.225554	-3.263996	0.556142
34	1	0	1.382822	-0.196958	1.956470
35	1	0	-0.588728	3.460447	-0.723379
36	1	0	-0.579667	1.748842	-1.176812
37	1	0	0.688841	2.837773	-1.783094
38	1	0	2.316846	3.396843	1.566351
39	1	0	1.152416	4.429331	0.727943
40	1	0	2.507850	3.700958	-0.171401
41	1	0	-4.336313	-0.944688	1.636650

42	1	0	-6.380210	-0.226004	0.407885
43	1	0	-4.048502	0.233183	-3.162660
44	1	0	-2.025177	-0.485371	-1.931652
45	1	0	-6.541218	1.590267	-2.443133
46	1	0	-7.498691	0.345072	-1.636323
47	1	0	-6.689049	-0.008847	-3.168358
48	35	0	5.434343	-0.399831	-0.756921

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3932.517841
Sum of electronic and thermal Energies=	-3932.492405
Sum of electronic and thermal Enthalpies=	-3932.491461
Sum of electronic and thermal Free Energies=	-3932.577189

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.065926	0.462203	-1.249968
2	6	0	2.487076	-0.935082	-0.936915
3	6	0	1.893911	1.068955	0.154675
4	6	0	2.059971	-1.297033	0.324376
5	6	0	-1.829894	1.170919	2.528735
6	6	0	2.137729	-2.667270	0.918496
7	6	0	1.561057	-0.149481	0.946966
8	7	0	-0.530260	0.120967	0.617738
9	7	0	-0.002362	2.232232	1.417329
10	6	0	0.227745	2.693462	-0.946319
11	6	0	0.989385	2.333821	0.340781
12	6	0	1.898827	3.509645	0.710366
13	6	0	-0.748633	1.191518	1.473194
14	6	0	-2.979139	-0.738810	-0.089994
15	6	0	-4.160109	-0.917197	0.611341
16	6	0	-5.363758	-0.526293	0.028627
17	6	0	-5.393153	0.041378	-1.241847
18	6	0	-4.186923	0.205474	-1.931741
19	6	0	-2.983532	-0.181791	-1.365489
20	6	0	-6.689064	0.484733	-1.871013
21	16	0	-1.408025	-1.229741	0.634882
22	8	0	-0.790045	-2.150829	-0.308933
23	8	0	-1.724096	-1.741256	1.970412
24	1	0	1.080690	0.396384	-1.731622
25	1	0	2.766451	0.992618	-1.892398
26	1	0	2.822705	-1.630669	-1.692746
27	1	0	2.918106	1.321887	0.474980
28	1	0	-1.787332	2.117664	3.061892
29	1	0	-1.693232	0.331734	3.210962
30	1	0	-2.814477	1.054978	2.066927
31	1	0	1.793145	-2.662069	1.954373
32	1	0	3.171940	-3.022593	0.892568
33	1	0	1.502001	-3.359768	0.362678
34	1	0	1.357743	-0.096727	2.011156
35	1	0	-0.331836	3.615221	-0.772180
36	1	0	-0.476438	1.901434	-1.204844
37	1	0	0.915705	2.852323	-1.781227
38	1	0	2.400729	3.303102	1.658577
39	1	0	1.303523	4.417668	0.829041
40	1	0	2.660183	3.669708	-0.059016
41	1	0	-4.120087	-1.356144	1.601604

42	1	0	-6.292521	-0.663435	0.572723
43	1	0	-4.197808	0.643137	-2.925043
44	1	0	-2.045127	-0.059362	-1.894580
45	1	0	-6.703625	1.569586	-2.005445
46	1	0	-7.543745	0.209561	-1.251605
47	1	0	-6.821274	0.030157	-2.855921
48	35	0	5.159426	-0.449462	-0.764340

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3932.096477
Sum of electronic and thermal Energies=	-3932.071886
Sum of electronic and thermal Enthalpies=	-3932.070942
Sum of electronic and thermal Free Energies=	-3932.152556

Cartesian coordinates of Transition State D-3e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.464466	1.083033	-0.097500
2	6	0	-1.646970	1.634128	-0.703530
3	6	0	-0.664405	0.966090	1.375099
4	7	0	-0.911368	-1.145461	-0.370963
5	6	0	-2.640133	1.592917	0.214509
6	6	0	1.709276	-1.546899	-0.442126
7	6	0	1.986525	-2.352385	0.660710
8	6	0	-2.207498	0.952420	1.512812
9	7	0	-3.169323	-1.087935	0.341894
10	6	0	-2.901334	-0.455338	1.645790
11	6	0	-2.783831	-2.111129	-1.766714
12	6	0	-2.265853	-1.421080	-0.515248
13	6	0	3.156062	-2.141940	1.381412
14	6	0	4.056466	-1.130702	1.021136
15	6	0	3.762912	-0.347928	-0.097223
16	6	0	-4.297864	-0.214048	2.258454
17	6	0	-2.133910	-1.417066	2.573818
18	6	0	2.599079	-0.554219	-0.834631
19	6	0	5.295590	-0.870994	1.843833
20	16	0	0.194786	-1.829891	-1.386385
21	8	0	0.026944	-3.294415	-1.475100
22	8	0	0.343682	-1.089309	-2.654793
23	6	0	-1.709316	2.090070	-2.126231

24	1	0	0.477471	0.974515	-0.598849
25	1	0	-0.257842	1.874081	1.828550
26	1	0	-0.150440	0.108676	1.800298
27	1	0	-3.655268	1.923786	0.028775
28	1	0	1.297511	-3.141734	0.934244
29	1	0	-2.516594	1.547628	2.379798
30	1	0	-3.871262	-2.127428	-1.725086
31	1	0	-2.395651	-3.129382	-1.831154
32	1	0	-2.449860	-1.582718	-2.664118
33	1	0	3.373592	-2.770708	2.239737
34	1	0	4.438933	0.447228	-0.392228
35	1	0	-4.224568	0.179940	3.277900
36	1	0	-4.851421	-1.155568	2.279143
37	1	0	-4.872117	0.490274	1.650752
38	1	0	-1.185913	-1.720025	2.131647
39	1	0	-1.940583	-0.955651	3.548655
40	1	0	-2.736443	-2.315493	2.735040
41	1	0	2.378685	0.053184	-1.703173
42	1	0	5.661321	-1.786275	2.316912
43	1	0	5.088500	-0.148078	2.640758
44	1	0	6.100754	-0.457571	1.231792
45	1	0	-1.375367	1.289115	-2.792682
46	1	0	-2.723786	2.384274	-2.406044
47	1	0	-1.032135	2.937993	-2.261887
48	35	0	1.165821	3.558062	-0.190006

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3932.516414
Sum of electronic and thermal Energies=	-3932.490944
Sum of electronic and thermal Enthalpies=	-3932.490000
Sum of electronic and thermal Free Energies=	-3932.574391

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.407228	1.132835	-0.075809
2	6	0	-1.696578	1.672768	-0.448879
3	6	0	-0.395566	0.819189	1.385183
4	7	0	-0.899166	-1.038100	-0.501162
5	6	0	-2.538039	1.481216	0.580996
6	6	0	1.649732	-1.407937	-0.681226
7	6	0	1.898531	-2.386205	0.276526
8	6	0	-1.903137	0.716005	1.716448
9	7	0	-3.028982	-1.195827	0.468630
10	6	0	-2.544746	-0.714446	1.771849
11	6	0	-2.857162	-1.924268	-1.794203
12	6	0	-2.238835	-1.373210	-0.527321
13	6	0	3.012050	-2.268376	1.092273
14	6	0	3.877165	-1.175248	0.972680
15	6	0	3.612899	-0.216803	-0.001462
16	6	0	-3.809328	-0.596144	2.635341
17	6	0	-1.614645	-1.743438	2.427146
18	6	0	2.506276	-0.330550	-0.839187
19	6	0	5.051574	-1.028230	1.905905
20	16	0	0.137999	-1.536285	-1.636880
21	8	0	-0.032572	-2.950057	-1.981064
22	8	0	0.257072	-0.587335	-2.747373
23	6	0	-1.966564	2.212630	-1.812715

24	1	0	0.401180	1.009311	-0.768277
25	1	0	0.038496	1.672898	1.907171
26	1	0	0.192201	-0.069501	1.606261
27	1	0	-3.590611	1.741659	0.566067
28	1	0	1.218207	-3.225727	0.364273
29	1	0	-2.103354	1.187838	2.684542
30	1	0	-3.937054	-1.949661	-1.668813
31	1	0	-2.473578	-2.925724	-1.994308
32	1	0	-2.585935	-1.297740	-2.648505
33	1	0	3.212533	-3.028468	1.841111
34	1	0	4.263198	0.645086	-0.101527
35	1	0	-3.560103	-0.345743	3.671168
36	1	0	-4.347715	-1.545348	2.612625
37	1	0	-4.475277	0.172893	2.235062
38	1	0	-0.764866	-1.969972	1.784230
39	1	0	-1.245083	-1.371499	3.388672
40	1	0	-2.172993	-2.666192	2.604032
41	1	0	2.304621	0.419725	-1.595572
42	1	0	5.782208	-0.321472	1.510189
43	1	0	5.549775	-1.986909	2.066500
44	1	0	4.722268	-0.657053	2.880495
45	1	0	-1.639928	1.479330	-2.557088
46	1	0	-3.027789	2.423497	-1.953170
47	1	0	-1.382533	3.123694	-1.964693
48	35	0	1.008480	3.450958	-0.106469

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3932.098090
Sum of electronic and thermal Energies=	-3932.073471
Sum of electronic and thermal Enthalpies=	-3932.072527
Sum of electronic and thermal Free Energies=	-3932.153154

Cartesian coordinates of Transition State A-4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.120197	-1.350143	2.248842
2	16	0	2.128803	-1.480244	-0.792146
3	7	0	0.620116	-1.367580	-0.217423
4	6	0	0.220983	-1.674725	1.073490
5	7	0	-0.940711	-2.146127	1.359575
6	6	0	-1.245160	0.934659	-0.041321
7	6	0	3.114239	-0.014511	-0.336910
8	8	0	2.855889	-2.622371	-0.206492
9	6	0	-1.884128	-2.686600	0.361338

10	6	0	-0.870861	0.116881	-1.101281
11	8	0	2.010778	-1.383146	-2.255981
12	6	0	4.652364	2.240617	0.327496
13	6	0	3.024942	1.144468	-1.107009
14	6	0	4.747892	1.060949	1.070437
15	6	0	3.989552	-0.061145	0.743906
16	6	0	5.452544	3.465487	0.700981
17	6	0	-1.220830	-3.758764	-0.535458
18	6	0	-0.422823	2.131375	0.366177
19	6	0	-1.774911	-0.950939	-1.624949
20	6	0	-3.313322	-0.502638	0.280921
21	6	0	-2.619453	-1.620631	-0.522559
22	6	0	-2.948127	-3.422134	1.211835
23	6	0	-2.418676	0.642354	0.638229
24	6	0	3.785412	2.259419	-0.771306
25	1	0	0.576456	-1.546588	3.171272
26	1	0	1.441735	-0.305253	2.221661
27	1	0	2.015404	-1.976469	2.215690
28	1	0	-0.055891	0.418235	-1.746473
29	1	0	2.388884	1.153841	-1.983007
30	1	0	5.431894	1.013586	1.912512
31	1	0	4.090887	-0.981334	1.304377
32	1	0	5.821481	3.986948	-0.186491
33	1	0	6.312356	3.205136	1.322790
34	1	0	4.841190	4.178389	1.265517
35	1	0	-0.426829	-3.348330	-1.153127
36	1	0	-1.971331	-4.227517	-1.182067
37	1	0	-0.784896	-4.536697	0.096670
38	1	0	-0.184234	2.107204	1.434027
39	1	0	-0.997664	3.043567	0.176321
40	1	0	0.518364	2.176300	-0.183592
41	1	0	-2.466224	-0.458192	-2.328274
42	1	0	-1.196333	-1.670531	-2.201054
43	1	0	-4.123439	-0.078282	-0.322405
44	1	0	-3.789927	-0.882079	1.186026
45	1	0	-3.406958	-2.186860	-1.034346
46	1	0	-2.461268	-4.222863	1.773641
47	1	0	-3.733788	-3.860898	0.587145
48	1	0	-3.405568	-2.753111	1.941786
49	1	0	-2.650793	1.192713	1.538114
50	1	0	3.711255	3.156063	-1.379252
51	35	0	-4.130966	2.857233	-0.056159

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3971.807925
Sum of electronic and thermal Energies=	-3971.781373
Sum of electronic and thermal Enthalpies=	-3971.780428
Sum of electronic and thermal Free Energies=	-3971.868098

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.736094	-1.454190	2.381501
2	16	0	2.084780	-1.821853	-0.463060
3	7	0	0.531937	-1.629712	-0.117248
4	6	0	-0.037257	-1.794802	1.129512
5	7	0	-1.272427	-2.101639	1.282004
6	6	0	-0.919997	0.870536	0.016259

7	6	0	2.903467	-0.231573	-0.245314
8	8	0	2.761666	-2.743823	0.449732
9	6	0	-2.118268	-2.541300	0.159984
10	6	0	-0.559329	0.074026	-1.055499
11	8	0	2.161276	-2.068402	-1.900285
12	6	0	4.023139	2.305357	0.102014
13	6	0	3.001859	0.636286	-1.327458
14	6	0	3.956642	1.402567	1.163331
15	6	0	3.407817	0.136676	0.995323
16	6	0	4.570856	3.695049	0.300022
17	6	0	-1.483701	-3.681364	-0.659685
18	6	0	0.020599	1.876843	0.622205
19	6	0	-1.539450	-0.821616	-1.742033
20	6	0	-3.215177	-0.209239	-0.027667
21	6	0	-2.589854	-1.393287	-0.778031
22	6	0	-3.360656	-3.142643	0.843839
23	6	0	-2.194724	0.723181	0.551372
24	6	0	3.557027	1.896943	-1.148486
25	1	0	0.083157	-1.592024	3.240138
26	1	0	1.066999	-0.412771	2.331146
27	1	0	1.618280	-2.090691	2.469761
28	1	0	0.356388	0.296594	-1.592222
29	1	0	2.658483	0.303787	-2.299901
30	1	0	4.343696	1.693751	2.134434
31	1	0	3.381202	-0.572612	1.813197
32	1	0	5.227602	3.739988	1.170300
33	1	0	3.756985	4.408357	0.457209
34	1	0	5.135195	4.023862	-0.574828
35	1	0	-0.593003	-3.372219	-1.199067
36	1	0	-2.219800	-4.074790	-1.369031
37	1	0	-1.201671	-4.489327	0.019967
38	1	0	0.102177	1.735625	1.703852
39	1	0	-0.381903	2.879911	0.448927
40	1	0	1.021162	1.804566	0.192672
41	1	0	-2.064785	-0.203083	-2.485761
42	1	0	-1.000045	-1.599146	-2.282046
43	1	0	-3.809623	0.382238	-0.730554
44	1	0	-3.899942	-0.529278	0.757112
45	1	0	-3.375612	-1.841197	-1.398024
46	1	0	-3.052193	-4.013620	1.426167
47	1	0	-4.110213	-3.457335	0.110899
48	1	0	-3.808261	-2.433896	1.540291
49	1	0	-2.400892	1.161550	1.517981
50	1	0	3.627618	2.576685	-1.991582
51	35	0	-3.342060	3.124494	-0.063945

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.370733
Sum of electronic and thermal Energies=	-3971.345279
Sum of electronic and thermal Enthalpies=	-3971.344335
Sum of electronic and thermal Free Energies=	-3971.426277

Cartesian coordinates of Transition State D-4e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.048766	-2.744626	1.664505
2	16	0	0.866013	-1.736033	-1.238126
3	7	0	-0.407542	-1.271480	-0.350182
4	6	0	-0.948450	-2.002510	0.694813
5	7	0	-2.205999	-2.018884	0.967142
6	6	0	-0.835417	1.107280	1.254272
7	6	0	2.385231	-1.021680	-0.533198
8	8	0	1.070243	-3.198367	-1.206739
9	6	0	-3.240001	-1.470129	0.071592
10	6	0	-0.941980	1.038199	-0.178590
11	8	0	0.731805	-1.072771	-2.543177
12	6	0	4.721032	0.100158	0.547117
13	6	0	2.778797	0.263633	-0.905296
14	6	0	4.321671	-1.194771	0.889524
15	6	0	3.164459	-1.757695	0.355021
16	6	0	5.959747	0.720966	1.148061
17	6	0	-3.151345	-2.060466	-1.355410
18	6	0	0.508388	1.360021	1.882067
19	6	0	-2.260965	0.824022	-0.857390
20	6	0	-3.323119	0.759451	1.402678
21	6	0	-3.312050	0.097270	0.010578
22	6	0	-4.570586	-1.985573	0.674553
23	6	0	-1.955804	0.927979	1.987493
24	6	0	3.934643	0.815139	-0.363672
25	1	0	-0.662018	-3.162123	2.461586
26	1	0	0.699784	-2.069585	2.090627
27	1	0	0.479530	-3.547279	1.146006
28	1	0	-0.065188	1.146916	-0.787647
29	1	0	2.192659	0.815166	-1.629334
30	1	0	4.928146	-1.777023	1.577083
31	1	0	2.876558	-2.771482	0.601698
32	1	0	6.549622	1.245991	0.391316
33	1	0	6.599032	-0.034106	1.611785
34	1	0	5.698324	1.453534	1.919679
35	1	0	-2.228566	-1.788445	-1.859927
36	1	0	-4.001076	-1.721336	-1.958860
37	1	0	-3.193534	-3.151262	-1.294516
38	1	0	0.437402	1.349098	2.972650
39	1	0	0.880082	2.336843	1.560434
40	1	0	1.236289	0.605731	1.574282
41	1	0	-2.645173	1.820861	-1.095684
42	1	0	-2.086035	0.319232	-1.805546
43	1	0	-3.768254	1.762712	1.307013

44	1	0	-3.959467	0.213031	2.101070
45	1	0	-4.280922	0.305747	-0.459198
46	1	0	-4.559651	-3.078048	0.674130
47	1	0	-5.436182	-1.643941	0.096354
48	1	0	-4.688247	-1.668764	1.712280
49	1	0	-1.880847	0.969402	3.071414
50	1	0	4.228600	1.818226	-0.656705
51	35	0	-0.641188	3.787688	-0.576105

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-3971.809539
Sum of electronic and thermal Energies=	-3971.783308
Sum of electronic and thermal Enthalpies=	-3971.782363
Sum of electronic and thermal Free Energies=	-3971.866960

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.560885	-2.595309	1.742359
2	16	0	0.414535	-1.927092	-1.212756
3	7	0	-0.705669	-1.197353	-0.332837
4	6	0	-1.345419	-1.763299	0.755268
5	7	0	-2.566681	-1.510614	1.043245
6	6	0	-0.456218	1.110961	1.201036
7	6	0	2.012765	-1.388161	-0.586724
8	8	0	0.392464	-3.384052	-1.066030
9	6	0	-3.432806	-0.766400	0.116116
10	6	0	-0.601953	1.075015	-0.243858
11	8	0	0.337757	-1.355385	-2.553838
12	6	0	4.349961	-0.377916	0.558269
13	6	0	2.559298	-0.200143	-1.062230
14	6	0	3.813131	-1.592049	0.986866
15	6	0	2.648600	-2.101161	0.421343
16	6	0	5.576473	0.203903	1.213080
17	6	0	-3.487268	-1.404978	-1.284556
18	6	0	0.917736	0.988578	1.792868
19	6	0	-1.951899	1.193419	-0.894609
20	6	0	-2.938127	1.427248	1.379861
21	6	0	-3.120034	0.758882	0.009201
22	6	0	-4.843909	-0.921208	0.714716
23	6	0	-1.564179	1.233101	1.946718
24	6	0	3.716185	0.301594	-0.483478
25	1	0	-1.212403	-2.865537	2.570468
26	1	0	0.290144	-2.014536	2.112332
27	1	0	-0.175057	-3.493061	1.256585
28	1	0	0.255921	0.900737	-0.864486
29	1	0	2.077884	0.322270	-1.880825
30	1	0	4.311310	-2.144587	1.777337
31	1	0	2.230967	-3.045684	0.749847
32	1	0	5.299412	1.019740	1.886546
33	1	0	6.263902	0.611284	0.468842
34	1	0	6.108570	-0.549080	1.796875
35	1	0	-2.532705	-1.368230	-1.801876
36	1	0	-4.243788	-0.896176	-1.891985
37	1	0	-3.779808	-2.453113	-1.182692
38	1	0	0.872843	1.053187	2.881832
39	1	0	1.548953	1.794719	1.409807
40	1	0	1.382170	0.038632	1.518408

41	1	0	-2.092334	2.249259	-1.136861
42	1	0	-1.926554	0.641501	-1.833328
43	1	0	-3.099922	2.508997	1.265669
44	1	0	-3.682448	1.072317	2.093702
45	1	0	-4.019779	1.186457	-0.449389
46	1	0	-5.093644	-1.983706	0.747641
47	1	0	-5.594987	-0.401273	0.112017
48	1	0	-4.884376	-0.550521	1.739635
49	1	0	-1.462661	1.245801	3.029015
50	1	0	4.121331	1.243634	-0.838379
51	35	0	0.334870	3.499694	-0.624001

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.377190
Sum of electronic and thermal Energies=	-3971.351678
Sum of electronic and thermal Enthalpies=	-3971.350734
Sum of electronic and thermal Free Energies=	-3971.432779

artesian coordinates of Intermediate Cmplx-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.870352	-0.319967	-0.160626
2	6	0	1.875850	0.671813	-1.337784
3	6	0	0.645988	-0.106214	0.747479
4	6	0	1.988466	-1.805008	-0.586429
5	6	0	1.922472	2.107181	-0.809136
6	6	0	0.912765	2.360705	0.276317
7	6	0	0.323487	1.358230	0.947647
8	35	0	5.264230	0.821074	0.170221
9	7	0	-0.550968	-0.884920	0.192207
10	6	0	-3.224391	-0.181564	0.423272
11	6	0	2.186746	-2.718138	0.643261
12	6	0	3.183438	-2.014952	-1.534269
13	7	0	0.765702	-2.221342	-1.299379
14	6	0	-0.367179	-1.800103	-0.905226
15	6	0	-4.504353	-0.733761	0.451998
16	6	0	-5.570703	-0.016779	-0.091479
17	6	0	-5.376826	1.244904	-0.666308

18	6	0	-4.078977	1.777803	-0.679292
19	6	0	-3.003144	1.077703	-0.138961
20	6	0	-6.527754	2.005440	-1.282673
21	16	0	-1.879475	-1.086326	1.218163
22	8	0	-2.293924	-2.496649	1.258262
23	8	0	-1.564399	-0.405218	2.479342
24	6	0	-1.595103	-2.186085	-1.700262
25	6	0	0.642282	3.802452	0.625098
26	1	0	2.761740	-0.070775	0.434229
27	1	0	1.000571	0.520340	-1.986240
28	1	0	2.776225	0.506350	-1.932677
29	1	0	0.855256	-0.535045	1.730726
30	1	0	1.781345	2.830503	-1.626910
31	1	0	2.938981	2.272727	-0.410046
32	1	0	-0.362766	1.584485	1.760028
33	1	0	2.250348	-3.764029	0.322062
34	1	0	1.363429	-2.644293	1.361580
35	1	0	3.120199	-2.450431	1.150871
36	1	0	3.379393	-3.087469	-1.656228
37	1	0	4.074470	-1.512769	-1.137381
38	1	0	2.967688	-1.608472	-2.526976
39	1	0	-4.653799	-1.716490	0.886317
40	1	0	-6.569137	-0.448189	-0.070271
41	1	0	-3.906464	2.757014	-1.120761
42	1	0	-2.000253	1.495332	-0.160211
43	1	0	-7.492649	1.632449	-0.923630
44	1	0	-6.525511	1.911419	-2.376961
45	1	0	-6.470476	3.075273	-1.051855
46	1	0	-2.115297	-1.294709	-2.070458
47	1	0	-2.304528	-2.769288	-1.108220
48	1	0	-1.255506	-2.784522	-2.547096
49	1	0	-0.080793	3.901392	1.442443
50	1	0	0.261339	4.357073	-0.244768
51	1	0	1.572683	4.302575	0.927728

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3971.853378
Sum of electronic and thermal Energies=	-3971.827698
Sum of electronic and thermal Enthalpies=	-3971.826754
Sum of electronic and thermal Free Energies=	-3971.909279

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.832881	-0.368136	-0.050390
2	6	0	1.835066	0.658755	-1.186063
3	6	0	0.626817	-0.173671	0.871534
4	6	0	1.893051	-1.826794	-0.544490
5	6	0	1.896793	2.070483	-0.616307
6	6	0	0.914567	2.291149	0.495498
7	6	0	0.330872	1.280776	1.142879
8	35	0	5.316258	0.801701	-0.024215
9	7	0	-0.569640	-0.883802	0.270102
10	6	0	-3.197886	-0.156401	0.425902
11	6	0	1.980475	-2.802840	0.637535
12	6	0	3.098505	-2.048760	-1.458144
13	7	0	0.680085	-2.135815	-1.317968
14	6	0	-0.428434	-1.702251	-0.900896

15	6	0	-4.457933	-0.725823	0.306163
16	6	0	-5.473010	0.006550	-0.296798
17	6	0	-5.238959	1.292735	-0.782869
18	6	0	-3.960821	1.838715	-0.646488
19	6	0	-2.935025	1.124285	-0.042635
20	6	0	-6.334968	2.061978	-1.473707
21	16	0	-1.905243	-1.092261	1.236909
22	8	0	-2.332702	-2.480227	1.222544
23	8	0	-1.615617	-0.457291	2.507529
24	6	0	-1.672472	-1.951227	-1.715678
25	6	0	0.660424	3.720800	0.884184
26	1	0	2.732808	-0.170913	0.544869
27	1	0	0.945590	0.535953	-1.817222
28	1	0	2.724688	0.504359	-1.796992
29	1	0	0.827208	-0.657803	1.829168
30	1	0	1.730500	2.815455	-1.403322
31	1	0	2.914116	2.236906	-0.232917
32	1	0	-0.341452	1.483033	1.970530
33	1	0	2.065269	-3.823887	0.259589
34	1	0	1.095584	-2.758639	1.276806
35	1	0	2.867705	-2.572243	1.233381
36	1	0	3.208927	-3.117777	-1.658392
37	1	0	4.008639	-1.651903	-0.999058
38	1	0	2.949686	-1.547300	-2.414902
39	1	0	-4.624466	-1.732473	0.670222
40	1	0	-6.461144	-0.430479	-0.397448
41	1	0	-3.764359	2.837204	-1.022328
42	1	0	-1.936444	1.541855	0.044968
43	1	0	-7.304762	1.864772	-1.013492
44	1	0	-6.401311	1.772794	-2.526403
45	1	0	-6.147274	3.135759	-1.434589
46	1	0	-2.129483	-1.002241	-2.008093
47	1	0	-2.412281	-2.534647	-1.167488
48	1	0	-1.362663	-2.498970	-2.602199
49	1	0	-0.024178	3.796710	1.730885
50	1	0	0.243370	4.280337	0.039934
51	1	0	1.604342	4.206316	1.150549

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.429103
Sum of electronic and thermal Energies=	-3971.403108
Sum of electronic and thermal Enthalpies=	-3971.402164
Sum of electronic and thermal Free Energies=	-3971.486702

Cartesian coordinates of Intermediate Cmplx-1_d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.041865	2.108089	-0.359811
2	6	0	0.909003	1.067254	-1.450110
3	6	0	-0.246289	2.393833	0.495935
4	6	0	2.270971	1.743143	0.497064
5	6	0	1.139917	-0.224070	-1.208968
6	6	0	1.378988	-0.706744	0.205400
7	6	0	2.085401	-2.069382	0.252869
8	7	0	-0.003640	-0.774170	0.919948
9	6	0	2.272022	0.289565	1.004151
10	7	0	-0.482295	1.524064	1.660619
11	6	0	-1.509001	2.392307	-0.386180
12	6	0	-0.108250	3.808548	1.111100
13	6	0	-0.711028	-0.222685	3.258357
14	6	0	-0.424795	0.271567	1.850300
15	6	0	-2.590435	-1.046940	-0.187665
16	6	0	-3.592667	-0.564491	0.654543
17	6	0	-4.704931	0.067803	0.101344
18	6	0	-4.839118	0.218309	-1.285566
19	6	0	-3.829414	-0.295376	-2.110706
20	6	0	-2.707889	-0.924183	-1.572887
21	6	0	-6.033017	0.931476	-1.876096
22	16	0	-1.164482	-1.927221	0.490086
23	8	0	-0.638332	-2.732453	-0.615961
24	8	0	-1.672903	-2.597747	1.697634
25	1	0	1.249901	3.065265	-0.857881
26	1	0	0.696352	1.405863	-2.463162
27	1	0	3.161665	1.845797	-0.134311
28	1	0	2.380577	2.438786	1.337961
29	1	0	1.127328	-0.968164	-2.000434
30	1	0	3.076782	-1.922030	-0.197586
31	1	0	1.545713	-2.845953	-0.286813
32	1	0	2.220212	-2.386066	1.294093
33	1	0	2.029447	0.218770	2.069878
34	1	0	3.299103	-0.071709	0.871522
35	1	0	-2.397862	2.605514	0.217770
36	1	0	-1.647363	1.432449	-0.883966
37	1	0	-1.423014	3.168214	-1.157168
38	1	0	-0.987427	4.033909	1.723714
39	1	0	-0.019577	4.570224	0.326893
40	1	0	0.773100	3.874437	1.756338
41	1	0	-1.048564	0.616105	3.869811
42	1	0	0.217146	-0.631234	3.679125
43	1	0	-1.440361	-1.034128	3.278013
44	1	0	-3.512960	-0.702243	1.727355
45	1	0	-5.486566	0.442748	0.758586
46	1	0	-3.922998	-0.205640	-3.190814
47	1	0	-1.931081	-1.328918	-2.211771
48	1	0	-6.917909	0.829860	-1.238393
49	1	0	-6.282639	0.541226	-2.868761
50	1	0	-5.835135	2.005894	-1.989778
51	35	0	5.222608	-0.234264	-0.912783

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3971.806574
Sum of electronic and thermal Energies= -3971.781196

Sum of electronic and thermal Enthalpies= -3971.780252
Sum of electronic and thermal Free Energies= -3971.861614

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.109773	2.099383	-0.291983
2	6	0	1.256273	1.110858	-1.428584
3	6	0	-0.323341	2.277869	0.322001
4	6	0	2.168885	1.769947	0.773560
5	6	0	1.477293	-0.176073	-1.196044
6	6	0	1.431875	-0.678181	0.227560
7	6	0	2.046970	-2.067145	0.393143
8	7	0	-0.043559	-0.669399	0.663272
9	6	0	2.214619	0.280734	1.155570
10	7	0	-0.578924	1.495067	1.548689
11	6	0	-1.406279	1.996332	-0.721012
12	6	0	-0.456119	3.735189	0.788825
13	6	0	-0.752545	-0.352545	3.050811
14	6	0	-0.491962	0.246150	1.688434
15	6	0	-2.597651	-1.061723	-0.217573
16	6	0	-3.459780	-0.618301	0.776156
17	6	0	-4.629565	0.035880	0.412610
18	6	0	-4.952729	0.238694	-0.929528
19	6	0	-4.083112	-0.245046	-1.907614
20	6	0	-2.905228	-0.892648	-1.560501
21	6	0	-6.203451	0.984907	-1.315028
22	16	0	-1.066380	-1.890202	0.201313
23	8	0	-0.553499	-2.457118	-1.031526
24	8	0	-1.382765	-2.768967	1.317531
25	1	0	1.351466	3.084609	-0.703916
26	1	0	1.268229	1.492490	-2.444326
27	1	0	3.145575	2.017053	0.350363
28	1	0	2.013461	2.387941	1.662751
29	1	0	1.681024	-0.888907	-1.985805
30	1	0	3.097430	-1.983904	0.097977
31	1	0	1.561224	-2.815382	-0.229427
32	1	0	1.990514	-2.375332	1.441299
33	1	0	1.906596	0.111125	2.190504
34	1	0	3.254209	-0.040512	1.064354
35	1	0	-2.402908	2.049311	-0.271986
36	1	0	-1.262482	1.014445	-1.162797
37	1	0	-1.339595	2.738513	-1.522118
38	1	0	-1.421063	3.877062	1.280140
39	1	0	-0.378975	4.422950	-0.057132
40	1	0	0.329217	3.974878	1.509636
41	1	0	-1.135502	0.422626	3.710837
42	1	0	0.197853	-0.733068	3.438287
43	1	0	-1.425100	-1.208446	3.014024
44	1	0	-3.228409	-0.789857	1.819775
45	1	0	-5.304504	0.391495	1.183835
46	1	0	-4.328823	-0.108469	-2.955399
47	1	0	-2.215795	-1.263191	-2.309833
48	1	0	-6.978190	0.876035	-0.554437
49	1	0	-6.599816	0.624000	-2.265583
50	1	0	-5.991894	2.052180	-1.426173
51	35	0	5.213208	-0.147517	-0.742641

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.389429
Sum of electronic and thermal Energies=	-3971.363965
Sum of electronic and thermal Enthalpies=	-3971.363021
Sum of electronic and thermal Free Energies=	-3971.445308

Cartesian coordinates of Intermediate Cmplx-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.902275	-0.486502	-0.048972
2	6	0	-1.875355	0.801417	-0.899688
3	6	0	-1.975295	-1.827885	-0.785633
4	6	0	-0.692290	-0.349278	0.897789
5	6	0	-1.256195	1.788626	0.064729
6	6	0	-1.544472	3.251312	-0.050963
7	6	0	-0.574182	1.154032	1.032039
8	7	0	0.532214	-1.009792	0.271191
9	7	0	-0.699039	-2.137956	-1.453087
10	6	0	-3.081025	-1.776537	-1.854230
11	6	0	-2.285118	-2.971411	0.204197
12	6	0	1.677782	-2.121853	-1.683040
13	6	0	0.408020	-1.780673	-0.933486
14	6	0	3.137117	-0.032613	0.436744
15	6	0	2.784816	1.235662	-0.027551
16	6	0	3.770563	2.054148	-0.575821
17	6	0	5.105291	1.632747	-0.659473
18	6	0	5.430164	0.355005	-0.185431
19	6	0	4.456831	-0.479123	0.362556
20	6	0	6.170918	2.540930	-1.227609
21	16	0	1.913768	-1.089878	1.240307
22	8	0	1.560949	-0.463986	2.519052
23	8	0	2.472358	-2.450407	1.238924
24	1	0	-2.802028	-0.368050	0.571046
25	1	0	-2.897371	1.091741	-1.168787
26	1	0	-1.264766	0.710044	-1.812212
27	1	0	-0.856373	-0.841631	1.857885
28	1	0	-1.024698	3.844224	0.710476
29	1	0	-2.630490	3.375167	0.070835
30	1	0	-1.281850	3.643254	-1.043709
31	1	0	-0.062239	1.622406	1.866988

32	1	0	-3.261573	-2.775990	-2.268820
33	1	0	-2.785458	-1.120698	-2.679070
34	1	0	-4.006028	-1.376814	-1.421411
35	1	0	-2.279505	-3.933987	-0.319980
36	1	0	-1.544737	-3.024008	1.010596
37	1	0	-3.274021	-2.820746	0.651274
38	1	0	1.377500	-2.619811	-2.605997
39	1	0	2.329363	-2.783209	-1.106813
40	1	0	2.247811	-1.218656	-1.928733
41	1	0	1.751091	1.567721	0.024438
42	1	0	3.495718	3.038261	-0.948613
43	1	0	6.458033	0.004278	-0.250641
44	1	0	4.704781	-1.473467	0.718020
45	1	0	6.669527	3.112576	-0.432994
46	1	0	5.747035	3.264884	-1.931457
47	1	0	6.946340	1.971227	-1.751646
48	35	0	-5.143052	1.199163	0.233055

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3932.555759
Sum of electronic and thermal Energies=	-3932.531082
Sum of electronic and thermal Enthalpies=	-3932.530137
Sum of electronic and thermal Free Energies=	-3932.611336

Cartesian coordinates of Intermediate Cmplx-2_d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.994754	0.162405	1.810744
2	6	0	0.342592	0.693889	0.776591
3	6	0	1.990557	-0.888014	1.360231
4	6	0	0.766659	0.019751	-0.524458
5	6	0	0.821553	0.924353	-1.752402
6	6	0	2.168713	-0.483904	-0.116219
7	6	0	1.519148	-2.392134	1.520406
8	7	0	1.123421	-3.035002	0.257033
9	6	0	2.721082	-3.219394	2.022089
10	6	0	0.354323	-2.557336	2.516766
11	6	0	0.401330	-2.565531	-0.676405
12	6	0	0.198531	-3.439054	-1.901422

13	7	0	-0.148206	-1.221847	-0.741888
14	6	0	-2.512053	0.208934	-0.400032
15	6	0	-2.789199	1.444263	-0.979583
16	6	0	-3.454346	2.414507	-0.228164
17	6	0	-3.854308	2.161399	1.089012
18	6	0	-3.589791	0.895754	1.637001
19	6	0	-2.925177	-0.080363	0.902607
20	6	0	-4.539758	3.226661	1.911919
21	16	0	-1.719573	-1.081476	-1.372713
22	8	0	-1.725774	-0.623345	-2.770989
23	8	0	-2.422152	-2.331482	-1.032124
24	1	0	0.859562	0.446243	2.851045
25	1	0	-0.389314	1.491297	0.821608
26	1	0	2.932421	-0.773677	1.909801
27	1	0	1.137002	0.357870	-2.635291
28	1	0	1.560022	1.714583	-1.547191
29	1	0	-0.142763	1.386343	-1.979721
30	1	0	2.828272	0.395832	-0.169695
31	1	0	2.568502	-1.266684	-0.765485
32	1	0	3.564239	-3.124399	1.328545
33	1	0	2.455076	-4.280112	2.087413
34	1	0	3.049529	-2.873437	3.010008
35	1	0	0.074029	-3.614170	2.591300
36	1	0	-0.521339	-1.986673	2.195937
37	1	0	0.645873	-2.206620	3.514352
38	1	0	0.564496	-2.915235	-2.792858
39	1	0	-0.855318	-3.673299	-2.064320
40	1	0	0.759432	-4.364453	-1.760688
41	1	0	-2.491062	1.635001	-2.004373
42	1	0	-3.663922	3.383382	-0.674955
43	1	0	-3.908669	0.675555	2.653429
44	1	0	-2.729539	-1.060216	1.324302
45	1	0	-5.350248	2.806234	2.518370
46	1	0	-4.961706	4.013320	1.278101
47	1	0	-3.833097	3.705556	2.602494
48	35	0	3.658027	2.906023	-0.352054

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3932.518967
Sum of electronic and thermal Energies= -3932.494579
Sum of electronic and thermal Enthalpies= -3932.493635
Sum of electronic and thermal Free Energies= -3932.573391

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.098423	0.226836	1.620655
2	6	0	0.436495	0.703636	0.575372
3	6	0	1.991169	-0.934845	1.227912
4	6	0	0.731390	-0.146718	-0.657006
5	6	0	0.746644	0.584790	-1.988700
6	6	0	2.125943	-0.670021	-0.278674
7	6	0	1.413873	-2.367554	1.542920
8	7	0	1.031059	-3.126642	0.342149
9	6	0	2.520460	-3.196881	2.202283
10	6	0	0.195767	-2.328559	2.472838
11	6	0	0.289868	-2.692745	-0.579925
12	6	0	0.010671	-3.575865	-1.771206

13	7	0	-0.229027	-1.341604	-0.652398
14	6	0	-2.403885	0.242640	-0.316844
15	6	0	-2.572074	1.434860	-1.005288
16	6	0	-2.982800	2.560405	-0.303798
17	6	0	-3.236863	2.498985	1.067173
18	6	0	-3.099781	1.274043	1.723454
19	6	0	-2.685017	0.141735	1.038833
20	6	0	-3.672186	3.733357	1.812277
21	16	0	-1.808242	-1.201401	-1.169766
22	8	0	-1.910851	-0.932326	-2.595625
23	8	0	-2.513806	-2.353885	-0.624484
24	1	0	1.059486	0.634288	2.623388
25	1	0	-0.204134	1.575726	0.561285
26	1	0	2.960842	-0.844128	1.723747
27	1	0	1.014107	-0.105466	-2.793051
28	1	0	1.493527	1.381536	-1.911827
29	1	0	-0.217026	1.028739	-2.235959
30	1	0	2.804178	0.175703	-0.428028
31	1	0	2.459582	-1.519887	-0.874738
32	1	0	3.392074	-3.240853	1.544325
33	1	0	2.170934	-4.216561	2.377739
34	1	0	2.823331	-2.748329	3.152562
35	1	0	-0.141901	-3.347671	2.674954
36	1	0	-0.617199	-1.771970	2.006559
37	1	0	0.452846	-1.845450	3.419351
38	1	0	0.376260	-3.080717	-2.675228
39	1	0	-1.057356	-3.753722	-1.897490
40	1	0	0.525028	-4.522448	-1.624458
41	1	0	-2.376262	1.471026	-2.069388
42	1	0	-3.094236	3.504805	-0.825417
43	1	0	-3.305190	1.212040	2.786402
44	1	0	-2.571883	-0.811087	1.540887
45	1	0	-4.709832	3.982082	1.572515
46	1	0	-3.052801	4.589229	1.537915
47	1	0	-3.599148	3.589370	2.890649
48	35	0	3.333746	2.872142	-0.477757

Level: M06-2X/6-311G**
 Sum of electronic and zero-point Energies= -3932.117067
 Sum of electronic and thermal Energies= -3932.092478
 Sum of electronic and thermal Enthalpies= -3932.091534
 Sum of electronic and thermal Free Energies= -3932.172702

Cartesian coordinates of Intermediate Cmplx-3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.814725	-0.941108	-1.651613
2	6	0	0.989805	-2.071117	-1.100919
3	6	0	1.961494	-0.015453	-0.418472
4	6	0	0.426246	-1.790013	0.078237
5	6	0	-1.486458	2.255572	-1.413068
6	6	0	-0.291378	-2.761610	0.969159
7	6	0	0.746598	-0.347706	0.472141
8	7	0	-0.401923	0.616417	0.175919
9	7	0	0.887420	2.044885	-1.248577
10	6	0	3.257064	1.724064	-1.711003
11	6	0	2.133221	1.484768	-0.693070
12	6	0	2.478673	2.231404	0.611796
13	6	0	-0.235405	1.655981	-0.813496
14	6	0	-3.121076	0.117453	0.482137
15	6	0	-4.349453	0.654807	0.856643
16	6	0	-5.516406	0.149707	0.290381
17	6	0	-5.476026	-0.885076	-0.648866
18	6	0	-4.226806	-1.398195	-1.016315
19	6	0	-3.051168	-0.908687	-0.456430
20	6	0	-6.745346	-1.448144	-1.240709
21	16	0	-1.636282	0.738458	1.313547
22	8	0	-1.317200	-0.188003	2.397338
23	8	0	-1.908033	2.139884	1.636524
24	1	0	1.321886	-0.454562	-2.503498
25	1	0	2.799648	-1.279025	-1.985495
26	1	0	0.919219	-3.040509	-1.586382
27	1	0	2.855696	-0.367521	0.113441
28	1	0	-1.163498	2.937056	-2.197459
29	1	0	-2.067539	2.808607	-0.674165
30	1	0	-2.129722	1.483044	-1.842293
31	1	0	0.254613	-2.874828	1.912104
32	1	0	-0.352034	-3.743961	0.492365
33	1	0	-1.296944	-2.437651	1.243393
34	1	0	0.979542	-0.249276	1.530322
35	1	0	3.406588	2.799390	-1.846779
36	1	0	2.996548	1.299998	-2.683832
37	1	0	4.183505	1.261039	-1.359780
38	1	0	1.700219	2.110388	1.369604
39	1	0	2.584680	3.301001	0.410154
40	1	0	3.421768	1.845308	1.006805
41	1	0	-4.383654	1.470609	1.567655
42	1	0	-6.472808	0.574046	0.578779
43	1	0	-4.169549	-2.190012	-1.756396
44	1	0	-2.089778	-1.301263	-0.765647
45	1	0	-7.054913	-2.355085	-0.709614
46	1	0	-6.610029	-1.716775	-2.291360
47	1	0	-7.567789	-0.732314	-1.175807
48	35	0	5.447669	-0.898488	0.337018

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3932.550883
Sum of electronic and thermal Energies=	-3932.525489
Sum of electronic and thermal Enthalpies=	-3932.524545
Sum of electronic and thermal Free Energies=	-3932.609552

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.814708	-0.941575	-1.647893
2	6	0	0.991892	-2.071932	-1.094779
3	6	0	1.960994	-0.013860	-0.416276
4	6	0	0.428661	-1.789758	0.084287
5	6	0	-1.489901	2.251844	-1.412625
6	6	0	-0.286316	-2.761235	0.977504
7	6	0	0.746964	-0.346229	0.475468
8	7	0	-0.403021	0.615771	0.177907
9	7	0	0.884209	2.044200	-1.248624
10	6	0	3.253820	1.725209	-1.712203
11	6	0	2.130934	1.486147	-0.693155
12	6	0	2.476383	2.235026	0.610421
13	6	0	-0.237977	1.654419	-0.812689
14	6	0	-3.121369	0.114930	0.484168
15	6	0	-4.350399	0.648305	0.861085
16	6	0	-5.517216	0.138381	0.298113
17	6	0	-5.475364	-0.895115	-0.641971
18	6	0	-4.225408	-1.408931	-1.007151
19	6	0	-3.050396	-0.914605	-0.451066
20	6	0	-6.739768	-1.426600	-1.272481
21	16	0	-1.637382	0.737704	1.315632
22	8	0	-1.317057	-0.187210	2.400356
23	8	0	-1.910653	2.139163	1.637213
24	1	0	1.320517	-0.457103	-2.500180
25	1	0	2.799939	-1.278556	-1.981812
26	1	0	0.922657	-3.042289	-1.578499
27	1	0	2.855890	-0.364254	0.115563
28	1	0	-1.167908	2.933049	-2.197655
29	1	0	-2.071709	2.804716	-0.674173
30	1	0	-2.132056	1.477972	-1.841095
31	1	0	0.260919	-2.871988	1.920025
32	1	0	-0.345588	-3.744457	0.502330
33	1	0	-1.292187	-2.438782	1.252371
34	1	0	0.980144	-0.245575	1.533392
35	1	0	3.402273	2.800504	-1.849411
36	1	0	2.992911	1.299723	-2.684304
37	1	0	4.180937	1.263358	-1.361215
38	1	0	1.698631	2.114061	1.368961
39	1	0	2.580907	3.304477	0.407242
40	1	0	3.420254	1.850700	1.005281
41	1	0	-4.386297	1.460771	1.575827
42	1	0	-6.474808	0.555216	0.593306
43	1	0	-4.167863	-2.208155	-1.739295
44	1	0	-2.088718	-1.309696	-0.756170
45	1	0	-6.877177	-1.019658	-2.280288
46	1	0	-7.620773	-1.158387	-0.685503
47	1	0	-6.710875	-2.515598	-1.363510
48	35	0	5.448857	-0.895865	0.331160

Level: M06-2x/6-311G**

Sum of electronic and zero-point Energies=	-3932.550946
Sum of electronic and thermal Energies=	-3932.526428
Sum of electronic and thermal Enthalpies=	-3932.525483
Sum of electronic and thermal Free Energies=	-3932.607626

Cartesian coordinates of Intermediate Cmplx-3_d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.681530	0.671530	-0.042709
2	6	0	-1.619738	1.798850	-0.452730
3	6	0	-0.835318	0.651826	1.478748
4	7	0	-1.079015	-0.642532	-0.653339
5	6	0	-2.518240	1.993240	0.520263
6	6	0	1.557502	-1.463351	-0.506868
7	6	0	1.741425	-2.590337	0.302187
8	6	0	-2.322441	1.007529	1.662665
9	7	0	-3.351417	-0.822580	0.183953
10	6	0	-3.284368	-0.220235	1.518602
11	6	0	-2.925876	-1.767635	-1.948368
12	6	0	-2.452299	-1.051373	-0.692561
13	6	0	2.850033	-2.643420	1.141632
14	6	0	3.767448	-1.580712	1.198846
15	6	0	3.548157	-0.462991	0.387590
16	6	0	-4.722842	0.256162	1.821774
17	6	0	-2.931825	-1.342238	2.520565
18	6	0	2.462241	-0.402218	-0.485580
19	6	0	4.968976	-1.646544	2.112982
20	16	0	0.130908	-1.422576	-1.595673
21	8	0	-0.297107	-2.816905	-1.792479
22	8	0	0.460001	-0.593092	-2.762017
23	6	0	-1.408875	2.536839	-1.734494
24	1	0	0.339836	0.910469	-0.338915
25	1	0	-0.202226	1.456632	1.867537
26	1	0	-0.518444	-0.292934	1.928074
27	1	0	-3.311793	2.736157	0.496429
28	1	0	1.029813	-3.407901	0.259273
29	1	0	-2.515523	1.456684	2.646958
30	1	0	-4.016421	-1.731347	-1.950290
31	1	0	-2.595289	-2.807828	-1.965686
32	1	0	-2.534881	-1.287778	-2.852050
33	1	0	3.001967	-3.517927	1.771526
34	1	0	4.195103	0.408306	0.445043
35	1	0	-4.801345	0.651858	2.842466
36	1	0	-5.424314	-0.577578	1.712085
37	1	0	-5.025102	1.040670	1.120729
38	1	0	-1.966985	-1.801797	2.290485
39	1	0	-2.891752	-0.948135	3.544025
40	1	0	-3.694837	-2.127796	2.482911

41	1	0	2.317472	0.503726	-1.068738
42	1	0	4.796364	-2.322963	2.957828
43	1	0	5.216538	-0.657162	2.512302
44	1	0	5.857285	-2.011567	1.578689
45	1	0	-1.391261	1.849655	-2.590793
46	1	0	-2.182564	3.294545	-1.904587
47	1	0	-0.421540	3.019686	-1.688657
48	35	0	2.091447	2.971193	-0.104557

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies=	-3932.545534
Sum of electronic and thermal Energies=	-3932.521004
Sum of electronic and thermal Enthalpies=	-3932.520060
Sum of electronic and thermal Free Energies=	-3932.599999

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.681530	0.671530	-0.042709
2	6	0	-1.619738	1.798850	-0.452730
3	6	0	-0.835318	0.651826	1.478748
4	7	0	-1.079015	-0.642532	-0.653339
5	6	0	-2.518240	1.993240	0.520263
6	6	0	1.557502	-1.463351	-0.506868
7	6	0	1.741425	-2.590337	0.302187
8	6	0	-2.322441	1.007529	1.662665
9	7	0	-3.351417	-0.822580	0.183953
10	6	0	-3.284368	-0.220235	1.518602
11	6	0	-2.925876	-1.767635	-1.948368
12	6	0	-2.452299	-1.051373	-0.692561
13	6	0	2.850033	-2.643420	1.141632
14	6	0	3.767448	-1.580712	1.198846
15	6	0	3.548157	-0.462991	0.387590
16	6	0	-4.722842	0.256162	1.821774
17	6	0	-2.931825	-1.342238	2.520565
18	6	0	2.462241	-0.402218	-0.485580
19	6	0	4.968976	-1.646544	2.112982
20	16	0	0.130908	-1.422576	-1.595673
21	8	0	-0.297107	-2.816905	-1.792479
22	8	0	0.460001	-0.593092	-2.762017
23	6	0	-1.408875	2.536839	-1.734494
24	1	0	0.339836	0.910469	-0.338915
25	1	0	-0.202226	1.456632	1.867537
26	1	0	-0.518444	-0.292934	1.928074
27	1	0	-3.311793	2.736157	0.496429
28	1	0	1.029813	-3.407901	0.259273
29	1	0	-2.515523	1.456684	2.646958
30	1	0	-4.016421	-1.731347	-1.950290
31	1	0	-2.595289	-2.807828	-1.965686
32	1	0	-2.534881	-1.287778	-2.852050
33	1	0	3.001967	-3.517927	1.771526
34	1	0	4.195103	0.408306	0.445043
35	1	0	-4.801345	0.651858	2.842466
36	1	0	-5.424314	-0.577578	1.712085
37	1	0	-5.025102	1.040670	1.120729
38	1	0	-1.966985	-1.801797	2.290485
39	1	0	-2.891752	-0.948135	3.544025
40	1	0	-3.694837	-2.127796	2.482911

41	1	0	2.317472	0.503726	-1.068738
42	1	0	4.796364	-2.322963	2.957828
43	1	0	5.216538	-0.657162	2.512302
44	1	0	5.857285	-2.011567	1.578689
45	1	0	-1.391261	1.849655	-2.590793
46	1	0	-2.182564	3.294545	-1.904587
47	1	0	-0.421540	3.019686	-1.688657
48	35	0	2.091447	2.971193	-0.104557

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3932.138551
Sum of electronic and thermal Energies=	-3932.114317
Sum of electronic and thermal Enthalpies=	-3932.113373
Sum of electronic and thermal Free Energies=	-3932.192067

Cartesian coordinates of Intermediate Cmplx-4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.014998	-0.826869	2.595306
2	16	0	2.112076	-1.570912	0.087836
3	7	0	0.483468	-1.190631	0.151103
4	6	0	-0.337515	-1.525671	1.305814
5	7	0	-1.367162	-2.262750	1.267874
6	6	0	-1.102503	0.505024	-0.711501
7	6	0	2.989067	0.000118	0.014668
8	8	0	2.460101	-2.226426	1.354830
9	6	0	-1.839662	-3.053651	0.118273
10	6	0	-0.169775	-0.629994	-1.086108
11	8	0	2.382670	-2.244033	-1.191860
12	6	0	4.327550	2.459976	-0.112612
13	6	0	3.490240	0.452037	-1.205572
14	6	0	3.831056	1.973148	1.106417
15	6	0	3.165231	0.753615	1.178168
16	6	0	5.009745	3.805486	-0.182378
17	6	0	-0.828316	-4.190426	-0.161769
18	6	0	-0.491380	1.850462	-0.408003
19	6	0	-0.878174	-1.716723	-1.899040
20	6	0	-3.094513	-1.021607	-0.976133

21	6	0	-2.135756	-2.224497	-1.177372
22	6	0	-3.146958	-3.721804	0.602265
23	6	0	-2.425658	0.294882	-0.671095
24	6	0	4.154581	1.677790	-1.260077
25	1	0	-0.687608	-1.139440	3.369439
26	1	0	-0.059672	0.258489	2.458378
27	1	0	1.033220	-1.071812	2.909827
28	1	0	0.656502	-0.226617	-1.682517
29	1	0	3.368909	-0.159848	-2.092651
30	1	0	3.965600	2.560357	2.011824
31	1	0	2.792820	0.384604	2.127347
32	1	0	5.621914	3.898806	-1.085343
33	1	0	5.655957	3.973825	0.686607
34	1	0	4.271632	4.617996	-0.199313
35	1	0	0.155658	-3.823258	-0.456765
36	1	0	-1.203611	-4.842548	-0.960759
37	1	0	-0.703560	-4.798379	0.740866
38	1	0	0.214901	1.794028	0.433730
39	1	0	-1.275128	2.581417	-0.166354
40	1	0	0.086193	2.222178	-1.269081
41	1	0	-1.183142	-1.266317	-2.853485
42	1	0	-0.177124	-2.521886	-2.135241
43	1	0	-3.689974	-0.893278	-1.894769
44	1	0	-3.834312	-1.229598	-0.194158
45	1	0	-2.632092	-2.941265	-1.847180
46	1	0	-2.939964	-4.337498	1.483869
47	1	0	-3.574722	-4.363538	-0.178053
48	1	0	-3.894874	-2.979345	0.892048
49	1	0	-3.078676	1.138780	-0.421409
50	1	0	4.543129	2.030929	-2.212446
51	35	0	-3.799288	3.629639	0.213660

Level: B3LYP/6-311G**//B3LYP/6-31G*

Sum of electronic and zero-point Energies= -3971.837739
Sum of electronic and thermal Energies= -3971.812222
Sum of electronic and thermal Enthalpies= -3971.811278
Sum of electronic and thermal Free Energies= -3971.893832

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.014998	-0.826869	2.595306
2	16	0	2.112076	-1.570912	0.087836
3	7	0	0.483468	-1.190631	0.151103
4	6	0	-0.337515	-1.525671	1.305814
5	7	0	-1.367162	-2.262750	1.267874
6	6	0	-1.102503	0.505024	-0.711501
7	6	0	2.989067	0.000118	0.014668
8	8	0	2.460101	-2.226426	1.354830
9	6	0	-1.839662	-3.053651	0.118273
10	6	0	-0.169775	-0.629994	-1.086108
11	8	0	2.382670	-2.244033	-1.191860
12	6	0	4.327550	2.459976	-0.112612
13	6	0	3.490240	0.452037	-1.205572
14	6	0	3.831056	1.973148	1.106417
15	6	0	3.165231	0.753615	1.178168
16	6	0	5.009745	3.805486	-0.182378
17	6	0	-0.828316	-4.190426	-0.161769

18	6	0	-0.491380	1.850462	-0.408003
19	6	0	-0.878174	-1.716723	-1.899040
20	6	0	-3.094513	-1.021607	-0.976133
21	6	0	-2.135756	-2.224497	-1.177372
22	6	0	-3.146958	-3.721804	0.602265
23	6	0	-2.425658	0.294882	-0.671095
24	6	0	4.154581	1.677790	-1.260077
25	1	0	-0.687608	-1.139440	3.369439
26	1	0	-0.059672	0.258489	2.458378
27	1	0	1.033220	-1.071812	2.909827
28	1	0	0.656502	-0.226617	-1.682517
29	1	0	3.368909	-0.159848	-2.092651
30	1	0	3.965600	2.560357	2.011824
31	1	0	2.792820	0.384604	2.127347
32	1	0	5.621914	3.898806	-1.085343
33	1	0	5.655957	3.973825	0.686607
34	1	0	4.271632	4.617996	-0.199313
35	1	0	0.155658	-3.823258	-0.456765
36	1	0	-1.203611	-4.842548	-0.960759
37	1	0	-0.703560	-4.798379	0.740866
38	1	0	0.214901	1.794028	0.433730
39	1	0	-1.275128	2.581417	-0.166354
40	1	0	0.086193	2.222178	-1.269081
41	1	0	-1.183142	-1.266317	-2.853485
42	1	0	-0.177124	-2.521886	-2.135241
43	1	0	-3.689974	-0.893278	-1.894769
44	1	0	-3.834312	-1.229598	-0.194158
45	1	0	-2.632092	-2.941265	-1.847180
46	1	0	-2.939964	-4.337498	1.483869
47	1	0	-3.574722	-4.363538	-0.178053
48	1	0	-3.894874	-2.979345	0.892048
49	1	0	-3.078676	1.138780	-0.421409
50	1	0	4.543129	2.030929	-2.212446
51	35	0	-3.799288	3.629639	0.213660

Level: M06-2X/6-311G**

Sum of electronic and zero-point Energies=	-3971.412187
Sum of electronic and thermal Energies=	-3971.386904
Sum of electronic and thermal Enthalpies=	-3971.385959
Sum of electronic and thermal Free Energies=	-3971.467119

Cartesian coordinates of Intermediate Cmplx-4_d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.252737	-2.391003	1.764493
2	16	0	0.102761	-1.513129	-1.139384
3	7	0	-0.894478	-0.694331	-0.041358
4	6	0	-1.842335	-1.422079	0.766814
5	7	0	-3.099116	-1.230848	0.776303
6	6	0	-0.971492	1.304132	1.396989
7	6	0	1.773847	-1.466253	-0.485413
8	8	0	-0.345634	-2.915120	-1.127761
9	6	0	-3.849769	-0.393365	-0.177555
10	6	0	-0.918948	0.808357	-0.040057
11	8	0	0.089666	-0.744143	-2.387796
12	6	0	4.352744	-1.374172	0.592302
13	6	0	2.515686	-0.287822	-0.580153
14	6	0	3.593216	-2.552379	0.651540
15	6	0	2.303231	-2.606180	0.124920
16	6	0	5.748501	-1.319513	1.169396
17	6	0	-3.767694	-1.028661	-1.585799
18	6	0	0.323500	1.304448	2.162509
19	6	0	-2.066024	1.372468	-0.879094
20	6	0	-3.436945	1.825746	1.154940
21	6	0	-3.429248	1.115891	-0.221773
22	6	0	-5.324538	-0.499469	0.275620
23	6	0	-2.127752	1.751503	1.901931
24	6	0	3.790837	-0.247591	-0.021629
25	1	0	-2.061437	-2.867738	2.321938
26	1	0	-0.593696	-1.854945	2.458217
27	1	0	-0.659133	-3.156786	1.259085
28	1	0	0.024060	1.156234	-0.476364
29	1	0	2.134593	0.626381	-1.035064
30	1	0	4.014169	-3.438995	1.122065
31	1	0	1.717024	-3.517747	0.170839
32	1	0	6.506901	-1.288044	0.375629
33	1	0	5.961040	-2.193203	1.795439
34	1	0	5.889429	-0.420167	1.780111
35	1	0	-2.751707	-1.060218	-1.980286
36	1	0	-4.391275	-0.465244	-2.291624
37	1	0	-4.143145	-2.056944	-1.545243
38	1	0	0.178606	1.656744	3.190745
39	1	0	1.049491	1.952616	1.647391
40	1	0	0.765336	0.299249	2.202126
41	1	0	-1.899864	2.454399	-0.959044
42	1	0	-2.008554	0.968485	-1.892796
43	1	0	-3.682116	2.888707	0.993510
44	1	0	-4.241927	1.442006	1.794090
45	1	0	-4.198689	1.594692	-0.844405
46	1	0	-5.637843	-1.548642	0.257931
47	1	0	-5.985239	0.072101	-0.388241
48	1	0	-5.461845	-0.138348	1.299096
49	1	0	-2.141988	2.134260	2.923920
50	1	0	4.317185	0.703488	-0.059445
51	35	0	2.090711	3.132964	-0.592272

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies= -3971.848141
Sum of electronic and thermal Energies= -3971.822727

Sum of electronic and thermal Enthalpies= -3971.821783
Sum of electronic and thermal Free Energies= -3971.903072

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.252737	-2.391003	1.764493
2	16	0	0.102761	-1.513129	-1.139384
3	7	0	-0.894478	-0.694331	-0.041358
4	6	0	-1.842335	-1.422079	0.766814
5	7	0	-3.099116	-1.230848	0.776303
6	6	0	-0.971492	1.304132	1.396989
7	6	0	1.773847	-1.466253	-0.485413
8	8	0	-0.345634	-2.915120	-1.127761
9	6	0	-3.849769	-0.393365	-0.177555
10	6	0	-0.918948	0.808357	-0.040057
11	8	0	0.089666	-0.744143	-2.387796
12	6	0	4.352744	-1.374172	0.592302
13	6	0	2.515686	-0.287822	-0.580153
14	6	0	3.593216	-2.552379	0.651540
15	6	0	2.303231	-2.606180	0.124920
16	6	0	5.748501	-1.319513	1.169396
17	6	0	-3.767694	-1.028661	-1.585799
18	6	0	0.323500	1.304448	2.162509
19	6	0	-2.066024	1.372468	-0.879094
20	6	0	-3.436945	1.825746	1.154940
21	6	0	-3.429248	1.115891	-0.221773
22	6	0	-5.324538	-0.499469	0.275620
23	6	0	-2.127752	1.751503	1.901931
24	6	0	3.790837	-0.247591	-0.021629
25	1	0	-2.061437	-2.867738	2.321938
26	1	0	-0.593696	-1.854945	2.458217
27	1	0	-0.659133	-3.156786	1.259085
28	1	0	0.024060	1.156234	-0.476364
29	1	0	2.134593	0.626381	-1.035064
30	1	0	4.014169	-3.438995	1.122065
31	1	0	1.717024	-3.517747	0.170839
32	1	0	6.506901	-1.288044	0.375629
33	1	0	5.961040	-2.193203	1.795439
34	1	0	5.889429	-0.420167	1.780111
35	1	0	-2.751707	-1.060218	-1.980286
36	1	0	-4.391275	-0.465244	-2.291624
37	1	0	-4.143145	-2.056944	-1.545243
38	1	0	0.178606	1.656744	3.190745
39	1	0	1.049491	1.952616	1.647391
40	1	0	0.765336	0.299249	2.202126
41	1	0	-1.899864	2.454399	-0.959044
42	1	0	-2.008554	0.968485	-1.892796
43	1	0	-3.682116	2.888707	0.993510
44	1	0	-4.241927	1.442006	1.794090
45	1	0	-4.198689	1.594692	-0.844405
46	1	0	-5.637843	-1.548642	0.257931
47	1	0	-5.985239	0.072101	-0.388241
48	1	0	-5.461845	-0.138348	1.299096
49	1	0	-2.141988	2.134260	2.923920
50	1	0	4.317185	0.703488	-0.059445
51	35	0	2.090711	3.132964	-0.592272

Level: M06-2X/6-311G**
Sum of electronic and zero-point Energies= -3971.429862
Sum of electronic and thermal Energies= -3971.404416
Sum of electronic and thermal Enthalpies= -3971.403471
Sum of electronic and thermal Free Energies= -3971.485776

Cartesian coordinates of Compound 4aa (Prd-1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.762360	1.361280	-1.199049
2	6	0	2.521100	2.784560	-0.692799
3	6	0	2.881039	0.366950	-0.030709
4	6	0	1.466810	2.856600	0.382001
5	6	0	0.942441	4.228031	0.714671
6	6	0	1.594179	0.370470	0.816991
7	7	0	2.123198	-1.615840	-1.273669
8	6	0	3.228238	-1.079980	-0.467759
9	6	0	4.493438	-1.128411	-1.339189
10	6	0	3.448318	-1.998701	0.753701
11	6	0	-0.195102	-1.960259	-1.748219
12	6	0	0.925638	-1.392079	-0.914139
13	7	0	0.567179	-0.559349	0.195251
14	16	0	-0.723972	-1.043199	1.211781
15	8	0	-0.792032	-2.501439	1.250551
16	6	0	-2.217921	-0.460628	0.393501
17	6	0	-2.310281	0.854952	-0.056359
18	6	0	-3.301952	-1.327527	0.302251
19	6	0	-4.492141	-0.866457	-0.254659
20	8	0	-0.554951	-0.294249	2.453871
21	6	0	-5.894421	0.932084	-1.351649
22	6	0	-3.503740	1.294523	-0.614539
23	6	0	-4.613061	0.444713	-0.722729
24	6	0	1.043160	1.763671	1.024341
25	1	0	3.669080	1.344979	-1.805739
26	1	0	1.940029	1.061060	-1.855479
27	1	0	2.238561	3.437980	-1.527079
28	1	0	3.454780	3.208429	-0.295019
29	1	0	3.676289	0.725579	0.635061
30	1	0	0.213671	4.198511	1.526761
31	1	0	0.469191	4.689711	-0.159759
32	1	0	1.759651	4.894480	1.014451
33	1	0	1.829409	-0.033250	1.802751

34	1	0	4.741538	-2.168931	-1.558569
35	1	0	5.344899	-0.669211	-0.827059
36	1	0	4.341219	-0.623701	-2.293539
37	1	0	3.682888	-3.008681	0.410881
38	1	0	2.564148	-2.067600	1.388291
39	1	0	4.285488	-1.639421	1.360191
40	1	0	-0.890032	-1.177149	-2.060469
41	1	0	-0.758252	-2.716309	-1.199689
42	1	0	0.256128	-2.422999	-2.623359
43	1	0	-1.457630	1.519232	0.013501
44	1	0	-3.208892	-2.345697	0.657681
45	1	0	-5.339042	-1.540526	-0.325099
46	1	0	-6.127120	1.952864	-1.038729
47	1	0	-6.738081	0.293134	-1.084749
48	1	0	-5.814561	0.936424	-2.443949
49	1	0	-3.577140	2.316993	-0.970139
50	1	0	0.301940	1.854351	1.810011

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-1397.604975
Sum of electronic and thermal Energies=	-1397.580977
Sum of electronic and thermal Enthalpies=	-1397.580033
Sum of electronic and thermal Free Energies=	-1397.658171

Cartesian coordinates of Direct substitution product of Prd-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.289331	1.873309	-0.818465
2	6	0	1.929254	0.969773	-1.975571
3	6	0	1.126728	2.231747	0.185426
4	6	0	3.513521	1.283537	-0.090260
5	6	0	1.950948	-0.355916	-1.859694
6	6	0	2.232402	-0.987642	-0.513234
7	6	0	2.684201	-2.454998	-0.628624
8	7	0	0.964935	-0.876212	0.341935
9	6	0	3.382697	-0.225083	0.214600
10	7	0	0.996902	1.337132	1.351183
11	6	0	-0.227820	2.334800	-0.533741
12	6	0	1.449783	3.611923	0.800379
13	6	0	0.756625	-0.521841	2.820703
14	6	0	0.882116	0.081475	1.436855
15	6	0	-1.820438	-0.867584	-0.037236
16	6	0	-2.506596	-0.486258	1.112694
17	6	0	-3.666906	0.270711	0.990140
18	6	0	-4.163918	0.639766	-0.264795
19	6	0	-3.467995	0.219418	-1.403869
20	6	0	-2.300629	-0.528605	-1.300010
21	6	0	-5.412415	1.477327	-0.386315

22	16	0	-0.360152	-1.917864	0.067628
23	8	0	-0.171108	-2.500800	-1.259531
24	8	0	-0.554949	-2.788191	1.226141
25	1	0	2.587763	2.835728	-1.245060
26	1	0	1.668655	1.430531	-2.923809
27	1	0	4.382259	1.436558	-0.735520
28	1	0	3.709490	1.835098	0.831692
29	1	0	1.704599	-1.010711	-2.687650
30	1	0	3.611069	-2.485075	-1.207724
31	1	0	1.950181	-3.079657	-1.128654
32	1	0	2.886348	-2.868136	0.362777
33	1	0	3.305725	-0.407822	1.287659
34	1	0	4.302828	-0.719360	-0.100502
35	1	0	-1.011046	2.602809	0.178786
36	1	0	-0.500414	1.397068	-1.011388
37	1	0	-0.184590	3.112184	-1.302347
38	1	0	0.690302	3.868604	1.540935
39	1	0	1.470273	4.388876	0.030857
40	1	0	2.416098	3.602121	1.310073
41	1	0	0.596793	0.274462	3.544544
42	1	0	1.687928	-1.048057	3.058737
43	1	0	-0.031100	-1.270699	2.886036
44	1	0	-2.159175	-0.797222	2.088681
45	1	0	-4.203250	0.565207	1.885853
46	1	0	-3.848736	0.472980	-2.387574
47	1	0	-1.773846	-0.869131	-2.181817
48	1	0	-6.080763	1.322872	0.463229
49	1	0	-5.962329	1.243564	-1.300504
50	1	0	-5.162388	2.543360	-0.417947

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-1397.562128
Sum of electronic and thermal Energies=	-1397.538431
Sum of electronic and thermal Enthalpies=	-1397.537487
Sum of electronic and thermal Free Energies=	-1397.614456

Cartesian coordinates of compound 4ka (Prod-2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.308397	-0.942264	-1.519887
2	6	0	-3.289431	-1.820399	-0.285331
3	6	0	-2.197560	0.103177	-1.253032
4	6	0	-2.179719	-1.618027	0.425292

5	6	0	-1.255888	-0.642052	-0.273632
6	7	0	-0.454026	0.287065	0.581496
7	6	0	-3.363794	2.271394	-1.794037
8	7	0	-1.570606	2.240006	-0.190953
9	6	0	-2.703896	1.449703	-0.673001
10	6	0	-3.691521	1.317071	0.506383
11	16	0	0.835359	-0.446693	1.450876
12	6	0	-4.391241	-2.789221	0.006540
13	6	0	-0.584330	1.697033	0.400911
14	6	0	0.492152	2.617683	0.921043
15	6	0	2.456402	-1.214513	-0.658572
16	6	0	2.311942	-0.346495	0.424166
17	6	0	3.329551	0.541299	0.763564
18	6	0	3.613284	-1.155178	-1.426130
19	6	0	4.484763	0.580231	-0.011263
20	6	0	5.882447	-0.183930	-1.976340
21	6	0	4.641722	-0.254673	-1.122145
22	8	0	0.482492	-1.858512	1.532734
23	8	0	1.072215	0.339578	2.652772
24	1	0	-4.286995	-0.486226	-1.698914
25	1	0	-3.081064	-1.536995	-2.415120
26	1	0	-1.655974	0.350032	-2.169927
27	1	0	-1.889604	-2.144095	1.322903
28	1	0	-0.531690	-1.212702	-0.867608
29	1	0	-3.665367	3.245365	-1.403743
30	1	0	-4.247319	1.770608	-2.199435
31	1	0	-2.655798	2.442332	-2.609022
32	1	0	-3.958644	2.319762	0.847353
33	1	0	-3.250888	0.778150	1.344892
34	1	0	-4.609408	0.802987	0.211461
35	1	0	-5.351812	-2.270590	0.107306
36	1	0	-4.204520	-3.346639	0.926210
37	1	0	-4.508974	-3.509488	-0.811588
38	1	0	0.190452	3.625856	0.647738
39	1	0	1.461974	2.402472	0.467928
40	1	0	0.601708	2.541218	2.001971
41	1	0	1.693373	-1.950371	-0.876157
42	1	0	3.223325	1.172006	1.636290
43	1	0	3.726573	-1.832564	-2.265806
44	1	0	5.280614	1.265394	0.260241
45	1	0	5.726861	0.484887	-2.829774
46	1	0	6.148427	-1.165367	-2.375004
47	1	0	6.734855	0.198000	-1.411221

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-1358.304626
Sum of electronic and thermal Energies=	-1358.281852
Sum of electronic and thermal Enthalpies=	-1358.280908
Sum of electronic and thermal Free Energies=	-1358.356839

Cartesian coordinates of Direct Substitution Product Prd-2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.753804	0.576726	0.436898
2	6	0	-2.949445	1.226841	-0.673851
3	6	0	-3.319471	-0.659192	0.666664
4	6	0	-2.469533	-0.015810	-1.451463
5	6	0	-1.807399	2.105080	-0.047705
6	6	0	-2.257224	-1.068607	-0.345707
7	6	0	-2.492753	-2.520570	-0.784115
8	6	0	-0.798706	2.566214	-1.116228
9	7	0	-1.078830	1.461978	1.053321
10	6	0	-2.451599	3.363700	0.573509
11	6	0	-0.069354	-0.095629	2.538424
12	6	0	-0.694704	0.265516	1.205467
13	7	0	-0.897378	-0.848472	0.301666
14	6	0	1.875436	-0.698106	-0.115880
15	6	0	2.823253	-0.820237	0.896039
16	6	0	3.969760	-0.033208	0.851304
17	6	0	4.190104	0.867974	-0.195012
18	6	0	3.236879	0.944057	-1.218249
19	6	0	2.088710	0.162917	-1.190437
20	6	0	5.418445	1.742232	-0.219822
21	16	0	0.454142	-1.808072	-0.150698
22	8	0	0.692065	-2.846757	0.850524
23	8	0	0.249874	-2.182938	-1.550133
24	1	0	-4.512384	1.091631	1.013273
25	1	0	-3.551154	1.887406	-1.305254
26	1	0	-3.643827	-1.327298	1.455583
27	1	0	-3.274320	-0.346946	-2.113584
28	1	0	-1.575270	0.125254	-2.055568
29	1	0	-1.922186	-2.788203	-1.668914
30	1	0	-3.557895	-2.629896	-1.001844
31	1	0	-2.238656	-3.217413	0.018432
32	1	0	-0.054951	3.223771	-0.661014
33	1	0	-1.312182	3.121650	-1.906545
34	1	0	-0.271437	1.729224	-1.571019
35	1	0	-1.676529	3.988892	1.020395
36	1	0	-3.152481	3.093455	1.365580
37	1	0	-2.984414	3.947991	-0.182412
38	1	0	0.593114	-0.955768	2.493319
39	1	0	-0.886806	-0.369375	3.214710
40	1	0	0.445935	0.768613	2.953395
41	1	0	2.674663	-1.539571	1.690431
42	1	0	4.709776	-0.131544	1.638257
43	1	0	3.402830	1.612798	-2.056035

44	1	0	1.381505	0.195745	-2.008441
45	1	0	5.744067	1.943691	-1.242638
46	1	0	6.248327	1.280654	0.318928
47	1	0	5.214381	2.708020	0.255088

Level : B3LYP/6-311G**

Sum of electronic and zero-point Energies= -1358.274794
Sum of electronic and thermal Energies= -1358.252017
Sum of electronic and thermal Enthalpies= -1358.251073
Sum of electronic and thermal Free Energies= -1358.326520

Cartesian coordinates of compound 40a (Prd-3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.887851	1.835849	-1.066075
2	6	0	-1.858689	2.754929	-0.463342
3	6	0	-3.015418	0.731041	0.015377
4	6	0	-1.195007	2.204092	0.557089
5	6	0	-0.203818	2.889051	1.449260
6	6	0	-1.660599	0.761693	0.762754
7	7	0	-0.705735	-0.249865	0.167564
8	7	0	-2.321728	-1.222278	-1.303668
9	6	0	-3.404218	-0.672241	-0.476184
10	6	0	-4.669508	-0.623027	-1.345180
11	6	0	2.076099	-0.392852	0.353299
12	6	0	3.167684	-1.236898	0.547916
13	6	0	-1.113585	-1.055057	-0.952632
14	6	0	-3.644130	-1.625677	0.713127
15	6	0	-0.028661	-1.680646	-1.792275
16	6	0	4.394060	-0.897535	-0.012491
17	6	0	4.549585	0.271231	-0.766478
18	6	0	3.432447	1.092280	-0.955224
19	6	0	2.198459	0.772456	-0.397494
20	6	0	5.891801	0.642082	-1.345962
21	16	0	0.537909	-0.819864	1.189123
22	8	0	0.441186	-0.030233	2.414591
23	8	0	0.484113	-2.277299	1.268052
24	1	0	-3.842264	2.339193	-1.246584
25	1	0	-2.556849	1.433742	-2.030614

26	1	0	-1.700484	3.769681	-0.814327
27	1	0	-3.763133	1.073102	0.738612
28	1	0	-0.576250	2.913551	2.479066
29	1	0	-0.035679	3.917616	1.121198
30	1	0	0.755749	2.372249	1.496806
31	1	0	-1.776744	0.517269	1.816818
32	1	0	-4.926431	-1.631577	-1.676055
33	1	0	-4.512072	-0.012213	-2.235867
34	1	0	-5.515568	-0.212969	-0.785094
35	1	0	3.050099	-2.151211	1.115473
36	1	0	-2.762053	-1.712383	1.349967
37	1	0	-4.481315	-1.275485	1.324229
38	1	0	-3.883672	-2.624488	0.341871
39	1	0	-0.515251	-2.178609	-2.628188
40	1	0	0.542459	-2.418219	-1.226518
41	1	0	0.666968	-0.926826	-2.167429
42	1	0	5.242932	-1.556960	0.134095
43	1	0	3.525801	1.993285	-1.551973
44	1	0	1.337650	1.405433	-0.571916
45	1	0	5.786674	1.314803	-2.199337
46	1	0	6.442550	-0.242486	-1.673676
47	1	0	6.508283	1.151956	-0.597858

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-1358.304322
Sum of electronic and thermal Energies=	-1358.281417
Sum of electronic and thermal Enthalpies=	-1358.280473
Sum of electronic and thermal Free Energies=	-1358.356349

Cartesian coordinates for Direct Substitution product from 3o.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.383987	-0.677292	-1.173627
2	6	0	-2.904455	-0.595377	-1.147302
3	6	0	-0.979322	0.705181	-1.704691
4	7	0	-0.862586	-0.967080	0.196542
5	6	0	-3.276560	0.686152	-1.170165
6	6	0	1.931553	-0.828600	0.038301
7	6	0	2.420188	-0.114783	1.132090
8	6	0	-2.079137	1.617194	-1.137638
9	7	0	-1.689630	1.039495	1.330218
10	6	0	-1.786749	2.095972	0.321695
11	6	0	-1.354141	-0.888508	2.665175

12	6	0	-1.283740	-0.160852	1.333440
13	6	0	3.491657	0.751256	0.951741
14	6	0	4.089474	0.915432	-0.304752
15	6	0	3.589233	0.174119	-1.379596
16	6	0	-2.948838	3.002088	0.783345
17	6	0	-0.483161	2.919834	0.391017
18	6	0	2.514407	-0.696279	-1.218667
19	6	0	5.238011	1.875563	-0.488649
20	16	0	0.541207	-1.950583	0.258369
21	8	0	0.651286	-2.520098	1.592952
22	8	0	0.487723	-2.810644	-0.919930
23	6	0	-3.756203	-1.820747	-1.063330
24	1	0	-1.033689	-1.495547	-1.798449
25	1	0	-1.044172	0.694023	-2.796154
26	1	0	0.036644	0.987000	-1.431955
27	1	0	-4.303352	1.031601	-1.141146
28	1	0	1.985042	-0.253683	2.113412
29	1	0	-2.222717	2.512815	-1.750249
30	1	0	-1.959122	-0.278287	3.331807
31	1	0	-0.369593	-1.035103	3.109078
32	1	0	-1.792789	-1.880441	2.549188
33	1	0	3.877232	1.301303	1.803661
34	1	0	4.051327	0.269774	-2.356312
35	1	0	-3.065240	3.860409	0.114896
36	1	0	-2.753401	3.365882	1.793477
37	1	0	-3.888769	2.447800	0.807387
38	1	0	0.396626	2.319586	0.155843
39	1	0	-0.528616	3.760041	-0.308004
40	1	0	-0.355156	3.317969	1.399726
41	1	0	2.144758	-1.285242	-2.048214
42	1	0	5.784604	1.672436	-1.411286
43	1	0	5.942371	1.817075	0.344744
44	1	0	4.876941	2.908393	-0.537491
45	1	0	-3.504157	-2.408377	-0.174369
46	1	0	-4.817517	-1.568596	-1.018197
47	1	0	-3.592510	-2.474572	-1.927123

Level: B3LYP/6-311G**
 Sum of electronic and zero-point Energies= -1358.293435
 Sum of electronic and thermal Energies= -1358.270485
 Sum of electronic and thermal Enthalpies= -1358.269541
 Sum of electronic and thermal Free Energies= -1358.346475

Cartesian coordinates of compound 4la (Prd-4)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.801464	-0.810350	-0.932085
2	6	0	-2.954644	-1.326402	-0.093603
3	6	0	-2.174861	0.449663	-1.712218
4	7	0	-0.576691	-0.597824	-0.074534
5	6	0	-3.948402	-0.503299	0.246943
6	6	0	2.187891	-0.670394	-0.190433
7	6	0	-4.047607	0.947646	-0.143552
8	6	0	3.075297	-0.891897	0.857524
9	6	0	-2.773587	1.526530	-0.802435
10	7	0	-1.294811	1.254125	1.275182
11	6	0	-1.744990	2.147577	0.197517
12	6	0	-0.225611	-0.521094	2.437896
13	6	0	-0.725085	0.127213	1.166263
14	6	0	4.247070	-0.142236	0.923103
15	6	0	4.546783	0.818976	-0.046041
16	6	0	3.644963	1.002844	-1.103395
17	6	0	-2.391009	3.353984	0.913072
18	6	0	-0.503918	2.679032	-0.554800
19	6	0	2.472654	0.263855	-1.185289
20	6	0	5.802407	1.649163	0.045230
21	16	0	0.719505	-1.695527	-0.336283
22	8	0	0.788920	-2.715040	0.709639
23	8	0	0.592621	-2.108644	-1.733456
24	6	0	-2.906531	-2.775655	0.310423
25	1	0	-1.510511	-1.578123	-1.647905
26	1	0	-2.923480	0.161194	-2.458207
27	1	0	-1.306553	0.814379	-2.262592
28	1	0	-4.776060	-0.895273	0.834850
29	1	0	-4.885081	1.055292	-0.847696
30	1	0	-4.337812	1.533490	0.732082
31	1	0	2.856012	-1.654014	1.593940
32	1	0	-3.082787	2.365266	-1.435823
33	1	0	-0.573261	0.090007	3.267539
34	1	0	0.865272	-0.557486	2.469792
35	1	0	-0.584074	-1.546027	2.536917
36	1	0	4.941421	-0.315927	1.737961
37	1	0	3.869855	1.728414	-1.877799
38	1	0	-2.745490	4.098194	0.193627
39	1	0	-1.653341	3.823962	1.566325
40	1	0	-3.227342	3.047760	1.542418
41	1	0	0.073481	1.879371	-1.014613
42	1	0	-0.802606	3.387420	-1.333502
43	1	0	0.149309	3.201377	0.147489
44	1	0	1.797103	0.394196	-2.020939
45	1	0	5.584260	2.635233	0.469161
46	1	0	6.245972	1.809674	-0.940240
47	1	0	6.549873	1.174006	0.683138
48	1	0	-1.974528	-3.018150	0.830568
49	1	0	-3.741617	-3.033262	0.964997
50	1	0	-2.948042	-3.428115	-0.569675

Level: B3LYP/6-311G**

Sum of electronic and zero-point Energies=	-1397.591035
Sum of electronic and thermal Energies=	-1397.567306
Sum of electronic and thermal Enthalpies=	-1397.566362
Sum of electronic and thermal Free Energies=	-1397.643578