
Supplementary information

Control of stereogenic oxygen in a helically chiral oxonium ion

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Supporting Information for:

Control of Stereogenic Oxygen in a Helically Chiral Oxonium Ion

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Contents

1	General Information.....	2
2	Experimental Procedures for the synthesis of oxonium ions.....	3
2.1	Xanthene-derived oxonium ion synthesis	3
2.2	Dibenzodidehydrooxepane derived oxonium ion synthesis	9
3	Experimental data for resolution of <i>rac</i> - 16	14
4	X-ray Crystallography	19
4.1	1,3,6-Trimethyl-8 <i>H</i> -benzofuro[3,2,1- <i>de</i>]xanthen-13-ium tetrafluoroborate, 10	20
4.2	11,13-Dimethyl-4,5-dihydrobenzo[<i>b</i>]benzo[6,7]oxepino[3,2,1- <i>hi</i>] benzofuran-10-ium tetrafluoroborate, <i>rac</i> - 16	21
4.3	11,13-Dimethyl-4,5-dihydrobenzo[<i>b</i>]benzo[6,7]oxepino[3,2,1- <i>hi</i>] benzofuran-10-ium tetrafluoroborate, <i>enantioenriched</i> - 16	22
5	Inversion Barrier Measurements	23
5.1	1,3,6-Trimethyl-8 <i>H</i> -benzofuro[3,2,1- <i>de</i>]xanthen-13-ium tetrafluoroborate, 10	23
5.2	Equilibration of 11,13-Dimethyl-4,5-dihydrobenzo[<i>b</i>]benzo[6,7]oxepino[3,2,1- <i>hi</i>]benzofuran-10-ium, [<i>P</i> , (<i>R</i>) _o]-bis-(<i>R</i>)-BINOL borate, 18	25
5.3	Enantiomeric ratio erosion study of 11,13-dimethyl-4,5-dihydrobenzo[<i>b</i>]benzo[6,7]oxepino[3,2,1- <i>hi</i>]benzofuran-10-ium hexafluorophosphate, <i>enantioenriched</i> -[<i>M</i> , (<i>S</i>) _o]- 17	30
6	Computational Studies	33
6.1	Computational details	33
6.2	Hyperhomodesmotic bond separation reactions.....	35
6.3	NBO analysis on ring size influence	37
6.4	Comparison between triaryl oxonium ions and triaryl amines	38
6.5	Thermochemical data.....	40
6.6	Cartesian coordinates for stationary points	45
7	NMR Spectra	88
8	References.....	112

1 General Information

Reagents were purchased from major commercial suppliers and were used without further purification. Anhydrous reaction solvents (CH_2Cl_2 , 1,4-dioxane, DMF, THF, PhMe, Et_3N , $i\text{-Pr}_2\text{NH}$) were obtained from an MBraun SPS5 solvent purification system having been dried over activated alumina columns. All other solvents were used without prior drying. Unless specified, the synthetic reactions were carried out without using dried glassware or an inert atmosphere. The glassware for reactions conducted using an inert atmosphere was flame-dried under vacuum and then placed under N_2 unless H_2O was used as a solvent in the procedure. Solvents were degassed by sparging with Argon for 10 minutes as stated in the procedures. Reactions were heated using a DrySyn® heating block and contact thermometer. Room Temperature (r.t.) is defined as 20-25 °C.

Reactions were monitored by Thin Layer Chromatography (TLC) using silica gel on pre-coated 0.25 mm aluminium sheets (Merck Kieselgel 60 F_{254}) and visualized with UV irradiation ($\lambda = 254 \text{ nm}$) followed by a basic KMnO_4 solution. Flash column chromatography was carried out on Silica Gel 60 (0.043-0.063 mm, VWR) under pressure (0.2-0.4 bar) from the house N_2 supply. A UltrawaveU1250D Ultrasonic water bath (50-60 Hz) was used for sonication.

NMR spectra were recorded on Bruker AVIII/AVIIHD (700, 600, 500 and 400 MHz (^1H)) and Bruker NEO (600 MHz (^1H)) spectrometers in the deuterated solvent specified. NMR data are reported as chemical shifts (δ) and quoted in parts per million (ppm). ^1H NMR were referenced to the non-deuterated residual solvent peak, ^{13}C NMR were referenced to the residual solvent peak and ^{19}F NMR were referenced externally to $\text{CFCl}_3 = 0 \text{ ppm}$. Chemical shifts are quoted in ppm with splitting assigned as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), septet (sept), and multiplet (m) or combinations of the above. The abbreviation br is used to denote broad signals. Coupling constants, J , are measured to the nearest 0.1 Hz and are presented as observed. NMR Spectra were processed using MestReNova 11.0 and where spectra are assigned, this was carried out with the aid of COSY, HSQC and HMBC experiments.

Melting points (M.P.) were determined using a Reichert melting point apparatus and are uncorrected. Unless otherwise stated, the solid material analysed was obtained from *in vacuo* removal of the solvent system used for flash column chromatography. Fourier Transform Infra-red spectra were recorded on a Bruker Tensor 27 FTIR spectrometer equipped with a diamond ATR module. Absorption maxima (ν_{max}) are reported in wavenumbers (cm^{-1}) for the range 3500 – 600 cm^{-1} . Low-resolution mass spectra were recorded on a Micro Mass LCT Premier spectrometer under conditions of electrospray ionization (ESI). High resolution mass spectra using electrospray ionization (ESI) were recorded on a Thermo Exactive orbitrap spectrometer equipped with a Waters Acquity LC system. High resolution mass spectra using atmospheric pressure chemical ionization (APCI) or electron ionization (EI) were recorded on an Agilent 7200 Accurate Mass Q-TOF GC-MS spectrometer connected to a 7890 GC system DIP solid/liquid state thermal probe and a CTC Analytics HTS PAL Sample Manager. Optical rotations were recorded on a Schmidt-Haensch Unipol L2000 polarimeter at 25 °C using 589 nm radiation. Concentrations are quoted in g/100 mL and $[\alpha]_D^{25}$ values are quoted in $[\text{° mL g}^{-1} \text{ dm}^{-1}]$. The absolute configuration of enantioenriched **16** was confirmed by x-ray crystallography; see **Section 4** for further information. Compound names were

generated using ChemDraw 20.1.1 in accordance with the guidelines stipulated by the International Union of Pure and Applied Chemistry (IUPAC).

2 Experimental Procedures for the synthesis of oxonium ions

2.1 Xanthene-derived oxonium ion synthesis

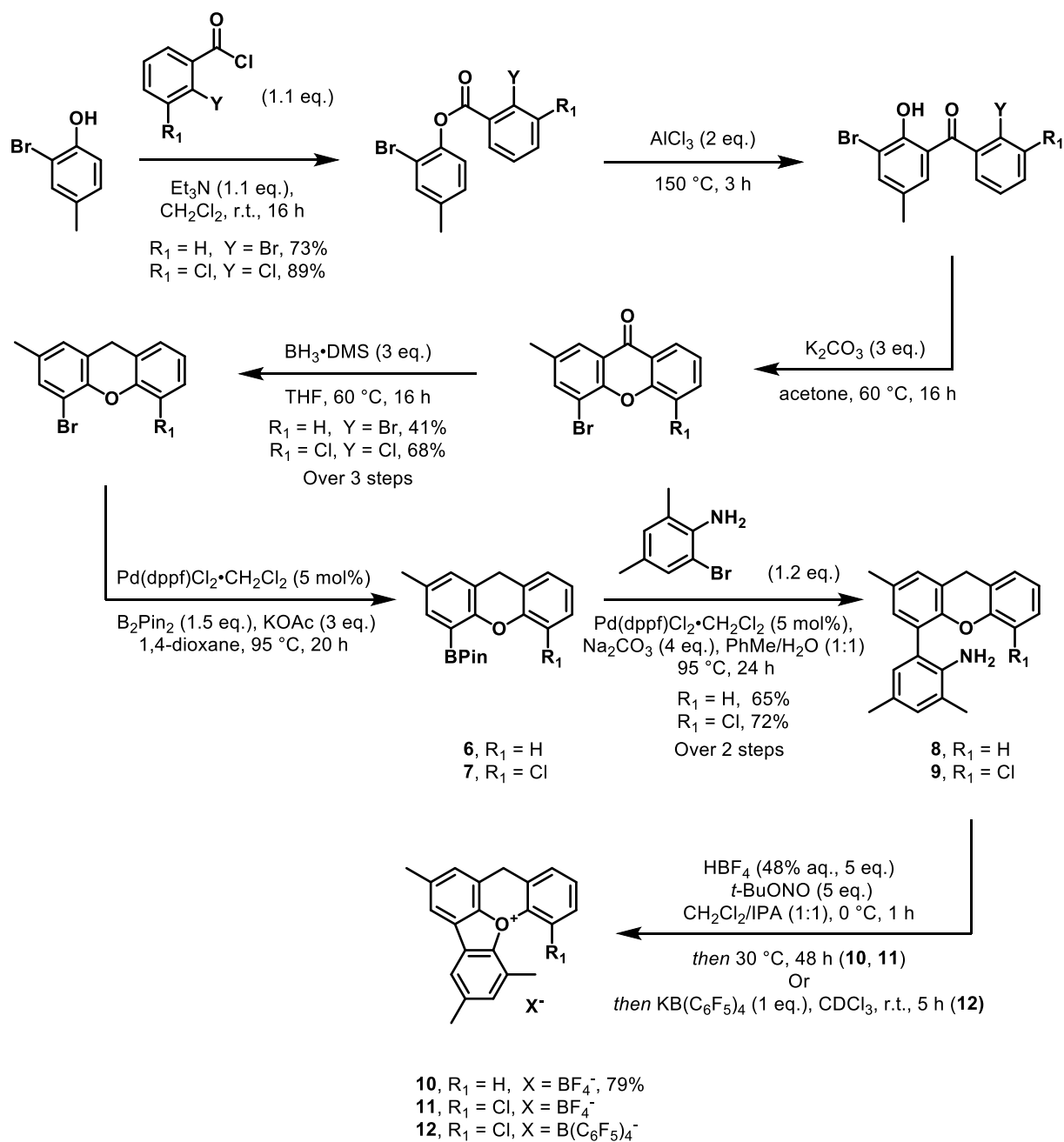
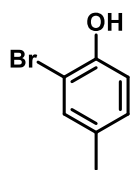


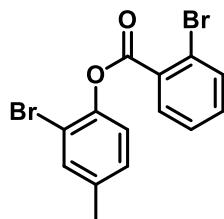
Figure S1. Synthetic approach to xanthene-derived oxonium ions

2-Bromo-4-methylphenol, **S1**:



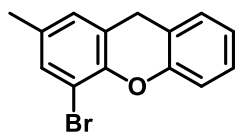
Bromine (2.37 mL, 7.39 g, 46.00 mmol, 1 eq.) in CHCl_3 (20 mL) was added *via* pressure equalising dropping funnel to a solution of *p*-cresol (5.00 g, 46.00 mmol, 1 eq.) in CHCl_3 (40 mL) at 0 °C. After 1 h, the organic layer was washed (Na_2SO_3 , sat. aq., 30 mL), dried (MgSO_4) and concentrated *in vacuo* to give the title compound as a pale yellow oil (7.53 g, 87%). $^1\text{H NMR}$ (400 MHz, CDCl_3): δ_{H} = 7.29 – 7.28 (m, 1H), 7.04 – 7.00 (m, 1H), 6.94 (d, J = 8.2 Hz, 1H), 5.58 (s, 1H), 2.28 (dd, J = 0.8 Hz, 0.8 Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ_{C} = 150.1, 132.3, 131.5, 129.9, 116.0, 110.0, 20.3. **FTIR** (neat) $\nu_{\text{max}}/\text{cm}^{-1}$ = 3503, 2922, 2360, 1609, 1494, 1407, 1330, 1283, 1252, 1210, 1180, 1041, 867, 814, 761, 671. **HRMS** (EI^+): m/z calculated for $\text{C}_7\text{H}_7^{79}\text{BrO}^+$, $[\text{M}]^+ = 185.9680$, m/z found = 185.9675. Δ = -2.69 ppm. *Spectra are consistent with literature values.¹

2-Bromo-4-methylphenyl 2-bromobenzoate, **S2**:



Triethylamine (1.53 mL, 1.11 g, 11.00 mmol, 1.1 eq.) was added to a solution of 2-bromo-4-methylphenol, **S1**, (1.86 g, 10.00 mmol, 1 eq.) in CH_2Cl_2 (20 mL) at 0 °C under N_2 . After 5 mins, 2-bromobenzoylchloride (1.40 mL, 2.41 g, 11.00 mmol, 1.1 eq.) was added and the reaction was warmed to r.t.. After 16 h, the reaction mixture was sequentially washed with HCl (3 M aq., 10 mL) and NaHCO_3 (sat. aq., 30 mL). The organics were dried (MgSO_4), concentrated *in vacuo* and the crude residue was purified by flash column chromatography (Et_2O :pentane, 5:95, R_f = 0.25) to give the title compound as a white solid (3.15 g, 73%). **M.P.** = 52–54 °C. $^1\text{H NMR}$ (500 MHz, CDCl_3): δ_{H} = 8.17 (dd, J = 7.6, 1.9 Hz, 1H), 7.75 (dd, J = 7.8, 1.4 Hz, 1H), 7.48 (d, J = 1.3 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.19 – 7.17 (m, 2H), 2.37 (s, 3H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ_{C} = 163.6, 145.9, 137.9, 134.8, 133.9, 133.5, 132.3, 130.8, 129.4, 127.5, 123.5, 122.8, 115.8, 20.8. **FTIR** (neat) $\nu_{\text{max}}/\text{cm}^{-1}$ = 2981, 2360, 1754, 1589, 1487, 1432, 1382, 1224, 1199, 1132, 1079, 1021, 954, 867, 806, 741, 683, 643. **HRMS** (ESI^+): m/z calculated for $\text{C}_{14}\text{H}_{10}^{79}\text{Br}_2\text{NaO}_2^+$, $[\text{M}+\text{Na}]^+ = 390.8940$, m/z found = 390.8939. Δ = - 0.26 ppm.

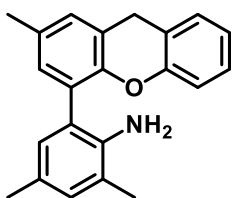
4-Bromo-2-methyl-9H-xanthene, **S3**:



Xanthene **S3** was prepared according to a modified literature procedure.² 2-Bromo-4-methylphenyl 2-bromobenzoate, **S2**, (2.00 g, 5.40 mmol, 1 eq.) and AlCl_3 (1.44 g, 10.80 mmol, 2.00 eq.) were heated to 150 °C under N_2 . After 3 h, the reaction was cooled to r.t. and then 0 °C HCl (6 M, aq., 40 mL) was added and decanted. The remaining residue was sonicated with $\text{H}_2\text{O}/\text{Et}_2\text{O}$ (5 × 10 mL/10 mL) until fully dissolved. All fractions were combined, extracted with Et_2O (2 × 50 mL), dried (MgSO_4) and concentrated *in vacuo*. The crude solid was dissolved in acetone (20 mL), K_2CO_3 (2.24 g, 16.21 mmol, 3 eq.) was added and the reaction was heated to 60 °C. After 16 h, the acetone was removed *in vacuo*. H_2O (50 mL) was added and the mixture was extracted with Et_2O (3 × 50 mL), dried (MgSO_4) and concentrated *in vacuo*. $\text{BH}_3\cdot\text{DMS}$ (1.54 mL, 1.23 g, 16.20 mmol, 3 eq.) was added to a solution of the crude residue in THF (20 mL) under N_2 and the reaction was heated to 60 °C. After 16 h, MeOH (5 mL) was slowly added to the reaction. The solvent was removed by a steady stream of N_2 and the crude residue was purified by flash column chromatography (pentane, R_f = 0.3) to give the title

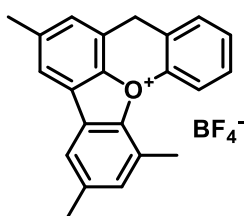
compound as a pale yellow solid (605 mg, 41%). **M.P.** = 125-128 °C. **¹H NMR** (500 MHz, CDCl₃): δ_H = 7.25 (s, 1H), 7.23 – 7.18 (m, 1H), 7.18 – 7.12 (m, 2H), 7.04 (td, *J* = 7.4, 1.4 Hz, 1H), 6.91 (s, 1H), 4.01 (s, 2H), 2.28 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 152.0, 146.8, 133.5, 131.9, 128.8, 128.6, 127.9, 123.5, 122.2, 120.5, 117.0, 110.4, 28.4, 20.5. **FTIR** (neat) ν_{max}/cm⁻¹ = 2898, 1663, 1613, 1596, 1469, 1411, 1314, 1271, 1238, 1196, 1110, 1039, 929, 891, 843, 755, 713, 647. **HRMS (ESI⁺)**: *m/z* calculated for C₁₄H₁₀⁷⁹BrO⁺, [M-H]⁺ = 272.9910; *m/z* found = 272.9911. Δ = 0.61 ppm.

2,4-Dimethyl-6-(2-methyl-9H-xanthen-4-yl)aniline, 8:



1,4-Dioxane (10 mL) was added to a mixture of 4-bromo-2-methyl-9H-xanthene, **S3**, (280 mg, 1.02 mmol, 1 eq.), B₂Pin₂ (387 mg, 1.53 mmol, 1.5 eq.), Pd(dppf)Cl₂·CH₂Cl₂ (24.9 mg, 0.03 mmol, 3 mol%) and KOAc (300 mg, 3.05 mmol, 3 eq.) under N₂. Argon was bubbled through the solution for 10 minutes and the reaction was heated to 95 °C. After 20 h, H₂O (10 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 10 mL). The organic extracts were dried (MgSO₄) and concentrated *in vacuo*. The crude residue was suspended in pentane (15 mL), filtered through Celite® (2 mL), eluted (pentane, 3 × 5 mL) and concentrated *in vacuo*.³ The crude solid was added as a solution in PhMe (5 mL) to a suspension of 2-bromo-4,6-dimethylaniline (245 mg, 1.22 mmol, 1.2 eq.), Pd(dppf)Cl₂·CH₂Cl₂ (41.6 mg, 0.05 mmol, 5 mol%) and Na₂CO₃ (428 mg, 4.08 mmol, 4 eq.) in H₂O (5 mL) under N₂. Argon was bubbled through the solution for 10 mins and the reaction was heated to 95 °C. After 24 h, the reaction was extracted with CH₂Cl₂ (3 × 10 mL). The organic extracts were dried (MgSO₄), concentrated *in vacuo* and the crude residue was purified by flash column chromatography (Et₂O:pentane, 5:95, R_f = 0.2) to give the title compound as a tan solid (210 mg, 65%). **M.P.** = 118-119 °C. **¹H NMR** (400 MHz, CDCl₃): δ_H = 7.23 – 7.13 (m, 2H), 7.07 – 7.02 (m, 3H), 7.01 – 6.94 (m, 2H), 6.91 (d, *J* = 2.1 Hz, 1H), 4.09 (s, 2H), 3.74 (br s, 2H), 2.37 (s, 3H), 2.33 (s, 3H), 2.29 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 152.3, 147.3, 139.8, 132.6, 130.7, 130.7, 129.5, 128.8, 128.7, 127.5, 127.3, 124.2, 123.1, 122.8, 121.4, 121.2, 117.0, 28.5, 20.7, 20.6, 18.1. **FTIR** (neat) ν_{max}/cm⁻¹ = 3384, 2917, 1620, 1584, 1484, 1456, 1292, 1265, 1239, 1209, 1189, 1154, 1098, 1033, 1012, 908, 879, 860, 827, 755, 730, 646. **HRMS (ESI⁺)**: *m/z* calculated for C₂₂H₂₂NO⁺, [M+H]⁺ = 316.1696, *m/z* found = 316.1697. Δ = 0.32 ppm.

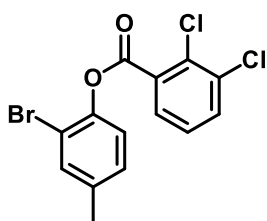
1,3,6-Trimethyl-8H-benzofuro[3,2,1-de]xanthen-13-ium tetrafluoroborate, 10:



t-BuONO (94 μL, 81 mg, 0.79 mmol, 5 eq.) was added to a solution of 2,4-dimethyl-6-(2-methyl-9H-xanthen-4-yl)aniline, **8**, (50 mg, 0.16 mmol, 1 eq.) and HBF₄ (48% aq., 103 μL, 145 mg, 0.79 mmol, 5 eq.) in CH₂Cl₂:IPA (1:1, 2 mL) at 0 °C. After 1 h, the reaction mixture was diluted with CH₂Cl₂ (3 mL), washed with H₂O (1 mL) and heated to 30 °C. After 48 h, the solvent was removed by a steady stream of N₂ and Et₂O (3 mL) was added. The Et₂O layer was passed through a Celite® filter (1 mL). The solid precipitate was washed and the solvent passed through the Celite® (Et₂O, 4 × 1 mL). The solid precipitate was dissolved in MeCN (2 mL), passed through the Celite® and eluted (MeCN, 3 × 2 mL). The solvent was removed by a steady stream of N₂ to give the title compound as a white solid (48 mg, 79%). **M.P.** = 157 °C (MeCN, dec.). **¹H NMR** (400 MHz, CD₃CN): δ_H = 7.96 – 7.91 (m, 1H), 7.83 (dd, *J* = 1.7, 0.9 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.64 – 7.58 (m,

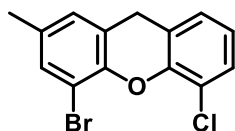
2H), 7.58 – 7.52 (m, 3H), 4.40 (br s, 2H), 2.62 (s, 3H), 2.58 (s, 3H), 2.54 (s, 3H). **¹³C NMR** (126 MHz, CD₃CN): δ_c = 159.6, 156.4, 155.2, 143.4, 142.9, 134.6, 132.7, 131.1, 129.9, 129.9, 127.7, 125.7, 124.4, 123.5, 122.0, 121.7, 115.1, 29.9, 21.6, 21.3, 18.4. One quaternary carbon was not observed. **¹⁹F NMR** (377 MHz, CD₃CN): δ_F = -151.8. **FTIR** (neat) $\nu_{\max}/\text{cm}^{-1}$ = 1475, 1452, 1386, 1285, 1171, 1051, 1036, 854, 825, 786, 766, 734, 700, 670, 644. **HRMS** (ESI⁺): m/z calculated for C₂₂H₁₉O⁺, [M+H]⁺ = 299.1430, m/z found = 299.1432. Δ = 0.67 ppm.

2-Bromo-4-methylphenyl 2,3-dichlorobenzoate, **S4**:



DMF (5 drops) was added to a solution of 2,3-dichlorobenzoic acid (1.50 g, 7.85 mmol, 1 eq.) and oxalyl chloride (0.797 mL, 1.20 g, 9.42 mmol, 1.2 eq.) in CH₂Cl₂ (40 mL) at r.t.. After 2 h, the solvent was removed *in vacuo*. Triethylamine (1.23 mL, 880 mg, 8.64 mmol, 1.1 eq.) was added to a solution of 2-bromo-4-methylphenol, **S1**, (1.46 g, 7.85 mmol, 1 eq.) and the crude residue in CH₂Cl₂ (40 mL) under N₂ at 0 °C and the reaction was allowed to warm to r.t.. After 16 h, the reaction mixture was sequentially washed with HCl (3 M aq., 10 mL) and NaHCO₃ (sat. aq., 30 mL). The organics were dried (MgSO₄), concentrated *in vacuo* to give the title compound as a white solid (2.52 g, 89%). **M.P.** = 103-105 °C. **¹H NMR** (400 MHz, CDCl₃): δ_H = 7.95 (dd, J = 7.8, 1.6 Hz, 1H), 7.59 (dd, J = 8.0, 1.6 Hz, 1H), 7.39 (dt, J = 1.4, 0.8 Hz, 1H), 7.27 (t, J = 7.9 Hz, 1H), 7.12 – 7.06 (m, 2H), 2.28 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃): δ_c = 162.8, 145.8, 138.1, 135.1, 134.1, 133.9, 132.6, 131.5, 130.0, 129.4, 127.4, 123.4, 115.7, 20.8. **FTIR** (neat) $\nu_{\max}/\text{cm}^{-1}$ = 2922, 1747, 1693, 1579, 1492, 1414, 1311, 1279, 1244, 1197, 1155, 1124, 1097, 1046, 889, 867, 808, 743, 711, 687, 671. **HRMS** (APCI⁺): m/z calculated for C₁₄H₁₀⁷⁹Br³⁵Cl₂O₂⁺, [M+H]⁺ = 358.9236, m/z found = 358.9235. Δ = -0.28 ppm.

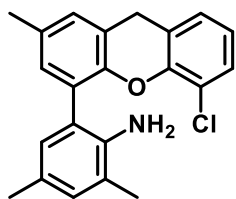
4-Bromo-5-chloro-2-methyl-9H-xanthene, **S5**:



Xanthene **S5** was prepared according to a modified literature procedure.² 2-Bromo-4-methylphenyl 2,3-dichlorobenzoate, **S4**, (1.80 g, 5.00 mmol, 1 eq.) and AlCl₃ (1.33 g, 10.00 mmol, 2 eq.) were heated to 150 °C under N₂. After 3 h, the reaction was cooled to r.t. and then 0 °C. HCl (6 M, aq., 40 mL) was added and decanted. The remaining residue was sonicated with H₂O/Et₂O (5 × 10 mL/10 mL) until fully dissolved. All fractions were combined, extracted with Et₂O (2 × 50 mL), dried (MgSO₄) and concentrated *in vacuo*. The crude solid was dissolved in acetone (20 mL), K₂CO₃ (2.07 g, 15.00 mmol, 3 eq.) was added and the reaction was heated to 60 °C. After 16 h, the acetone was removed *in vacuo*. H₂O (50 mL) was added and the mixture was extracted with Et₂O (3 × 50 mL), dried (MgSO₄) and concentrated *in vacuo*. BH₃·DMS (1.42 mL, 1.14 g, 15.00 mmol, 3 eq.) was added to a solution of the crude residue in THF (20 mL) under N₂ and the reaction was heated to 60 °C. After 16 h, MeOH (5 mL) was slowly added to the reaction. The solvent was removed by a steady stream of N₂ and the crude residue was purified by flash column chromatography (pentane, R_f = 0.3) to give the title compound as a pale yellow solid (1.05 g, 68%). **M.P.** = 111-113 °C. **¹H NMR** (400 MHz, CDCl₃): δ_H = 7.32 – 7.26 (m, 2H), 7.07 (ddt, J = 7.6, 1.8, 1.0 Hz, 1H), 6.98 (t, J = 7.7 Hz, 1H), 6.94 – 6.89 (m, 1H), 4.03 (s, 2H), 2.31 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ_c = 148.0, 146.5, 134.2, 132.1, 128.7, 128.3, 127.0, 123.6, 122.4, 122.3, 121.8, 110.8, 28.6, 20.5. **FTIR** (neat) $\nu_{\max}/\text{cm}^{-1}$ = 2918, 1589, 1567, 1457,

1377, 1322, 1302, 1265, 1251, 1235, 1216, 1181, 1146, 1128, 1064, 919, 875, 847, 831, 761, 715, 697, 624. **HRMS** (ESI⁻): m/z calculated for C₁₄H₉⁷⁹Br³⁵ClO⁻, [M-H]⁻ = 306.9520, m/z found = 306.9521. Δ = 0.33 ppm.

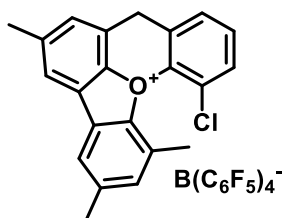
2-(5-Chloro-2-methyl-9H-xanthen-4-yl)-4,6-dimethylaniline, **9**:



1,4-Dioxane (10 mL) was added to a mixture of 4-bromo-5-chloro-2-methyl-9H-xanthene, **S5**, (248 mg, 0.80 mmol, 1 eq.), B₂Pin₂ (305 mg, 1.20 mmol, 1.5 eq.), Pd(dppf)Cl₂·CH₂Cl₂ (20.0 mg, 0.02 mmol, 3 mol%) and KOAc (235 mg, 2.40 mmol, 3 eq.) under N₂. Argon was bubbled through the solution for 10 minutes and the reaction was heated to 95 °C. After 20 h, H₂O (10 mL) was added and the mixture was extracted with CH₂Cl₂ (3 × 10 mL). The organic extracts were dried (MgSO₄) and concentrated *in vacuo*. The crude residue was suspended in pentane (15 mL), filtered through Celite® (2 mL), eluted (pentane, 3 × 5 mL) and concentrated *in vacuo*.³ The crude solid was added as a solution in PhMe (5 mL) to a suspension of 2-bromo-4,6-dimethylaniline (194 mg, 0.96 mmol, 1.2 eq.), Pd(dppf)Cl₂·CH₂Cl₂ (32.6 mg, 0.04 mmol, 5 mol%) and Na₂CO₃ (336 mg, 3.20 mmol, 4 eq.) in H₂O (5 mL) under N₂. Argon was bubbled through the solution for 10 mins and the reaction was heated to 95 °C. After 24 h, the reaction was extracted with CH₂Cl₂ (3 × 10 mL). The organic extracts were dried (MgSO₄), concentrated *in vacuo* and the crude residue was purified by flash column chromatography (Et₂O:pentane, 10:90, R_f = 0.2) to give the title compound as a viscous yellow oil (202 mg, 72%).

¹H NMR (500 MHz, CDCl₃): δ_H = 7.20 (dd, J = 7.9, 1.5 Hz, 1H), 7.10 – 7.05 (m, 2H), 6.99 (d, J = 2.0 Hz, 1H), 6.95 – 6.91 (m, 2H), 6.90 (d, J = 2.1 Hz, 1H), 4.05 (s, 2H), 3.53 (s, 2H), 2.34 (s, 3H), 2.28 (s, 3H), 2.23 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 148.3, 146.8, 140.2, 133.5, 130.8, 130.7, 129.6, 128.5, 128.4, 128.0, 127.1, 127.0, 123.5, 123.2, 123.1, 122.9, 122.2, 121.0, 28.7, 20.8, 20.6, 18.1. **FTIR** (neat) ν_{max}/cm^{-1} = 2917, 1621, 1454, 1250, 1207, 1184, 1146, 909, 859, 767, 737, 714, 635. **HRMS** (ESI⁺): m/z calculated for C₂₂H₂₁³⁵ClNO⁺, [M+H]⁺ = 350.1306, m/z found = 350.1307. Δ = 0.29 ppm.

12-Chloro-1,3,6-trimethyl-8H-benzofuro[3,2,1-de]xanthen-13-ium tetrakis(perfluorophenyl)borate, **12**:



t-BuONO (59 μ L, 52 mg, 0.50 mmol, 5 eq.) was added to a solution of 2-(5-chloro-2-methyl-9H-xanthen-4-yl)-4,6-dimethylaniline, **9**, (35 mg, 0.10 mmol, 1 eq.) and HBF₄ (48% aq., 65 μ L, 91 mg, 0.50 mmol, 5 eq.) in CH₂Cl₂:IPA (1:1, 2 mL) at 0 °C. After 1 h, the reaction mixture was diluted with CH₂Cl₂ (3 mL) and washed with H₂O (1 mL). The organics were removed by a steady stream of N₂, Et₂O (5 mL) was added and the precipitated diazonium salt was collected by suction filtration. KB(C₆F₅)₄ (44 mg, 0.06 mmol, 1 eq.) was added to a solution of the precipitated diazonium salt (26 mg, 0.06 mmol, 1 eq.) in CDCl₃ (0.5 mL) at r.t.. After 30 mins, the reaction was filtered through a Celite® filter (0.2 mL) and eluted with CDCl₃ (3 × 0.5 mL). After 5 h, the reaction mixture was subjected to NMR analysis. **¹H NMR** (500 MHz, CDCl₃): δ_H = 7.70 (d, J = 1.9 Hz, 1H), 7.62 (s, 1H), 7.52 (d, J = 7.3 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 7.36 (s, 1H), 7.33 (s, 1H), 7.31 – 7.27 (m, 1H), 4.41 (d, J = 17.7 Hz, 1H), 4.15 (d, J = 17.7 Hz, 1H), 2.55 (s, 3H), 2.54 (s,

3H), 2.52 (s, 3H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 160.4, 158.0, 156.5, 143.0, 142.5, 134.7, 132.8, 130.5, 130.1, 128.3, 128.3, 126.2, 124.4, 124.0, 123.0, 122.3, 121.0, 120.3, 30.5, 21.7, 21.4, 16.0. **¹⁹F NMR** (377 MHz, CDCl₃): δ_F = -131.9 – -133.1 (m), -162.8 (t, *J* = 21.3 Hz), -166.5 – -167.0 (m). **FTIR** (neat) ν_{max}/cm⁻¹ = 1643, 1513, 1461, 1275, 1086, 978, 909, 853, 775, 756, 734, 684, 661.

2.2 Dibenzodidehydrooxepane derived oxonium ion synthesis

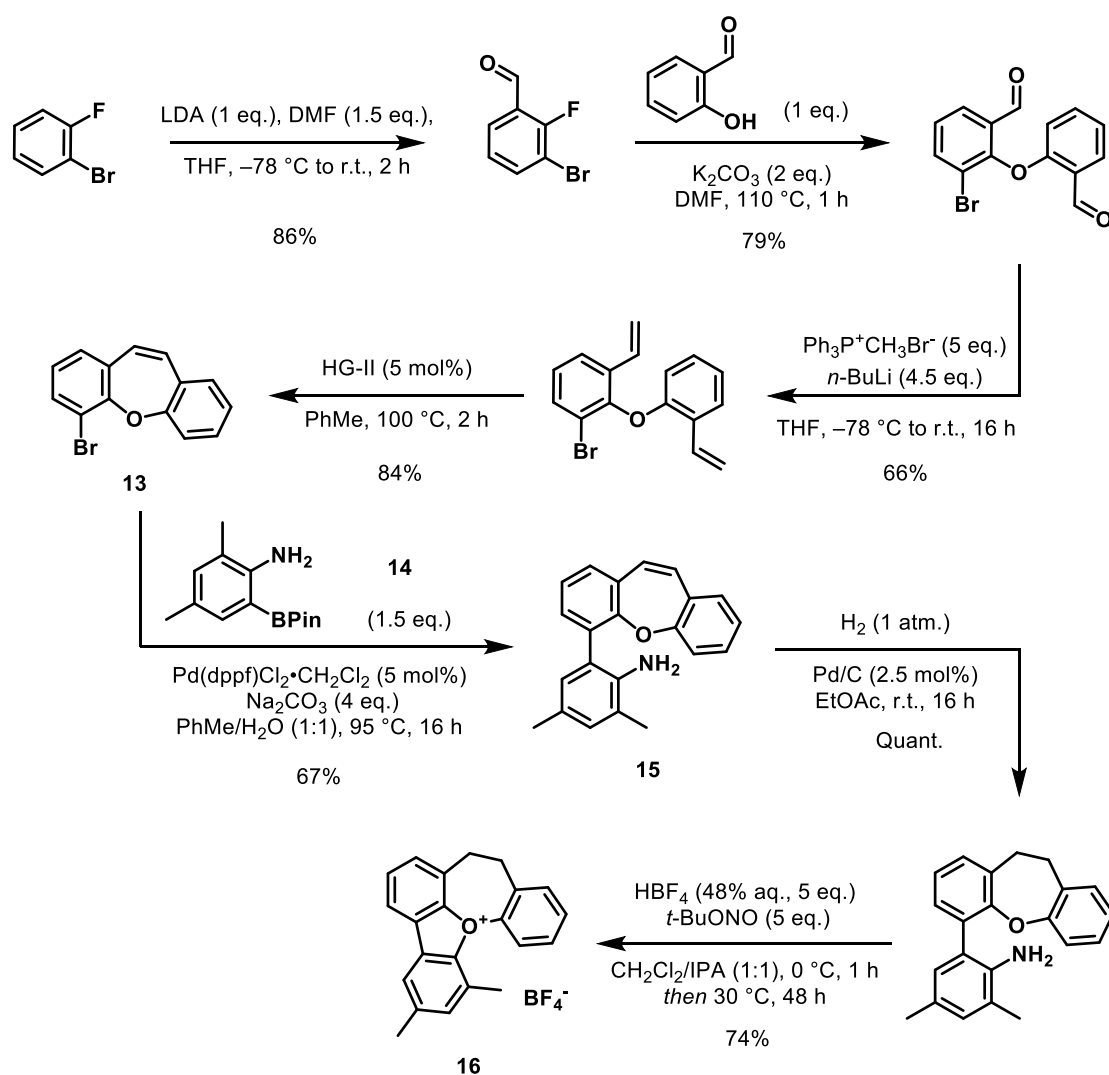
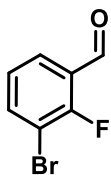


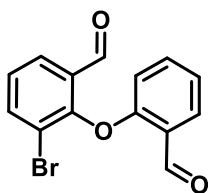
Figure S2. Synthetic approach to dihydrobenzooxepine-derived oxonium ions

3-bromo-2-fluorobenzaldehyde, **S6**:



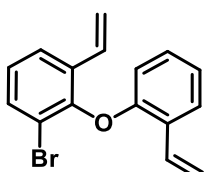
Aldehyde **S6** was prepared according to a literature procedure.^{4,5} *n*-BuLi (1.6 M, 7.5 mL, 12.00 mmol, 1.2 eq.) was added to a stirred solution of diisopropylamine (1.82 mL, 1.32 g, 13.00 mmol, 1.3 eq.) in THF (10 mL) at $-78\text{ }^{\circ}\text{C}$ under N_2 . After 30 mins, 1-fluoro-2-bromobenzene (1.09 mL, 1.75 g, 10.00 mmol, 1 eq.) was added dropwise and the resulting solution was stirred at $-78\text{ }^{\circ}\text{C}$ for 1 h. DMF (1.16 mL, 1.10 g, 15.00 mmol, 1.5 eq.) was added and, after 10 mins at $-78\text{ }^{\circ}\text{C}$, the reaction mixture was warmed to r.t.. After 1 h, water (50 mL) was added and the reaction mixture was extracted with EtOAc ($3 \times 15\text{ mL}$). The organic extracts were dried (MgSO_4), concentrated *in vacuo* and purified by flash column chromatography (Et_2O :Pentane, 5:95, $R_f = 0.3$) to give the title compound as a white solid (1.75 g, 86%). **M. P.** = $40\text{--}41\text{ }^{\circ}\text{C}$. **^1H NMR** (400 MHz, CDCl_3): $\delta_{\text{H}} = 10.30$ (d, $J = 0.8\text{ Hz}$, 1H), 7.78 (d, $J = 7.9\text{ Hz}$, 1H), 7.77 (d, $J = 7.8\text{ Hz}$, 1H), 7.15 (tt, $J = 7.9, 0.9\text{ Hz}$, 1H). **^{13}C NMR** (101 MHz, CDCl_3): $\delta_{\text{C}} = 186.2$ (d, $J = 6.1\text{ Hz}$), 161.0 (d, $J = 259.1\text{ Hz}$), 139.5 (d, $J = 1.5\text{ Hz}$), 127.8 (d, $J = 1.6\text{ Hz}$), 125.7 (d, $J = 4.6\text{ Hz}$), 125.3 (d, $J = 9.0\text{ Hz}$), 110.3 (d, $J = 20.3\text{ Hz}$). **^{19}F NMR (377 MHz, CDCl_3): $\delta_{\text{F}} = -116.1$. **FTIR (neat) $\nu_{\text{max}}/\text{cm}^{-1}$** = 2360, 1715, 1694, 1601, 1575, 1451, 1398, 1249, 1172, 1127, 855, 782, 709, 661. **HRMS**: Mass not found by ESI, APCI or EI.**

3-bromo-2-(2-formylphenoxy)benzaldehyde, **S7**:



3-Bromo-2-fluorobenzaldehyde, **S6**, (3.00 g, 11.40 mmol, 1 eq.), salicylaldehyde (1.21 mL, 1.39 g, 11.40 mmol, 1 eq.) and K_2CO_3 (3.15 g, 22.80 mmol, 2 eq.) were added to DMF (15 mL) and heated to $110\text{ }^{\circ}\text{C}$ under N_2 . After 24 h, H_2O (100 mL) was added and the reaction mixture was extracted with Et_2O ($3 \times 60\text{ mL}$). The combined organic layers were washed with H_2O (100 mL), dried (MgSO_4) and concentrated *in vacuo*. The crude residue was purified by flash column chromatography (Et_2O :pentane, 15:85, $R_f = 0.3$) to give the title compound as a white solid (2.72 g, 79%). **M.P.** = $100\text{--}102\text{ }^{\circ}\text{C}$. **^1H NMR** (400 MHz, CDCl_3): $\delta_{\text{H}} = 10.76$ (s, 1H), 10.20 (s, 1H), 8.01 – 7.92 (m, 3H) 7.44 (ddd, $J = 8.5, 7.5, 2.0\text{ Hz}$, 1H), 7.36 (t, $J = 8.0\text{ Hz}$, 1H), 7.19 (t, $J = 7.5\text{ Hz}$, 1H), 6.45 (d, $J = 8.5\text{ Hz}$, 1H). **^{13}C NMR** (101 MHz, CDCl_3): $\delta_{\text{C}} = 189.0, 188.0, 160.2, 153.3, 140.3, 136.1, 131.6, 129.5, 128.8, 127.9, 125.1, 123.5, 118.7, 114.5$. **FTIR (neat) $\nu_{\text{max}}/\text{cm}^{-1}$** = 2862, 1687, 1601, 1585, 1477, 1439, 1391, 1280, 1231, 1205, 1186, 1157, 1122, 1098, 879, 825, 786, 759, 707. **HRMS** (ESI^+): m/z calculated for $\text{C}_{14}\text{H}_{10}^{79}\text{BrO}_3^+$, $[\text{M}+\text{H}]^+ = 304.9808$; m/z found = 304.9810. $\Delta = 0.66\text{ ppm}$.

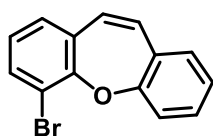
1-Bromo-3-vinyl-2-(2-vinylphenoxy)benzene, **S8**:



n-BuLi (1.6 M, 14.3 mL, 23.00 mmol, 4 eq.) was added to a suspension of methyltriphenylphosphonium bromide (9.37 g, 26.20 mmol, 4.5 eq.) in THF (200 mL) at $-78\text{ }^{\circ}\text{C}$. Once the addition was complete, the reaction mixture was warmed to $0\text{ }^{\circ}\text{C}$ for 10 mins before being cooled back to $-78\text{ }^{\circ}\text{C}$. 3-bromo-2-(2-formylphenoxy)benzaldehyde, **S7**, (1.75 g, 5.74 mmol, 1 eq.) in THF (20 mL) was added and the reaction was allowed to warm to r.t.. After 16 h, H_2O (150 mL) was added, the mixture was extracted with Et_2O ($3 \times 50\text{ mL}$). The organic extracts were dried (MgSO_4), concentrated *in vacuo*

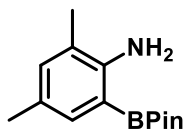
and purified by flash column chromatography (Et₂O:pentane, 5:95, *R_f* = 0.6) to give the title compound as a viscous colourless oil (1.14 g, 66%). **¹H NMR** (500 MHz, CDCl₃): δ_H = 7.59 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.56 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.30 (dd, *J* = 17.8, 11.2 Hz, 1H), 7.12 (t, *J* = 7.9 Hz, 1H), 7.09 – 7.04 (m, 1H), 7.00 (td, *J* = 7.5, 1.2 Hz, 1H), 6.76 (dd, *J* = 17.6, 11.1 Hz, 1H), 6.29 (dd, *J* = 8.2, 1.2 Hz, 1H), 5.88 (dd, *J* = 17.7, 1.4 Hz, 1H), 5.76 (dd, *J* = 17.7, 1.0 Hz, 1H), 5.39 (dd, *J* = 11.2, 1.4 Hz, 1H), 5.25 (dd, *J* = 11.0, 1.0 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 154.8, 149.1, 134.0, 133.3, 131.4, 130.8, 128.9, 127.0, 126.7, 126.7, 125.8, 122.4, 118.4, 117.3, 115.4, 113.6. **FTIR** (neat) ν_{max}/cm⁻¹ = 2981, 1626, 1601, 1577, 1557, 1481, 1451, 1436, 1409, 1310, 1259, 1227, 1183, 1123, 1100, 1022, 991, 914, 880, 829, 790, 773, 760, 746, 641. **HRMS** (ESI⁺): *m/z* calculated for C₁₆H₁₄⁷⁹BrO⁺, [M+H]⁺ = 301.0223; *m/z* found = 301.0224. Δ = 0.33 ppm.

4-Bromodibenzo[*b,f*]oxepine, **13**:



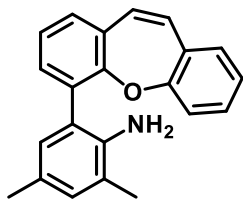
Oxepine **13** was prepared according to a literature procedure for a similar substrate.⁶ Hoveyda-Grubbs 2nd Generation Catalyst (52 mg, 0.083 mmol, 2.5 mol%) in degassed PhMe (5 mL) was added to a solution of 1-bromo-3-vinyl-2-(2-vinylphenoxy)benzene, **S7**, (1.00 g, 3.33 mmol, 1 eq.) in degassed PhMe (20 mL) at 100 °C over 5 mins. After 2 h, the reaction was cooled to r.t. and diluted (60 mL, 2:98, EtOAc:Pentane). The reaction mixture was filtered through Celite® (10 mL), eluted (EtOAc:Pentane, 2:98, 3 × 20 mL) and concentrated *in vacuo*. The crude residue was purified by flash column chromatography (Et₂O:pentane, 2:98, *R_f* = 0.3) to give the title compound as a viscous colourless oil (768 mg, 84%). **¹H NMR** (400 MHz, CDCl₃): δ_H = 7.56 – 7.49 (m, 2H), 7.33 (ddd, *J* = 8.0, 7.0, 2.0 Hz, 1H), 7.19 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.14 (td, *J* = 7.5, 1.0 Hz, 1H), 7.11 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.97 (t, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 11.5 Hz, 1H), 6.69 (d, *J* = 11.5 Hz, 1H). **¹³C NMR** (126 MHz, CDCl₃): δ_C = 157.2, 153.3, 133.3, 132.6, 131.1, 130.4, 130.3, 129.6, 129.4, 128.7, 125.9, 125.5, 122.6, 116.5. **FTIR** (neat) ν_{max}/cm⁻¹ = 3649, 2981, 2888, 2361, 1482, 1436, 1383, 1229, 1155, 1073, 956, 747. **HRMS** (ESI⁺): *m/z* calculated for C₁₄H₁₀⁷⁹BrO⁺, [M+H]⁺ = 272.9910; *m/z* found = 272.9910. Δ = 0.05 ppm.

2,4-Dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline, **14**:



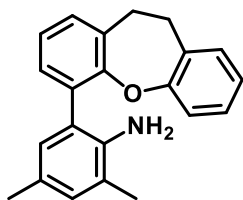
Aniline **14** was prepared according to a modified literature procedure.³ 1,4-Dioxane (40 mL) was added to a mixture of 2-bromo-4,6-dimethylaniline (1.00 g, 5.00 mmol, 1 eq.), Pd(dppf)Cl₂·CH₂Cl₂ (122 mg, 0.15 mmol, 3 mol%), KOAc (1.47 g, 15.00 mmol, 3 eq.) and B₂Pin₂ (1.90 g, 7.50 mmol, 1.5 eq.) under N₂. Argon was bubbled through the mixture for 10 mins and the reaction was heated to 95 °C. After 20 h, H₂O (30 mL) was added. The resulting mixture was extracted (CH₂Cl₂, 3 × 15 mL), the combined organic extracts were dried (MgSO₄) and concentrated *in vacuo*. The crude residue was suspended in pentane (30 mL), filtered through Celite® (8 mL), eluted (pentane, 3 × 10 mL) and concentrated *in vacuo*. The crude product was used without further purification.

2-(Dibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, **S9**:



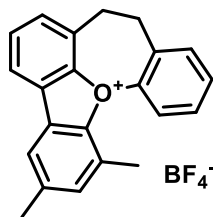
4-Bromodibenzo[*b,f*]oxepine, **13**, (600 mg, 2.21 mmol, 1 eq.) as a solution in PhMe (2 mL), 2,4-dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline, **14**, (3.32 mmol, 1.5 eq.) as a solution in PhMe (20 mL) and water (20 mL) were sequentially added to Pd(dppf)Cl₂·CH₂Cl₂ (90.2 mg, 0.11 mmol, 5 mol%) and Na₂CO₃ (937mg, 8.84 mmol, 4 eq.) under N₂ at r.t.. Argon was bubbled through the solution for 10 mins and the reaction mixture was heated to 95 °C. After 24 h, the reaction mixture was extracted (CH₂Cl₂, 3 × 20 mL), dried (MgSO₄) and concentrated *in vacuo*. The crude residue was purified by flash column chromatography (Et₂O:Pentane, 10:90, R_f = 0.3) to give the title compound as a viscous oil (463 mg, 67%). ¹H NMR (500 MHz, CDCl₃): δ_H = 7.29 (dd, *J* = 7.1, 2.2 Hz, 1H), 7.22 – 7.15 (m, 2H), 7.15 – 7.08 (m, 2H), 7.04 (td, *J* = 7.4, 1.3 Hz, 1H), 7.00 (d, *J* = 2.1 Hz, 1H, H18), 6.82 (d, *J* = 2.1 Hz, 1H), 6.79 (d, *J* = 11.4 Hz, 1H), 6.73 (d, *J* = 11.4 Hz, 1H), 6.36 (dd, *J* = 8.1, 1.3 Hz, 1H), 2.29 (s, 3H), 2.27 (s, 3H). ¹³C NMR (126 MHz, CDCl₃): δ_C = 157.0, 154.3, 140.2, 133.1, 132.0, 131.4, 130.8, 130.8, 130.3, 130.2, 129.7, 129.4, 129.0, 128.9, 126.9, 125.1, 124.9, 124.3, 122.6, 122.0, 20.6, 18.1. FTIR (neat) ν_{max}/cm⁻¹ = 3379, 3022, 2918, 2359, 1621, 1602, 1485, 1443, 1267, 1227, 1196, 1108, 1033, 893, 863, 820, 804, 775, 732. HRMS (ESI⁺): *m/z* calculated for C₂₂H₂₀NO⁺, [M+H]⁺ = 314.1539; *m/z* found = 314.1536. Δ = -0.96 ppm.

2-(10,11-Dihydrodibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, **15**:



H₂ was passed through a solution of Pd/C (10%, 40 mg, 2.5 mol%) and 2-(dibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, **S9**, (463 mg, 1.48 mmol, 1 eq.) in EtOAc (20 mL) under N₂ and kept under a positive pressure of H₂. After 16 h, N₂ was bubbled through the solution for 10 mins, the reaction was filtered (Celite®, 5 mL), eluted (EtOAc, 4 × 10 mL) and concentrated *in vacuo* to give the title compound as a viscous oil (466 mg, Quant.). ¹H NMR (500 MHz, CDCl₃): δ_H = 7.20 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.14 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.96 – 6.90 (m, 2H), 6.80 (d, *J* = 2.1 Hz, 1H), 6.44 (dd, *J* = 7.5, 1.9 Hz, 1H), 3.39 (ddd, *J* = 13.9, 10.5, 3.7 Hz, 1H), 3.19 – 3.10 (m, 1H), 3.03 – 2.91 (m, 2H), 2.42 (s, 3H), 2.28 (s, 3H). ¹³C NMR (126 MHz, CDCl₃): δ_C = 156.1, 154.7, 134.8, 133.4, 131.6, 131.0, 130.8, 130.6, 129.8, 129.6, 129.4, 128.1, 127.0, 126.8, 124.8, 124.5, 123.7, 121.6, 31.2, 30.4, 20.6, 18.6. FTIR (neat) ν_{max}/cm⁻¹ = 2920, 2360, 1757, 1621, 1575, 1487, 1446, 1225, 1204, 1103, 1030, 901, 862, 802, 771, 670. HRMS (ESI⁺): *m/z* calculated for C₂₂H₂₂NO⁺, [M+H]⁺ = 316.1696, *m/z* found = 316.1698. Δ = 0.63 ppm.

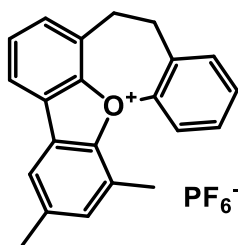
11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium tetrafluoroborate, *rac*-**16**:



t-BuONO (0.51 mL, 442 mg, 4.28 mmol, 5 eq.) was added to a solution of 2-(10,11-dihydrodibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, **15**, (270 mg, 0.86 mmol, 1 eq.) and HBF₄ (48% aq., 0.56 mL, 783 mg, 4.28 mmol, 5 eq.) in CH₂Cl₂:IPA (1:1, 8 mL) at 0 °C. After 1 h, the reaction mixture was diluted with CH₂Cl₂ (10 mL), washed with H₂O (2 × 5 mL) and heated to 30 °C. After 48 h, the solvent was removed by a steady stream of N₂ and Et₂O (10 mL) was added. The Et₂O layer was passed through

a Celite® filter (5 mL). The solid precipitate was washed and the solvent passed through the Celite® (Et₂O, 4 x 5 mL). The solid precipitate was dissolved in MeCN (10 mL), passed through the Celite® and eluted (MeCN, 3 x 10 mL). The solvent was removed by a steady stream of N₂ to give the title compound as a white solid (244 mg, 74%). **M.P.** = 145-147 °C (CHCl₃/Et₂O, dec.) **¹H NMR** (500 MHz, CD₃CN): δ_H = 8.01 – 7.94 (m, 2H), 7.76 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.70 – 7.60 (m, 2H), 7.48 (dq, *J* = 7.8, 1.1 Hz, 1H), 7.46 – 7.44 (m, 1H), 7.39 (ddd, *J* = 9.0, 7.4, 1.8 Hz, 1H), 7.17 (dd, *J* = 8.8, 1.0 Hz, 1H), 4.10 (td, *J* = 14.1, 3.9 Hz, 1H), 3.56 – 3.47 (m, 1H), 3.27 (dt, *J* = 14.2, 3.7 Hz, 1H), 3.21 – 3.09 (m, 1H), 2.56 (s, 3H), 2.17 (s, 3H). **¹³C NMR** (126 MHz, CD₃CN): δ_C = 162.2, 161.0, 153.7, 143.3, 134.7, 133.6, 133.5, 132.9, 132.6, 131.7, 130.5, 127.3, 126.1, 125.2, 123.9, 122.9, 122.3, 115.6, 30.1, 27.9, 21.3, 16.8. **¹⁹F NMR** (471 MHz, CD₃CN): δ_F = -151.8. **FTIR** (neat) ν_{max}/cm⁻¹ = 1481, 1455, 1407, 1051, 900, 828, 799, 773, 734, 613. **HRMS** (ESI⁺): *m/z* calculated for C₂₂H₁₉O⁺, [M]⁺ = 299.1430 *m/z* found = 299.1432. Δ = -1.34 ppm.

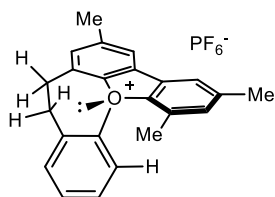
11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium hexafluorophosphate, *rac*-17:



11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium, tetrafluoroborate, ***rac*-16**, (15 mg, 0.04 mmol, 1 eq.) and potassium hexafluorophosphate (35 mg, 0.19 mmol, 5 eq.) were dissolved in MeCN (1 mL). After 1 min, the solvent was removed by a steady stream of N₂. CH₂Cl₂ (1 mL) was added and the mixture was washed with H₂O (2 x 1 mL). The organic layers were dried (MgSO₄) and the solvent was removed by a steady stream of N₂.

Et₂O (4 mL) was added and the solvent was removed by a steady stream of N₂. **M.P.** = 149-151 °C (CHCl₃/Et₂O, dec.) **¹H NMR** (600 MHz, CD₃CN): δ_H = 8.00 – 7.94 (m, 2H), 7.76 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.50 – 7.45 (m, 2H), 7.39 (ddd, *J* = 9.0, 7.5, 2.0 Hz, 1H), 7.19 – 7.15 (m, 1H), 4.10 (td, *J* = 14.0, 4.0 Hz, 1H), 3.51 (dt, *J* = 18.0, 3.5 Hz, 1H), 3.27 (dt, *J* = 14.0, 3.5 Hz, 1H), 3.21 – 3.09 (m, 1H), 2.57 (s, 3H), 2.17 (s, 3H). **¹³C NMR** (151 MHz, CD₃CN): δ_C 162.3, 161.0, 153.7, 143.4, 134.8, 133.6, 133.5, 132.9, 132.7, 131.7, 130.5, 127.3, 126.1, 125.2, 123.9, 122.9, 122.3, 115.6, 30.1, 27.9, 21.3, 16.8. **¹⁹F NMR** (376 MHz, CD₃CN): δ_F = -71.7 – -72.1 (m), -73.6 – -74.0 (m). **FTIR** (neat) ν_{max}/cm⁻¹ = 3057, 2917, 2849, 2360, 2342, 2263, 1423, 1267, 1189, 1017, 896, 846, 792, 736, 704, 668. **HRMS** (ESI⁺): *m/z* calculated for C₂₂H₁₉O⁺, [M]⁺ = 299.1430 *m/z* found = 299.1427. Δ = -1.15 ppm.

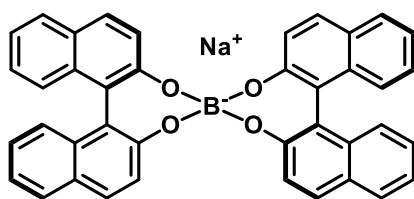
(*M*, (*S*)_o)-11,13-dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium hexafluorophosphate, enantioenriched-17 (97:3):



$$[\alpha]_D^{25} = -2.82 \text{ (} c = 1.0, \text{CHCl}_3 \text{)}$$

Purified by semi-preparative chiral HPLC (2x Chiralpak IC, 90% 250 mM NaPF₆ in MeOH, 10% H₂O, 1.0 mL min⁻¹, λ = 270 nm τ_R (major) = 22.2 min, τ_R (minor) = 23.6 min).

Sodium bis-(*R*)-BINOL borate, **S10**:



NaBH₄ (500 mg, 13.21 mmol, 1 eq.) was slowly added to MeOH (25 mL) at r.t. over 10 mins. After 30 mins the reaction was heated to reflux. After 1 h, the solvent was removed *in vacuo* and the white solid was dried at 80 °C for 16 h to give NaB(OMe)₄ as a white solid (2.09 g, Quant.) that was used without further

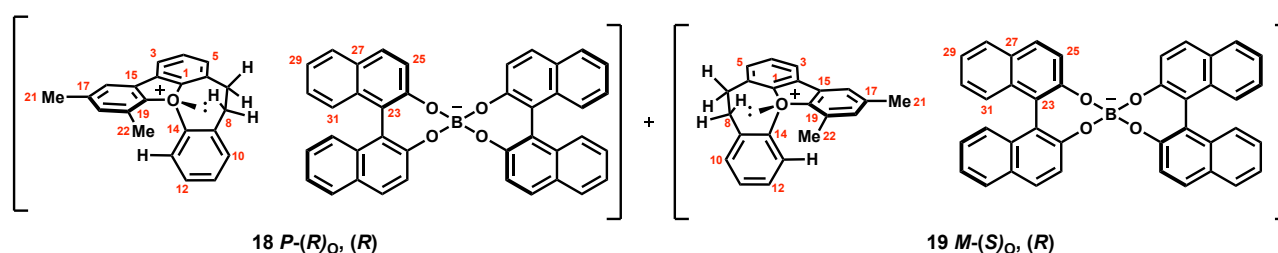
purification. Sodium bis-(*R*)-BINOL borate, **S10**, was prepared according to a modified literature procedure for racemic sodium bis-BINOL borate.⁷ (*R*)-BINOL (1.00 g, 3.50 mmol, 2.94 eq.) and NaB(OMe)₄ (2.84 g, 1.80 mmol, 1 eq.) were dissolved in THF (30 mL) and heated to reflux. After 20 h, the reaction was cooled to 40 °C and B(OMe)₃ (0.25 mL, 235 mg, 2.27 mmol, 1.26 eq.) was added. After 1 h, the reaction was heated to reflux. After 3 h, the reaction was cooled to r.t. and left for 16 h to crystallise. The precipitate was collected by suction filtration and sequentially washed with THF (2 × 20 mL), Et₂O (2 × 20 mL) and pentane (2 × 20 mL). The crude product consisted of sodium bis-(*R*)-BINOL borate·xTHF adduct where x = 2.5. The crude product was dried at 80 °C under vacuum for 7 d to give the title compound as a white solid (501 mg, 46%). **M.P.** = >250 °C. **¹H NMR** (400 MHz, DMSO-d₆): δ_H = 7.98 (d, *J* = 8.8 Hz, 4H), 7.94 (d, *J* = 8.2 Hz, 4H), 7.36 (d, *J* = 8.7 Hz, 4H), 7.30 (ddd, *J* = 8.0, 5.7, 2.2 Hz, 4H), 7.22 – 7.12 (m, 8H). **¹³C NMR** (101 MHz, DMSO-d₆): δ_C = 156.1, 132.8, 128.9, 128.2, 128.0, 125.8, 124.8, 124.6, 122.4, 121.8. **FTIR** (film) ν_{max}/cm⁻¹ = 3053, 2162, 1618, 1590, 1505, 1464, 1428, 1366, 1331, 1266, 1246, 1155, 1071, 986, 948, 910, 828, 812, 744, 720, 665, 633. **LRMS** (ESI⁻): *m/z* calculated for C₂₀H₁₃O₂⁻, [M-C₂₀H₁₁BO₂]⁻ = 285; *m/z* found = 285. [α]_D²⁵ = -284 (c = 1.04, DMSO). *Spectra are consistent with literature values.⁷

3 Experimental data for resolution of *rac*-16

11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium, bis-(*R*)-BINOL borate, **18** and **19**:

11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium, tetrafluoroborate, **rac-16**, (50 mg, 0.13 mmol, 1 eq.) and sodium [bis-(*R*)-BINOL borate] (78 mg, 0.13 mmol, 1 eq.) were dissolved in MeCN (8 mL). After 1 min, the solvent was removed by a steady stream of N₂. CH₂Cl₂ (8 mL) was added and the mixture was washed with H₂O (2 × 4 mL). The organic layers were dried (MgSO₄) and the solvent was removed by a steady stream of N₂. Et₂O (4 mL) was added and the solvent was removed by a steady stream of N₂. Data for the 1:1 mixture of diastereoisomeric oxonium ion/ bis-(*R*)-BINOL borate ion pairs **18** and **19** was obtained at this point.

Data for 1:1 mixture of diastereoisomers*

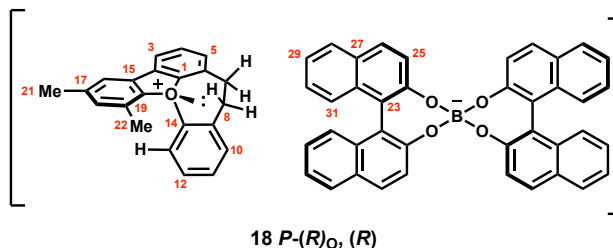


* This compound was found to display particularly concentration-dependant ¹H NMR chemical shifts.

M.P. = 180 °C (CHCl₃/Et₂O, dec.) **¹H NMR** (400 MHz, CD₂Cl₂): δ_H = 7.84 (td, *J* = 7.5, 1.0 Hz, 16H, H₂₈, H₂₆), 7.77 (dd, *J* = 9.0, 1.0 Hz, 1H, H_{Ar}), 7.55 (dt, *J* = 2.0, 1.0 Hz, 1H, H₁₆), 7.48 (ddd, *J* = 7.5, 1.5, 1.0 Hz, 2H, H_{Ar}), 7.42 – 7.33 (m, 9H, H₃₀, H_{Ar}), 7.32 – 7.08 (m, 21H, H₃₁, H₂₉, H_{Ar}), 7.08 – 6.98 (m, 10H, H₂₅, H_{Ar}), 6.98 – 6.96 (m, 1H, H_{Ar}), 6.95 – 6.89 (m, 1H, H_{Ar}), 6.76 (dq, *J* = 7.5, 1.0 Hz, 1H, H_{Ar}), 6.66 – 6.55 (m, 3H, H₁₈, H₁₃, H₃), 3.72 (ddd, *J* = 14.0, 12.0, 6.0 Hz, 1H, H_{8A}), 3.48 (td, *J* = 15.5, 4.0 Hz, 1H, H_{8A'}), 3.07 – 2.98 (m, 1H, H_{8B'}), 2.74 – 2.52 (m, 3H, H_{8B}, H_{7B'}, H_{7A'}), 2.49 – 2.40 (m, 2H, H_{7B}, H_{7A}), 2.38 (d, *J* = 0.5 Hz, 3H, H₂₂), 2.31 (d, *J* = 1.0 Hz, 3H, H_{22'}), 1.78 (d, *J* = 1.0 Hz, 3H, H_{21'}), 1.61 (s, 3H, H₂₁). **¹³C NMR** (151 MHz, CD₂Cl₂): δ_C = 161.0 (C_{Ar}), 160.7 (C_{Ar}), 160.2 (C_{Ar}), 160.1 (C_{Ar}), 156.8 (C₂₄), 152.6 (C₂₀), 152.4 (C₂₀), 142.3 (C_{Ar}), 142.0 (C_{Ar}), 134.0 (C_{Ar}), 133.6 (C_{Ar}), 133.6 (C₃₂), 132.7 (C_{Ar}), 132.6 (C_{Ar}), 132.4 (C_{Ar}), 132.3 (C_{Ar}), 132.1 (C_{Ar}), 131.9 (C_{Ar}), 131.8 (C_{Ar}), 131.7 (C_{Ar}), 130.6 (C_{Ar}), 130.1 (C_{Ar}), 129.8 (C₂₇), 129.2 (C_{Ar}), 129.1 (C_{Ar}), 128.5 (C_{28/26}), 128.2 (C_{28/26}), 127.2 (C_{Ar}), 127.0 (C₃₁), 125.6 (C_{Ar}), 125.6 (C_{Ar}), 125.3 (C₃₀), 124.8 (C₂₅), 124.6 (C_{Ar}), 124.6 (C_{Ar}), 124.3 (C_{Ar}), 124.3 (C_{Ar}), 123.8 (C_{Ar}), 122.8 (C₂₉), 122.6 (C₂₃), 122.1 (C_{Ar}), 121.6 (C_{Ar}), 121.4 (C_{Ar}), 121.1 (C_{Ar}), 113.9 (C₁₃), 113.8 (C₁₃), 29.3 (C₇), 29.1 (C₇), 27.3 (C₈), 27.2 (C₈), 21.3 (C₂₁), 21.3 (C₂₁), 16.5 (C₂₂). **FTIR** (film) ν_{max}/cm⁻¹ = 3505, 3058, 2360, 2341, 1619, 1593, 1506, 1464, 1432, 1383, 1333, 1272, 1247, 1212, 1171, 1145, 1127, 1070, 1006, 953, 909, 864, 816, 791, 748, 712, 678, 666, 627. **HRMS** (ESI⁺): *m/z* calculated for C₂₂H₁₉O, [M]⁺ = 299.1431, *m/z* found = 299.1430. Δ = -0.12 ppm. **¹⁹F NMR** (377 MHz, CD₂Cl₂): δ_F = No peaks were observed, indicating the loss of the BF₄ counterion.

The mixture was dissolved in CHCl₃ (3 mL) and concentrated to approximately 1 mL by a steady stream of N₂. After standing for 1 h at r.t, the mixture was filtered through Celite® (0.2 mL) and the solid precipitate was washed with CHCl₃ (6 × 0.2 mL). The solid precipitate was eluted from the Celite® with CH₂Cl₂ (4 × 0.5 mL) and the solvent was removed by a steady stream of nitrogen. The solid was dried under vacuum for 2 h to give the title compound as a white solid. Maximum theoretical yield of each diastereoisomer = 56.8 mg. Isolated yield of *P*, (*R*)_O, [B((*R*)-BINOL)₂] diastereoisomer **18** = 25.8 mg, 96:4 d.r. (46% of theoretical).

Data for major diastereoisomer from resolution, 18 *P-(R)*_O, (*R*):



M.P. = 120-124 °C (CHCl₃/Et₂O, dec.) **¹H NMR** (400 MHz, CD₂Cl₂) δ 7.87 – 7.81 (m, 8H, H₂₈, H₂₆), 7.55 – 7.50 (m, 1H, H₁₆), 7.45 (dd, *J* = 7.5, 1.5 Hz, 1H, H₃), 7.37 – 7.30 (m, 5H, H₁₀, H₂₅), 7.27 – 7.16 (m, 9H, H₃₁, H₂₉, H_{Ar}), 7.13 – 7.03 (m, 5H, H₃₀, H_{Ar}), 6.98 (ddd, *J* = 9.0, 7.5, 2.0 Hz, 1H, H₄), 6.72 (dd, *J* = 8.0, 1.5 Hz, 1H, H₅), 6.55 (dd, *J* = 5.0, 3.5 Hz, 2H, H₁₈, H₁₃), 3.68 (ddd, *J* = 14.0, 11.5, 6.5 Hz, 1H, H_{8A}), 2.63 (dt, *J* = 14.0, 3.5 Hz, 1H, H_{8B}), 2.41 – 2.38 (m, 2H, H₇), 2.36 (s, 3H, H₂₁), 1.57 (s, 3H, H₂₂). **¹³C NMR** (101 MHz, CD₂Cl₂): δ_C = 160.7 (C₁₄), 160.2 (C₁), 156.9 (C_{Ar}), 152.6 (C₂₀), 142.0 (C_{Ar}), 133.7 (C_{Ar}), 133.6 (C₁₈), 132.6 (C_{Ar}), 132.4 (C_{Ar}), 132.1 (C_{Ar}), 131.8 (C_{Ar}), 130.1 (C_{Ar}), 129.8 (C_{Ar}), 129.0 (C₄), 128.4 (C_{Ar}), 128.3 (C_{Ar}), 127.1 (C_{Ar}), 125.6 (C_{Ar}), 125.3 (C₂₅), 124.9 (C_{Ar}), 124.8 (C_{Ar}), 124.3 (C_{Ar}), 122.7 (C_{Ar}), 122.6 (C_{Ar}), 121.6 (C₁₆), 121.1 (C₃), 113.9 (C₁₃), 78.0 (C_{Ar}), 29.1 (C₇), 27.3 (C₈), 21.4 (C₂₁), 16.5 (C₂₂). **FTIR** (film) ν_{max}/cm⁻¹ = 3056, 2918, 2360, 2341, 1617, 1591, 1505, 1481, 1464, 1429, 1366, 1335, 1272, 1249, 1211, 1142, 1127, 1070, 988, 947, 928, 910, 849, 816, 791, 747, 711, 677, 668, 649, 634, 611. **HRMS** (ESI⁺): *m/z* calculated for C₂₂H₁₉O, [M]⁺ = 299.1431, *m/z* found = 299.1430. Δ = -0.22 ppm.

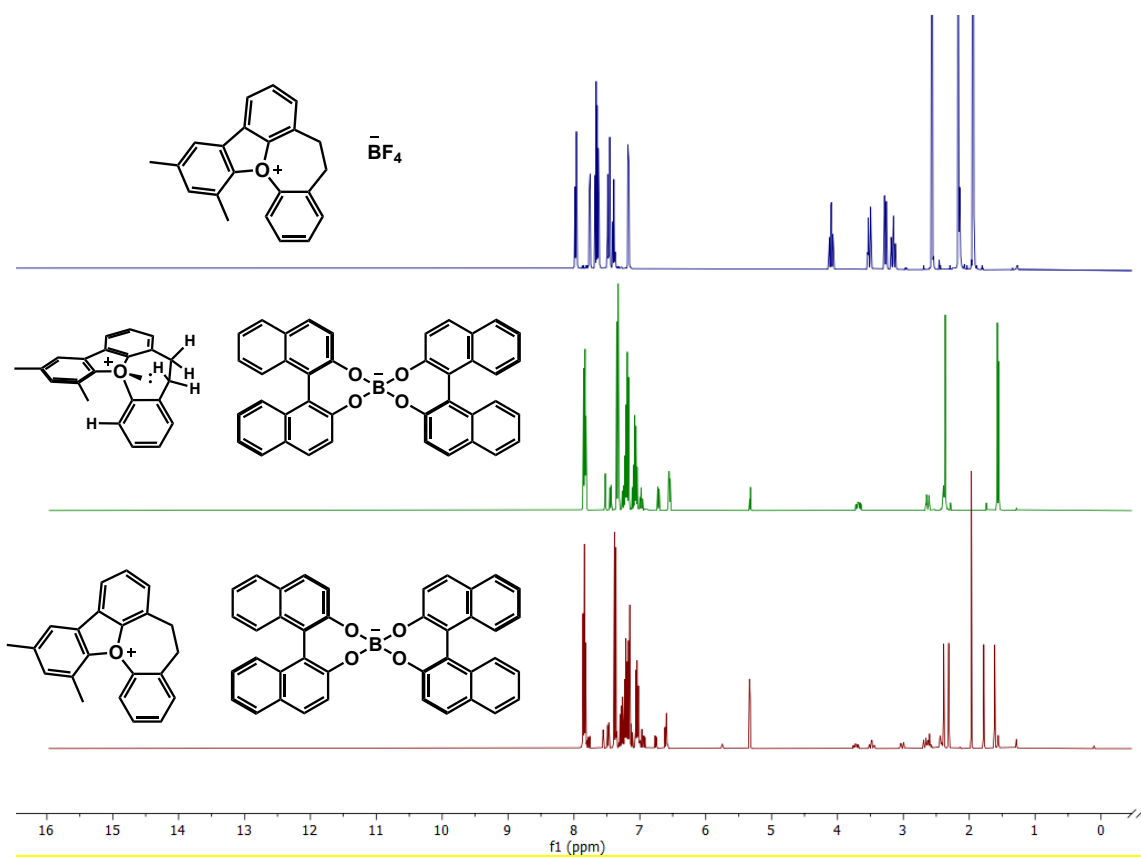


Figure S3: ^1H NMR spectra of *rac*-**16** (top), diastereoisomerically enriched **18** (d.r. 94:6, middle) and 1:1 mixture of diastereoisomers **18** & **19** (bottom).

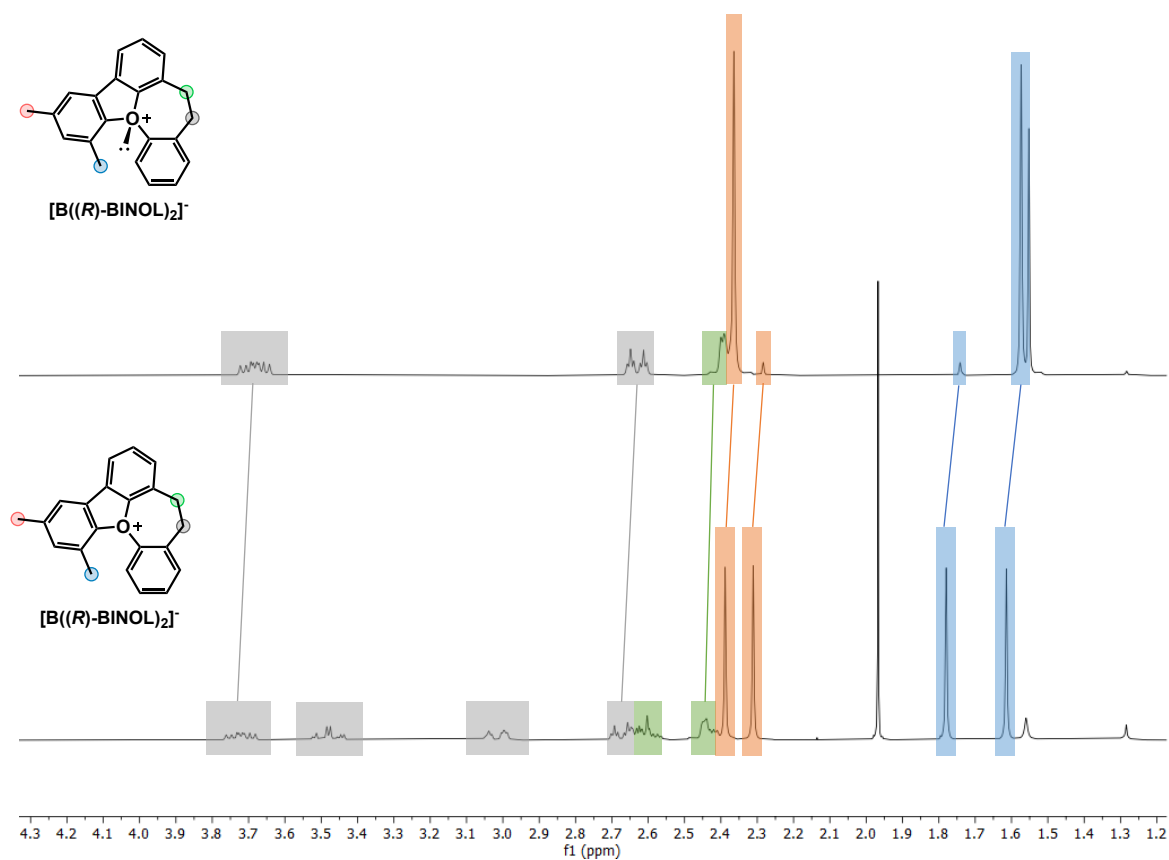


Figure S4: Expansion of ^1H NMR spectra of diastereoisomerically enriched **18** (d.r. 94:6, top) and 1:1 mixture of diastereoisomers **18** & **19** (bottom).

The resolution process in pictures (read in context of experimental procedure above):

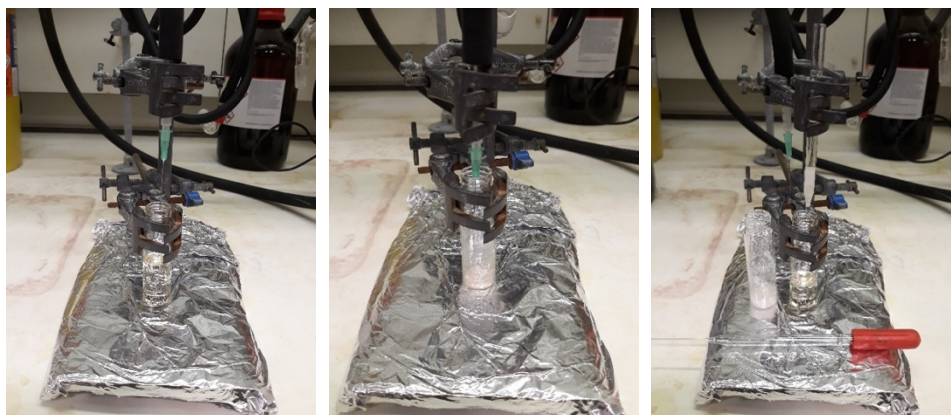


Figure S5. *Left:* Sodium bis-(*R*)-BINOL borate, **S10**, is poorly soluble in CH_2Cl_2 so the formation of the salt mixture must be carried out in MeCN. *Centre:* The MeCN is removed by a steady stream of N_2 . *Right:* Addition of CH_2Cl_2 leads to precipitation of some NaBF_4 , though multiple water washes are necessary to remove it entirely (this can be validated by ^{19}F NMR analysis). The CH_2Cl_2 layers are dried over MgSO_4 and filtered using a pipette filter.

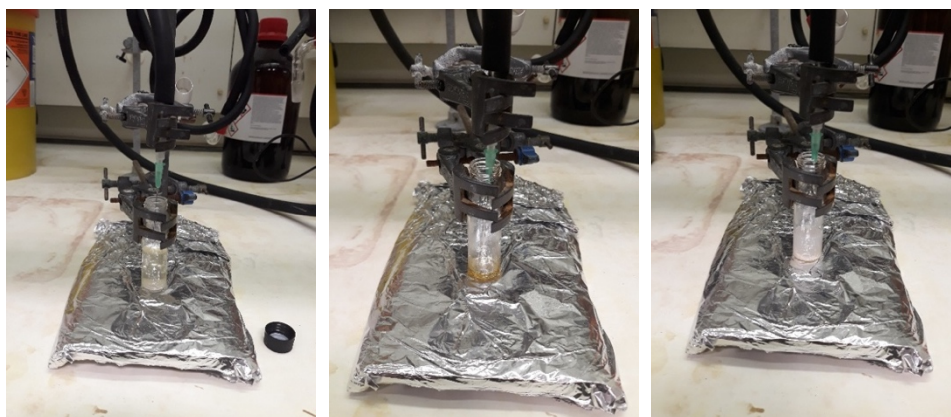


Figure S6. *Left:* The CH_2Cl_2 is removed by a steady stream of N_2 . *Centre:* After concentration of the oxonium-borate solution, extended periods under vacuum may be required to remove the CH_2Cl_2 , which can interfere in the resolution if not removed fully. This can be enabled by the sequential addition and then removal of Et_2O . This provides a convenient solution to the removal of CH_2Cl_2 , and yields a white powder (*Right*).

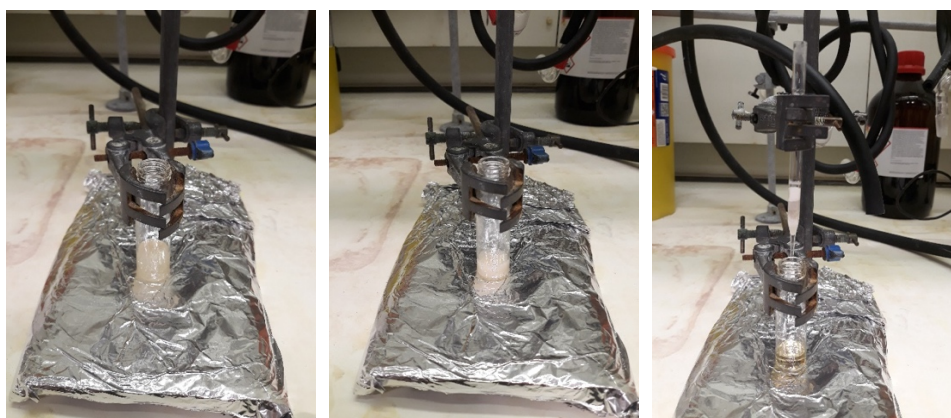


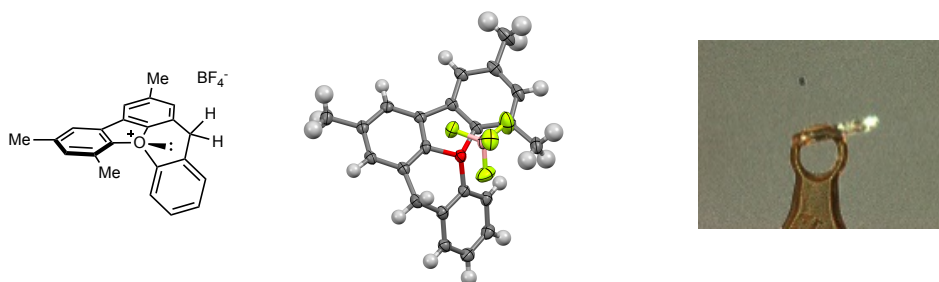
Figure S7. *Left:* Some precipitation is observed after the addition of CHCl_3 (3 mL). *Centre:* Upon concentration to 1 mL, the less soluble diastereomeric ion-pair precipitates from the mother liquor. *Right:* Celite® filtration is used to isolate the diastereoenriched oxonium ion. Washing the solid obtained with CHCl_3 reliably gives the oxonium ion in high diastereoselectivity. It is then eluted from the Celite® using CH_2Cl_2 .

4 X-ray Crystallography

Single crystal X-ray diffraction was carried out by Owen A. Smith using a (Rigaku) Oxford Diffraction/Agilent Supernova A diffractometer (Cu-K α radiation, λ = 1.54184 Å) within the Department of Chemistry, University of Oxford. Samples were mounted in perfluoropoly-ethyl ether oil and flash-cooled to 150 K by a N₂ Cryostream open-flow cooling device.⁸ The raw frame data was integrated and reduced using CrysAlisPro. SuperFlip⁹ embedded within CRYSTALS^{10,11} was used to obtain an ab initio solution using CRYSTALS and for structure refinement.

Molecular graphics of the structure solutions are shown with displacement ellipsoid plots of the best fit model drawn at 50% probability. Raw frame data, unprocessed cif files and completed cif files for all structures are available on request.

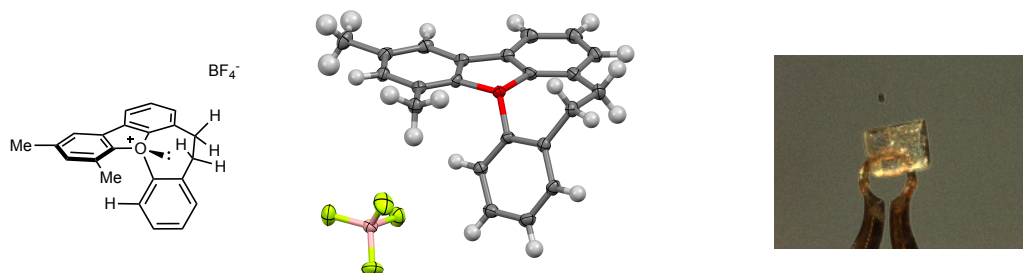
4.1 1,3,6-Trimethyl-8*H*-benzofuro[3,2,1-*de*]xanthen-13-ium tetrafluoroborate, **10**:



Vapour diffusion of Et₂O into a solution of **10** (5 mg) in CH₂Cl₂ (0.6 mL) over 16 h gave colourless needles suitable for single crystal x-ray analysis.

Identification Code	001os20 (CCDC 2124020)
Empirical Formula	C ₂₂ H ₁₉ B F ₄ O
<i>M_r</i>	386.20
Temperature	150 K
Wavelength	λ = 1.54180 Å (Cu K _α)
Crystal System	Monoclinic
Space Group	P 2 ₁ /c
Unit Cell Dimensions	a = 8.0432(3) Å α = 90° B = 12.6195(5) Å β = 96.911(3)° c = 18.0018(7) Å γ = 90°
Volume	1813.93(12) (Å ³)
Z	4
Density (Calculated)	1.414 Mg m ⁻³
Absorption Coefficient	0.954 mm ⁻¹
Crystal Size	0.05 x 0.06 x 0.35 mm ³
Theta range for data collection	4.289 to 75.949°
Index Ranges	-10 ≤ h ≤ 9, -14 ≤ k ≤ 15, -15 ≤ l ≤ 22
Reflections Collected	11627
Independent Reflections	3735 [R(int) = 0.046]
Completeness to theta = 73.671°	99.6%
Absorption Correction	multi-scan
Refinement method	Full-matrix least-squares on F ²
Goodness-of-fit on F²	1.0103
Final R indices [I > 2σ(I)]	R1 = 0.0692, wR2 = 0.1373
R indices (all data)	R1 = 0.0506, wR2 = 0.1213

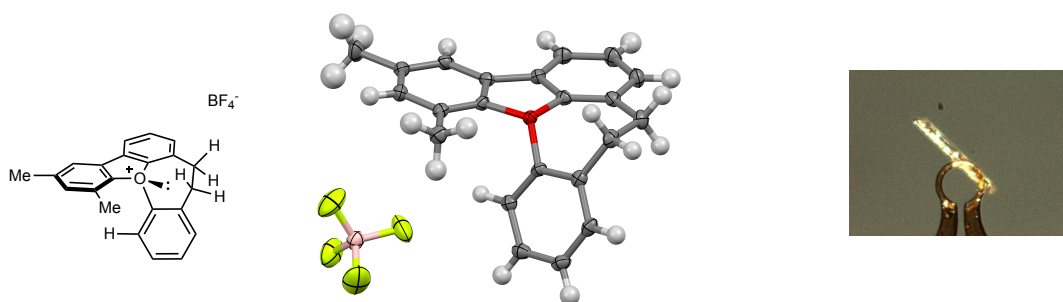
4.2 11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*] benzofuran-10-ium tetrafluoroborate, ***rac*-16**:



Vapour diffusion of Et₂O into a solution of ***rac*-16** (5 mg) in CH₂Cl₂ (0.6 mL) over 16 h gave colourless blocks suitable for single crystal x-ray analysis.

Identification Code	027os21 (CCDC 2124019)
Empirical Formula	C ₂₂ H ₁₉ B F ₄ O
<i>M_r</i>	386.20
Temperature	150 K
Wavelength	λ = 1.54184 Å (Cu K _α)
Crystal System	Triclinic
Space Group	P $\bar{1}$
Unit Cell Dimensions	a = 8.2151(2) Å α = 75.869(2)° b = 9.8320(2) Å β = 76.543(2)° c = 11.9880(3) Å γ = 88.198(2)°
Volume	912.87(4) (Å ³)
Z	2
Density (Calculated)	1.405 Mg m ⁻³
Absorption Coefficient	0.948 mm ⁻¹
Crystal Size	0.10 x 0.18 x 0.21 mm ³
Theta range for data collection	3.909 to 76.160°
Index Ranges	-10 ≤ h ≤ 8, -12 ≤ k ≤ 12, -15 ≤ l ≤ 14
Reflections Collected	19078
Independent Reflections	3781 [R(int) = 0.021]
Completeness to theta = 73.875°	99.6%
Absorption Correction	multi-scan
Refinement method	Full-matrix least-squares on F ²
Goodness-of-fit on F ²	1.0033
Final R indices [I > 2σ(I)]	R1 = 0.0361, wR2 = 0.0900
R indices (all data)	R1 = 0.0346, wR2 = 0.0855

4.3 11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*] benzofuran-10-ium tetrafluoroborate, *enantioenriched*-**16**:



Oxonium ion bis-(*R*)-BINOL borate salt, **18**, 94:6 d.r. (3 mg) was dissolved in CH₂Cl₂ (0.5 mL). The organic layer was washed with 48% aq. HBF₄ (3 × 0.5 mL), dried (MgSO₄) and the solvent was removed by a steady stream of N₂. Vapour diffusion of Et₂O into a solution of the crude residue in CH₂Cl₂ (0.6 mL) over 16 h gave a mixture of an amorphous solid and colourless needles. The colourless needles were subjected to single crystal x-ray diffraction analysis. The Flack x parameter^{12,13} was refined to -0.04(10), with a Parsons' q of -0.03(3).¹⁴ Bayesian analysis of the Bijvoet pairs was used to give the Hooft y parameter¹⁵ as -0.02(4). Two further crystals were measured and the same absolute structure was found in each case (Flack x parameters: 0.08(12) and -0.06(12), Parsons' q parameters: 0.03(4) and -0.03(3), Hooft y parameters: 0.04(5) and -0.05(4) respectively) allowing us to assign the absolute structure as (*P*, *R*_O).

Identification Codes	037os21, 035os21, 038os21 (CCDC 21911038-2191040)
Empirical Formula	C22 H19 B F4 O
<i>M</i>_r	386.19
Temperature	150 K
Wavelength	λ = 1.54180 Å (Cu Kα)
Crystal System	Orthorhombic
Space Group	P 21 21 21
Unit Cell Dimensions	a = 6.9568(1) Å α = 90° B = 14.0648(1) Å β = 90° c = 18.5135(1) Å γ = 90°
Volume	1811.47(3) (Å ³)
Z	4
Density (Calculated)	1.416 Mg m ⁻³
Absorption Coefficient	0.956 mm ⁻¹
Crystal Size	0.05 x 0.06 x 0.410 mm ³
Theta range for data collection	3.947 to 76.072°
Index Ranges	-8<=h<=8, -17<=k<=17, -23<=l<=22
Reflections Collected	41603
Independent Reflections	3765 [R(int) = 0.044]
Completeness to theta = 74.550°	99.8%
Absorption Correction	multi-scan
Refinement method	Full-matrix least-squares on F ²
Goodness-of-fit on F²	0.9966
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0788
R indices (all data)	R1 = 0.0308, wR2 = 0.0802
Flack x parameter	-0.04(10)
Parsons' q parameter	0.03(4)
Hooft y parameter	-0.02(4)

5 Inversion Barrier Measurements

5.1 1,3,6-Trimethyl-8*H*-benzofuro[3,2,1-*de*]xanthen-13-ium tetrafluoroborate, **10**:

The barrier to enantiomerization of **10** was estimated using a Bruker AVIIIHD 500 MHz (¹H) spectrometer equipped with a BCU-II temperature regulation unit. Calculations were performed and graphs generated in Microsoft Excel.

Using the method presented by Clayden¹⁶, the enantiomerization constant, k_{ent} , for a diastereotopic AB system can be approximated using equation (1) and substitution of k_{ent} into the Eyring equation (2) gives the enantiomerization barrier, $\Delta G_{ent}^\ddagger$, at the coalescence temperature, T_c .

$$(1) k_{ent} = \pi \sqrt{\frac{(\Delta\nu)^2 + 6(J_{AB})^2}{2}}$$

$$J_{AB} = (\nu_1 - \nu_2) = (\nu_3 - \nu_4) \text{ and } \Delta\nu = \sqrt{(\nu_1 - \nu_4)(\nu_2 - \nu_3)}$$

$$(2)^\dagger \Delta G_{ent}^\ddagger(T_c) = \kappa RT_c \ln \left(\frac{k_B T_c}{h k_{ent}} \right)$$

$$R = 8.314 \text{ JK}^{-1}\text{mol}^{-1}, k_B = 1.3806 \times 10^{-23} \text{ JK}^{-1} \text{ and } h = 6.626 \times 10^{-34} \text{ Js}$$

Oxonium ion **10** (10 mg) in CD₂Cl₂ (0.5 mL) was cooled to −40 °C (233 K), the sample was allowed to equilibrate for 20 mins and a ¹H NMR spectrum was recorded from which values for J_{AB} and $\Delta\nu$ were obtained. The sample was subsequently warmed in 10 °C intervals from −40 °C (233 K) to 20 °C (293 K) and then in 1 °C intervals from 20 °C (293 K) to 22 °C (295 K) to obtain the coalescence temperature, T_c . In each case, the sample was equilibrated at the desired temperature for 20 minutes and a ¹H NMR spectrum was recorded.

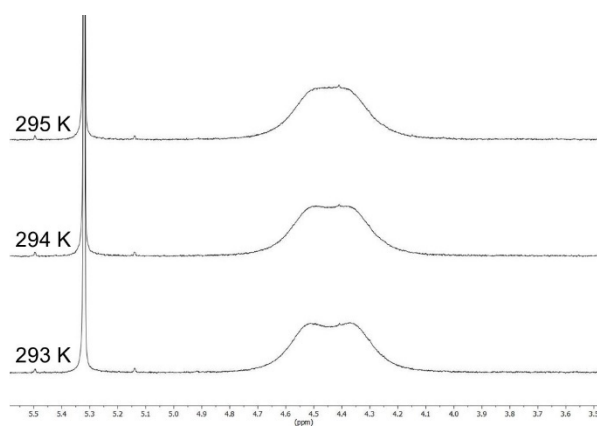
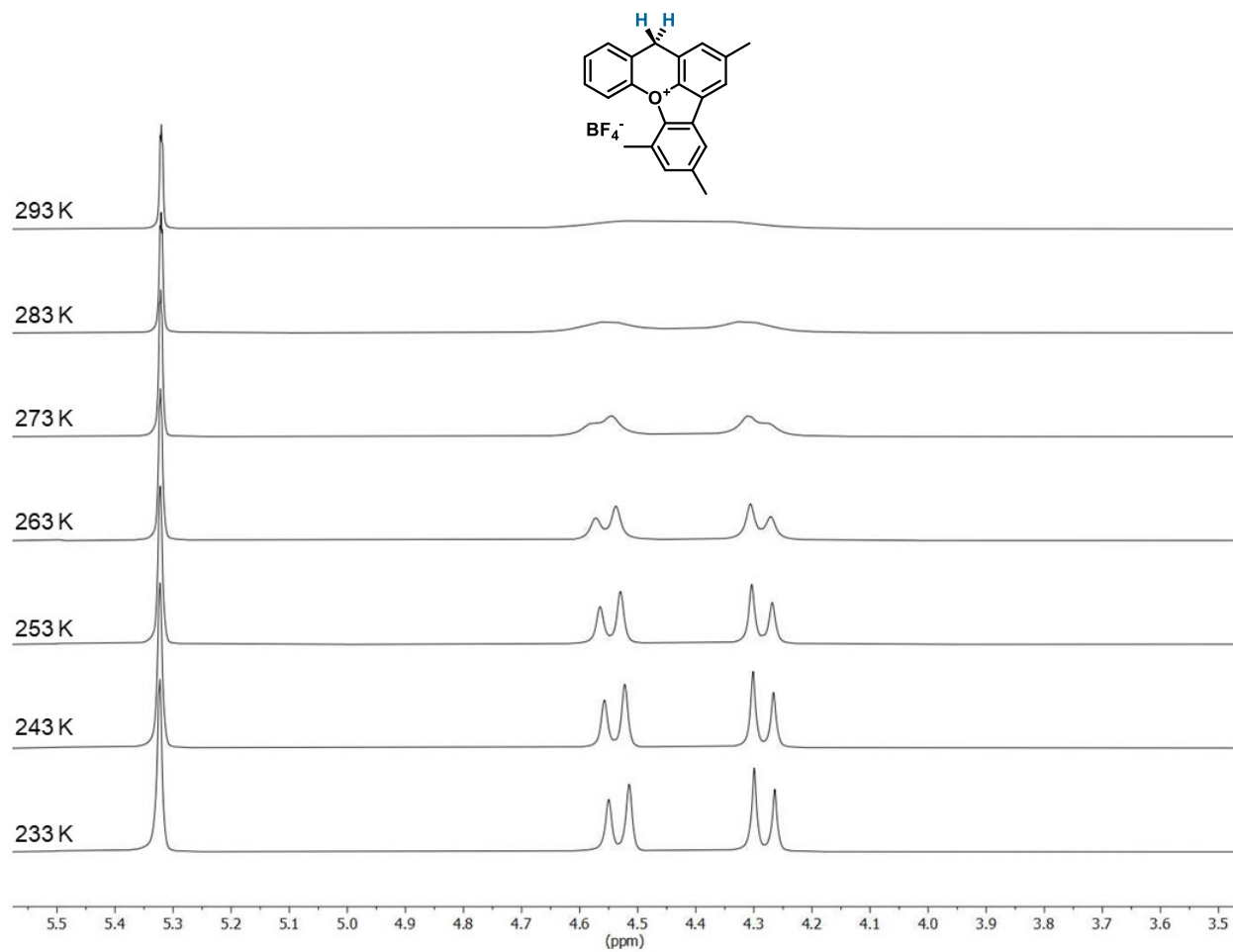
The following values were obtained: $\Delta\nu = 124.1 \text{ Hz}$, $J_{AB} = 17.6 \text{ Hz}$ and $T_c = 295 \text{ K}$.

$$(1) k_{ent} = \pi \sqrt{\frac{(\Delta\nu)^2 + 6(J_{AB})^2}{2}} = 2918 \text{ s}^{-1}$$

$$(2) \Delta G_{ent}^\ddagger(T_c) = RT_c \ln \left(\frac{k_B T_c}{h k_{ent}} \right)$$

$$\Delta G_{ent}^\ddagger(295) = 58302 \text{ Jmol}^{-1} = 58.3 \text{ kJmol}^{-1} = 13.9 \text{ kcalmol}^{-1}$$

[†] In this equation the transmission coefficient $\kappa = 1$ in the absence of other information.



$\nu_1 = 4.5499$ ppm

$\nu_2 = 4.5148$ ppm

$\nu_3 = 4.2994$ ppm

$\nu_4 = 4.2641$ ppm

$\Delta\nu = 0.2481$ ppm = 124.058 Hz (500 MHz)

Average $J_{AB} = 0.0352$ ppm = 17.6 Hz (500 MHz)

Figure S8: Variable temperature ^1H NMR spectra of **10** (233 to 295 K) and values for T_c , $\Delta\nu$ and J_{AB} .

5.2 Equilibration of 11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium, [*P*, (*R*)_o]-bis-(*R*)-BINOL borate, **18**:

The barrier to diastereomerization of **18** is quoted as an average of three experiments:

Experiment 1:

Oxonium ion **18** (8.8 mg, 0.01 mmol) at 94:6 d.r. was dissolved in CD₂Cl₂ (0.45 mL) in an NMR tube fitted with a J. Young valve. CH₂Br₂ (0.005 mmol) in CD₂Cl₂ (0.05 mL) was added as an internal standard and the diastereomeric ratio was monitored by ¹H NMR using a Bruker AVII 500 MHz spectrometer. The sample was maintained at 298 K for the duration of the experiment (using a Cambridge Reactor Design Polar Bear Plus). ¹H NMR spectra with extended relaxation times were recorded at 24 h intervals

Experiment 2:

Oxonium ion **18** (8.8 mg, 0.01 mmol) at 97:3 d.r. was dissolved in CD₂Cl₂ (0.5 mL) in an NMR tube fitted with a J. Young valve under Argon. 1,2,4,5-Tetramethylbenzene (0.005 mmol) in CD₂Cl₂ (0.01 mL) was added as an internal standard and the diastereomeric ratio was monitored by ¹H NMR using a Bruker AVII 400 MHz spectrometer. The sample was maintained at 298 K for the duration of the experiment (using a Cambridge Reactor Design Polar Bear Plus).

Experiment 3:

Oxonium ion **18** (8.8 mg, 0.01 mmol) at 93:7 d.r. was dissolved in CD₂Cl₂ (0.5 mL) in an NMR tube fitted with a J. Young valve under Argon. 1,2,4,5-Tetramethylbenzene (0.005 mmol) in CD₂Cl₂ (0.01 mL) was added as an internal standard and the diastereomeric ratio was monitored by ¹H NMR using a Bruker AVII 500 MHz spectrometer. The sample was maintained at 298 K for the duration of the experiment (using a Cambridge Reactor Design Polar Bear Plus).

To prepare the internal standard stock solution **Experiment 1:**

- (1) CH₂Br₂ (10.5 μL, 26.1 mg, 0.15 mmol) was dissolved in CD₂Cl₂ (0.3 mL).
- (2) 0.1 mL of (1) (0.05 mmol CH₂Br₂) was diluted with CD₂Cl₂ (0.4 mL).

To prepare the internal standard stock solution **Experiment 2 and 3:**

- (1) 1,2,4,5-tetramethylbenzene (67.1 mg, 0.5 mmol) was dissolved in CD₂Cl₂ (1 mL). Integration of the signals at 3.70 and 3.44 ppm, belonging to the H₈ residue in the major and minor diastereoisomeric salt pair respectively, relative to the internal standard were used to calculate the ratio.

The sum of the integrals of the resonances at 3.70 and 3.44 ppm were monitored over the course of the experiment and no change was observed.

A sample of **18** was left to equilibrate for 5 weeks and the ratio of diastereoisomers was found to be 1.02 by integration of the NMR peaks at 3.70 and 3.44. Using the method presented by Schurig,¹⁷ the diastereomerization constants, $k_{A \rightarrow B}$ and $k_{B \rightarrow A}$, for a diastereotopic AB system can be calculated using the equilibrium constant, K_{eq} , and the rate constant for equilibration, $k_{A \rightarrow B}$, using equation (4). Substitution of $k_{A \rightarrow B}$ and $k_{B \rightarrow A}$ into the Eyring equation (5) gives the diastereomerization barriers, $\Delta G_{A \rightarrow B}^\ddagger$ and $\Delta G_{B \rightarrow A}^\ddagger$, respectively. The free energies are given as an average over three experiments (designated 1-3 below).

$$A \rightleftharpoons B$$

$$(3) K_{eq} = \frac{k_{A \rightarrow B}}{k_{B \rightarrow A}} = \frac{[B_{eq}]}{[A_{eq}]}$$

$$(4) k_{A \rightarrow B} = k_{A \rightarrow B} \left(1 + \frac{1}{K_{eq}} \right) = k_{B \rightarrow A} (1 + K_{eq})$$

$$(5) \Delta G_{A \rightarrow B}^\ddagger(T) = RT_c \ln \left(\frac{k_B T}{h k_{A \rightarrow B}} \right)$$

$$T = 298 \text{ K}, R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}, k_B = 1.3806 \times 10^{-23} \text{ J K}^{-1} \text{ and } h = 6.626 \times 10^{-34} \text{ Js}$$

$$\Delta G_{A \rightarrow B}^\ddagger(298) = 26.7 \text{ kcal mol}^{-1}, \Delta G_{B \rightarrow A}^\ddagger(298) = 26.7 \text{ kcal mol}^{-1}$$

Experiment 1						
time (s)	major (3.70 ppm)	minor (3.44 ppm)	sum	dr	de	ln(d0/de)
0	2.06	0.13	2.19	94.06	88.13	0
86400	2.04	0.15	2.19	93.15	86.30	0.020943174
172800	2.02	0.17	2.19	92.24	84.47	0.042334364
259200	2	0.19	2.19	91.32	82.65	0.064193158
354600	1.96	0.22	2.18	89.91	79.82	0.099058223
432000	1.94	0.24	2.18	88.99	77.98	0.122315085
518400	1.9	0.27	2.17	87.56	75.12	0.159765612
604800	1.87	0.29	2.16	86.57	73.15	0.186301834
k_{rac}				3.12697E-07	s-1	
Experiment 2						
time (s)	major (3.70 ppm)	minor (3.44 ppm)	sum	dr	de	ln(d0/de)
0	1.12	0.03	1.15	97.39	94.78	0
87480	1.17	0.06	1.23	95.12	90.24	0.049069908
168720	1.12	0.06	1.18	94.92	89.83	0.053661284
264720	1.02	0.08	1.1	92.73	85.45	0.103601337
331980	1.01	0.08	1.09	92.66	85.32	0.105164143
419280	1	0.1	1.1	90.91	81.82	0.147086449
530220	0.99	0.12	1.11	89.19	78.38	0.190037837
k_{rac}				3.39823E-07	s-1	
Experiment 3						
time (s)	major (3.70 ppm)	minor (3.44 ppm)	sum	dr	de	ln(d0/de)
0	0.83	0.06	0.89	93.26	86.52	0
121560	0.86	0.07	0.93	92.47	84.95	0.018320693
192540	0.83	0.08	0.91	91.21	82.42	0.048540445
261540	0.84	0.09	0.93	90.32	80.65	0.070280432
347820	0.74	0.09	0.83	89.16	78.31	0.09962239
434220	0.77	0.1	0.87	88.51	77.01	0.116384551
520440	0.74	0.11	0.85	87.06	74.12	0.154685582
k_{rac}				3.01899E-07	s-1	

Table S1: Integration of the peaks at δ 3.70 and δ 3.44 in the ^1H NMR spectrum of **18** over time for experiments 1, 2 and 3, and calculated dr, de and $\ln(\text{de}_0/\text{de}_t)$.

	Experiment 1	Experiment 2	Experiment 3	
K_{eq}	1.02	1.02	1.02	
k_{a-eq}	3.13E-07	3.40E-07	3.02E-07	
k_{a-b}	1.58E-07	1.72E-07	1.52E-07	
Free energy	111786.8697	111584.6757	111877.8762	J
	26.71770309	26.66937755	26.73945415	Kcal mol ⁻¹
Average free energy		26.70884493		Kcal mol ⁻¹
Half-life	2213160.402	2039728.443	2295960.858	s
	614.7667784	566.5912342	637.7669051	h
	25.61528243	23.60796809	26.57362105	d
K_{eq}	1.02	1.02	1.02	
k_{a-eq}	3.13E-07	3.40E-07	3.02E-07	
k_{b-a}	1.55E-07	1.68E-07	1.49E-07	
Free energy	111835.9351	111633.7411	111926.9415	J
	26.72943	26.68110446	26.75118106	Kcal mol ⁻¹
Average free energy		26.72057184		Kcal mol ⁻¹
Half-life	2213160.402	2039728.443	2295960.858	s
	614.7667784	566.5912342	637.7669051	h
	25.61528243	23.60796809	26.57362105	d

Table S2: Free energy and half-life calculated from the rate constants, k_{A-to-B} and k_{B-to-A} , and the equilibrium constant, K_{eq} for **18**.

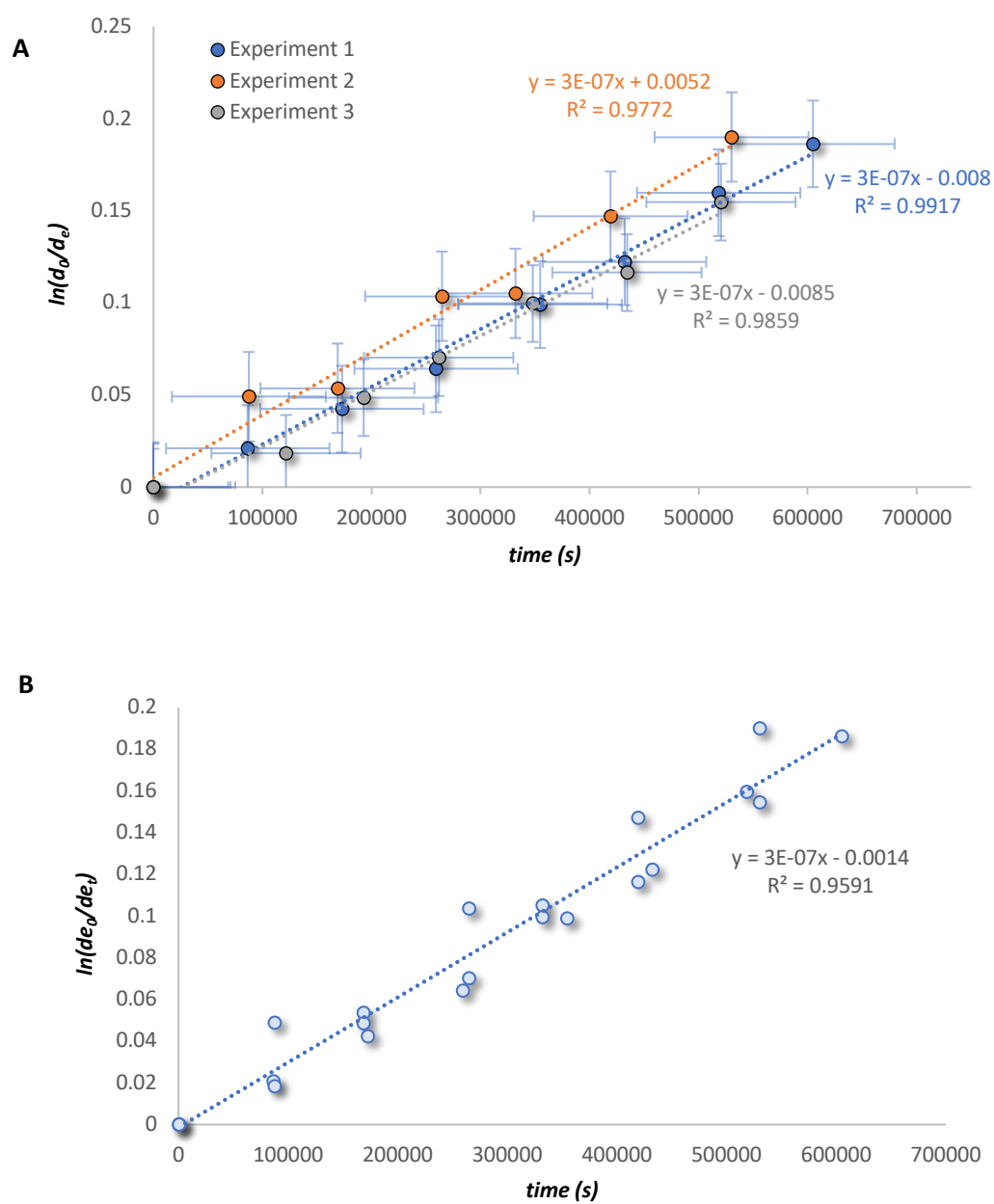


Figure S9: Graphs to show the correlation between $\ln(d_o/d_e)$ and time for inversion barrier experiments 1, 2 and 3 for **18**.
A linear correlations for each of the three experiments; **B** correlation for all three combined datasets.

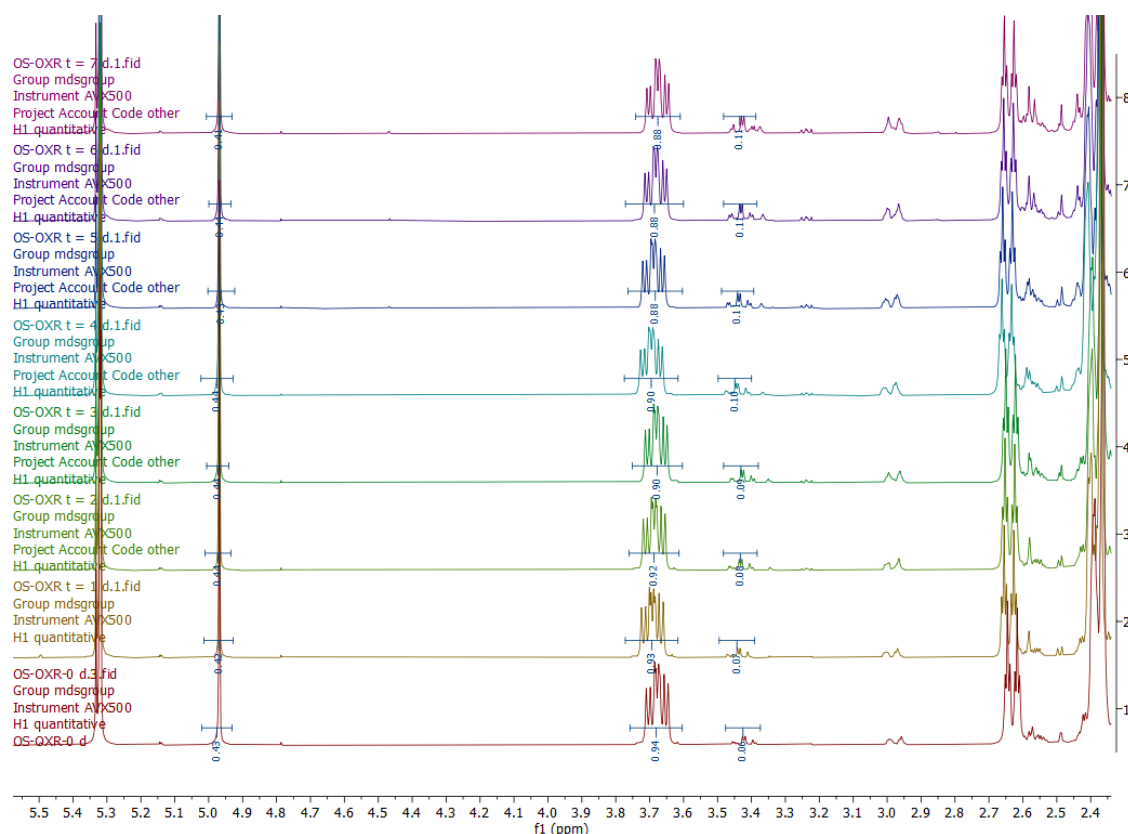


Figure S10: ^1H NMR spectra to show the thermal equilibration at 298K of enriched diastereomer **18** over 7 days (starting dr 94:6).

5.3 Enantiomeric ratio erosion study of 11,13-dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium hexafluorophosphate, enantioenriched-[*M*, (*S*)_o]-**17**:[‡]

Three samples were prepared from the same enantioenriched material **17** at 97:3 e.r., and were dissolved in CH_2Cl_2 in a screw cap vial. The samples were maintained at 298 K for the duration of the experiment (using a Cambridge Reactor Design Polar Bear Plus). Aliquots were taken from each sample over 5 days and dissolved in MeOH. The e.r. was monitored by HPLC.

Chiral HPLC: (2x Chiralpak IC, 95% 100 mM NaPF_6 in MeOH, 5% H_2O , 1.0 mL min^{-1} , $\lambda = 270 \text{ nm}$) τ_R (major) = 22.1 min, τ_R (minor) = 23.4 min).

[‡] The absolute configuration of the major enantiomer in this 97:3 ratio was correlated with the known absolute configuration of **18** separated in the resolution process. This was achieved by comparing the HPLC retention times (under the above conditions: MeOH/ H_2O , 10:1, 100mM NaPF_6) of the major/minor enantiomers of **17** with that of a sample of highly diastereoenriched **18** under these conditions. We assume that complete counterion metathesis to generate enantioenriched **17** occurs under these conditions.

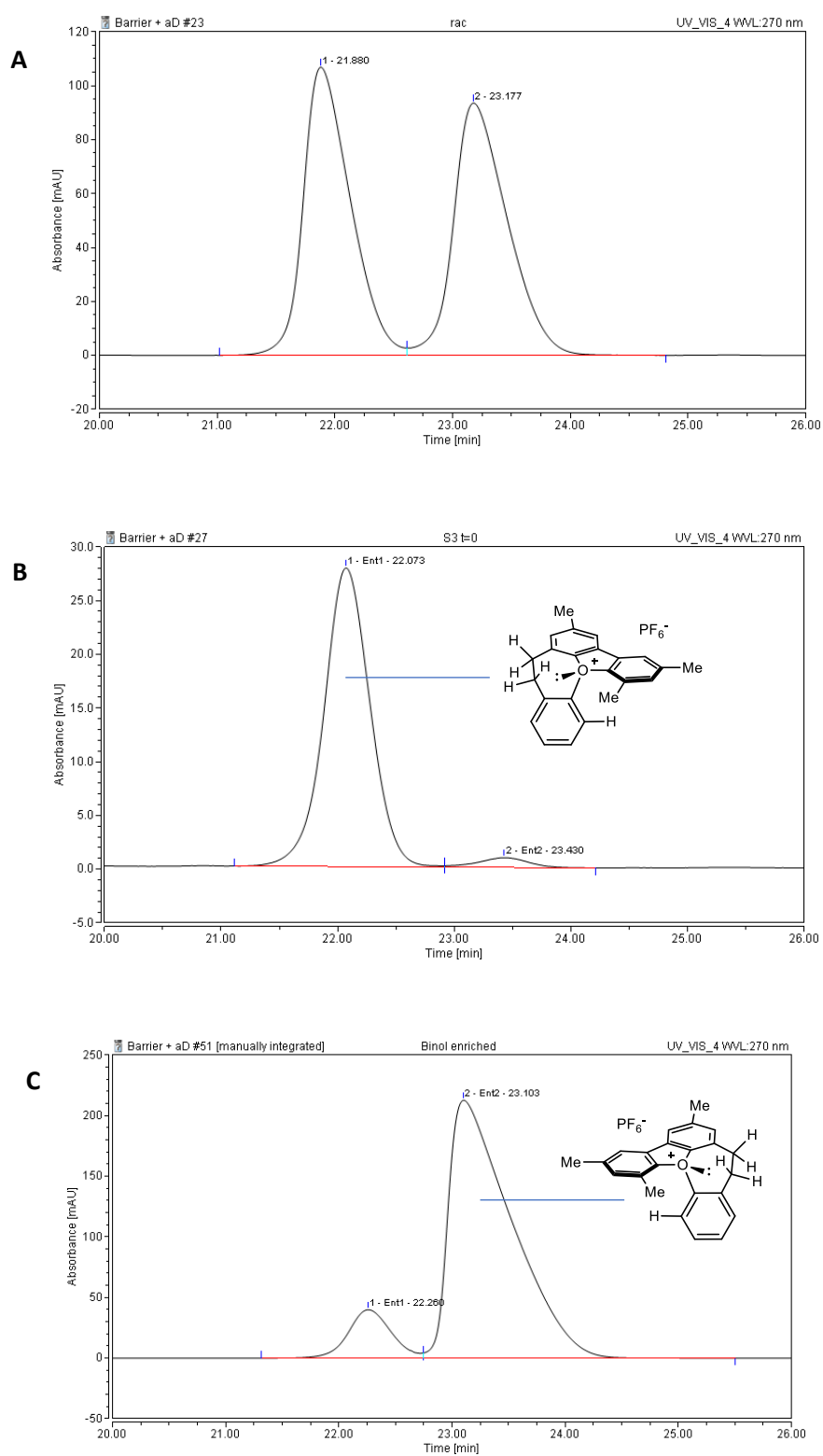


Figure S11: HPLC chromatograms (2x Chiralpak IC, 95% 100 mM NaPF₆ in MeOH, 5% H₂O, 1.0 mL min⁻¹, λ = 270 nm). **A** racemic **17**; **B** enantioenriched **17** (major enantiomer [*M*, (*S*)_O] after preparative HPLC separation. **C** **18** after *in-situ* counterion metathesis to [PF₆]⁻ salt (showing absolute configuration: [*P*, (*R*)_O]).

		ee			
	Time (h)	S1	S2	S3	Average
S=0	0	92.09	93.11	93.03	92.74
S=1	12.25	91.43	91.65	90.7	91.26
S=2	39.45	86.72	87.52	87.31	87.18
S=3	61.25	82.67	85.46	85.27	84.47
S=4	85.4	78.7	82.8	82.58	81.36
S=5	113.5	73.45	80.14	78.38	77.32

Table S3: Measured erosion of e.r. of enantioenriched **17** over time (3 samples)

	Average $\ln(ee(0)/ee(t))$	Standard deviation	Standard error (SE)
S=0	0	0.567215	0.327481976
S=1	0.016123246	0.497293	0.287112057
S=2	0.06182264	0.414769	0.239467001
S=3	0.093478842	1.558856	0.900006173
S=4	0.130952069	2.306252	1.331515427
S=5	0.181840057	3.467915	2.002201566
k_{rac}	4.4259E-07	s^{-1}	
k_{ent}	2.21295E-07	s^{-1}	
Free energy	111.0	$kJ\ mol^{-1}$	
	26.5	$Kcal\ mol^{-1}$	
Half life	1566115.667	s	
	435.0321296	h	
	18.12633873	d	

Table S4: Calculated $\ln(de_0/d_t)$, k_{rac} , k_{ent} , standard errors, free energy and half life from the measured e.r. of **17**.

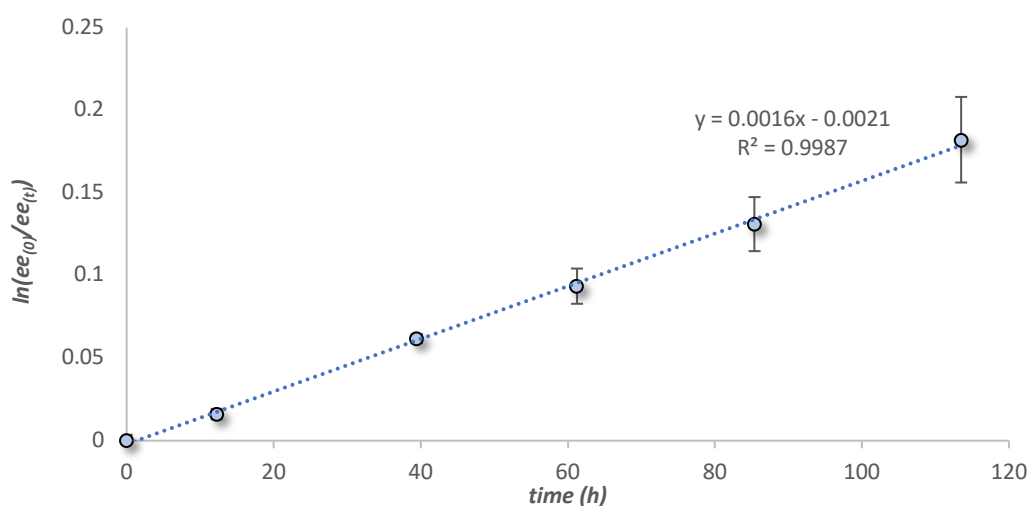


Figure S12: Graph to show the correlation between $\ln(de_0/de_t)$ and time for inversion barrier experiments 1, 2 and 3 for compound **17**.

6 Computational Studies

6.1 Computational details

Gaussian 16 version C.01¹⁸ was employed for all density functional theory (DFT) calculations, using an “ultrafine” pruned (99,590) grid for numerical integration of the exchange-correlation functional and its derivatives. Vibrational frequency calculations were used to verify that stationary points were either minima or first-order saddle points on the potential energy surface, and to calculate thermal corrections to Gibbs free energies (G). Intrinsic reaction coordinate (IRC)¹⁹ calculations were performed to ensure that the transition structures connected to their corresponding starting and final geometries and were used to construct **Figure 4** in the main article. The computed thermochemistry data were corrected following Grimme’s quasi-harmonic (QHA)²⁰ model for entropy with a frequency cut-off value of 100.0 cm⁻¹ using the GoodVibes²¹ program at 298.15 K (25°C). Molecular graphics were generated using CYLview²².

The B3LYP²³ functional in conjunction with Grimme’s D3 dispersion correction method with Becke–Johnson damping²⁴ and Pople’s double- ζ 6-31+G(d,p) basis set²⁵ were used in this study, as it performed best in benchmarking optimization against experimentally determined crystal structure of compound **10** (**Table S3**). Inversion barrier height computed for compound **10** also showed little variation with respect to the level of theory and basis set (**Table S4**). The inclusion of solvation effects with implicit solvation models (PCM,²⁶ CPCM²⁷ and SMD²⁸; solvent=dichloromethane), also did not significantly influence the computed barrier heights (**Table S4**), lowering the barriers by 0.3 to 0.4 kcal·mol⁻¹ relative to the gas phase barrier. This can be rationalised based on the small change in dipole moment between the ground state (1.08 D) and transition state (1.16 D) structures. Similarly, the influence of the tetrafluoroborate (BF₄⁻) non-coordinating counterion was investigated. Grimme’s CREST²⁹ conformational search workflow was used to sample the conformational space of oxonium ion **10** in the presence of the BF₄⁻ counterion, using an energy window of 12 kcal·mol⁻¹. The resulting conformational ensembles for the ground state (**10-BF₄-GS**) and transition state (**10-BF₄-TS**) were then filtered using the in-built *CREGEN* function and further optimised at the B3LYP/6-31+G(d,p)-SMD(CH₂Cl₂) level of theory. Further thermochemical corrections and Boltzmann averaging was applied using the *Goodvibes* program. The final conformational space that was studied can be visualised in **Figure S11**. The computed inversion barrier in the presence of the counterion, obtained as an ensemble average over all of the ion-pair conformations, was found to be very similar as the computed barrier in gas phase at the B3LYP/6-31+G(d,p) in the absence of the counterion (13.1 kcal/mol). As such, further computational investigations were performed in the gas phase in the absence of the counterion.

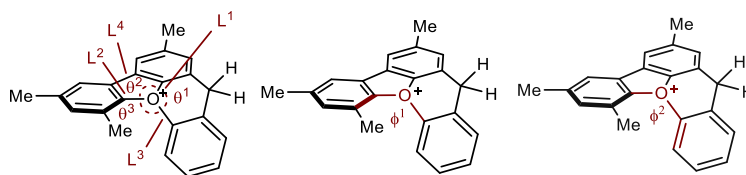


Figure S13: Diagram showing selected bonds, angles and dihedral angles used in benchmarking studies

Theory	Basis Set	L ¹ / Å	L ² / Å	L ³ / Å	L ⁴ / Å	Θ ¹	Θ ²	Θ ³	Φ ¹	Φ ²
Experimental		1.459	1.476	1.491	1.458	110.1	104.3	123.9	9.5	-62.3
M06-2X-D3 ³⁰	6-31+G(d,p)	1.444	1.460	1.471	1.466	111.2	105.2	124.2	5.9	-62.7
M06-2X-D3	Def2-TZVPP ³¹	1.440	1.457	1.467	1.462	111.4	105.2	124.6	6.0	-61.7
B3LYP-D3(BJ)	6-31+G(d,p)	1.456	1.477	1.485	1.464	111.0	105.0	124.6	6.8	-63.3
B3LYP-D3(BJ)	Def2-TZVPP	1.452	1.474	1.480	1.460	111.1	105.0	124.9	6.9	-62.9
wb97x-D ³²	6-31+G(d,p)	1.442	1.462	1.472	1.464	111.2	105.2	124.6	5.6	-63.0
wb97x-D	Def2-TZVPP	1.437	1.458	1.467	1.460	111.3	105.2	125.0	5.7	-62.3

Table S5: Compiled selected bond lengths, angles and dihedrals of compound **10** obtained experimentally and computationally at various levels of theory.

Optimization Method	Optimization Basis Set	Single Point Correction Method	Single Point Correction Basis Set	ΔG / kcal·mol ⁻¹
Experimental				13.9
B3LYP-D3(BJ)	6-31+G(d,p)	N/A		13.1
B3LYP-D3(BJ)-SMD(CH₂Cl₂)^(a)	6-31+G(d,p)	N/A		13.1 ^(b)
B3LYP-D3(BJ)	6-31+G(d,p)	B3LYP-D3(BJ)-SMD(CH ₂ Cl ₂)	6-31+G(d,p)	12.7
B3LYP-D3(BJ)	6-31+G(d,p)	B3LYP-D3(BJ)-PCM(CH ₂ Cl ₂)	6-31+G(d,p)	12.8
B3LYP-D3(BJ)	6-31+G(d,p)	B3LYP-D3(BJ)-CPCM(CH ₂ Cl ₂)	6-31+G(d,p)	12.8
B3LYP-D3(BJ)	6-31+G(d,p)	B3LYP-D3(BJ)	6-31+G(d,p)	12.8
B3LYP-D3(BJ)	6-31+G(d,p)	B3LYP-D3(BJ)	Def2-TZVPP	12.4
B3LYP-D3(BJ)	6-31+G(d,p)	M06-2X-D3	Def2-TZVPP	14.4
B3LYP-D3(BJ)	6-31+G(d,p)	wb97xd	Def2-TZVPP	13.8

Table S6: Compiled free energy of inversion for compound **10** obtained experimentally and computationally at various levels of theory; (a) Calculations include an explicit BF₄⁻ counterion; (b) Gibbs free energy Boltzmann averaged across conformational ensemble.

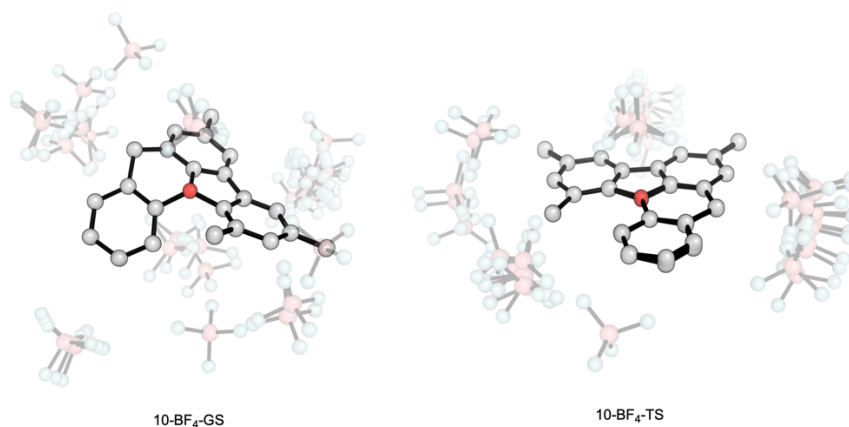


Figure S14: Conformational space sampled for compound **10** when the non-coordinating BF₄⁻ counterion is included. Graphics show several optimised ion-pair conformations superimposed for ground and transition state structures, generated with PyMol³³.

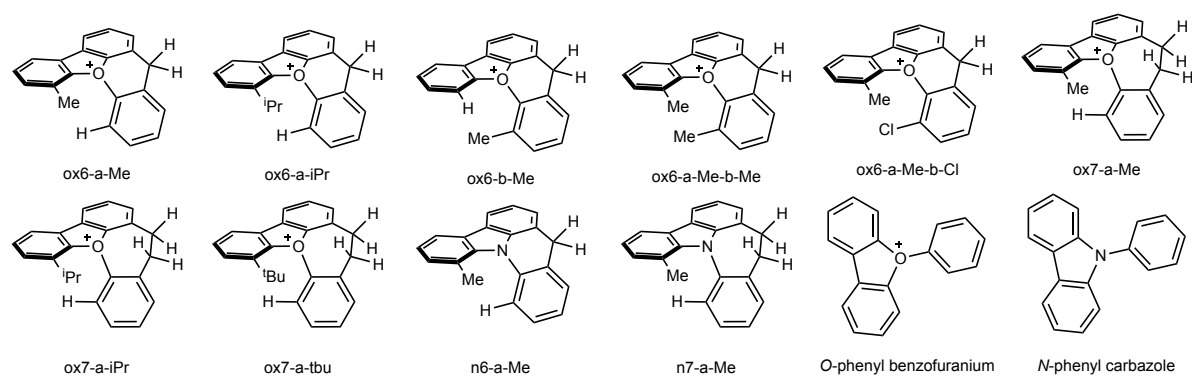


Figure S15: Oxonium ion and triarylamine structures computed in this study.

6.2 Hyperhomodesmotic bond separation reactions

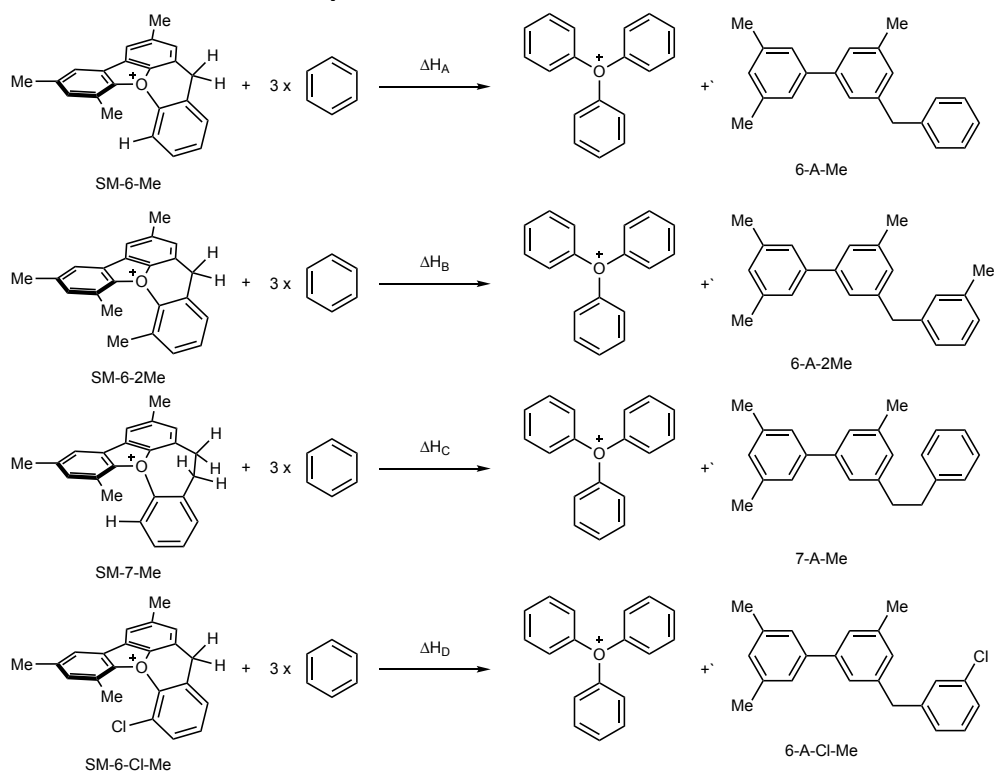


Figure S16: Hyperhomodesmotic transformations used in the estimation of ring strain

Single Point Correction Level of Theory	ΔH_A	ΔH_B	ΔH_C	ΔH_D	$\Delta\Delta(H_A/H_B)$	$\Delta\Delta(H_A/H_C)$	$\Delta\Delta(H_A/H_D)$
N/A	-8.7	-13.0	-4.9	-19.6	4.3	-3.8	10.9
B3LYP-D3(BJ)/6-311+G(d,p)	-8.4	-12.4	-4.7	-18.9	4.0	-3.7	10.5
B3LYP-D3(BJ)/Def2-TZVPP	-6.9	-11.4	-3.4	-17.3	4.5	-3.5	10.4
M06-2X-D3/Def2-TZVPP	-7.1	-11.5	-3.5	-18.1	4.4	-3.6	11.0
wb97x-D ²⁹ /Def2-TZVPP	-5.6	-10.0	-2.5	-17.2	4.4	-3.1	11.6

Table S7: Compiled reaction enthalpies ($\text{kcal} \cdot \text{mol}^{-1}$) for hyperhomodesmotic transformations; geometries were optimised at the B3LYP-D3(BJ)/6-31+G(d,p) level of theory

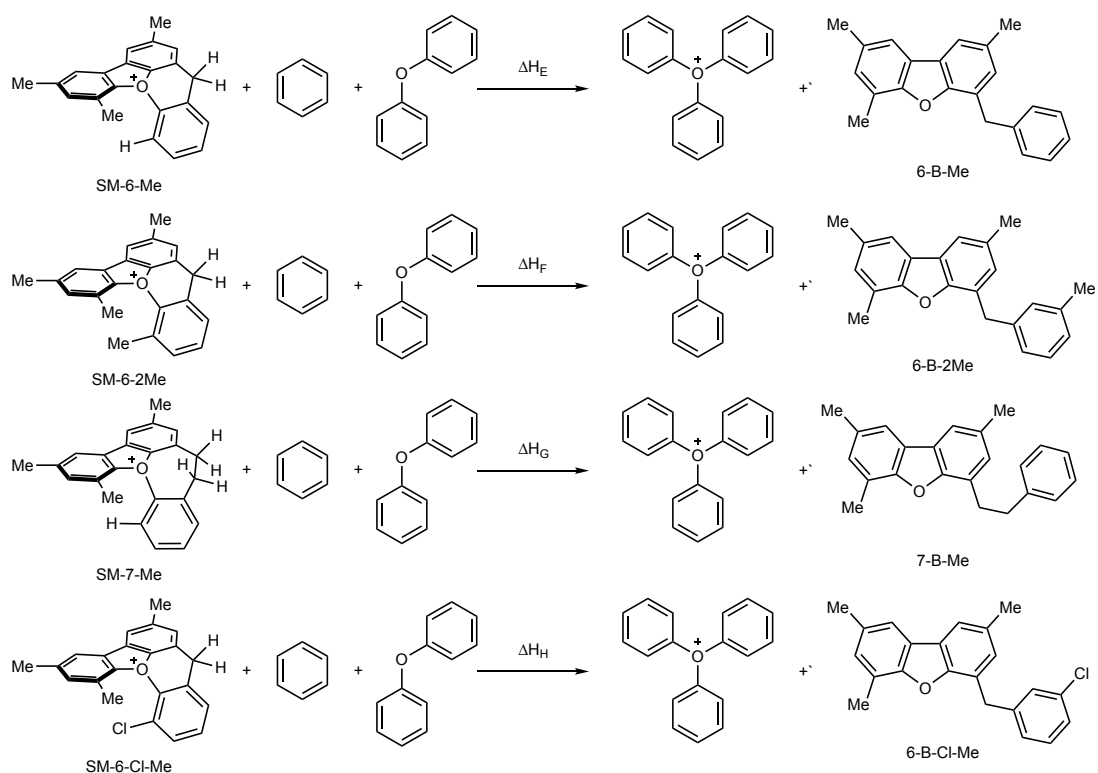


Figure S17: Hyperhomodesmotic transformations used in the estimation of ring strain

Single Point Correction Level of Theory	ΔH_E	ΔH_F	ΔH_G	ΔH_H	$\Delta\Delta(H_E/H_F)$	$\Delta\Delta(H_E/H_G)$	$\Delta\Delta(H_E/H_H)$
N/A	-10.6	-14.9	-7.4	-21.8	4.3	-3.2	11.2
B3LYP-D3(BJ)/6-311+G(d,p)	-10.3	-14.4	-7.3	-21.0	4.1	-3.0	10.7
B3LYP-D3(BJ)/Def2-TZVPP	-9.4	-13.9	-6.4	-20.0	4.5	-3.0	10.6
M06-2X-D3/Def2-TZVPP	-9.4	-13.9	-6.3	-20.6	4.5	-3.1	11.2
wb97xD/Def2-TZVPP	-9.3	-13.9	-6.6	-21.0	4.6	-2.7	11.7

Table S8: Compiled reaction enthalpies ($\text{kcal} \cdot \text{mol}^{-1}$) for hyperhomodesmotic transformations; geometries were optimised at the B3LYP-D3(BJ)/6-31+G(d,p) level of theory

6.3 NBO analysis on ring size influence

In order to further deconvolute the influence of ring size on the enantiomerization activation energy barrier, natural bonding orbital (NBO) analysis was performed for the oxonium ions ox6-a-Me and ox7-a-Me. Calculations used NBO7³⁴ interfaced with Gaussian 16 version C.01. Second-order perturbation theory analysis of the Fock matrices was used to estimate donor-acceptor (i.e. filled to empty) interactions in the NBO basis. Delocalization energies of the oxygen lone pair into adjacent π^* orbitals (for both GS and TS structures) have been compiled in **Table S9**. These results suggest that for ox6-a-Me, the increasing planarity about oxygen in the TS results in a stabilization from increased delocalization by 14.0 kcal mol⁻¹ relative to the GS. In contrast, for ox7-a-Me, there is very little change in delocalization between GS and TS, with the stabilization reduced to 2.9 kJ mol⁻¹.

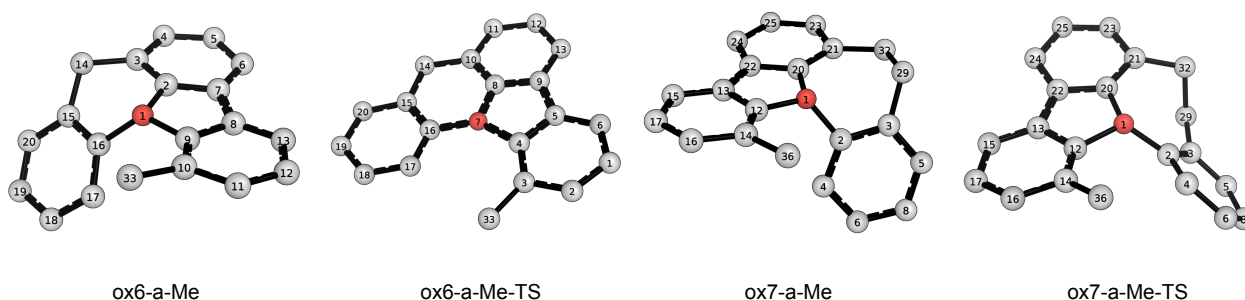


Figure S18: Three-dimensional structures of ox6-a-Me, ox6-a-Me-TS, ox7-a-Me and ox7-a-Me-TS generated using PyMol, together with their corresponding atom indices.

Entry	Donor	Acceptor	E / kcal mol ⁻¹
ox6-a-Me	LP(1)O1	BD*(1)C2-C7	0.77
		BD*(2)C2-C7	7.43
		BD*(1)C8-C9	0.77
		BD*(2)C9-C10	6.59
		BD*(2)C16-C17	0.96
		BD*(2)C16-C17	7.65
		RY*(5)C2	0.72
ox6-a-Me-TS	LP(1)O7	BD*(2)C3-C4	9.55
		BD*(2)C8-C10	14.61
		BD*(2)C15-C16	11.50
ox7-a-Me	LP(1)O1	BD*(1)C2-C3	0.79
		BD*(1)C2-C4	2.59
		BD*(2)C2-C4	3.87
		BD*(1)C12-C13	0.85
		BD*(2)C12-C14	6.82
		BD*(2)C20-C21	6.45
ox7-a-Me-TS	LP(1)O1	BD*(1)C2-C3	1.54
		BD*(2)C2-C3	5.80
		BD*(1)C12-C13	0.55
		BD*(2)C12-C14	5.61
		BD*(2)C20-C22	8.51
		RY(3)C2	0.59

Table S9: Second-order perturbative estimates of the oxygen lone pair delocalization energies for compounds ox6-a-Me and ox7-a-Me

6.4 Comparison between triaryl oxonium ions and triaryl amines

To elucidate the influence of the heteroatom on the activation energy barrier of enantiomerization, the corresponding nitrogen-containing triaryl amines were also investigated computationally (**Figure S19**) at the same level of theory.

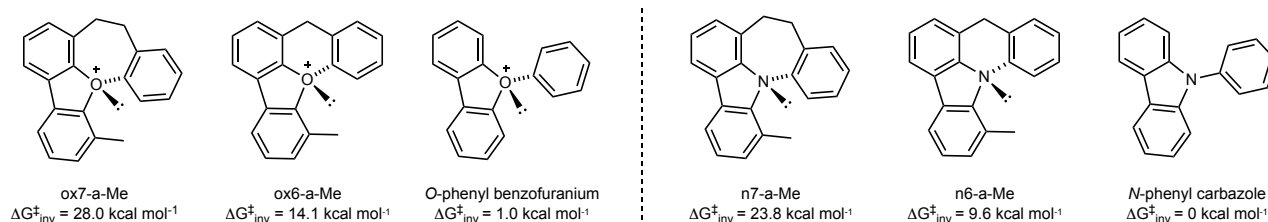


Figure S19: Three-dimensional structures of ox6-a-Me, ox6-a-Me-TS, ox7-a-Me, and ox7-a-Me-TS, together with their corresponding atom indices.

The computed barriers to enantiomerization for the triaryl amines were found to be consistently higher than their oxonium counterpart. The ground state structure of *N*-phenyl carbazole is completely planar. NBO calculations performed on these structures revealed increased delocalization of the heteroatom lone pair in the triarylamine heterocycles, as evidenced by shortened C-N bond lengths, larger C-N Wiberg bond orders (WBO), and decreased nitrogen lone pair orbital occupancy compared to the corresponding oxonium ions (**Figure S20**). Consequently, due to the increased delocalization of the nitrogen atom lone pair, there is little change in lone pair hybridization between GS and TS structures. For n6-a-Me, the p-character of the nitrogen atom changes from 96%p to 100%p from GS to TS, while for n7-a-Me, the p-character changes from 96%p to 97%p. On the other hand, ox6-a-Me has a much larger change in the hybridization of the oxygen atom from 86%p to 100%p on going from GS to TS, while the ox7-a-Me compound has a more modest change from 86%p to 89%p. Compared to triaryl amines, the ground state structures of oxonium ions are characterized by lower lone-pair p-character, less delocalization, and greater pyramidalization of the central heteroatom. Consequently, there is an increase in enantiomerization activation energy barrier due to the associated increase in structural distortion necessary to achieve planarity (or near planarity) in the TS.

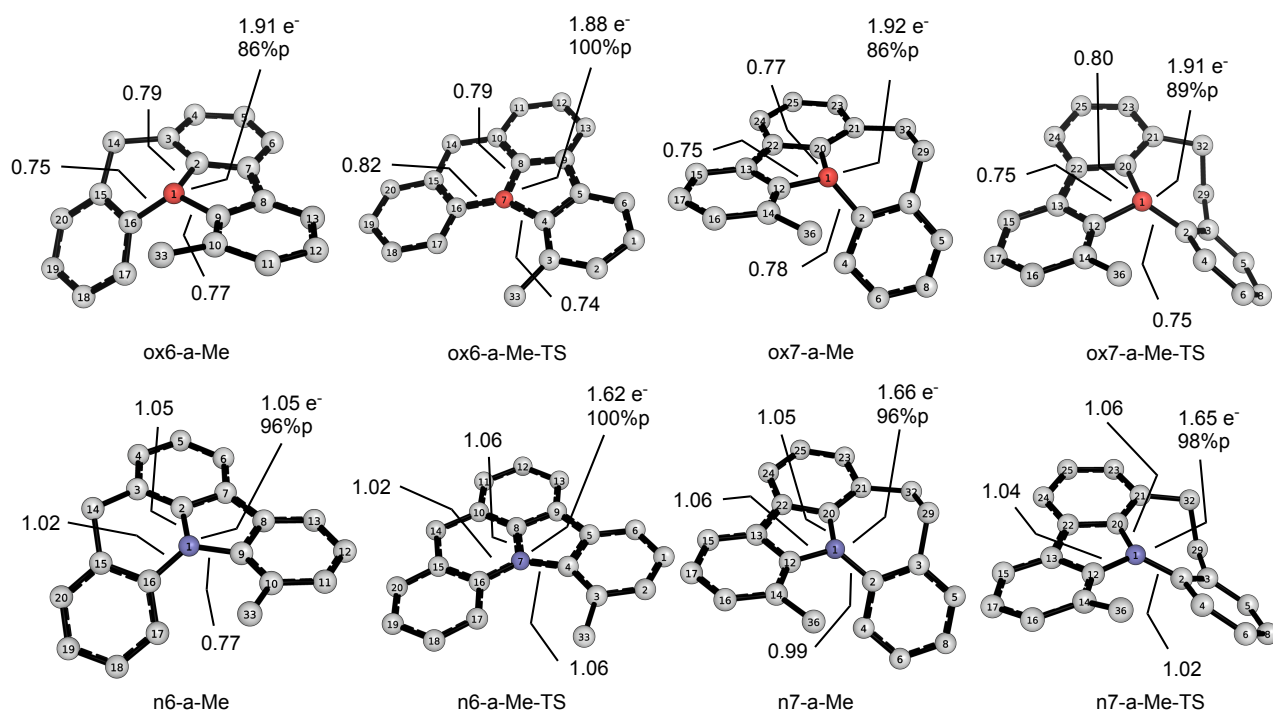


Figure S20: Optimised structures of ox6-a-Me, ox6-a-Me-TS, ox7-a-Me, ox7-a-Me-TS, n6-a-Me, n6-a-Me-TS, n7-a-Me and n7-a-Me-TS generated using PyMol, together with corresponding Wiberg bond orders, lone pair occupancy and %p character of the heteroatom

6.5 Thermochemical data

Name	$E / a.u.$	$ZPE / a.u.$	$H / a.u.$	$T \cdot S / a.u.$	$G / a.u.$	ν_{imag} / cm^{-1}
10-BF4-GS_1	-1349.647827	0.360068	-1349.261207	0.078266	-1349.339474	
10-BF4-GS_10	-1349.645530	0.359786	-1349.259180	0.078147	-1349.337328	
10-BF4-GS_13	-1349.645485	0.359716	-1349.259063	0.078851	-1349.337914	
10-BF4-GS_16	-1349.645767	0.359804	-1349.259553	0.077781	-1349.337333	
10-BF4-GS_17	-1349.644987	0.359797	-1349.258602	0.078106	-1349.336708	
10-BF4-GS_18	-1349.644419	0.359666	-1349.258016	0.079540	-1349.337556	
10-BF4-GS_19	-1349.644428	0.359845	-1349.257889	0.079429	-1349.337318	
10-BF4-GS_20	-1349.644633	0.359890	-1349.258089	0.079022	-1349.337112	
10-BF4-GS_21	-1349.644645	0.359891	-1349.258083	0.079001	-1349.337085	
10-BF4-GS_22	-1349.643938	0.359979	-1349.257334	0.078844	-1349.336178	
10-BF4-GS_23	-1349.644177	0.359459	-1349.257844	0.080491	-1349.338335	
10-BF4-GS_24	-1349.644151	0.359679	-1349.257674	0.080862	-1349.338535	
10-BF4-GS_25	-1349.644165	0.359672	-1349.257667	0.079862	-1349.337529	
10-BF4-GS_26	-1349.644167	0.359713	-1349.257657	0.079620	-1349.337277	
10-BF4-GS_27	-1349.644157	0.359763	-1349.257638	0.079574	-1349.337212	
10-BF4-GS_28	-1349.644219	0.359753	-1349.257698	0.079539	-1349.337237	
10-BF4-GS_30	-1349.644164	0.359601	-1349.257680	0.080204	-1349.337884	
10-BF4-GS_31	-1349.644067	0.359633	-1349.257637	0.079305	-1349.336943	
10-BF4-GS_32	-1349.644171	0.359809	-1349.257647	0.079216	-1349.336864	
10-BF4-GS_34	-1349.644235	0.359781	-1349.257668	0.079521	-1349.337189	
10-BF4-GS_37	-1349.644270	0.359976	-1349.257671	0.078788	-1349.336459	
10-BF4-GS_38	-1349.644184	0.359697	-1349.257670	0.079568	-1349.337239	
10-BF4-GS_39	-1349.644195	0.359916	-1349.257595	0.079117	-1349.336712	
10-BF4-GS_40	-1349.644204	0.359955	-1349.257567	0.079188	-1349.336754	
10-BF4-GS_41	-1349.644179	0.359716	-1349.257660	0.079621	-1349.337281	
10-BF4-GS_42	-1349.644183	0.359901	-1349.257591	0.079010	-1349.336601	
10-BF4-GS_44	-1349.644238	0.359950	-1349.257609	0.079234	-1349.336842	
10-BF4-GS_45	-1349.644160	0.359785	-1349.257622	0.079295	-1349.336917	
10-BF4-GS_46	-1349.643071	0.359835	-1349.256573	0.079092	-1349.335665	
10-BF4-GS_47	-1349.643269	0.359666	-1349.256829	0.079707	-1349.336536	
10-BF4-GS_48	-1349.643310	0.359620	-1349.256933	0.079236	-1349.336169	
10-BF4-GS_49	-1349.642484	0.359874	-1349.255911	0.079493	-1349.335405	
10-BF4-GS_5	-1349.647653	0.359938	-1349.261098	0.078359	-1349.339456	
10-BF4-GS_50	-1349.642421	0.359892	-1349.255959	0.079114	-1349.335073	
10-BF4-GS_51	-1349.642450	0.359855	-1349.255911	0.079470	-1349.335381	
10-BF4-GS_52	-1349.645826	0.359770	-1349.259388	0.078956	-1349.338344	
10-BF4-GS_58	-1349.644542	0.359660	-1349.258131	0.079434	-1349.337565	
10-BF4-GS_59	-1349.644189	0.359582	-1349.257784	0.079694	-1349.337478	
10-BF4-TS_1	-1349.627011	0.359991	-1349.241060	0.076973	-1349.318033	-70.95
10-BF4-TS_10	-1349.623734	0.359872	-1349.237683	0.078886	-1349.316570	-86.95
10-BF4-TS_11	-1349.623805	0.359580	-1349.237970	0.078647	-1349.316618	-70.89

10-BF4-TS_13	-1349.623778	0.359739	-1349.237814	0.078542	-1349.316356	-66.59
10-BF4-TS_14	-1349.623744	0.359891	-1349.237699	0.078829	-1349.316528	-88.54
10-BF4-TS_15	-1349.623648	0.359828	-1349.237692	0.078355	-1349.316047	-93.80
10-BF4-TS_17	-1349.623725	0.359713	-1349.237803	0.078495	-1349.316298	-93.99
10-BF4-TS_18	-1349.623733	0.360133	-1349.237491	0.078109	-1349.315600	-84.02
10-BF4-TS_19	-1349.623262	0.359958	-1349.237208	0.077963	-1349.315172	-69.06
10-BF4-TS_2	-1349.626868	0.359745	-1349.241029	0.077417	-1349.318446	-73.54
10-BF4-TS_20	-1349.623782	0.359983	-1349.237642	0.078407	-1349.316049	-78.69
10-BF4-TS_22	-1349.623729	0.360018	-1349.237637	0.077679	-1349.315316	-83.71
10-BF4-TS_24	-1349.623364	0.360135	-1349.237205	0.077640	-1349.314845	-86.02
10-BF4-TS_26	-1349.623418	0.359867	-1349.237348	0.078598	-1349.315946	-81.21
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10-BF4-TS_29	-1349.623616	0.360006	-1349.237483	0.078083	-1349.315566	-82.48
10-BF4-TS_3	-1349.626768	0.359721	-1349.240961	0.077426	-1349.318387	-78.36
10-BF4-TS_30	-1349.623646	0.360039	-1349.237523	0.078031	-1349.315554	-84.67
10-BF4-TS_31	-1349.623675	0.359973	-1349.237582	0.078248	-1349.315830	-88.51
10-BF4-TS_32	-1349.622935	0.359664	-1349.237081	0.078361	-1349.315442	-73.21
10-BF4-TS_37	-1349.622948	0.359691	-1349.237084	0.078242	-1349.315326	-82.01
10-BF4-TS_38	-1349.626993	0.359879	-1349.241063	0.077388	-1349.318452	-76.15
10-BF4-TS_39	-1349.623516	0.359571	-1349.237749	0.078124	-1349.315873	-66.26
10-BF4-TS_4	-1349.623999	0.359513	-1349.238216	0.078330	-1349.316545	-95.99
10-BF4-TS_40	-1349.622669	0.359702	-1349.236820	0.078024	-1349.314844	-86.99
10-BF4-TS_41	-1349.622666	0.359634	-1349.236826	0.078285	-1349.315111	-86.01
10-BF4-TS_42	-1349.622513	0.359362	-1349.236877	0.079019	-1349.315897	-94.87
10-BF4-TS_43	-1349.622520	0.359527	-1349.236797	0.078641	-1349.315438	-90.38
10-BF4-TS_45	-1349.623733	0.359831	-1349.237741	0.078279	-1349.316020	-82.10
10-BF4-TS_46	-1349.623827	0.359614	-1349.237942	0.078675	-1349.316617	-66.43
10-BF4-TS_47	-1349.622722	0.359740	-1349.236830	0.078068	-1349.314898	-88.32
10-BF4-TS_50	-1349.623806	0.359555	-1349.237979	0.078697	-1349.316677	-69.77
10-BF4-TS_51	-1349.621643	0.359393	-1349.236005	0.078998	-1349.315004	-87.97
10-BF4-TS_52	-1349.622102	0.359545	-1349.236195	0.080104	-1349.316300	-74.20
10-BF4-TS_53	-1349.623212	0.359721	-1349.237265	0.078912	-1349.316177	-77.55
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10-BF4-TS_6	-1349.623688	0.360018	-1349.237593	0.077816	-1349.315408	-79.56
10-BF4-TS_7	-1349.623793	0.360040	-1349.237613	0.078659	-1349.316272	-77.55
10-BF4-TS_9	-1349.623619	0.359952	-1349.237532	0.078706	-1349.316237	-54.14
6-A-2Me-1	-891.105543	0.399508	-890.682287	0.074518	-890.756805	
6-A-2Me-10	-891.104883	0.399443	-890.681639	0.075190	-890.756829	
6-A-2Me-11	-891.104877	0.399440	-890.681632	0.075336	-890.756968	
6-A-2Me-12	-891.105029	0.399454	-890.681790	0.075060	-890.756850	
6-A-2Me-13	-891.105442	0.399496	-890.682178	0.074729	-890.756907	
6-A-2Me-14	-891.105032	0.399451	-890.681796	0.074964	-890.756760	
6-A-2Me-2	-891.104877	0.399441	-890.681632	0.075353	-890.756985	
6-A-2Me-3	-891.105529	0.399501	-890.682266	0.074564	-890.756831	
6-A-2Me-4	-891.105430	0.399487	-890.682161	0.074863	-890.757025	

6-A-2Me-5	-891.104824	0.399539	-890.681602	0.074319	-890.755921
6-A-2Me-6	-891.105033	0.399438	-890.681806	0.075006	-890.756812
6-A-2Me-7	-891.104970	0.399476	-890.681727	0.074811	-890.756538
6-A-2Me-8	-891.105175	0.399506	-890.681918	0.074771	-890.756689
6-A-2Me-9	-891.105123	0.399486	-890.681867	0.074892	-890.756759
6-A-Me-1	-851.779186	0.372214	-851.385088	0.070890	-851.455978
6-A-Me-2	-851.778684	0.372221	-851.384595	0.070803	-851.455398
6-A-Me-3	-851.778795	0.372232	-851.384705	0.070748	-851.455453
6-A-Me-4	-851.778835	0.372245	-851.384731	0.070727	-851.455458
6-A-Me-5	-851.778796	0.372238	-851.384704	0.070674	-851.455378
6-A-Me-6	-851.779186	0.372217	-851.385090	0.070845	-851.455935
6-A-Me-7	-851.778833	0.372230	-851.384730	0.071365	-851.456096
6-A-Me-Cl-1	-1311.377860	0.362643	-1310.992157	0.073546	-1311.065703
6-A-Me-Cl-10	-1311.377387	0.362660	-1310.991648	0.073839	-1311.065487
6-A-Me-Cl-11	-1311.377352	0.362656	-1310.991618	0.073952	-1311.065570
6-A-Me-Cl-12	-1311.377387	0.362634	-1310.991687	0.073820	-1311.065507
6-A-Me-Cl-13	-1311.377784	0.362678	-1310.992038	0.073730	-1311.065768
6-A-Me-Cl-14	-1311.377390	0.362600	-1310.991695	0.074353	-1311.066048
6-A-Me-Cl-2	-1311.377352	0.362657	-1310.991618	0.073950	-1311.065568
6-A-Me-Cl-3	-1311.377847	0.362627	-1310.992136	0.073712	-1311.065847
6-A-Me-Cl-4	-1311.377767	0.362649	-1310.992018	0.074180	-1311.066198
6-A-Me-Cl-5	-1311.377352	0.362659	-1310.991621	0.073926	-1311.065548
6-A-Me-Cl-6	-1311.377401	0.362652	-1310.991707	0.073444	-1311.065151
6-A-Me-Cl-7	-1311.377502	0.362674	-1310.991770	0.073649	-1311.065419
6-A-Me-Cl-8	-1311.377539	0.362623	-1310.991836	0.073985	-1311.065821
6-A-Me-Cl-9	-1311.377514	0.362635	-1310.991792	0.074061	-1311.065853
6-B-2Me-1	-965.126357	0.382722	-964.720376	0.072753	-964.793129
6-B-2Me-2	-965.126236	0.382638	-964.720305	0.072919	-964.793225
6-B-2Me-3	-965.125936	0.382701	-964.719957	0.072625	-964.792583
6-B-2Me-4	-965.126074	0.382833	-964.720003	0.072734	-964.792736
6-B-2Me-5	-965.126357	0.382844	-964.720268	0.072641	-964.792909
6-B-Me-1	-925.799939	0.355459	-925.423132	0.068512	-925.491644
6-B-Me-2	-925.799929	0.355610	-925.422998	0.068370	-925.491368
6-B-Me-Cl-1	-1385.399415	0.345997	-1385.030925	0.070913	-1385.101838
6-B-Me-Cl-2	-1385.398792	0.345852	-1385.030377	0.071409	-1385.101787
6-B-Me-Cl-3	-1385.398042	0.345866	-1385.029583	0.071763	-1385.101347
6-B-Me-Cl-4	-1385.398686	0.346050	-1385.030103	0.071334	-1385.101437
6-B-Me-Cl-5	-1385.399415	0.345997	-1385.030925	0.070912	-1385.101837
7-A-Me-1	-812.449082	0.346400	-812.083391	0.065097	-812.148488
7-A-Me-10	-812.449076	0.346386	-812.083384	0.065178	-812.148562
7-A-Me-11	-812.454213	0.346933	-812.088313	0.063302	-812.151615
7-A-Me-12	-812.453528	0.346856	-812.087666	0.063639	-812.151305
7-A-Me-13	-812.451793	0.346679	-812.086026	0.064313	-812.150339
7-A-Me-14	-812.451712	0.346672	-812.085954	0.064201	-812.150155
7-A-Me-2	-812.451027	0.346650	-812.085290	0.064207	-812.149496

7-A-Me-3	-812.451793	0.346701	-812.086019	0.064129	-812.150148	
7-A-Me-4	-812.451004	0.346655	-812.085258	0.064245	-812.149503	
7-A-Me-5	-812.450989	0.346645	-812.085242	0.064316	-812.149558	
7-A-Me-6	-812.451022	0.346670	-812.085270	0.064195	-812.149465	
7-A-Me-7	-812.451028	0.346650	-812.085289	0.064204	-812.149493	
7-A-Me-8	-812.449135	0.346402	-812.083447	0.065045	-812.148492	
7-A-Me-9	-812.449125	0.346381	-812.083440	0.065234	-812.148674	
7-B-Me-1	-886.472193	0.329645	-886.123715	0.063494	-886.187209	
7-B-Me-2	-886.473973	0.329806	-886.125481	0.063038	-886.188520	
7-B-Me-3	-886.476271	0.330017	-886.127782	0.061762	-886.189545	
C6H6	-232.287286	0.100497	-232.181441	0.032824	-232.214265	
E	-576.702089					
F	-576.706658					
G	-616.021128					
H	-616.008193					
N-phenyl-carbazole	-748.642493	0.257501	-748.370553	0.053691	-748.424245	
O-phenyl-benzoduranium-TS	-768.798989	0.255859	-768.529083	0.052896	-768.581980	-40.70
O-phenyl-benzoduranium	-768.800035	0.256076	-768.529167	0.054445	-768.583611	
Ph2O	-538.594283	0.185231	-538.398110	0.046503	-538.444612	
Ph3O+	-770.000999	0.277311	-769.707535	0.057346	-769.764881	
SM-6-2Me	-964.219667	0.373436	-963.824456	0.067934	-963.892390	
SM-6-Cl-Me	-1384.480878	0.335461	-1384.123813	0.068005	-1384.191818	
SM-6-Me	-924.900062	0.345769	-924.534185	0.064773	-924.598959	
SM-7-Me	-885.575527	0.320362	-885.237813	0.059031	-885.296844	
n6-a-Me-TS	-826.069407	0.293082	-825.761280	0.054456	-825.815736	-94.65
n6-a-Me	-826.083509	0.292610	-825.775061	0.056052	-825.831113	
n7-a-Me-1	-865.409317	0.321654	-865.070747	0.058156	-865.128903	
n7-a-Me-TS	-865.372893	0.322196	-865.034747	0.056126	-865.090874	-92.16
ox6-H-TS	-806.908696	0.263096	-806.631421	0.052936	-806.684357	-79.91
ox6-H	-806.915549	0.263659	-806.637337	0.053585	-806.690922	
ox6-a-Cl-b-Me-TS	-1305.784390	0.278039	-1305.488644	0.060177	-1305.548821	-26.82
ox6-a-Cl-b-Me	-1305.824625	0.281069	-1305.525896	0.059899	-1305.585795	
ox6-a-Me-TS	-846.221794	0.291309	-845.914881	0.055553	-845.970434	-93.77
ox6-a-Me-b-Me-TS	-885.507343	0.318349	-885.171898	0.058242	-885.230140	-93.64
ox6-a-Me-b-Me	-885.563552	0.319020	-885.226689	0.059833	-885.286522	
ox6-a-Me	-846.243659	0.291333	-845.936126	0.056759	-845.992885	
ox6-a-iPr-TS	-924.862654	0.347859	-924.496413	0.061016	-924.557429	-65.44
ox6-a-iPr	-924.890632	0.348172	-924.523553	0.061993	-924.585546	
ox6-b-Me-TS	-846.214393	0.291320	-845.907679	0.055022	-845.962701	-86.31
ox6-b-Me	-846.234364	0.291359	-845.926865	0.056534	-845.983399	
ox7-a-Me-1	-885.575527	0.320362	-885.237813	0.059031	-885.296844	
ox7-a-Me-2	-885.562895	0.320097	-885.225276	0.059437	-885.284713	
ox7-a-Me-TS	-885.532520	0.320647	-885.195555	0.056739	-885.252294	-73.17
ox7-a-Me-flip-TS	-885.562366	0.319888	-885.225635	0.058113	-885.283748	-96.30

ox7-a-iPr-1	-964.222406	0.377222	-963.825127	0.064209	-963.889336	
ox7-a-iPr-2	-964.210020	0.376933	-963.812859	0.064637	-963.877496	
ox7-a-iPr-TS	-964.174714	0.377021	-963.778512	0.062345	-963.840857	-50.55
ox7-a-tBu-1	-1003.539358	0.405399	-1003.112789	0.066004	-1003.178793	
ox7-a-tBu-2	-1003.528463	0.405092	-1003.102037	0.066417	-1003.168455	
ox7-a-tBu-TS	-1003.481295	0.405314	-1003.055651	0.064334	-1003.119985	-46.01

Table S10: Compiled thermochemical data for structures computed at the B3LYP-D3/6-31+G(d,p) level of theory

6.6 Cartesian coordinates for stationary points

47			C	-1.656998	-0.473760	-0.633039	C	2.812645	-3.239069	-0.333838	
10-BF4-GS_1	Eopt		C	-2.702605	-1.373652	-0.621338	C	3.062697	2.131753	-1.146875	
-1349.647827			C	-3.905993	-0.820747	-0.135882	H	2.796567	2.870658	-1.783840	
O	-0.119303	-0.311896	-0.365234	C	-4.047902	0.524028	0.239120	H	2.129223	4.926650	0.140436
C	-0.373447	1.113682	-0.330469	C	-2.959189	1.400917	0.090099	H	1.789808	5.276850	-1.556666
C	-1.653422	1.594955	-0.233440	C	-5.361464	1.030652	0.776436	H	0.518915	5.487128	-0.335437
C	-1.730964	2.992730	-0.237821	C	-2.646446	-2.794383	-1.118713	H	-1.002886	3.699057	0.095548
C	-0.574197	3.798614	-0.335379	C	2.322733	-0.609218	-2.125861	H	-4.575211	-1.905232	-0.264335
C	-0.718469	5.300533	-0.309345	C	1.903227	-1.732708	-1.194897	H	-3.334018	2.115880	0.642364
C	0.698700	3.213811	-0.450242	C	0.623762	-1.792971	-0.646169	H	-6.190167	-0.309445	0.544525
C	0.806054	1.818261	-0.456951	C	0.207579	-2.680080	0.323968	H	-5.385780	0.230675	2.023990
C	1.890668	0.840013	-0.528086	C	1.131739	-3.646327	0.738142	H	-5.753871	1.400625	0.753488
C	1.343035	-0.447017	-0.436042	C	2.414980	-3.669506	0.190546	H	-2.155367	-3.609808	-0.770755
C	2.047250	-1.616178	-0.226038	C	2.799645	-2.712257	-0.751464	H	-1.489688	-2.780560	-2.185345
C	3.445314	-1.439151	-0.278547	H	3.125534	2.159793	-2.051842	H	-3.232484	-3.068405	-2.059615
C	4.065845	-0.193457	-0.455363	H	2.458847	4.657497	-2.148715	H	3.377107	0.302434	-2.197442
C	3.276753	0.964720	-0.550439	H	1.148676	5.199866	-1.080402	H	2.042232	-0.079406	-3.287868
C	5.568953	-0.091949	-0.513755	H	2.638748	4.536529	-0.394157	H	-0.460415	-2.650314	0.404463
C	1.440670	-2.954337	0.099024	H	-0.565691	3.668111	-0.392200	H	1.359435	-4.267917	0.890842
C	-2.765896	0.579329	-0.171034	H	-4.771920	-1.473371	-0.082272	H	3.617132	-3.931008	-0.107260
C	-2.411097	-0.593851	-1.064330	H	-3.065751	2.458336	0.307728	H	4.060675	-1.950848	-1.534036
C	-1.092851	-1.021040	-1.219196	H	-5.559215	2.054131	0.439447	B	1.343207	0.055782	2.636098
C	-0.661837	-1.981734	-2.110523	H	-6.192241	0.393161	0.463984	F	1.219203	1.083374	3.601399
C	-1.641447	-2.629813	-2.869979	H	-5.344197	1.044125	1.873214	F	0.088960	-0.165005	2.025620
C	-2.985247	-2.281452	-2.725674	H	-1.793814	-2.964053	-1.779611	F	2.287935	0.441359	1.660773
C	-3.359615	-1.262958	-1.845763	H	-3.559436	-3.018764	-1.674289	F	1.774820	-1.133495	3.268406
H	-2.705282	3.467375	-0.164312	H	-2.579932	-3.506194	-0.289759	47			
H	0.228767	5.793977	-0.541974	H	3.406137	-0.488105	-2.094250	10-BF4-GS_16	Eopt		
H	-1.469610	5.637533	-1.031572	H	2.048894	-0.855928	-3.160589	-1349.645767			
H	-1.043028	5.641325	0.680881	H	-0.771417	-2.618627	0.774788	O	0.566560	-0.312099	-1.248351
H	1.582399	3.837714	-0.531856	H	0.840047	-4.358016	1.500479	C	1.096348	0.968292	-0.816219
H	4.066113	-2.318782	-0.132653	H	3.130054	-4.415406	0.520776	C	2.449024	1.175817	-0.744856
H	3.736973	1.945708	-0.607542	H	3.813550	-2.699171	-1.134730	C	2.798401	2.448898	-0.279361
H	5.910269	-0.024621	-1.554185	B	1.331357	0.649182	2.502461	C	1.817425	3.400605	0.079538
H	5.924601	0.803081	0.005772	F	0.178075	-0.022399	2.036441	C	2.256107	4.751561	0.591362
H	6.044293	-0.967488	-0.063397	F	2.420690	0.378801	1.647239	C	0.449530	3.092327	-0.017199
H	1.432255	-3.613588	-0.775588	F	1.084806	2.040763	2.532280	C	0.070608	1.825273	-0.474148
H	0.420527	-2.858074	0.472633	F	1.636449	0.201340	3.809719	C	-1.186136	1.122222	-0.722666
H	2.041817	-3.440529	0.872143	47				C	-0.898637	-0.153553	-1.221970
H	-3.717351	1.013485	-0.483531	10-BF4-GS_13	Eopt			C	-1.802933	-1.030635	-1.785545
H	-2.877198	0.237157	0.865669	-1349.645485				C	-3.139537	-0.599805	-1.668338
H	0.385056	-2.220120	-2.231589	O	-0.253562	-0.513680	-1.267672	C	-3.513225	0.624018	-1.092302
H	-1.341002	-3.397674	-3.574654	C	0.236102	0.851293	-1.181052	C	-2.519986	1.510615	-0.645392
H	-3.743064	-2.786755	-3.315507	C	1.483858	1.175225	-1.645117	C	-4.969240	0.987961	-0.957417
H	-4.400251	-0.964288	-1.764957	C	1.821550	2.520676	-1.456903	C	-1.454012	-2.306041	-2.503336
B	-0.905347	-0.915276	2.934148	C	0.932032	3.427477	-0.839013	C	3.345468	0.024698	-1.129628
F	-1.301618	-1.840724	1.941373	C	1.361170	4.860232	-0.639292	C	2.705726	-1.274498	-0.675141
F	-0.696439	-1.595719	4.154285	C	-0.328198	2.999678	-0.386485	C	1.323260	-1.445664	-0.665045
F	0.290090	-0.276316	2.539383	C	-0.689725	1.658706	-0.553736	C	0.648512	-2.517721	-0.119610
F	-1.923549	0.053187	3.100927	C	-1.856538	0.831452	-0.252810	C	1.428650	-3.561237	0.387080
47				C	-1.615340	-0.471585	-0.707181	C	2.822214	-3.480010	0.352715
10-BF4-GS_10	Eopt			C	-2.547573	-1.484807	-0.806821	C	3.449643	-2.339844	-0.154086
-1349.645530				C	-3.794090	-1.150407	-0.238245	H	3.849420	2.706213	-0.183145
O	-0.303786	-0.749080	-1.150644	C	-4.081595	0.104714	0.318484	H	2.808290	4.648340	1.533329
C	0.342867	0.547654	-1.238462	C	-3.109199	1.117976	0.280499	H	2.921224	5.246614	-0.125648
C	1.623330	0.661516	-1.712171	C	-5.430134	0.371720	0.937003	H	1.396395	5.403867	0.770920
C	2.112768	1.972631	-1.702994	C	-2.334159	-2.807204	-1.493670	H	-0.298258	3.822759	0.272118
C	1.329372	3.052958	-1.238963	C	2.313312	0.060677	-2.232299	H	-3.912259	-1.246259	-2.073674
C	1.922100	4.439367	-1.218370	C	2.050328	-1.215485	-1.454082	H	-2.783643	2.488067	-0.256451
C	0.025407	2.838414	-0.761561	C	0.799569	-1.496650	-0.909036	H	-5.119302	2.069729	-1.056506
C	-0.485849	1.536045	-0.749748	C	0.510016	-2.540983	-0.057114	H	-5.579575	0.476396	-1.710447
C	-1.745317	0.899139	-0.364658	C	1.547106	-3.435647	0.221259	H	-5.342766	0.690508	0.034346

H -1.620383 -3.181533 -1.866788
H -0.413657 -2.319720 -2.832672
H -2.094209 -2.412488 -3.382913
H 4.333957 0.128163 -0.679256
H 3.483112 0.016692 -2.219601
H -0.428770 -2.532264 -0.041032
H 0.935092 -4.422019 0.825955
H 3.422411 -4.291875 0.750213
H 4.531484 -2.253475 -0.127536
B -1.162948 -0.532772 2.630329
F -0.914131 -1.069865 3.915466
F 0.063376 -0.183673 2.022024
F -1.827951 -1.500562 1.843057
F -1.973468 0.618907 2.749825

47
10-BF4-GS_17 Eopt
-1349.644987

O 0.239247 -1.000463 -1.088682
C 0.657465 0.378369 -1.279605
C 1.963456 0.680297 -1.559462
C 2.209417 2.054350 -1.681667
C 1.180761 3.007318 -1.518865
C 1.507335 4.477079 -1.615719
C -0.132439 2.600675 -1.222350
C -0.405374 1.236867 -1.086678
C -1.581792 0.418196 -0.802230
C -1.211760 -0.932697 -0.831149
C -2.073483 -2.011916 -0.834077
C -3.419888 -1.647137 -0.626857
C -3.853894 -0.319750 -0.494080
C -2.925424 0.726888 -0.616767
C -5.307866 -0.014802 -0.239689
C -1.686749 -3.445228 -1.084195
C 2.933570 -0.470514 -1.656302
C 2.552633 -1.526844 -0.635430
C 1.224450 -1.768287 -0.290051
C 0.797619 -2.591872 0.729972
C 1.781243 -3.302016 1.424475
C 3.128132 -3.143629 1.093329
C 3.506950 -2.251941 0.087661
H 3.219270 2.391961 -1.896194
H 0.622544 5.063358 -1.878419
H 1.877812 4.849042 -0.652545
H 2.284303 4.664447 -2.362816
H -0.915731 3.338087 -1.083458
H -4.155716 -2.446083 -0.598099
H -3.248266 1.762077 -0.583291
H -5.947372 -0.853778 -0.527057
H -5.474235 0.183413 0.826246
H -5.628440 0.874484 -0.790883
H -0.724757 -3.529698 -1.593807
H -2.448114 -3.919402 -1.709364
H -1.627085 -4.013560 -0.150221
H 3.958354 -0.138407 -1.480285
H 2.896038 -0.895792 -2.668719
H -0.243577 -2.665635 1.008268
H 1.483876 -3.959830 2.233944
H 3.888984 -3.691846 1.639255
H 4.557350 -2.090829 -0.134842
B -0.033010 1.467526 2.669507
F -1.430040 1.592771 2.492306
F 0.605850 2.651975 2.238415
F 0.248061 1.253699 4.039980
F 0.443870 0.370846 1.918480

47
10-BF4-GS_19 Eopt
-1349.644428

O 1.260516 -0.571243 0.488524
C 0.446167 0.596197 0.183121
C -0.921254 0.524745 0.244450
C -1.563228 1.717421 -0.110919
C -0.829852 2.863761 -0.493700
C -1.576261 4.127069 -0.844999
C 0.574925 2.835036 -0.548518
C 1.242945 1.652877 -0.207258
C 2.633805 1.207851 -0.114304
C 2.653154 -0.118598 0.337859
C 3.762765 -0.815181 0.775229
C 4.971328 -0.117838 0.573289
C 5.039172 1.179132 0.041396
C 3.852568 1.860993 -0.276770

10-BF4-GS_18 Eopt
-1349.644419
O -1.283651 0.584220 0.678406
C -0.443858 -0.600190 0.569551
C 0.883187 -0.545469 0.906170
C 1.562702 -1.752964 0.710408
C 0.906880 -2.898282 0.204781
C 1.692330 -4.172927 0.024726
C -0.457133 -2.852338 -0.134516
C -1.160407 -1.655323 0.042001
C -2.533182 -1.190906 -0.162496
C -2.623534 0.144794 0.251231
C -3.787375 0.864966 0.432687
C -4.939371 0.179404 -0.004867
C -4.916365 -1.128968 -0.514425
C -3.701510 -1.831517 -0.564373
C -6.189707 -1.784278 -0.985978
C -3.881608 2.220728 1.078076
C 1.422013 0.785325 1.369612
C 0.748915 1.885658 0.571454
C -0.579406 1.787570 0.162440
C -1.228920 2.659349 -0.686788
C -0.504930 3.775950 -1.119650
C 0.817702 3.957009 -0.709722
C 1.439367 3.014040 0.111849
H 2.623079 -1.800726 0.935914
H 2.583469 -3.996503 -0.586732
H 2.034584 -4.559503 0.991966
H 1.089108 -4.946294 -0.457539
H -0.950195 -3.731427 -0.535855
H -5.893417 0.688869 0.092865
H -3.674612 -2.868204 -0.883655
H -6.202126 -2.850089 -0.735271
H -7.069678 -1.309769 -0.541696
H -6.280295 -1.702292 -2.077208
H -4.755963 2.248640 1.733304
H -4.003782 3.012307 0.331209
H -2.997299 2.453441 1.676533
H 2.502507 0.834372 1.238082
H 1.208857 0.913511 2.439744
H -2.242216 2.489498 -1.021833
H -0.981222 4.488364 -1.784452
H 1.377020 4.821055 -1.052714
H 2.483190 3.128220 0.386112
B 4.982416 -0.174486 -0.365282
F 4.737134 -0.172284 1.029400
F 4.014600 0.624860 -1.012927
F 6.270548 0.348098 -0.615900
F 4.905651 -1.498963 -0.851979

47
10-BF4-GS_19 Eopt
-1349.644428
O 1.260516 -0.571243 0.488524
C 0.446167 0.596197 0.183121
C -0.921254 0.524745 0.244450
C -1.563228 1.717421 -0.110919
C -0.829852 2.863761 -0.493700
C -1.576261 4.127069 -0.844999
C 0.574925 2.835036 -0.548518
C 1.242945 1.652877 -0.207258
C 2.633805 1.207851 -0.114304
C 2.653154 -0.118598 0.337859
C 3.762765 -0.815181 0.775229
C 4.971328 -0.117838 0.573289
C 5.039172 1.179132 0.041396
C 3.852568 1.860993 -0.276770

47
10-BF4-GS_20 Eopt
-1349.644633
O 1.265183 0.572346 -0.635824
C 0.472506 -0.638087 -0.478544
C -0.869649 -0.630567 -0.753280
C -1.499817 -1.857808 -0.513454
C -0.780755 -2.974778 -0.030537
C -1.514545 -4.271879 0.200928
C 0.594649 -2.881635 0.242715
C 1.248985 -1.663346 0.021710
C 2.613226 -1.152349 0.154385
C 2.637870 0.182969 -0.270441
C 3.768232 0.940248 -0.511214
C 4.961313 0.295106 -0.129250
C 5.008252 -1.008466 0.386482
C 3.821281 -1.751443 0.501925
C 6.325715 -1.618374 0.795540
C 3.785494 2.297757 -1.161870
C -1.472214 0.676129 -1.205771
C -0.804096 1.806618 -0.445989
C 0.543977 1.755360 -0.095962
C 1.200419 2.652873 0.720527
C 0.460836 3.749648 1.174946
C -0.882996 3.884838 0.822254
C -1.509670 2.915157 0.035389
H -2.568552 -1.941697 -0.686331
H -0.866132 -5.017704 0.667716
H -2.384894 -4.117927 0.848236
H -1.884169 -4.684682 -0.745022
H 1.135999 -3.739743 0.626530
H 5.892358 0.835607 -0.276748
H 3.844908 -2.785815 0.827497

C 6.375147 1.846220 -0.164694
C 3.735094 -2.157402 1.455946
C -1.524774 -0.804829 0.622657
C -0.690268 -1.911575 0.006346
C 0.691900 -1.796235 -0.131111
C 1.510560 -2.672484 -0.813170
C 0.904555 -3.813893 -1.348997
C -0.469190 -4.014808 -1.202400
C -1.257396 -3.065056 -0.548071
H -2.648403 1.754251 -0.101725
H -0.906408 4.878807 -1.270505
H -2.373739 3.923520 -1.567056
H -2.049171 4.557475 0.045490
H 1.128921 3.715539 -0.856232
H 5.890656 -0.608837 0.880225
H 3.879927 2.891176 -0.616225
H 7.138017 1.419806 0.492350
H 6.714441 1.712437 -1.199356
H 6.313525 2.922218 0.023288
H 2.756070 -2.378407 1.886933
H 4.475179 -2.169593 2.260466
H 3.989164 -2.964877 0.761387
H -2.557531 -0.881986 0.283083
H -1.531310 -0.904052 1.716760
H 2.567019 -2.487505 -0.946681
H 1.514530 -4.531729 -1.886819
H -0.934933 -4.900384 -1.622160
H -2.332338 -3.197823 -0.477031
B -5.332319 0.173155 0.334923
F -4.955822 1.367663 -0.323119
F -4.813334 0.178542 1.649525
F -6.738969 0.079423 0.378995
F -4.806022 -0.935216 -0.372211

47
10-BF4-GS_20 Eopt
-1349.644633

O 1.265183 0.572346 -0.635824
C 0.472506 -0.638087 -0.478544
C -0.869649 -0.630567 -0.753280
C -1.499817 -1.857808 -0.513454
C -0.780755 -2.974778 -0.030537
C -1.514545 -4.271879 0.200928
C 0.594649 -2.881635 0.242715
C 1.248985 -1.663346 0.021710
C 2.613226 -1.152349 0.154385
C 2.637870 0.182969 -0.270441
C 3.768232 0.940248 -0.511214
C 4.961313 0.295106 -0.129250
C 5.008252 -1.008466 0.386482
C 3.821281 -1.751443 0.501925
C 6.325715 -1.618374 0.795540
C 3.785494 2.297757 -1.161870
C -1.472214 0.676129 -1.205771
C -0.804096 1.806618 -0.445989
C 0.543977 1.755360 -0.095962
C 1.200419 2.652873 0.720527
C 0.460836 3.749648 1.174946
C -0.882996 3.884838 0.822254
C -1.509670 2.915157 0.035389
H -2.568552 -1.941697 -0.686331
H -0.866132 -5.017704 0.667716
H -2.384894 -4.117927 0.848236
H -1.884169 -4.684682 -0.745022
H 1.135999 -3.739743 0.626530
H 5.892358 0.835607 -0.276748
H 3.844908 -2.785815 0.827497

H	6.337721	-2.695846	0.607915	F	6.407447	0.163043	0.685960	C	5.283438	0.031078	0.049981
H	7.159865	-1.160008	0.257289	47				C	4.364899	1.058506	-0.223783
H	6.499386	-1.468203	1.868297	10-BF4-GS_22			Eopt	C	6.759625	0.263933	-0.146699
H	3.914156	3.094860	-0.422018	-1349.643938				C	3.015682	-2.801288	1.339729
H	2.868059	2.498897	-1.719334	O	-1.135548	0.584399	0.315240	C	-1.574916	0.148444	0.631465
H	4.627921	2.354185	-1.856250	C	-0.195685	-0.349990	-0.287065	C	-1.125402	-1.137223	-0.036144
H	-2.548771	0.698729	-1.035213	C	1.106893	0.016421	-0.505772	C	0.224079	-1.452614	-0.184865
H	-1.304704	0.800133	-2.285261	C	1.876518	-0.983079	-1.112053	C	0.730632	-2.516892	-0.901786
H	2.232461	2.516455	1.011040	C	1.323236	-2.237649	-1.454194	C	-0.201081	-3.392012	-1.469900
H	0.941579	4.481657	1.814133	C	2.211711	-3.283007	-2.081511	C	-1.568858	-3.159147	-1.318862
H	-1.455103	4.733409	1.182146	C	-0.033769	-2.514125	-1.212418	C	-2.024801	-2.034870	-0.624907
H	-2.567493	2.993153	-0.193557	C	-0.830245	-1.530484	-0.614218	H	-1.846282	2.959710	0.037276
B	-5.091054	-0.152419	0.193706	C	-2.222927	-1.411680	-0.183121	H	0.791790	5.449410	-0.978919
F	-6.427647	-0.178822	0.646124	C	-2.406942	-0.154259	0.408152	H	-0.875994	4.998416	-1.385929
F	-4.857604	1.046677	-0.523472	C	-3.505498	0.248036	1.142075	H	-0.459179	5.417601	0.276014
F	-4.212874	-0.215962	1.298954	C	-4.561522	-0.686103	1.118404	H	2.351214	3.684836	-0.687166
F	-4.856860	-1.258555	-0.658933	C	-4.484428	-1.928725	0.471049	H	5.540804	-1.966888	0.802208
47				C	-3.287860	-2.307722	-0.160566	H	4.708513	2.043966	-0.520090
10-BF4-GS_21			Eopt	C	-5.667480	-2.863078	0.473761	H	7.031213	1.298508	0.082585
-1349.644645				C	-3.597941	1.513903	1.951238	H	7.354283	-0.401283	0.485519
O	-1.266146	-0.573204	-0.639191	C	1.504024	1.416335	-0.110168	H	7.041243	0.072125	-1.189313
C	-0.470033	0.635994	-0.484861	C	0.346456	2.352966	-0.399929	H	3.047923	-3.623426	0.616927
C	0.872083	0.624954	-0.763638	C	-0.978865	1.945091	-0.255566	H	2.002920	-2.745037	1.744111
C	1.505605	1.850773	-0.527176	C	-2.090368	2.668816	-0.635004	H	3.696950	-3.055734	2.156016
C	0.790832	2.969683	-0.042167	C	-1.865764	3.952949	-1.142152	H	-2.580850	0.411252	0.303816
C	1.528220	4.266000	0.185768	C	-0.563638	4.440663	-1.266540	H	-1.614583	0.010555	1.720816
C	-0.584581	2.879921	0.234731	C	0.527266	3.641717	-0.915751	H	1.791991	-2.667599	-1.037218
C	-1.242318	1.663323	0.016772	H	2.924260	-0.788188	-1.315083	H	0.155839	-4.245966	-2.036777
C	-2.607149	1.155188	0.155284	H	2.722923	-2.884967	-2.964595	H	-2.287740	-3.839168	-1.764023
C	-2.636525	-0.180261	-0.268915	H	2.987020	-3.602954	-1.376185	H	-3.087531	-1.827005	-0.551303
C	-3.768455	-0.935460	-0.505934	H	1.638436	-4.163846	-2.381984	B	-5.502953	-0.009307	0.303603
C	-4.959595	-0.287570	-0.119677	H	-0.454287	-3.475758	-1.486704	F	-5.006723	-0.422255	1.561095
C	-5.001511	1.016934	0.396148	H	-5.466665	-0.432539	1.663402	F	-5.325931	-1.051577	-0.636637
C	-3.812446	1.757203	0.505980	H	-3.181334	-3.294802	-0.598376	F	-6.874411	0.302520	0.412614
C	-6.315818	1.628779	0.809486	H	-6.240001	-2.758441	-0.456186	F	-4.790126	1.135611	-0.127682
C	-3.791199	-2.292411	-1.156630	H	-5.346718	-3.906643	0.544864	47			
C	1.469751	-0.683521	-1.217137	H	-6.343210	-2.648001	1.305927	10-BF4-GS_24			Eopt
C	0.800610	-1.812172	-0.455322	H	-4.172523	2.284630	1.426777	-1349.644151			
C	-0.546062	-1.757150	-0.100472	H	-2.613299	1.925249	2.183692	O	-1.884480	0.243170	-0.636050
C	-1.202038	-2.652988	0.718102	H	-4.112032	1.303355	2.892687	C	-1.061200	-0.957670	-0.673712
C	-0.462966	-3.751050	1.170948	H	2.395123	1.741678	-0.647849	C	-1.641253	-2.194360	-0.777083
C	0.879085	-3.890304	0.812728	H	1.749272	1.433526	0.959609	C	-0.719359	-3.249728	-0.760251
C	1.505593	-2.922296	0.024214	H	-3.090429	2.266625	-0.558392	C	0.668378	-3.016950	-0.641133
H	2.573633	1.932297	-0.702994	H	-2.714613	4.556897	-1.444298	C	1.623345	-4.184866	-0.662560
H	2.400378	4.109896	0.829476	H	-0.393991	5.436998	-1.661446	C	1.170759	-1.708493	-0.512793
H	1.895070	4.676821	-0.761902	H	1.540657	4.005009	-1.055409	C	0.272698	-0.636509	-0.518565
H	0.882498	5.013406	0.653764	B	4.917993	-0.326774	1.051494	C	0.363226	0.821187	-0.424889
H	-1.122617	3.739631	0.619838	F	4.868900	0.513295	-0.086372	C	-0.925598	1.361581	-0.531401
H	-5.892363	-0.825838	-0.263376	F	6.112633	-0.081047	1.764825	C	-1.240801	2.692392	-0.715997
H	-3.832508	2.791948	0.831774	F	3.807899	-0.056895	1.884363	C	-0.119433	3.543986	-0.625970
H	-6.484733	1.482685	1.883604	F	4.882435	-1.677701	0.639214	C	1.190983	3.082663	-0.432659
H	-6.328046	2.705947	0.619094	47				C	1.439292	1.700481	-0.361479
H	-7.153807	1.170265	0.277376	10-BF4-GS_23			Eopt	C	2.337817	4.055517	-0.330269
H	-3.919085	-3.088932	-0.416188	-1349.644177				C	-2.610122	3.229385	-1.035288
H	-2.876261	-2.495390	-1.716880	O	1.147054	-0.487219	0.469987	C	-3.148374	-2.244710	-0.833217
H	-4.636277	-2.347228	-1.848083	C	0.734495	0.884949	0.221679	C	-3.706945	-1.169599	0.081452
H	2.546345	-0.708594	-1.048236	C	-0.588090	1.238205	0.299729	C	-3.060704	0.054923	0.246032
H	1.299960	-0.807446	-2.295634	C	-0.827044	2.586921	0.006819	C	-3.400884	1.025699	1.165365
H	-2.232642	-2.513562	1.012749	C	0.224531	3.467092	-0.336721	C	-4.536846	0.787517	1.946110
H	-0.943436	-4.482302	1.812052	C	-0.092189	4.913149	-0.624692	C	-5.258322	-0.397584	1.793453
H	1.450051	-4.740597	1.171003	C	1.551178	3.005714	-0.412115	C	-4.835446	-1.370199	0.884088
H	2.562185	-3.004063	-0.209225	C	1.818522	1.660793	-0.131890	H	-1.084686	-4.270215	-0.830332
B	5.080717	0.153759	0.206138	C	3.003393	0.805399	-0.074422	H	1.179073	-5.068733	-0.195306
F	4.180752	0.240298	1.291551	C	2.612444	-0.480749	0.321468	H	1.881345	-4.451717	-1.694961
F	4.844331	-1.046820	-0.506137	C	3.452745	-1.503602	0.715334	H	2.553521	-3.943726	-0.141734
F	4.881997	1.255309	-0.659682	C	4.818472	-1.203896	0.527752	H	2.236050	-1.540801	-0.399468

H	-0.289681	4.610588	-0.744017	F	4.616353	0.746204	-0.089884	C	-1.204038	2.691294	-0.712839
H	2.453310	1.324241	-0.280707	F	4.610429	-1.554760	0.075033	C	-0.069624	3.525123	-0.618801
H	2.694427	4.119331	0.704696	F	3.760297	-0.272731	1.795709	C	1.232135	3.044158	-0.416394
H	3.184694	3.730557	-0.942537	47				C	1.457657	1.658558	-0.336522
H	2.039979	5.058126	-0.648287	10-BF4-GS_26			Eopt	C	2.394252	3.998800	-0.315401
H	-2.521248	4.027281	-1.777431	-1349.644167				C	-2.561258	3.250642	-1.045026
H	-3.091294	3.656196	-0.149154	O	-1.884157	0.234253	-0.637622	C	-3.184385	-2.220145	-0.833294
H	-3.269603	2.458394	-1.439505	C	-1.042241	-0.953157	-0.685021	C	-3.739541	-1.132235	0.067993
H	-3.523961	-3.223413	-0.528862	C	-1.603353	-2.197995	-0.790910	C	-3.078038	0.083766	0.235935
H	-3.482873	-2.070654	-1.865164	C	-0.665099	-3.239330	-0.783049	C	-3.418465	1.063955	1.145096
H	-2.812508	1.923114	1.295607	C	0.719082	-2.985524	-0.668948	C	-4.568908	0.846058	1.910340
H	-4.840241	1.529808	2.676375	C	1.693904	-4.136683	-0.700538	C	-5.304747	-0.329582	1.753293
H	-6.137757	-0.579126	2.402543	C	1.201648	-1.669620	-0.536246	C	-4.882450	-1.312590	0.854968
H	-5.369888	-2.311413	0.801095	C	0.287363	-0.611820	-0.533714	H	-1.150516	-4.274588	-0.800875
B	4.794354	-0.348619	0.763019	C	0.355003	0.846799	-0.433481	H	1.667286	-4.630310	-1.614641
F	4.700759	0.843990	0.006391	C	-0.942532	1.367046	-0.532561	H	2.544392	-3.952343	-0.235446
F	6.075236	-0.437645	1.347245	C	-1.279954	2.693272	-0.711396	H	1.165627	-5.039959	0.028150
F	3.807951	-0.340016	1.774968	C	-0.172216	3.562459	-0.622474	H	2.205456	-1.591064	-0.350794
F	4.582515	-1.458339	-0.089153	C	1.146154	3.121299	-0.434915	H	-0.222203	4.593665	-0.742573
47				C	1.417088	1.743143	-0.370925	H	2.465441	1.267259	-0.250321
10-BF4-GS_25			Eopt	C	2.276667	4.112565	-0.327928	H	3.231275	3.665537	-0.936745
-1349.644165				C	-2.659302	3.208567	-1.023824	H	2.109124	5.007923	-0.624234
O	-1.883823	0.230652	-0.638484	C	-3.109725	-2.271408	-0.838935	H	2.760086	4.049431	0.716983
C	-1.032637	-0.949941	-0.694892	C	-3.679379	-1.210111	0.085134	H	-2.453236	4.039817	-1.793928
C	-1.584363	-2.198605	-0.801593	C	-3.051686	0.023857	0.250958	H	-3.038983	3.694749	-0.165564
C	-0.637738	-3.232683	-0.802409	C	-3.401912	0.985615	1.176044	H	-3.232768	2.488538	-1.445898
C	0.744731	-2.968267	-0.694876	C	-4.528950	0.725953	1.962870	H	-3.577648	-3.191676	-0.528492
C	1.729974	-4.110296	-0.734393	C	-5.231796	-0.470284	1.810313	H	-3.503121	-2.047256	-1.870416
C	1.217572	-1.648726	-0.560484	C	-4.799053	-1.432396	0.894451	H	-2.820315	1.954201	1.278675
C	0.295175	-0.598353	-0.549848	H	-1.015111	-4.264900	-0.855830	H	-4.872440	1.596651	2.632010
C	0.351636	0.860481	-0.445453	H	1.242257	-5.050218	-0.303320	H	-6.195450	-0.495526	2.350339
C	-0.950657	1.370379	-0.535389	H	2.010167	-4.343937	-1.730434	H	-5.428623	-2.246809	0.768827
C	-1.299924	2.694328	-0.708581	H	2.592251	-3.908954	-0.120863	B	4.833137	-0.348057	0.729125
C	-0.198986	3.572300	-0.623240	H	2.264560	-1.487236	-0.423849	F	3.917019	-0.287177	1.803487
C	1.123998	3.141430	-0.444167	H	-0.359853	4.626646	-0.736554	F	4.514063	-1.451664	-0.097729
C	1.406783	1.765430	-0.386344	H	2.437169	1.381969	-0.297450	F	4.745663	0.842959	-0.030096
C	2.246341	4.142152	-0.339387	H	3.143913	3.784674	-0.909072	F	6.144048	-0.495187	1.228763
C	-2.685289	3.198722	-1.012248	H	1.973643	5.102910	-0.678028	47			
C	-3.090270	-2.283963	-0.840766	H	2.604008	4.207697	0.714459	10-BF4-GS_28			Eopt
C	-3.662598	-1.230719	0.090852	H	-2.586268	4.011055	-1.762731	-1349.644219			
C	-3.044016	0.007842	0.256750	H	-3.144732	3.623316	-0.134228	O	-1.880222	0.264109	-0.629630
C	-3.396466	0.963825	1.186995	H	-3.307172	2.428364	-1.429353	C	-1.105295	-0.968748	-0.632947
C	-4.516314	0.692349	1.980070	H	-3.468495	-3.257676	-0.538627	C	-1.730689	-2.184071	-0.736985
C	-5.209977	-0.509349	1.828349	H	-3.452753	-2.096285	-1.867906	C	-0.852088	-3.273745	-0.689066
C	-4.775075	-1.464998	0.906770	H	-2.827797	1.892273	1.306138	C	0.541852	-3.093837	-0.543211
H	-0.980096	-4.260701	-0.876477	H	-4.840001	1.460503	2.697722	C	1.445781	-4.301731	-0.523333
H	1.272211	-5.041943	-0.390263	H	-6.104244	-0.668496	2.424236	C	1.092005	-1.805603	-0.420296
H	2.087585	-4.273763	-1.758585	H	-5.319125	-2.381503	0.810923	C	0.236178	-0.699139	-0.455239
H	2.604082	-3.898392	-0.112866	B	4.774315	-0.346986	0.779145	C	0.384724	0.754236	-0.379316
H	2.279378	-1.458179	-0.451721	F	4.603373	-1.553354	0.060335	C	-0.878980	1.345756	-0.518081
H	-0.396024	4.635226	-0.733368	F	6.057110	-0.322729	1.365780	C	-1.134101	2.686462	-0.721216
H	2.430412	1.412694	-0.320620	F	4.638416	0.747013	-0.109407	C	0.020646	3.491371	-0.616914
H	3.119793	3.815778	-0.911941	F	3.787880	-0.256794	1.786692	C	1.306561	2.978932	-0.394265
H	1.937996	5.127164	-0.699753	47				C	1.494857	1.588319	-0.302885
H	2.565947	4.249249	0.704294	10-BF4-GS_27			Eopt	C	2.494155	3.901768	-0.293704
H	-3.169098	3.608126	-0.119268	-1349.644157				C	-2.471844	3.281236	-1.071047
H	-3.328943	2.413673	-1.415211	O	-1.886432	0.251120	-0.629417	C	-3.236563	-2.176369	-0.830184
H	-2.623116	4.002838	-1.750386	C	-1.080929	-0.961817	-0.652452	C	-3.775507	-1.067962	0.055723
H	-3.439231	-3.274288	-0.542267	C	-1.677606	-2.191151	-0.758340	C	-3.086879	0.133287	0.221459
H	-3.441055	-2.107671	-1.866917	C	-0.771662	-3.258990	-0.729188	C	-3.415637	1.129524	1.117320
H	-2.829218	1.874914	1.316347	C	0.618789	-3.045787	-0.597421	C	-4.580191	0.945923	1.870133
H	-4.828880	1.422032	2.719117	C	1.552642	-4.230906	-0.599591	C	-5.341355	-0.213712	1.715004
H	-6.076804	-0.716757	2.447182	C	1.138670	-1.745031	-0.470108	C	-4.931637	-1.214418	0.830539
H	-5.287860	-2.418058	0.823663	C	0.255604	-0.659849	-0.487727	H	-1.254883	-4.280327	-0.758037
B	4.757864	-0.347694	0.797866	C	0.367889	0.796507	-0.401752	H	1.521918	-4.744769	-1.523621
F	6.034342	-0.307459	1.397285	C	-0.911781	1.356339	-0.520293	H	2.453613	-4.034400	-0.196679

H	1.056842	-5.074808	0.147451	B	4.780876	-0.344374	0.772587	C	0.348866	0.835620	-0.401172
H	2.160972	-1.673488	-0.295618	F	4.626184	0.743088	-0.120790	C	-0.944346	1.363143	-0.517639
H	-0.103064	4.562656	-0.748485	F	6.064771	-0.298340	1.355855	C	-1.270843	2.690892	-0.705753
H	2.490416	1.172592	-0.196839	F	3.795797	-0.264586	1.782354	C	-0.158598	3.553256	-0.606797
H	2.967953	3.814821	0.690356	F	4.626255	-1.556184	0.059208	C	1.154802	3.104853	-0.403098
H	3.254098	3.642648	-1.038566	47				C	1.416040	1.725238	-0.330460
H	2.202156	4.944204	-0.443999	10-BF4-GS_31			Eopt	C	2.290398	4.089551	-0.289854
H	-2.335387	4.054247	-1.832121	-1349.644067				C	-2.642294	3.215071	-1.037320
H	-2.939888	3.754695	-0.201612	O	1.749979	0.207606	0.551920	C	-3.127203	-2.266430	-0.841962
H	-3.164608	2.533879	-1.463238	C	0.937458	-0.975606	0.310378	C	-3.706340	-1.196880	0.066559
H	-3.657199	-3.135555	-0.523197	C	1.448973	-2.226580	0.530207	C	-3.074576	0.034299	0.237981
H	-3.538372	-2.003724	-1.872400	C	0.548993	-3.260738	0.237051	C	-3.435530	1.001694	1.153028
H	-2.799248	2.007199	1.249964	C	-0.752379	-2.994134	-0.241293	C	-4.577632	0.751973	1.921061
H	-4.874682	1.710450	2.580844	C	-1.680115	-4.139974	-0.562301	C	-5.284909	-0.440626	1.760854
H	-6.242758	-0.353176	2.302692	C	-1.184316	-1.671151	-0.451825	C	-4.841667	-1.408880	0.856629
H	-5.498288	-2.136563	0.746150	C	-0.304287	-0.620153	-0.177285	H	-1.043089	-4.269866	-0.821974
B	4.843781	-0.348808	0.693210	C	-0.352544	0.841407	-0.225672	H	1.213886	-5.054647	-0.197614
F	6.133148	-0.734391	1.116703	C	0.866149	1.350562	0.243167	H	1.956987	-4.398043	-1.660643
F	4.425926	-1.183742	-0.371276	C	1.127828	2.664692	0.574630	H	2.573850	-3.917098	-0.076806
F	3.933337	-0.470410	1.767329	C	0.075431	3.540606	0.235115	H	2.245684	-1.507262	-0.359876
F	4.870626	0.993621	0.249357	C	-1.140323	3.115005	-0.320614	H	-0.338394	4.618086	-0.727074
47				C	-1.368365	1.743443	-0.526198	H	2.432952	1.357390	-0.246993
10-BF4-GS_30			Eopt	C	-2.214454	4.114375	-0.666422	H	1.995363	5.081206	-0.643062
-1349.644164				C	2.362512	3.159854	1.279345	H	2.611901	4.183892	0.754391
O	-1.886662	0.229177	-0.637638	C	2.878066	-2.309272	1.007527	H	3.159241	3.755885	-0.865322
C	-1.035656	-0.951766	-0.685577	C	3.685456	-1.216448	0.330209	H	-2.554039	4.014148	-1.778249
C	-1.586883	-2.200386	-0.794059	C	3.125839	0.026682	0.035646	H	-3.135547	3.636951	-0.155479
C	-0.640495	-3.234870	-0.785651	C	3.726428	1.021643	-0.707992	H	-3.290896	2.438242	-1.448003
C	0.741066	-2.970803	-0.668408	C	5.036937	0.787244	-1.137579	H	-3.495029	-3.249056	-0.540602
C	1.727043	-4.112481	-0.698295	C	5.672131	-0.417305	-0.831188	H	-3.453734	-2.096564	-1.877159
C	1.213405	-1.650934	-0.533037	C	4.995509	-1.412333	-0.121354	H	-2.858786	1.905620	1.289430
C	0.291319	-0.600493	-0.530919	H	0.863182	-4.290356	0.381516	H	-4.897130	1.491415	2.647343
C	0.347346	0.858454	-0.427968	H	-1.579942	-4.433237	-1.614770	H	-6.169286	-0.631204	2.359950
C	-0.953712	1.368914	-0.528845	H	-1.453002	-5.017773	0.049212	H	-5.365611	-2.355412	0.767661
C	-1.300709	2.692927	-0.707386	H	-2.723608	-3.859033	-0.396651	B	4.830757	-0.341834	0.732185
C	-0.199786	3.570103	-0.615510	H	-2.186122	-1.470882	-0.813732	F	4.587294	-1.551004	0.039360
C	1.121590	3.138769	-0.424940	H	0.212571	4.596019	0.454212	F	6.152584	-0.336959	1.224375
C	1.402685	1.762808	-0.361861	H	-2.331198	1.382714	-0.870318	F	4.651188	0.746912	-0.154811
C	2.242896	4.139693	-0.311283	H	-2.048284	5.069498	-0.161064	F	3.920825	-0.224257	1.807005
C	-2.683332	3.197889	-1.022437	H	-2.229156	4.303634	-1.746805	47			
C	-3.092525	-2.285292	-0.844560	H	-3.203724	3.738350	-0.388609	10-BF4-GS_34			Eopt
C	-3.671472	-1.230272	0.081062	H	3.061560	3.632619	0.581337	-1349.644235			
C	-3.053742	0.008437	0.249193	H	2.891048	2.355625	1.795484	O	-1.853356	0.251586	-0.608907
C	-3.412506	0.966049	1.175305	H	2.077522	3.912413	2.019390	C	-1.082408	-0.979187	-0.504445
C	-4.538304	0.696452	1.960591	H	3.314324	-3.285355	0.787486	C	-1.692781	-2.196475	-0.660965
C	-5.231304	-0.505205	1.805865	H	2.907080	-2.174229	2.097442	C	-0.826846	-3.284100	-0.492952
C	-4.790031	-1.462630	0.889138	H	3.211144	1.936030	-0.966529	C	0.540506	-3.099817	-0.186555
H	-0.982719	-4.262857	-0.860489	H	5.545396	1.548865	-1.718868	C	1.433199	-4.307326	-0.038421
H	2.119960	-4.254253	-1.712683	H	6.688455	-0.594644	-1.167347	C	1.073647	-1.809137	-0.020894
H	2.579723	-3.913931	-0.043257	H	5.474773	-2.366369	0.075530	C	0.228886	-0.704060	-0.175631
H	1.258098	-5.050756	-0.389287	B	-4.817178	-0.326616	0.107908	C	0.367304	0.751130	-0.108681
H	2.274689	-1.460592	-0.418415	F	-3.991472	0.135209	1.156635	C	-0.872468	1.336698	-0.402163
H	-0.395130	4.632954	-0.729555	F	-4.233638	0.018171	-1.136933	C	-1.103877	2.671516	-0.663163
H	2.424975	1.408484	-0.286511	F	-4.944686	-1.731452	0.189876	C	0.031557	3.481907	-0.448348
H	2.530183	4.273286	0.738842	F	-6.091484	0.273340	0.208962	C	1.284615	2.977642	-0.071684
H	3.132472	3.797312	-0.848218	47				C	1.461462	1.589972	0.073588
H	1.948086	5.115942	-0.705348	10-BF4-GS_32			Eopt	C	2.455524	3.904482	0.133839
H	-2.614825	4.002143	-1.759828	-1349.644171				C	-2.395377	3.252503	-1.173672
H	-3.174383	3.607219	-0.133418	O	-1.890895	0.234916	-0.631121	C	-3.177475	-2.188743	-0.930732
H	-3.323926	2.413095	-1.430809	C	-1.055270	-0.957522	-0.662087	C	-3.812818	-1.072215	-0.122068
H	-3.444204	-3.275009	-0.547210	C	-1.621403	-2.199987	-0.771648	C	-3.146254	0.131440	0.104754
H	-3.435341	-2.110349	-1.873633	C	-0.688752	-3.245843	-0.747707	C	-3.570800	1.138136	0.947058
H	-2.845673	1.876957	1.307391	C	0.695363	-2.999024	-0.616454	C	-4.811914	0.962434	1.568106
H	-4.856019	1.427552	2.696037	C	1.663064	-4.156548	-0.631595	C	-5.551842	-0.199595	1.343420
H	-6.102797	-0.711156	2.418609	C	1.183095	-1.685352	-0.482676	C	-5.047613	-1.210638	0.521556
H	-5.302667	-2.415576	0.803806	C	0.274072	-0.622842	-0.495762	H	-1.219378	-4.292081	-0.593685

H	1.587861	-4.796093	-1.007663
H	2.412408	-4.027596	0.357320
H	0.986260	-5.048174	0.632989
H	2.119568	-1.673874	0.230924
H	-0.076311	4.549625	-0.618333
H	2.440157	1.178699	0.293130
H	2.187340	4.940507	-0.088266
H	2.810496	3.855004	1.169362
H	3.296163	3.617614	-0.506609
H	-2.176594	4.003594	-1.937456
H	-2.954614	3.749834	-0.373999
H	-3.042298	2.492710	-1.617337
H	-3.633987	-3.145021	-0.669371
H	-3.353415	-2.021823	-2.002335
H	-2.971920	2.017398	1.137917
H	-5.182944	1.734735	2.233214
H	-6.512739	-0.332603	1.829593
H	-5.602606	-2.133593	0.385403
B	4.954780	-0.330877	0.337003
F	4.795999	0.989160	0.819491
F	6.317720	-0.692223	0.382612
F	4.202808	-1.216648	1.145898
F	4.487268	-0.403239	-0.994693
47			
10-BF4-GS_37			Eopt
-1349.644270			
O	-1.869224	0.222250	-0.644960
C	-0.983959	-0.929230	-0.755891
C	-1.498800	-2.194128	-0.862350
C	-0.520797	-3.196372	-0.917322
C	0.856454	-2.888933	-0.860354
C	1.873258	-3.999268	-0.956799
C	1.290621	-1.557475	-0.723656
C	0.336197	-0.537833	-0.657174
C	0.351893	0.919433	-0.528539
C	-0.967849	1.389706	-0.556932
C	-1.362731	2.705152	-0.693346
C	-0.285863	3.614780	-0.637168
C	1.055872	3.222203	-0.518786
C	1.381302	1.854949	-0.495603
C	2.150599	4.255382	-0.441490
C	-2.773688	3.171621	-0.932994
C	-3.001516	-2.327202	-0.845587
C	-3.569149	-1.310193	0.127755
C	-2.985917	-0.054073	0.290597
C	-3.332606	0.873605	1.250992
C	-4.409784	0.551020	2.083166
C	-5.067709	-0.671464	1.938809
C	-4.638624	-1.596294	0.983688
H	-0.832794	-4.233909	-0.994376
H	2.809082	-3.720103	-0.465936
H	1.499221	-4.920125	-0.499678
H	2.101978	-4.221099	-2.006654
H	2.347165	-1.326900	-0.656706
H	-0.519157	4.672727	-0.721022
H	2.414344	1.525450	-0.473967
H	2.503325	4.361065	0.591617
H	3.012472	3.962095	-1.048607
H	1.800599	5.234508	-0.779240
H	-3.409992	2.372456	-1.319365
H	-2.765997	3.986314	-1.662041
H	-3.231469	3.555340	-0.015173
H	-3.307135	-3.333686	-0.554399
H	-3.397059	-2.142480	-1.853834
H	-2.791643	1.801150	1.374771
H	-4.716048	1.257363	2.847103

H	-5.900671	-0.918672	2.588726
H	-5.120651	-2.565686	0.904911
B	4.613213	-0.363968	0.933843
F	5.810670	0.202434	1.421490
F	4.754439	-1.766640	0.839137
F	3.549621	-0.053740	1.810653
F	4.330708	0.165027	-0.350365
47			
10-BF4-GS_38			Eopt
-1349.644184			
O	-1.877993	0.225756	-0.616812
C	-1.028707	-0.956987	-0.624319
C	-1.575639	-2.204783	-0.753388
C	-0.630165	-3.240438	-0.708906
C	0.745326	-2.977553	-0.540196
C	1.734288	-4.117009	-0.520204
C	1.213430	-1.656839	-0.391855
C	0.293223	-0.606377	-0.425767
C	0.348211	0.853107	-0.333335
C	-0.947535	1.365742	-0.481178
C	-1.283071	2.689536	-0.684640
C	-0.182793	3.563918	-0.565143
C	1.130691	3.130615	-0.329626
C	1.404433	1.754737	-0.244335
C	2.251264	4.129349	-0.193382
C	-2.651459	3.198194	-1.051391
C	-3.077362	-2.290913	-0.869294
C	-3.699248	-1.227403	0.017738
C	-3.087838	0.010973	0.211125
C	-3.492306	0.973421	1.113196
C	-4.657863	0.710097	1.840376
C	-5.345484	-0.490324	1.655217
C	-4.859498	-1.452774	0.767019
H	-0.970326	-4.267888	-0.798098
H	1.228096	-5.081729	-0.430754
H	2.327396	-4.129465	-1.442289
H	2.436202	-4.012768	0.312772
H	2.270628	-1.467467	-0.244212
H	-0.370904	4.625966	-0.697168
H	2.422665	1.395935	-0.142728
H	1.988463	5.088732	-0.647327
H	2.475670	4.309033	0.865209
H	3.168237	3.758176	-0.660332
H	-3.171928	3.613970	-0.182381
H	-3.280477	2.414336	-1.478805
H	-2.553284	3.998592	-1.789565
H	-3.440509	-3.277770	-0.576148
H	-3.374494	-2.128655	-1.914522
H	-2.932395	1.884270	1.270887
H	-5.011034	1.445393	2.555239
H	-6.248187	-0.691235	2.222816
H	-5.368908	-2.405307	0.659331
B	4.827906	-0.337458	0.654100
F	4.609893	-1.685672	0.286979
F	4.552043	0.497615	-0.455263
F	3.965781	0.003824	1.720955
F	6.169852	-0.164725	1.053530
47			
10-BF4-GS_39			Eopt
-1349.644195			
O	-1.861484	0.221369	-0.609915
C	-1.021534	-0.965930	-0.536349
C	-1.565634	-2.211377	-0.693598
C	-0.633647	-3.252586	-0.564056
C	0.725862	-2.995535	-0.290931
C	1.702608	-4.139586	-0.171340

C	1.190407	-1.675689	-0.121812
C	0.282953	-0.620380	-0.238015
C	0.339950	0.840158	-0.159743
C	-0.936957	1.357309	-0.418450
C	-1.248126	2.678809	-0.665158
C	-0.155365	3.550256	-0.470628
C	1.131712	3.114336	-0.124014
C	1.389505	1.737987	0.004371
C	2.249004	4.105741	0.078041
C	-2.581915	3.186820	-1.143221
C	-3.054863	-2.286120	-0.924836
C	-3.732070	-1.213268	-0.091258
C	-3.128670	0.023926	0.132242
C	-3.589127	0.997994	0.993977
C	-4.803550	0.747048	1.641475
C	-5.482399	-0.452678	1.422277
C	-4.941681	-1.426667	0.579168
H	-0.972223	-4.278910	-0.670282
H	2.229620	-4.104871	0.787923
H	1.196777	-5.105060	-0.253279
H	2.463550	-4.082963	-0.957728
H	2.235959	-1.491391	0.097843
H	-0.326594	4.611108	-0.631477
H	2.392172	1.375905	0.202213
H	2.527189	4.160053	1.137223
H	3.144533	3.804548	-0.474864
H	1.957282	5.107524	-0.247797
H	-3.159304	3.629699	-0.324785
H	-3.185177	2.395588	-1.593541
H	-2.424450	3.966285	-1.893472
H	-3.448921	-3.268537	-0.658665
H	-3.268625	-2.123785	-1.990242
H	-3.037375	1.908567	1.180252
H	-5.201490	1.491334	2.322796
H	-6.422602	-0.643572	1.929261
H	-5.447096	-2.378198	0.446556
B	4.901638	-0.325662	0.415297
F	4.539097	0.183535	-0.852818
F	6.286807	-0.152794	0.618503
F	4.184502	0.368604	1.418685
F	4.579780	-1.701498	0.478523
47			
10-BF4-GS_40			Eopt
-1349.644204			
O	-1.867228	0.255504	-0.618232
C	-1.098783	-0.978881	-0.537650
C	-1.718413	-2.192744	-0.679765
C	-0.853441	-3.285078	-0.533650
C	0.521231	-3.107509	-0.260402
C	1.417017	-4.316104	-0.145713
C	1.063946	-1.819008	-0.104419
C	0.221553	-0.710141	-0.238803
C	0.367351	0.744336	-0.170677
C	-0.876619	1.335802	-0.432454
C	-1.109667	2.672479	-0.681612
C	0.033360	3.478144	-0.490176
C	1.292951	2.967727	-0.144983
C	1.468250	1.578696	-0.010573
C	2.470906	3.890166	0.039002
C	-2.411437	3.259507	-1.157864
C	-3.209887	-2.178166	-0.909302
C	-3.818139	-1.061009	-0.080720
C	-3.139809	0.138686	0.131529
C	-3.535617	1.144106	0.989241
C	-4.759980	0.972126	1.643662
C	-5.511663	-0.185391	1.435270

C	-5.035251	-1.195994	0.596466	H	-2.917590	1.895974	1.268711	C	-0.522374	3.106688	-0.253296
H	-1.253355	-4.291018	-0.623975	H	-4.992509	1.469744	2.563725	C	-1.418941	4.314554	-0.136932
H	2.337061	-4.075693	0.392976	H	-6.241193	-0.661785	2.241508	C	-1.064011	1.817832	-0.095517
H	0.911940	-5.136781	0.373027	H	-5.377274	-2.383135	0.677593	C	-0.221532	0.709458	-0.232537
H	1.699885	-4.680800	-1.140872	B	4.832017	-0.338085	0.663330	C	-0.366452	-0.745189	-0.164436
H	2.114897	-1.689577	0.129009	F	3.961019	0.013592	1.719577	C	0.877397	-1.335808	-0.428986
H	-0.074749	4.547082	-0.652210	F	4.640354	-1.698576	0.329369	C	1.110178	-2.672328	-0.679560
H	2.449932	1.163630	0.186498	F	4.543911	0.464321	-0.466929	C	-0.032183	-3.478421	-0.486612
H	3.295833	3.605591	-0.622563	F	6.169598	-0.130092	1.061167	C	-1.291483	-2.968851	-0.139275
H	2.200093	4.928129	-0.170435	47				C	-1.467008	-1.579950	-0.003500
H	2.849613	3.833416	1.065600	10-BF4-GS_42			Eopt	C	-2.468745	-3.891827	0.046346
H	-3.071918	2.502906	-1.586748	-1349.644183				C	2.411204	-3.258761	-1.158566
H	-2.209558	4.012036	-1.924871	O	-1.864368	0.226647	-0.608871	C	3.207517	2.179137	-0.911737
H	-2.948397	3.756330	-0.342773	C	-1.031061	-0.966000	-0.551681	C	3.818471	1.062284	-0.084734
H	-3.663133	-3.133073	-0.637551	C	-1.584897	-2.207951	-0.702626	C	3.141285	-0.137662	0.129603
H	-3.414201	-2.008164	-1.975380	C	-0.656831	-3.254690	-0.590774	C	3.539618	-1.142814	0.986446
H	-2.927518	2.019852	1.166457	C	0.708635	-3.006243	-0.340040	C	4.765731	-0.970288	1.637448
H	-5.108712	1.743728	2.321510	C	1.680632	-4.156255	-0.240308	C	5.516516	0.187373	1.426579
H	-6.459445	-0.315476	1.947283	C	1.183664	-1.689520	-0.176230	C	5.037497	1.197671	0.588889
H	-5.598017	-2.116008	0.472893	C	0.280389	-0.628896	-0.275049	H	1.250496	4.290991	-0.622086
B	4.958038	-0.332687	0.414878	C	0.347480	0.830858	-0.194813	H	-0.909851	5.139443	0.371037
F	4.598600	-0.552603	-0.934394	C	-0.929867	1.356468	-0.429455	H	-1.713234	4.672089	-1.131371
F	4.820480	1.041660	0.719419	C	-1.235985	2.680919	-0.670867	H	-2.332819	4.076090	0.413053
F	4.102530	-1.085022	1.254807	C	-0.134460	3.544142	-0.496379	H	-2.114212	1.687520	0.140738
F	6.295082	-0.732613	0.621852	C	1.156604	3.099088	-0.173434	H	0.076179	-4.547182	-0.649589
47				C	1.406811	1.721670	-0.050565	H	-2.448607	-1.165176	0.194740
10-BF4-GS_41			Eopt	C	2.279474	4.086676	0.016025	H	-2.841731	-3.839937	1.075398
-1349.644179				C	-2.573967	3.197343	-1.127863	H	-3.297195	-3.603547	-0.609090
O	-1.879354	0.228710	-0.619631	C	-3.077897	-2.274172	-0.910917	H	-2.199482	-4.928899	-0.169479
C	-1.035505	-0.957860	-0.628256	C	-3.736804	-1.197373	-0.067704	H	2.949707	-3.756125	-0.344820
C	-1.589711	-2.204282	-0.752037	C	-3.122279	0.035374	0.150065	H	3.070800	-2.501684	-1.587964
C	-0.650538	-3.243574	-0.706627	C	-3.564782	1.010744	1.019703	H	2.208136	-4.010666	-1.925877
C	0.728275	-2.987277	-0.543284	C	-4.772690	0.767161	1.681955	H	3.661033	3.134273	-0.641217
C	1.704572	-4.137578	-0.537693	C	-5.462917	-0.427130	1.468685	H	3.409131	2.009154	-1.978328
C	1.203328	-1.670098	-0.398461	C	-4.939586	-1.403283	0.617218	H	2.932137	-2.018647	1.165460
C	0.287634	-0.613779	-0.433079	H	-1.003233	-4.278773	-0.693300	H	5.116604	-1.741571	2.314552
C	0.350285	0.845421	-0.341746	H	1.165443	-5.118726	-0.294620	H	6.465732	0.317826	1.935832
C	-0.943276	1.364221	-0.487354	H	2.414762	-4.114294	-1.052823	H	5.599705	2.117786	0.463522
C	-1.273128	2.689421	-0.690645	H	2.240037	-4.115030	0.700048	B	-4.960694	0.332376	0.407760
C	-0.168568	3.558705	-0.573688	H	2.233685	-1.511193	0.026702	F	-6.299077	0.728865	0.612916
C	1.143309	3.119304	-0.340501	H	-0.301059	4.605972	-0.655921	F	-4.818767	-1.039942	0.718609
C	1.410859	1.742193	-0.255239	H	2.410743	1.351818	0.123763	F	-4.601572	0.547559	-0.942332
C	2.268757	4.112862	-0.206505	H	3.224069	3.685498	-0.362412	F	-4.107826	1.091265	1.244697
C	-2.639876	3.204139	-1.054990	H	2.069791	5.031798	-0.492405	47			
C	-3.092341	-2.282551	-0.862085	H	2.421526	4.303915	1.081887	10-BF4-GS_45			Eopt
C	-3.705008	-1.214570	0.025885	H	-2.423264	3.979892	-1.876241	-1349.644160			
C	-3.086797	0.021157	0.214062	H	-3.138434	3.638358	-0.299514	O	1.885670	-0.229994	-0.613036
C	-3.482592	0.987458	1.115844	H	-3.186761	2.410951	-1.573888	C	1.050415	0.962384	-0.605350
C	-4.646033	0.731244	1.848901	H	-3.473396	-3.254234	-0.638168	C	1.611255	2.205663	-0.732883
C	-5.340149	-0.466292	1.669411	H	-3.306929	-2.111297	-1.973072	C	0.679743	3.250853	-0.672334
C	-4.862831	-1.432836	0.780973	H	-3.004169	1.916899	1.200776	C	-0.698930	3.003067	-0.493330
H	-0.995929	-4.269926	-0.790154	H	-5.156775	1.512820	2.369684	C	-1.666683	4.160517	-0.472803
H	2.036982	-4.363600	-1.558508	H	-6.398267	-0.612289	1.986646	C	-1.180958	1.688832	-0.347379
H	2.593298	-3.898264	0.051674	H	-5.453333	-2.350968	0.489164	C	-0.272386	0.626725	-0.395466
H	1.247129	-5.044215	-0.131101	B	4.887968	-0.329033	0.465733	C	-0.344446	-0.832240	-0.309236
H	2.261378	-1.485006	-0.252051	F	6.265647	-0.172367	0.724969	C	0.943526	-1.359611	-0.473506
H	-0.351967	4.621588	-0.705613	F	4.576782	-1.705199	0.365780	C	1.260845	-2.686100	-0.687623
H	2.427502	1.378677	-0.155171	F	4.137449	0.244970	1.518572	C	0.151616	-3.547921	-0.560229
H	3.183122	3.737444	-0.675165	F	4.555973	0.315628	-0.748621	C	-1.153996	-3.100369	-0.308504
H	2.009486	5.073424	-0.659994	47				C	-1.410340	-1.721608	-0.213162
H	2.496012	4.291526	0.851650	10-BF4-GS_44			Eopt	C	-2.284880	-4.086652	-0.166285
H	-2.539580	4.002435	-1.795166	-1349.644238				C	2.618571	-3.209003	-1.073163
H	-3.156060	3.624426	-0.185598	O	1.866768	-0.255253	-0.616985	C	3.112657	2.273861	-0.864711
H	-3.273859	2.422506	-1.479129	C	1.097972	0.978862	-0.534714	C	3.731270	1.197772	0.009170
H	-3.459744	-3.267066	-0.566414	C	1.716635	2.192942	-0.678397	C	3.107348	-0.034377	0.202224
H	-3.392406	-2.119798	-1.906393	C	0.851372	3.284878	-0.530250	C	3.510772	-1.007127	1.093637

C	4.687705	-0.762172	1.808786	H	-4.835105	1.333678	-1.473955	C	-3.729658	0.175155	-0.666040
C	5.387325	0.431200	1.623059	H	-3.358306	1.254118	-2.438309	C	-4.786811	-0.720736	-0.464867
C	4.902556	1.404800	0.746448	H	-0.350763	2.170623	1.618289	C	-4.560730	-2.042957	-0.020406
H	1.030772	4.275211	-0.757440	H	-1.417406	4.311314	2.279017	C	-5.735844	-2.973517	0.152632
H	-1.971899	4.423950	-1.493115	H	-3.543787	5.026780	1.195439	C	-3.257677	-2.494872	0.254326
H	-2.571098	3.909438	0.087063	H	-4.625906	3.571962	-0.498520	C	-2.181555	-1.618860	0.070730
H	-1.212290	5.049390	-0.025157	B	5.569158	0.242308	-0.791852	C	-0.727299	-1.678302	0.220111
H	-2.239076	1.509375	-0.193768	F	6.885110	0.562042	-1.191489	C	-0.182916	-0.448223	-0.168321
H	0.325685	-4.611384	-0.699609	F	5.331140	0.761222	0.503710	C	1.153023	-0.176756	-0.392055
H	-2.423891	-1.353313	-0.098716	F	4.647252	0.811512	-1.700975	C	2.001583	-1.239463	-0.022566
H	-2.031140	-5.051694	-0.613262	F	5.406225	-1.160893	-0.772471	C	1.534656	-2.472736	0.461108
H	-2.512549	-4.256258	0.893238	47				C	0.152982	-2.705421	0.553307
H	-3.197601	-3.709677	-0.636827	10-BF4-GS_47			Eopt	C	2.518191	-3.544833	0.855185
H	3.142519	-3.639393	-0.213366	-1349.643269				C	1.693260	1.083025	-1.013118
H	3.253054	-2.429382	-1.500195	O	-1.284133	0.461340	-0.464528	C	-3.772788	1.625961	-1.078236
H	2.502339	-4.001377	-1.817361	C	-2.477259	-0.365964	-0.411249	C	-2.725037	2.389241	-0.288590
H	3.491617	3.254375	-0.570506	C	-3.701167	0.153730	-0.745156	C	-1.506320	1.805618	0.055078
H	3.395778	2.113583	-1.914142	C	-4.755899	-0.757277	-0.609517	C	-0.557944	2.355898	0.891885
H	2.942241	-1.912442	1.251998	C	-4.537613	-2.080205	-0.163423	C	-0.813603	3.643593	1.375134
H	5.040380	-1.506096	2.514919	C	-5.708006	-3.027101	-0.062030	C	-1.993583	4.303293	1.027720
H	6.298858	0.617876	2.181331	C	-3.245922	-2.517594	0.179375	C	-2.944755	3.674081	0.220489
H	5.421804	2.352020	0.638772	C	-2.173177	-1.626370	0.062190	H	-5.804342	-0.387108	-0.647195
B	-4.886345	0.333607	0.617553	C	-0.729038	-1.670416	0.290382	H	-6.558888	-2.476419	0.675969
F	-4.669733	-0.762842	-0.251038	C	-0.178361	-0.430632	-0.056744	H	-6.118134	-3.299129	-0.822269
F	-4.003106	0.240016	1.717112	C	1.164823	-0.143272	-0.203733	H	-5.454983	-3.865800	0.717897
F	-4.639979	1.537903	-0.082281	C	2.003773	-1.201474	0.200074	H	-3.094078	-3.506403	0.610395
F	-6.220188	0.316785	1.076042	C	1.524698	-2.444535	0.644809	H	3.070170	-1.096721	-0.146898
47				C	0.142543	-2.691793	0.660695	H	-0.227202	-3.676690	0.852301
10-BF4-GS_46			Eopt	C	2.496051	-3.512143	1.079222	H	2.054936	-4.535178	0.835454
-1349.643071				C	1.727773	1.127831	-0.779676	H	3.386962	-3.548856	0.190877
O	-1.273267	0.494619	-0.324237	C	-3.742697	1.606996	-1.147935	H	2.888249	-3.367982	1.872491
C	-2.273954	-0.553665	-0.423881	C	-2.746323	2.377609	-0.301234	H	2.094878	1.763245	-0.255797
C	-3.506449	-0.291616	-0.964784	C	-1.540032	1.807628	0.103660	H	0.929238	1.618341	-1.581472
C	-4.367720	-1.395106	-0.963884	C	-0.643370	2.367205	0.989983	H	2.514943	0.829873	-1.686442
C	-3.966877	-2.645802	-0.441509	C	-0.940786	3.649022	1.464661	H	-4.760050	2.057898	-0.905567
C	-4.934942	-3.802720	-0.479152	C	-2.110002	4.294812	1.059385	H	-3.562238	1.705597	-2.153616
C	-2.686300	-2.813989	0.113270	C	-3.008987	3.657119	0.200845	H	0.336895	1.820858	1.177363
C	-1.806173	-1.725519	0.134664	H	-5.765989	-0.435007	-0.845742	H	-0.087196	4.114708	2.028371
C	-0.435117	-1.480179	0.581291	H	-6.039075	-3.341216	-1.059194	H	-2.186887	5.301803	1.405810
C	-0.090941	-0.156997	0.278682	H	-5.443481	-3.924970	0.502302	H	-3.881657	4.171500	-0.010398
C	1.177382	0.388770	0.322299	H	-6.561385	-2.548252	0.428862	B	5.668872	0.275670	-0.189278
C	2.134201	-0.480209	0.883507	H	-3.088502	-3.530169	0.535252	F	5.241583	0.336310	-1.535739
C	1.845080	-1.791588	1.294884	H	3.076101	-1.048129	0.129814	F	5.496943	-1.041526	0.297885
C	0.551928	-2.307267	1.112721	H	-0.243211	-3.670022	0.928311	F	7.032010	0.635030	-0.109609
C	2.930726	-2.644894	1.898936	H	2.055129	-4.509117	0.992159	F	4.897824	1.168139	0.590873
C	1.568934	1.738814	-0.214519	H	3.412820	-3.479526	0.484004	47			
C	-3.765672	1.121093	-1.426707	H	2.782584	-3.364030	2.127726	10-BF4-GS_49			Eopt
C	-3.088352	2.081055	-0.465878	H	2.578910	0.887283	-1.420291	-1349.642484			
C	-1.874161	1.766651	0.143325	H	2.094702	1.795280	0.006548	O	1.270033	-0.091846	-0.980186
C	-1.259085	2.501822	1.135490	H	0.988187	1.671878	-1.371160	C	2.175962	-1.016608	-0.321098
C	-1.875432	3.701127	1.508117	H	-4.742869	2.024742	-1.020167	C	2.062415	-2.367857	-0.524371
C	-3.068906	4.096379	0.901828	H	-3.481252	1.698833	-2.211073	C	2.985021	-3.126095	0.206408
C	-3.674827	3.285228	-0.060794	H	0.243518	1.843127	1.317258	C	3.927699	-2.517867	1.066049
H	-5.369345	-1.284252	-1.369523	H	-0.255344	4.126717	2.156245	C	4.912249	-3.385038	1.811199
H	-5.194816	-4.059965	-1.512235	H	-2.336350	5.288711	1.431240	C	3.953773	-1.121608	1.227857
H	-4.510015	-4.690617	-0.004499	H	-3.939464	4.142703	-0.076697	C	3.037686	-0.338232	0.516503
H	-5.867491	-3.550424	0.037633	B	5.709463	0.275542	-0.343128	C	2.740588	1.087997	0.384555
H	-2.388964	-3.773830	0.521964	F	7.101484	0.499778	-0.414055	C	1.700942	1.247521	-0.541094
H	3.155409	-0.119043	0.955455	F	5.465109	-1.026466	0.154342	C	1.288446	2.437944	-1.107275
H	0.329479	-3.342372	1.349961	F	5.119244	1.224838	0.522716	C	1.914448	3.566843	-0.540713
H	3.059670	-2.405496	2.961735	F	5.143560	0.397813	-1.633119	C	2.901613	3.491052	0.454165
H	2.686838	-3.708127	1.823572	47				C	3.341753	2.233481	0.899180
H	3.890414	-2.468538	1.405247	10-BF4-GS_48			Eopt	C	3.499124	4.750713	1.026825
H	0.828035	2.134842	-0.912183	-1349.643310				C	0.313436	2.572163	-2.246046
H	2.525019	1.651137	-0.735797	O	-1.298287	0.454035	-0.520816	C	0.957766	-2.832879	-1.440448
H	1.699780	2.466423	0.593427	C	-2.496161	-0.358479	-0.396015	C	-0.258048	-1.949373	-1.227643

C	-0.131435	-0.592332	-0.936402	H	1.544271	-3.375009	-1.207450	O	-1.269205	-0.081336	0.956183
C	-1.158848	0.254766	-0.577894	H	0.587410	-2.806858	0.174236	C	-2.179805	-1.025315	0.332018
C	-2.450163	-0.283062	-0.578993	H	-3.877768	0.773525	-0.045276	C	-2.039103	-2.372809	0.542833
C	-2.650969	-1.624514	-0.908141	H	-2.843501	-0.040257	1.137126	C	-2.970767	-3.151351	-0.154447
C	-1.565323	-2.449615	-1.211248	H	0.262040	-1.963592	-2.443808	C	-3.947262	-2.565073	-0.991249
H	2.968379	-4.208371	0.115552	H	-1.496850	-3.160312	-3.726001	C	-4.940828	-3.453400	-1.698532
H	4.404173	-4.215123	2.312938	H	-3.900107	-2.764977	-3.201013	C	-3.999347	-1.170811	-1.164347
H	5.644836	-3.820450	1.121329	H	-4.535421	-1.133957	-1.441995	C	-3.075516	-0.367432	-0.486249
H	5.457663	-2.809581	2.563476	B	-0.283101	-1.355419	2.911819	C	-2.795913	1.064205	-0.375480
H	4.669903	-0.662057	1.900610	F	0.782775	-2.242479	3.183356	C	-1.732740	1.247220	0.518510
H	1.628815	4.542437	-0.924224	F	0.236536	-0.107895	2.500710	C	-1.322599	2.448332	1.063290
H	4.155203	2.151494	1.612552	F	-1.094402	-1.894474	1.886437	C	-1.980201	3.563222	0.504950
H	2.947513	5.061595	1.922722	F	-1.062960	-1.177445	4.077724	C	-2.993620	3.464129	-0.461151
H	4.541856	4.597306	1.319461	47				C	-3.427948	2.196397	-0.882473
H	3.454603	5.574521	0.309110	10-BF4-GS_50			Eopt	C	-3.625745	4.709570	-1.027595
H	-0.679040	2.867080	-1.889678	-1349.642421				C	-0.321331	2.605099	2.175894
H	0.207969	1.642365	-2.808887	O	1.272267	-0.101079	-0.990834	C	-0.900827	-2.812901	1.429749
H	0.662391	3.350620	-2.929728	C	2.184067	-1.006153	-0.313716	C	0.294447	-1.912832	1.174082
H	0.699001	-3.875928	-1.250296	C	2.097735	-2.360761	-0.508427	C	0.137880	-0.560657	0.875214
H	1.295834	-2.762685	-2.483450	C	3.021803	-3.098891	0.240784	C	1.140453	0.299547	0.479684
H	-0.986464	1.282451	-0.291100	C	3.941511	-2.466661	1.110357	C	2.439754	-0.217662	0.448034
H	-3.287752	0.348894	-0.308081	C	4.929734	-3.312064	1.874972	C	2.671948	-1.552638	0.783263
H	-3.655212	-2.034018	-0.898833	C	3.942696	-1.069133	1.260110	C	1.608767	-2.392176	1.124310
H	-1.719760	-3.503912	-1.419362	C	3.024843	-0.305646	0.529978	H	-2.934920	-4.232422	-0.055051
B	-5.942514	0.217926	0.910811	C	2.705820	1.113650	0.385967	H	-5.657247	-3.877834	-0.985127
F	-5.337457	1.350266	0.311912	C	1.676030	1.250006	-0.553561	H	-5.504736	-2.897111	-2.451581
F	-6.065823	-0.810239	-0.051561	C	1.252699	2.428121	-1.134076	H	-4.437950	-4.291225	-2.192399
F	-5.136274	-0.232112	1.980731	C	1.853341	3.572741	-0.571454	H	-4.741420	-0.728175	-1.820144
F	-7.221161	0.569207	1.395037	C	2.828720	3.519845	0.436672	H	-1.698771	4.546171	0.872509
47				C	3.283843	2.270992	0.899572	H	-4.259964	2.096576	-1.571718
10-BF4-GS_5			Eopt	C	3.398547	4.791396	1.007756	H	-3.574662	5.540071	-0.318060
-1349.647653				C	0.287214	2.538909	-2.285447	H	-3.103219	5.021230	-1.940506
O	-0.199857	-0.251461	-0.383379	C	1.012386	-2.850520	-1.434602	H	-4.673474	4.537857	-1.290710
C	-0.552563	1.140932	-0.206550	C	-0.221045	-1.984271	-1.245425	H	-0.664267	3.383782	2.862345
C	-1.848004	1.506461	0.051385	C	-0.121715	-0.623575	-0.960668	H	0.657795	2.911076	1.793053
C	-2.028953	2.888964	0.175167	C	-1.165670	0.206853	-0.619086	H	-0.189068	1.681096	2.742690
C	-0.949545	3.791694	0.043095	C	-2.448811	-0.351034	-0.634493	H	-0.631695	-3.853552	1.240830
C	-1.199464	5.269784	0.217933	C	-2.622912	-1.697271	-0.959169	H	-1.209171	-2.738788	2.481685
C	0.345887	3.323574	-0.237409	C	-1.520892	-2.507589	-1.244305	H	0.942155	1.322029	0.191131
C	0.554728	1.946254	-0.375617	H	3.023780	-4.181861	0.159881	H	3.260307	0.425044	0.151161
C	1.696771	1.066204	-0.622235	H	5.452312	-2.723179	2.634019	H	3.682885	-1.943647	0.750293
C	1.254407	-0.263767	-0.589717	H	4.429928	-4.151498	2.370151	H	1.786110	-3.441936	1.337151
C	2.056416	-1.386553	-0.538673	H	5.684008	-3.735133	1.199508	B	6.023357	0.216775	-0.847975
C	3.427521	-1.096864	-0.695649	H	4.642204	-0.594212	1.940360	F	5.410478	1.337244	-0.235839
C	3.937822	0.203795	-0.822808	H	1.558051	4.539983	-0.964481	F	5.323937	-0.109479	-2.031961
C	3.062466	1.300493	-0.753988	H	4.089433	2.209936	1.622791	F	7.365197	0.526290	-1.158762
C	5.417717	0.427300	-1.005256	H	3.319399	5.618537	0.296961	F	5.983719	-0.881767	0.041120
C	1.577708	-2.789919	-0.281934	H	2.853639	5.080562	1.915796	47			
C	-2.868014	0.398740	0.131281	H	4.450932	4.666766	1.282010	10-BF4-GS_52			Eopt
C	-2.519572	-0.663960	-0.893138	H	0.207800	1.605381	-2.846046	-1349.645826			
C	-1.194852	-0.969087	-1.203259	H	0.629108	3.324014	-2.967900	O	-0.978516	-0.328403	0.874563
C	-0.782954	-1.817742	-2.209909	H	-0.715366	2.813146	-1.942202	C	-2.246282	0.100093	0.312808
C	-1.782306	-2.478229	-2.932423	H	0.767883	-3.894155	-1.237897	C	-3.319166	-0.753283	0.288024
C	-3.127616	-2.250515	-2.638785	H	1.361653	-2.783290	-2.474849	C	-4.459114	-0.206281	-0.312877
C	-3.488521	-1.340343	-1.642084	H	-1.014083	1.238593	-0.332155	C	-4.460922	1.106529	-0.836922
H	-3.023829	3.275209	0.377954	H	-3.300504	0.268311	-0.371565	C	-5.725605	1.649323	-1.455889
H	-1.400849	5.506174	1.269543	H	-3.621643	-2.124328	-0.964306	C	-3.302339	1.901424	-0.785662
H	-0.334858	5.858435	-0.099331	H	-1.654066	-3.562678	-1.447988	C	-2.144621	1.378427	-0.197254
H	-2.070129	5.594412	-0.361323	B	-5.913108	0.213681	0.937206	C	-0.785134	1.847933	0.072628
H	1.169003	4.022365	-0.343378	F	-6.122805	-0.722446	-0.102197	C	-0.087544	0.840628	0.750323
H	4.120616	-1.933438	-0.677414	F	-5.270614	1.363070	0.409839	C	1.132749	0.972560	1.382792
H	3.444556	2.315991	-0.769800	F	-7.157740	0.585409	1.494468	C	1.741288	2.221385	1.151977
H	5.655236	0.583026	-2.064964	F	-5.095143	-0.362514	1.939904	C	1.145892	3.249800	0.404517
H	5.752828	1.315328	-0.460778	47				C	-0.146973	3.071925	-0.113773
H	5.996013	-0.432941	-0.657640	10-BF4-GS_51			Eopt	C	1.888725	4.541007	0.174934
H	2.273676	-3.287000	0.398647	-1349.642450				C	1.772231	-0.062851	2.266235

C	-3.106303	-2.136465	0.853183	H	7.260258	0.327523	-0.399353	10-BF4-TS_1	Eopt		
C	-1.705369	-2.599864	0.495169	H	4.305760	-2.754561	1.846351	-1349.627011			
C	-0.637357	-1.705867	0.432592	H	3.466411	-3.408479	0.438230	C	-3.864694	-1.236826	-0.531287
C	0.626401	-1.987095	-0.040531	H	2.540845	-2.651997	1.743436	C	-2.969026	-2.300667	-0.679925
C	0.875037	-3.312677	-0.413493	H	-2.571100	-0.102334	1.179303	C	-1.560475	-2.197242	-0.748910
C	-0.135301	-4.271512	-0.323429	H	-1.312468	-0.375410	2.387474	C	-1.103279	-0.878338	-0.656400
C	-1.415597	-3.912673	0.107143	H	1.835709	-2.611141	-0.986852	C	-1.959755	0.223026	-0.523063
H	-5.360378	-0.808658	-0.383157	H	0.251109	-4.369526	-1.734500	C	-3.340182	0.050216	-0.460471
H	-6.122943	0.958868	-2.207424	H	-2.139828	-4.262028	-1.043156	O	0.309097	-0.258918	-0.648395
H	-6.503294	1.784939	-0.695110	H	-2.950817	-2.367023	0.339253	C	0.122697	1.172957	-0.574481
H	-5.549446	2.615457	-1.935374	B	-5.086829	0.062654	-0.281898	C	-1.222556	1.464478	-0.480399
H	-3.307448	2.903247	-1.201629	F	-6.326751	0.451760	-0.832146	C	1.131696	2.107220	-0.614487
H	2.717989	2.391668	1.595326	F	-4.069911	0.207026	-1.251799	C	0.709210	3.440457	-0.527431
H	-0.653035	3.880861	-0.630128	F	-4.788393	0.877584	0.836703	C	-0.643885	3.802187	-0.405584
H	2.572158	4.438917	-0.676912	F	-5.155788	-1.288681	0.132148	C	-1.621330	2.799067	-0.389359
H	1.200448	5.361655	-0.045851	47				C	2.559521	1.695652	-0.739754
H	2.491508	4.813304	1.046316	10-BF4-GS_59			Eopt	C	2.712323	0.216479	-0.971546
H	1.040481	-0.768803	2.665690	-1349.644189				C	1.693865	-0.735374	-0.882091
H	2.267541	0.433221	3.104939	O	1.146338	-0.480994	0.483699	C	1.932624	-2.091761	-0.955619
H	2.534526	-0.630523	1.724502	C	0.750535	0.897433	0.243477	C	3.227458	-2.547478	-1.198750
H	-3.842913	-2.841283	0.463285	C	-0.565318	1.270073	0.338327	C	4.269891	-1.635030	-1.350123
H	-3.225771	-2.105650	1.944890	C	-0.787675	2.621856	0.049491	C	4.001774	-0.276476	-1.225243
H	1.389758	-1.229506	-0.152856	C	0.271992	3.487372	-0.304993	H	-3.376968	-3.303925	-0.749422
H	1.859818	-3.575050	-0.783981	C	-0.027543	4.938990	-0.587171	H	-3.981774	0.918830	-0.354839
H	0.063886	-5.297184	-0.616449	C	1.590433	3.007634	-0.396656	H	1.467696	4.218295	-0.553892
H	-2.213618	-4.648591	0.127399	C	1.842091	1.658083	-0.122361	H	-2.673418	3.051669	-0.310052
B	4.232666	-0.404579	-0.869159	C	3.014986	0.784767	-0.081633	H	3.041696	2.248387	-1.552851
F	4.708171	0.567633	0.038339	C	2.609142	-0.496702	0.315680	H	3.098189	1.958903	0.178825
F	4.134942	-1.654016	-0.212217	C	3.439637	-1.533003	0.695317	H	1.150858	-2.803561	-0.806560
F	2.953595	-0.025728	-1.340881	C	4.806374	-1.252926	0.490578	H	3.404484	-3.616228	-1.254825
F	5.122998	-0.512508	-1.959593	C	5.283742	-0.023555	0.010838	H	5.281921	-1.976247	-1.541479
47				C	4.377166	1.018073	-0.248336	H	4.807763	0.447477	-1.303095
10-BF4-GS_58			Eopt	C	6.760795	0.186244	-0.204964	C	-0.840604	-3.512068	-0.918038
-1349.644542				C	2.991868	-2.826491	1.321551	H	-1.583747	-4.307106	-0.993539
O	1.205617	-0.532339	0.668808	C	-1.564582	0.194573	0.680827	H	-0.242280	-3.543414	-1.831199
C	0.590241	0.777113	0.512570	C	-1.142241	-1.097742	0.007039	H	-0.211255	-3.746605	-0.055270
C	-0.731576	0.964736	0.823846	C	0.200500	-1.431422	-0.160623	C	-5.346320	-1.488802	-0.430174
C	-1.185415	2.266829	0.583620	C	0.681786	-2.501319	-0.886379	H	-5.651217	-2.327209	-1.063430
C	-0.328982	3.264738	0.065088	C	-0.269302	-3.363637	-1.442382	H	-5.622194	-1.737954	0.601773
C	-0.876640	4.650938	-0.169482	C	-1.631572	-3.111881	-1.270363	H	-5.918292	-0.603815	-0.722414
C	1.011439	2.972272	-0.242000	C	-2.061572	-1.982792	-0.569068	C	-1.030245	5.253922	-0.274961
C	1.490778	1.675419	-0.021442	H	-1.801675	3.008717	0.092027	H	-0.890645	5.597729	0.757262
C	2.764093	0.973001	-0.181144	H	-0.351331	5.453109	0.325310	H	-0.412594	5.888775	-0.917683
C	2.609481	-0.346617	0.265020	H	0.853396	5.457390	-0.974175	H	-2.080095	5.409422	-0.538142
C	3.625476	-1.254188	0.492040	H	-0.836010	5.037562	-1.319228	B	0.652091	-0.479029	2.718297
C	4.888383	-0.791947	0.069061	H	2.397043	3.674908	-0.681113	F	1.693237	0.282709	2.140149
C	5.106572	0.484866	-0.471082	H	5.521050	-2.028216	0.752562	F	0.574353	-1.735170	2.074053
C	4.035284	1.388817	-0.567573	H	4.731738	1.999295	-0.546563	F	0.917401	-0.670563	4.093023
C	6.485172	0.891283	-0.925636	H	7.049481	1.219498	0.008945	F	-0.573170	0.205188	2.563341
C	3.465643	-2.590364	1.166197	H	7.354250	-0.480200	0.426814	47			
C	-1.498263	-0.238150	1.313207	H	7.027749	-0.020247	-1.248833	10-BF4-TS_10	Eopt		
C	-1.023446	-1.458498	0.546710	H	3.010117	-3.648255	0.597945	-1349.623734			
C	0.307869	-1.605268	0.161134	H	1.982434	-2.759276	1.732215	C	5.087303	-1.235148	0.173041
C	0.804695	-2.593058	-0.663673	H	3.675017	-3.089162	2.133738	C	5.074875	0.163511	0.197841
C	-0.100341	-3.571589	-1.089175	H	-2.569400	0.471763	0.362069	C	3.926007	0.985089	0.135536
C	-1.439818	-3.506524	-0.701813	H	-1.593995	0.055967	1.770243	C	2.735630	0.254822	0.038450
C	-1.897938	-2.451977	0.091529	H	1.739145	-2.667058	-1.036435	C	2.693414	-1.146700	0.009336
H	-2.224374	2.507890	0.786948	H	0.067314	-4.221127	-2.015174	C	3.866383	-1.895845	0.074404
H	-1.732470	4.620620	-0.852760	H	-2.365787	-3.782072	-1.705369	O	1.255234	0.676820	-0.053873
H	-1.226696	5.096213	0.768596	H	-3.120496	-1.764096	-0.477863	C	0.486276	-0.549334	-0.133981
H	-0.117903	5.310295	-0.598610	B	-5.500368	-0.017440	0.261425	C	1.337211	-1.634754	-0.094204
H	1.659667	3.740101	-0.650800	F	-4.740617	0.948222	-0.442298	C	-0.885091	-0.619727	-0.234942
H	5.736160	-1.458373	0.201791	F	-5.443876	-1.249986	-0.430722	C	-1.407721	-1.918288	-0.292883
H	4.197356	2.405129	-0.911258	F	-4.960358	-0.182431	1.557320	C	-0.594881	-3.065866	-0.252980
H	6.605789	0.699185	-1.999025	F	-6.840299	0.412514	0.355367	C	0.794299	-2.920744	-0.153339
H	6.657143	1.959168	-0.762224	47				C	-1.725481	0.611307	-0.279116

C	-0.905681	1.871388	-0.216815	C	-1.728172	1.940937	-0.204013	F	6.390073	1.207971	0.012542
C	0.485219	1.949102	-0.110086	H	-2.196146	2.925562	-0.225861	47			
C	1.168889	3.146538	-0.050548	H	-2.043525	1.420276	-1.110323	10-BF4-TS_14		Eopt	
C	0.455317	4.343298	-0.099980	H	-2.123730	1.422934	0.671707	-1349.623744			
C	-0.934220	4.321183	-0.208085	C	1.867459	5.359685	-0.069409	C	5.092963	-1.219422	0.173925
C	-1.590187	3.096897	-0.263840	H	1.398791	5.863002	0.783448	C	5.074040	0.179955	0.201191
H	6.026720	0.679528	0.271079	H	2.946594	5.523408	-0.014071	C	3.922441	0.995859	0.138144
H	3.809613	-2.978968	0.045170	H	1.492503	5.843347	-0.978211	C	2.734632	0.259947	0.038791
H	-2.485945	-2.025930	-0.368220	C	6.477280	-1.188075	0.250299	C	2.698625	-1.141015	0.011691
H	1.441532	-3.790714	-0.120286	H	7.000274	-0.228362	0.254919	C	3.875688	-1.885269	0.077959
H	-2.327479	0.618476	-1.194330	H	6.748720	-1.729644	1.163487	O	1.252294	0.675494	-0.051061
H	-2.442084	0.603308	0.548506	H	6.846652	-1.775440	-0.597668	C	0.488725	-0.554101	-0.128781
H	2.232841	3.177227	0.035045	B	-5.388910	0.217179	0.184085	C	1.344602	-1.635641	-0.087788
H	1.000255	5.280027	-0.052434	F	-6.561468	0.960106	0.441659	C	-0.882288	-0.630869	-0.230145
H	-1.501672	5.245068	-0.246534	F	-5.722908	-1.142556	-0.018606	C	-1.399097	-1.931887	-0.284937
H	-2.672393	3.059613	-0.345335	F	-4.755140	0.719865	-0.975251	C	-0.581161	-3.075748	-0.242442
C	4.208242	2.466456	0.184413	F	-4.509610	0.324387	1.286443	C	0.807397	-2.924217	-0.144020
H	5.285178	2.612197	0.278199	47				C	-1.727982	0.596301	-0.279261
H	3.896262	2.977841	-0.730013	10-BF4-TS_13		Eopt		C	-0.913963	1.860135	-0.217539
H	3.745438	2.945869	1.050653	-1349.623778				C	0.476409	1.944359	-0.109015
C	6.385884	-1.991357	0.276355	C	-1.486310	3.893571	-0.001876	C	1.154346	3.144979	-0.048175
H	6.282825	-3.007396	-0.113890	C	-0.159416	3.447677	-0.003171	C	0.435334	4.338406	-0.099217
H	7.184478	-1.484927	-0.273824	C	0.264209	2.099325	-0.003225	C	-0.953883	4.309798	-0.209825
H	6.704337	-2.065981	1.323303	C	-0.803600	1.194229	-0.002123	C	-1.604051	3.082457	-0.266113
C	-1.227587	-4.432850	-0.321064	C	-2.148278	1.586497	-0.000601	H	6.023558	0.699938	0.278718
H	-1.754421	-4.571479	-1.271969	C	-2.495633	2.936373	-0.000483	H	3.823459	-2.968650	0.053329
H	-0.477327	-5.222413	-0.227568	O	-0.865294	-0.352883	-0.001910	H	-2.476807	-2.044476	-0.360363
H	-1.965376	-4.561596	0.478304	C	-2.267965	-0.701552	-0.000012	H	1.458535	-3.791249	-0.109910
B	-5.334634	-0.333952	0.270310	C	-3.034947	0.446195	0.000854	H	-2.327429	0.598662	-1.196189
F	-6.677321	-0.600672	0.613938	C	-2.768838	-1.984731	0.000720	H	-2.446880	0.587167	0.546305
F	-4.577691	-0.123565	1.447190	C	-4.166850	-2.075198	0.002796	H	2.217979	3.180637	0.039600
F	-4.800524	-1.435019	-0.440000	C	-5.003118	-0.944132	0.003962	H	0.975819	5.277659	-0.050712
F	-5.272918	0.822765	-0.540185	C	-4.426920	0.331866	0.002892	H	-1.525568	5.231018	-0.249486
47				C	-1.863147	-3.170478	-0.000852	H	-2.685958	3.040126	-0.349025
10-BF4-TS_11		Eopt		C	-0.407348	-2.785498	-0.002464	C	4.196852	2.478536	0.190969
-1349.623805				C	0.103904	-1.484711	-0.002968	H	5.272868	2.629685	0.286884
C	1.540095	3.889422	-0.070477	C	1.456016	-1.209148	-0.004228	H	3.883801	2.990213	-0.722943
C	0.208821	3.461192	-0.132198	C	2.367709	-2.264272	-0.005090	H	3.729923	2.953599	1.057381
C	-0.232733	2.118679	-0.139269	C	1.909316	-3.580021	-0.004827	C	6.400284	-1.964329	0.247109
C	0.821484	1.199504	-0.081888	C	0.540212	-3.821369	-0.003513	H	6.948569	-1.702515	1.158738
C	2.169659	1.573976	-0.014747	H	0.628927	4.194015	-0.004042	H	6.239094	-3.045238	0.241848
C	2.535016	2.919184	-0.008811	H	-3.543724	3.216860	0.000784	H	7.042240	-1.709092	-0.603465
O	0.861420	-0.347320	-0.066285	H	-4.613194	-3.066156	0.003518	C	-1.207837	-4.445668	-0.307172
C	2.257052	-0.715494	0.011020	H	-5.048114	1.221306	0.003611	H	-1.943281	-4.576553	0.494020
C	3.038898	0.421676	0.044287	H	-2.068552	-3.795319	0.876075	H	-1.736104	-4.588077	-1.256715
C	2.739022	-2.005588	0.042735	H	-2.070704	-3.794563	-0.877822	H	-0.453847	-5.231714	-0.214100
C	4.133427	-2.115340	0.121885	H	1.826272	-0.207017	-0.004396	B	-5.334673	-0.332363	0.263730
C	4.984151	-0.995756	0.163119	H	3.427080	-2.036889	-0.005895	F	-4.582101	-0.120935	1.443275
C	4.426998	0.288029	0.121835	H	2.609861	-4.408496	-0.005537	F	-5.274984	0.825917	-0.544708
C	1.818529	-3.178807	-0.010977	H	0.165609	-4.840949	-0.003179	F	-4.794148	-1.430126	-0.446682
C	0.371077	-2.773188	-0.101082	C	1.758294	1.901724	-0.003782	F	-6.677369	-0.604709	0.602985
C	-0.121429	-1.465577	-0.123733	H	2.240108	2.879964	-0.003421	47			
C	-1.467707	-1.170909	-0.190326	H	2.107521	1.376728	0.887323	10-BF4-TS_15		Eopt	
C	-2.393471	-2.212362	-0.245791	H	2.107047	1.377627	-0.895719	-1349.623648			
C	-1.953081	-3.534391	-0.234984	C	-1.794168	5.368084	-0.001629	C	5.127534	-1.153614	0.158085
C	-0.589518	-3.795182	-0.162006	H	-1.365726	5.855729	0.881016	C	5.083554	0.245202	0.184345
H	-0.568056	4.218141	-0.177383	H	-1.364460	5.856389	-0.883271	C	3.917268	1.040258	0.124996
H	3.585168	3.186313	0.046136	H	-2.872540	5.545930	-0.002281	C	2.742434	0.283178	0.030325
H	4.564748	-3.112534	0.150638	C	-6.501231	-1.116205	0.006283	C	2.731354	-1.118254	0.006406
H	5.060165	1.168611	0.147321	H	-7.010486	-0.149104	0.007186	C	3.921909	-1.841134	0.068440
H	2.070352	-3.808397	-0.872202	H	-6.831907	-1.676249	-0.875578	O	1.252491	0.671977	-0.056683
H	1.960695	-3.803785	0.878357	H	-6.829134	-1.676452	0.889048	C	0.510375	-0.571436	-0.120703
H	-1.822590	-0.163493	-0.195230	B	5.391390	0.209047	0.004101	C	1.385678	-1.637404	-0.081683
H	-3.448995	-1.970317	-0.291014	F	4.600662	0.343550	-1.160467	C	-0.860073	-0.673373	-0.206380
H	-2.663863	-4.352983	-0.278362	F	4.574196	0.350589	1.149430	C	-1.354159	-1.983689	-0.247535
H	-0.229565	-4.819888	-0.146857	F	5.995089	-1.069322	0.014870	C	-0.515567	-3.112584	-0.208558

C	0.870971	-2.935689	-0.125732	H	2.476475	-4.523987	-0.322136	F	-4.735914	-0.636208	-1.338027
C	-1.727884	0.538187	-0.256113	H	3.171750	-2.139536	-0.391595	F	-4.683424	-1.024628	0.937367
C	-0.937061	1.816691	-0.195851	C	-3.690080	-2.980244	0.138426	F	-6.705016	-0.729891	-0.136988
C	0.452684	1.926513	-0.104527	H	-4.713311	-3.343056	0.242881	47			
C	1.109059	3.139579	-0.055263	H	-3.298074	-3.396496	-0.793300	10-BF4-TS_19		Eopt	
C	0.367420	4.319471	-0.095591	H	-3.122946	-3.373407	0.985654	-1349.623262			
C	-1.022586	4.265119	-0.184978	C	-6.723007	0.938052	0.376215	C	5.337370	0.033595	0.397337
C	-1.650496	3.025925	-0.233349	H	-6.805211	2.008227	0.169894	C	4.888800	-1.291859	0.357147
H	6.023686	0.782356	0.258488	H	-7.384167	0.399750	-0.310508	C	3.550763	-1.710818	0.181307
H	3.888519	-2.925340	0.046620	H	-7.092943	0.759847	1.392862	C	2.656509	-0.641518	0.039685
H	-2.430653	-2.115423	-0.307645	C	0.219174	4.891567	-0.262921	C	3.054380	0.702042	0.074699
H	1.538056	-3.790714	-0.092911	H	0.773533	5.143189	-1.173783	C	4.393791	1.044889	0.252579
H	-2.325069	0.529207	-1.174608	H	-0.683716	5.506701	-0.230026	O	1.131488	-0.575413	-0.176901
H	-2.448981	0.518747	0.567346	H	0.852418	5.166523	0.588090	C	0.788853	0.830164	-0.237855
H	2.173267	3.194950	0.014466	B	5.432037	0.263955	0.308520	C	1.929055	1.593107	-0.089769
H	0.891142	5.268564	-0.055877	F	4.632862	0.255719	1.476664	C	-0.482164	1.330099	-0.413978
H	-1.611768	5.175596	-0.215612	F	5.073446	1.368393	-0.497713	C	-0.567963	2.728327	-0.435183
H	-2.732445	2.963174	-0.302194	F	6.792855	0.360927	0.668434	C	0.555523	3.562562	-0.289958
C	4.165184	2.527595	0.178804	F	5.217901	-0.933973	-0.413861	C	1.819311	2.985434	-0.115956
H	5.238071	2.697831	0.277826	47				C	-1.658822	0.427018	-0.566820
H	3.845903	3.033596	-0.736230	10-BF4-TS_18		Eopt		C	-1.283783	-1.027745	-0.480715
H	3.686716	2.993679	1.043594	-1349.623733				C	0.003600	-1.540848	-0.306081
C	6.448258	-1.874930	0.226357	C	5.081753	-1.278531	-0.064336	C	0.274173	-2.892772	-0.252335
H	6.999346	-1.596279	1.131230	C	5.087534	0.121304	-0.076957	C	-0.775686	-3.803256	-0.366312
H	6.306194	-2.958536	0.230755	C	3.948415	0.956990	-0.054912	C	-2.080624	-3.342845	-0.533507
H	7.078570	-1.615277	-0.631597	C	2.745002	0.240092	-0.018161	C	-2.316083	-1.974007	-0.589578
C	-1.118204	-4.493786	-0.259881	C	2.684668	-1.160092	-0.005306	H	5.625467	-2.081067	0.471150
C	-0.349652	-5.265719	-0.168064	C	3.850525	-1.924225	-0.027064	H	4.677725	2.091615	0.276727
H	-1.845062	-4.632794	0.547744	O	1.264927	0.678144	0.008738	H	-1.549838	3.174935	-0.567431
H	-1.651024	-4.651448	-1.204476	C	0.479955	-0.539205	0.042174	H	2.701078	3.606896	-0.001228
B	-5.372421	-0.326171	0.234321	C	1.320128	-1.633464	0.031194	H	-2.409559	0.652275	0.197330
F	-5.279020	0.574512	-0.851411	C	-0.895329	-0.595399	0.081975	H	-2.147815	0.613420	-1.530020
F	-6.730022	-0.562709	0.538742	C	-1.432909	-1.888926	0.109145	H	1.270224	-3.257096	-0.127460
F	-4.745697	-1.546420	-0.112335	C	-0.631154	-3.044941	0.096074	H	-0.555463	-4.864549	-0.321753
F	-4.725100	0.229939	1.363150	C	0.762314	-2.913993	0.056364	H	-2.907675	-4.039799	-0.619055
47				C	-1.722952	0.645407	0.094963	H	-3.325171	-1.596184	-0.719039
10-BF4-TS_17		Eopt		C	-0.886793	1.896265	0.080191	C	3.353664	-3.207142	0.184305
-1349.623725				C	0.508233	1.957939	0.037169	H	4.322974	-3.684093	0.333726
C	-5.299033	0.466767	0.239444	C	1.208286	3.146988	0.016364	H	2.707264	-3.536805	1.001635
C	-5.003409	-0.901111	0.227915	C	0.507726	4.352117	0.042838	H	2.961157	-3.574286	-0.767334
C	-3.714659	-1.471412	0.122703	C	-0.885450	4.346123	0.089472	C	6.799171	0.337502	0.597177
C	-2.697748	-0.512810	0.025369	C	-1.558091	3.129649	0.106438	H	7.406657	-0.132205	-0.184188
C	-2.941357	0.867663	0.029706	H	6.048370	0.625371	-0.105394	H	6.984347	1.414425	0.575529
C	-4.239991	1.362707	0.136335	H	3.778284	-3.006655	-0.015064	H	7.149669	-0.051340	1.559807
O	-1.164545	-0.622837	-0.108929	H	-2.513723	-1.986784	0.144472	C	0.387731	5.060812	-0.321987
C	-0.662360	0.734913	-0.161749	H	1.402231	-3.790052	0.046110	H	-0.032934	5.386554	-1.279974
C	-1.715304	1.623339	-0.084224	H	-2.396725	0.651975	-0.768034	H	-0.299377	5.393674	0.463798
C	0.664957	1.086478	-0.266289	H	-2.369806	0.653492	0.978367	H	1.344558	5.569479	-0.178290
C	0.909529	2.465678	-0.297320	H	2.275509	3.163713	-0.020803	B	-5.532919	0.202189	0.496501
C	-0.119141	3.422665	-0.227003	H	1.065327	5.282435	0.026591	F	-5.627608	-1.068926	1.105621
C	-1.447765	2.993939	-0.118758	H	-1.443013	5.276559	0.110648	F	-6.777484	0.862637	0.577755
C	1.738970	0.054630	-0.333522	H	-2.643211	3.105281	0.140040	F	-4.546539	0.970219	1.160957
C	1.196551	-1.347574	-0.271128	C	4.251593	2.435608	-0.073066	F	-5.167926	0.046078	-0.861716
C	-0.148434	-1.710983	-0.171806	H	5.333811	2.567638	-0.104732	47			
C	-0.571565	-3.024159	-0.133794	H	3.844640	2.930559	-0.958710	10-BF4-TS_2		Eopt	
C	0.374233	-4.047179	-0.189317	H	3.895284	2.941917	0.827859	-1349.626868			
C	1.730162	-3.737459	-0.281272	C	6.378080	-2.045507	-0.090574	C	-3.784641	-1.032579	-0.804968
C	2.121078	-2.404112	-0.321149	H	6.998585	-1.792656	0.776344	C	-2.900691	-2.100828	-0.994385
H	-5.829889	-1.600318	0.307450	H	6.198352	-3.123479	-0.080738	C	-1.489948	-2.021360	-0.996001
H	-4.402542	2.435400	0.136856	H	6.957533	-1.801679	-0.987911	C	-1.015503	-0.721357	-0.788282
H	1.941551	2.796325	-0.377000	C	-1.280478	-4.405279	0.130363	C	-1.857538	0.383122	-0.606899
H	-2.259201	3.711696	-0.059794	H	-1.982018	-4.524241	-0.702486	C	-3.242909	0.233916	-0.613714
H	2.315448	0.175353	-1.257442	H	-0.534888	-5.202373	0.069105	O	0.405941	-0.129578	-0.683343
H	2.451699	0.201451	0.483964	H	-1.851934	-4.540499	1.055606	C	0.240385	1.292053	-0.488431
H	-1.606914	-3.275767	-0.061963	B	-5.350522	-0.332908	-0.100865	C	-1.102740	1.601442	-0.429184
H	0.033852	-5.076681	-0.158161	F	-5.270728	1.059098	0.135101	C	1.264778	2.205998	-0.391110

C	0.859465	3.533758	-0.203404	H	-2.249588	3.168582	0.055302	B	-4.943382	-0.348045	0.464452
C	-0.492615	3.911055	-0.116121	H	-1.036282	5.282691	-0.045236	F	-4.384158	0.017394	-0.786123
C	-1.484779	2.930436	-0.235967	H	1.464075	5.269237	-0.260327	F	-6.226009	0.227574	0.588982
C	2.691377	1.778019	-0.475048	H	2.653576	3.094080	-0.360346	F	-5.041625	-1.755020	0.537443
C	2.834452	0.312607	-0.789356	C	-4.221027	2.444816	0.173190	F	-4.108627	0.122387	1.502795
C	1.794801	-0.618822	-0.849320	H	-5.300316	2.581463	0.252105	47			
C	2.012799	-1.968442	-1.032738	H	-3.774556	2.931731	1.043982	10-BF4-TS_24		Eopt	
C	3.313237	-2.433779	-1.219682	H	-3.900964	2.955584	-0.738625	-1349.623364			
C	4.381633	-1.538861	-1.209019	C	-6.360854	-2.030868	0.280109	C	1.353139	2.986019	-0.131909
C	4.130199	-0.189617	-0.987746	H	-6.250446	-3.045359	-0.112169	C	0.062504	3.525155	-0.077024
H	-3.322448	-3.088925	-1.148898	H	-6.676837	-2.110019	1.327480	C	-1.143914	2.790494	-0.034278
H	-3.873460	1.104049	-0.464465	H	-7.164326	-1.529714	-0.267765	C	-0.935676	1.406101	-0.054773
H	1.630532	4.295016	-0.118669	C	1.269943	-4.410903	-0.339295	C	0.333199	0.814331	-0.105456
H	-2.535671	3.194729	-0.181025	H	1.800633	-4.539406	-1.289443	C	1.483733	1.600752	-0.144177
H	3.217959	2.368738	-1.232405	H	2.006292	-4.539265	0.461507	O	-1.908814	0.197818	-0.038088
C	3.191959	1.980557	0.479826	H	0.525340	-5.206606	-0.252892	C	-1.081614	-0.989653	-0.071559
H	1.206948	-2.668282	-1.012836	B	5.306474	-0.336843	0.275904	C	0.249970	-0.629059	-0.111081
H	3.473253	-3.497198	-1.362073	F	6.625861	-0.740934	0.573257	C	-1.552854	-2.283057	-0.062579
H	5.398577	-1.887848	-1.354874	F	5.312508	0.998441	-0.189054	C	-0.561003	-3.272166	-0.093226
H	4.952608	0.518895	-0.948681	F	4.767726	-1.179737	-0.724790	C	0.812314	-2.970786	-0.133703
C	-0.784543	-3.335947	-1.214876	F	4.510636	-0.424832	1.442286	C	1.222254	-1.631198	-0.143580
H	-1.536017	-4.113271	-1.359838	47				C	-3.016305	-2.575765	-0.026748
H	-0.156018	-3.327634	-2.108338	10-BF4-TS_22		Eopt		C	-3.852223	-1.325118	0.045186
H	-0.190036	-3.624027	-0.344393	-1349.623729				C	-3.372230	-0.012288	0.035738
C	-5.272807	-1.265984	-0.793241	C	-1.275436	3.090848	-0.348675	C	-4.203326	1.088527	0.087210
H	-5.580865	-1.897754	-1.632614	C	0.022275	3.582575	-0.187221	C	-5.583119	0.902250	0.158418
H	-5.574331	-1.777169	0.128734	C	1.199701	2.802684	-0.077072	C	-6.111562	-0.387363	0.177224
H	-5.820850	-0.321828	-0.849522	C	0.947568	1.430183	-0.145922	C	-5.246139	-1.473948	0.102519
C	-0.859171	5.354530	0.121045	C	-0.334892	0.884380	-0.303205	H	-0.037609	4.605938	-0.064383
H	-0.279417	6.021760	-0.524990	C	-1.450840	1.709310	-0.405776	H	2.457472	1.125802	-0.182165
H	-1.922148	5.528650	-0.066099	O	1.876024	0.185575	-0.084015	H	-0.877854	-4.311795	-0.084074
H	-0.649443	5.640704	1.158691	C	1.010944	-0.971063	-0.194677	H	2.275233	-1.375825	-0.174155
B	0.235975	-1.006404	2.661671	C	-0.301436	-0.560783	-0.328604	H	-3.303230	-3.145942	-0.918293
F	1.085709	0.043262	2.243602	C	1.431284	-2.279840	-0.170495	H	-3.249510	-3.213235	0.833628
F	0.601162	-1.416034	3.964247	C	0.407338	-3.232098	-0.294212	H	-3.811434	2.081870	0.074034
F	-1.102528	-0.555691	2.665083	C	-0.945133	-2.879388	-0.430942	H	-6.227884	1.773692	0.198545
F	0.363435	-2.097836	1.772795	C	-1.302327	-1.523057	-0.452705	H	-7.183250	-0.546304	0.234223
47				C	2.875068	-2.629395	-0.023750	H	-5.640019	-2.486011	0.132607
10-BF4-TS_20		Eopt		C	3.748385	-1.411820	0.131551	C	-2.395051	3.632895	0.030396
-1349.623782				C	3.319541	-0.081411	0.104589	H	-2.104974	4.684259	0.030652
C	-5.068468	-1.264267	0.176032	C	4.185145	0.985879	0.237470	H	-3.042166	3.480650	-0.837251
C	-5.067651	0.134498	0.196765	C	5.546896	0.746311	0.415194	H	-2.962450	3.459072	0.948340
C	-3.925562	0.965538	0.133800	C	6.023783	-0.562759	0.455499	C	2.555150	3.892713	-0.178669
C	-2.728990	0.244614	0.042032	C	5.125785	-1.614457	0.312926	H	2.555380	4.584893	0.670400
C	-2.675401	-1.156560	0.013589	H	0.156970	4.658100	-0.136290	H	3.482853	3.317223	-0.154979
C	-3.842152	-1.915207	0.079020	H	-2.433498	1.264522	-0.520157	H	2.549616	4.497590	-1.092680
O	-1.251584	0.678054	-0.045387	H	0.684975	-4.282534	-0.280428	C	1.826673	-4.085859	-0.175361
C	-0.473107	-0.541689	-0.130951	H	-2.338220	-1.222624	-0.558197	H	2.842166	-3.699852	-0.062888
C	-1.315524	-1.633724	-0.092503	H	3.014454	-3.284651	0.843585	H	1.642561	-4.813919	0.621915
C	0.898483	-0.600855	-0.236919	H	3.210921	-3.200579	-0.897419	H	1.772142	-4.625180	-1.128438
C	1.430775	-1.895170	-0.303144	H	3.832800	1.993814	0.205526	B	5.102237	-0.316974	0.162488
C	0.626905	-3.049121	-0.264018	H	6.218589	1.591632	0.519539	F	6.473429	-0.499473	0.441263
C	-0.762938	-2.915224	-0.158086	H	7.080938	-0.763300	0.594490	F	4.371704	-0.277264	1.372182
C	1.728920	0.637375	-0.273810	H	5.480272	-2.640704	0.338682	F	4.916920	0.897971	-0.537505
C	0.898164	1.890566	-0.218765	C	2.469800	3.598701	0.096885	F	4.633364	-1.388841	-0.633292
C	-0.492805	1.956396	-0.105777	H	2.218198	4.659885	0.095713	47			
C	-1.186361	3.147753	-0.040708	H	2.961133	3.388743	1.050490	10-BF4-TS_26		Eopt	
C	-0.483702	4.350653	-0.096727	H	3.174494	3.437980	-0.722883	-1349.623418			
C	0.905080	4.340478	-0.215902	C	-2.451144	4.024221	-0.468659	C	-1.342870	3.000501	-0.025981
C	1.571536	3.121894	-0.273149	H	-3.278533	3.691539	0.165821	C	-0.048144	3.532687	-0.016685
H	-6.024004	0.642740	0.265734	H	-2.180659	5.044574	-0.184932	C	1.155058	2.791688	-0.012554
H	-3.776666	-2.997847	0.050822	H	-2.821872	4.045261	-1.500343	C	0.938965	1.408417	-0.018951
H	2.509140	-1.994340	-0.386029	C	-2.010694	-3.941736	-0.526050	C	-0.333974	0.823520	-0.028483
H	-1.403343	-3.790238	-0.126483	H	-2.516989	-4.064718	0.438812	C	-1.481106	1.615971	-0.031487
H	2.434465	0.634449	0.563336	H	-2.775924	-3.667523	-1.258207	O	1.905699	0.195028	-0.023450
H	2.341946	0.649624	-1.181347	H	-1.585222	-4.908512	-0.808727	C	1.071693	-0.988056	-0.026746

C	-0.258209	-0.620028	-0.032680	H	-3.203075	-3.208388	-0.896411	H	1.526463	-4.973012	-0.060568
C	1.535297	-2.284253	-0.019710	H	-3.080562	-3.270084	0.852235	H	2.543576	-3.923206	-1.065186
C	0.537093	-3.267672	-0.022304	H	-3.852228	2.000992	0.141839	B	5.091825	-0.328540	0.121026
C	-0.835037	-2.958016	-0.032240	H	-6.252389	1.609241	0.341534	F	4.848031	-1.639555	-0.347370
C	-1.236650	-1.616231	-0.036491	H	-7.126567	-0.742156	0.385190	F	4.570305	0.603761	-0.808151
C	2.997455	-2.585022	-0.007790	H	-5.522342	-2.626937	0.218459	F	4.453252	-0.148720	1.369606
C	3.842237	-1.338473	0.017221	C	-2.484542	3.600956	0.059954	F	6.480904	-0.125362	0.264252
C	3.369793	-0.022877	0.004276	H	-2.229501	4.661322	0.056100	47			
C	4.208332	1.073559	0.010212	H	-3.155355	3.431289	-0.785948	10-BF4-TS_3		Eopt	
C	5.588615	0.879713	0.038152	H	-3.014978	3.404659	0.995397	-1349.626768			
C	6.109942	-0.412774	0.059187	C	2.456558	4.008066	-0.314196	C	-3.818977	-1.736847	-0.233856
C	5.237080	-1.494844	0.047708	H	2.891078	3.986447	-1.320516	C	-2.793353	-2.637738	-0.542646
H	0.058643	4.612775	-0.011699	H	2.171170	5.038865	-0.089115	C	-1.431273	-2.313231	-0.732271
H	-2.458247	1.146402	-0.037305	H	3.242658	3.701777	0.383223	C	-1.169415	-0.944526	-0.591894
H	0.847928	-4.309157	-0.015178	C	1.993618	-3.956864	-0.345894	C	-2.161979	-0.002117	-0.292560
H	-2.287413	-1.352247	-0.042415	H	2.703342	-3.752802	-1.153802	C	-3.487750	-0.391902	-0.110955
H	3.244300	-3.203072	0.863081	H	2.568702	-3.985977	0.586765	O	0.123153	-0.110931	-0.682032
H	3.263161	-3.178197	-0.890699	H	1.556769	-4.945881	-0.507296	C	-0.264409	1.265111	-0.476379
H	3.821518	2.068842	-0.007172	B	5.010081	-0.337797	0.302223	C	-1.619469	1.335168	-0.226917
H	6.239434	1.747582	0.042976	F	5.009067	-1.746162	0.408220	C	0.582374	2.347935	-0.545596
H	7.182022	-0.577489	0.082384	F	4.320557	0.219593	1.402937	C	-0.024483	3.590181	-0.320165
H	5.626132	-2.508739	0.061418	F	6.338343	0.138461	0.283357	C	-1.396259	3.727082	-0.041652
C	2.412291	3.627165	-0.000319	F	4.356468	0.041391	-0.896930	C	-2.203169	2.583467	-0.000540
H	2.128155	4.680302	0.003940	47				C	2.035318	2.173477	-0.833865
H	3.013774	3.455527	0.896000	10-BF4-TS_29		Eopt		C	2.384268	0.751747	-1.182294
H	3.024268	3.465838	-0.891638	-1349.623616				C	1.533862	-0.350824	-1.071076
C	-2.541436	3.912863	-0.030710	C	1.269124	3.065474	-0.092795	C	1.960463	-1.645890	-1.276368
H	-2.540201	4.551828	-0.921012	C	-0.037098	3.566996	-0.053795	C	3.276568	-1.879532	-1.671537
H	-3.470922	3.339831	-0.020212	C	-1.221735	2.796715	-0.024583	C	4.151797	-0.809028	-1.843033
H	-2.532270	4.572726	0.843957	C	-0.972914	1.419131	-0.039354	C	3.699651	0.481140	-1.589191
C	-1.858728	-4.065177	-0.045405	C	0.312912	0.865231	-0.077543	H	-3.052399	-3.686996	-0.642512
H	-1.680763	-4.774689	0.769972	C	1.440360	1.684726	-0.104632	H	-4.236298	0.357629	0.123229
H	-2.870655	-3.666860	0.058789	O	-1.911092	0.182611	-0.029694	H	0.600671	4.478180	-0.362108
H	-1.810305	-4.628682	-0.984565	C	-1.049473	-0.980698	-0.055543	H	-3.266680	2.662323	0.198953
B	-5.087539	-0.319149	0.040734	C	0.273151	-0.580169	-0.084756	H	2.340842	2.838537	-1.648442
F	-4.441650	-0.794101	1.205991	C	-1.480962	-2.285331	-0.049280	H	2.620386	2.467462	0.046041
F	-6.442781	-0.711957	0.056443	C	-0.457556	-3.246452	-0.074985	H	1.309207	-2.476359	-1.115328
F	-5.000810	1.091291	-0.001104	C	0.903664	-2.905101	-0.105658	H	3.602461	-2.902300	-1.827697
F	-4.449495	-0.861117	-1.099775	C	1.272703	-1.550844	-0.110637	H	5.178532	-0.976580	-2.151150
47				C	-2.934456	-2.623177	-0.018639	H	4.377041	1.324766	-1.684946
10-BF4-TS_28		Eopt		C	-3.808726	-1.398071	0.035262	C	-0.540392	-3.492104	-1.038436
-1349.623732				C	-3.368706	-0.071202	0.027595	H	-1.154575	-4.393123	-1.066517
C	1.274160	3.079312	-0.229329	C	-4.233726	1.004086	0.065062	H	-0.054501	-3.404882	-2.012857
C	-0.027598	3.575554	-0.124976	C	-5.608012	0.775958	0.117778	H	0.212770	-3.645711	-0.260864
C	-1.210535	2.799568	-0.051296	C	-6.097139	-0.529174	0.132144	C	-5.228745	-2.226632	-0.028729
C	-0.959105	1.425872	-0.092988	C	-5.198425	-1.589139	0.090815	H	-5.541544	-2.883699	-0.846871
C	0.327176	0.875522	-0.195198	H	-0.169920	4.644354	-0.045756	H	-5.305557	-2.803084	0.900652
C	1.448332	1.696700	-0.263452	H	2.427629	1.237620	-0.140298	H	-5.931291	-1.391525	0.032651
O	-1.891774	0.184189	-0.048377	H	-0.743931	-4.294477	-0.069434	C	-1.980152	5.091878	0.223927
C	-1.027396	-0.975586	-0.121694	H	2.317547	-1.264482	-0.131156	H	-3.070415	5.078525	0.143099
C	0.290623	-0.569941	-0.210288	H	-3.198687	-3.211941	-0.905052	H	-1.722933	5.431740	1.234467
C	-1.453091	-2.282310	-0.107911	H	-3.152646	-3.258144	0.847696	H	-1.589043	5.833839	-0.479464
C	-0.428371	-3.238774	-0.190141	H	-3.871177	2.008579	0.053319	B	1.578264	-0.744596	2.522605
C	0.928882	-2.891416	-0.279936	H	-6.279683	1.627304	0.146712	F	1.589658	0.578782	2.026716
C	1.291718	-1.535893	-0.293129	H	-7.164273	-0.720408	0.173727	F	0.469283	-1.438089	1.986455
C	-2.902679	-2.626551	-0.016960	H	-5.561735	-2.612647	0.099784	F	2.771237	-1.400862	2.145404
C	-3.778297	-1.405186	0.086395	C	-2.498080	3.601100	0.019992	F	1.478704	-0.717522	3.932437
C	-3.343753	-0.076457	0.071411	H	-2.239447	4.660683	0.020575	47			
C	-4.210198	0.994775	0.159487	H	-3.128258	3.426529	-0.855753	10-BF4-TS_30		Eopt	
C	-5.579803	0.760939	0.272919	H	-3.072145	3.413603	0.931061	-1349.623646			
C	-6.063164	-0.546192	0.296411	C	2.446760	4.004330	-0.122425	C	-1.319020	3.028867	-0.144344
C	-5.163468	-1.601987	0.203185	H	2.437885	4.669180	0.748384	C	-0.020919	3.548626	-0.080883
H	-0.162127	4.651886	-0.095222	H	3.389050	3.451720	-0.123595	C	1.173917	2.795033	-0.032180
H	2.433385	1.249147	-0.339474	H	2.418219	4.637445	-1.016459	C	0.944626	1.414116	-0.055381
H	-0.710091	-4.288132	-0.183306	C	1.965810	-3.974909	-0.135678	C	-0.332550	0.842386	-0.114324
H	2.331576	-1.239965	-0.366240	H	2.673864	-3.844881	0.689319	C	-1.470577	1.645947	-0.159849

O	1.899398	0.190148	-0.033257	H	-0.764702	-4.295568	-0.182054	C	4.619910	-4.008863	0.829854
C	1.054235	-0.984733	-0.073744	H	2.312654	-1.285710	-0.349407	H	4.947279	-4.017749	1.875818
C	-0.273204	-0.602316	-0.120612	H	-3.247496	-3.180437	-0.910728	H	4.064326	-4.930745	0.640123
C	1.503779	-2.283260	-0.068701	H	-3.123369	-3.260472	0.837050	H	5.521046	-4.015975	0.206976
C	0.494280	-3.258282	-0.112176	H	-3.839746	2.026452	0.130848	B	-5.144398	0.388411	0.925222
C	-0.871137	-2.935547	-0.157429	H	-6.241594	1.660087	0.353528	F	-6.257069	0.881730	1.643919
C	-1.259018	-1.586563	-0.162962	H	-7.139276	-0.681962	0.416830	F	-5.114230	-1.021739	1.009621
C	2.961625	-2.600879	-0.026390	H	-5.556024	-2.583944	0.240092	F	-5.252417	0.776667	-0.431511
C	3.817793	-1.363969	0.047825	C	-2.455825	3.610978	0.065050	F	-3.955956	0.920074	1.475271
C	3.359041	-0.043432	0.041573	H	-2.189159	4.668468	0.068680	47			
C	4.207860	1.043754	0.098101	H	-3.129447	3.455393	-0.781476	10-BF4-TS_37		Eopt	
C	5.584386	0.834845	0.169713	H	-2.987382	3.413398	0.999488	-1349.622948			
C	6.091860	-0.463248	0.184110	C	2.487122	3.968618	-0.327518	C	1.930151	-2.132555	-0.866708
C	5.209063	-1.535593	0.123330	H	2.214105	5.000624	-0.092792	C	2.184785	-0.762156	-0.973739
H	0.096035	4.627752	-0.066973	H	3.277196	3.649460	0.359356	C	1.240200	0.275980	-0.791705
H	-2.450082	1.184033	-0.209666	H	2.911333	3.949583	-1.338290	C	-0.036770	-0.202874	-0.487150
H	0.795057	-4.302277	-0.110026	C	1.942089	-3.994580	-0.342187	C	-0.349536	-1.564797	-0.373421
H	-2.307456	-1.314487	-0.196191	H	2.573874	-3.973534	0.552786	C	0.631129	-2.534539	-0.564298
H	3.180421	-3.241009	0.835928	H	1.489728	-4.986791	-0.418391	O	-1.387570	0.511517	-0.203037
H	3.242720	-3.177278	-0.915791	H	2.601332	-3.846877	-1.203770	C	-2.354566	-0.533467	0.045880
H	3.831580	2.043214	0.088056	B	5.040162	-0.331646	0.307821	C	-1.744564	-1.767576	-0.054257
H	6.243294	1.695461	0.213634	F	6.415292	-0.129694	0.551987	C	-3.684614	-0.329743	0.340280
H	7.160841	-0.639628	0.241008	F	4.818429	-1.670058	-0.089014	C	-4.431400	-1.497603	0.542831
H	5.586518	-2.553951	0.132523	F	4.303403	-0.060602	1.483201	C	-3.869927	-2.784158	0.454622
C	2.437882	3.617031	0.039607	F	4.610631	0.537943	-0.724358	C	-2.508916	-2.917801	0.153546
H	2.164898	4.672972	0.041293	47				C	-4.256798	1.045942	0.433501
H	2.998424	3.431972	0.959593	10-BF4-TS_32		Eopt		C	-3.235881	2.115267	0.145824
H	3.086156	3.456298	-0.825558	-1349.622935				C	-1.885709	1.905973	-0.148729
C	-2.509466	3.950429	-0.196817	C	-1.957267	-2.134659	-1.048111	C	-1.002306	2.938749	-0.387408
H	-2.510463	4.637202	0.656663	C	-2.202609	-0.763126	-1.174544	C	-1.459919	4.254818	-0.342812
H	-2.489482	4.560716	-1.106970	C	-1.264411	0.272033	-0.957913	C	-2.799072	4.516944	-0.058904
H	-3.443874	3.384588	-0.184695	C	-0.002510	-0.208878	-0.594228	C	-3.661300	3.452720	0.180232
C	-1.917821	-4.020363	-0.191324	C	0.299544	-1.569827	-0.455839	H	3.196513	-0.447638	-1.202787
H	-1.461160	-5.010096	-0.273822	C	-0.676242	-2.538114	-0.683565	H	0.368386	-3.583362	-0.471637
H	-2.528118	-3.999038	0.718458	O	1.335749	0.503793	-0.256326	H	-5.487301	-1.393075	0.778375
H	-2.598616	-3.880984	-1.037398	C	2.286226	-0.541861	0.048016	H	-2.051341	-3.898672	0.081589
B	-5.051874	-0.326569	0.178491	C	1.677394	-1.775035	-0.070574	H	-5.093545	1.149984	-0.266673
F	-4.414531	0.149833	1.347163	C	3.602467	-0.339922	0.400237	H	-4.672150	1.208019	1.435090
F	-4.834869	-1.717834	0.058138	C	4.335108	-1.508373	0.645741	H	0.027178	2.750330	-0.602005
F	-6.436577	-0.065420	0.253275	C	3.773832	-2.793963	0.543048	H	-0.757424	5.059692	-0.530317
F	-4.506501	0.331099	-0.950723	C	2.428084	-2.926197	0.179553	H	-3.167793	5.536572	-0.021632
47				C	4.176348	1.034320	0.503823	H	-4.707284	3.638686	0.406075
10-BF4-TS_31		Eopt		C	3.172701	2.104410	0.163403	C	1.797220	1.668711	-0.956882
-1349.623675				C	1.836421	1.897446	-0.190419	H	2.860614	1.591833	-1.181043
C	1.296078	3.051469	-0.237648	C	0.969266	2.931517	-0.478216	H	1.329435	2.203859	-1.787696
C	-0.000196	3.560768	-0.128955	C	1.429536	4.246250	-0.423519	H	1.711140	2.256701	-0.039940
C	-1.190654	2.796626	-0.053854	C	2.755143	4.505986	-0.080338	C	3.038980	-3.135746	-1.043877
C	-0.953236	1.420492	-0.098954	C	3.601116	3.440617	0.206638	H	2.665391	-4.060808	-1.492982
C	0.327465	0.857039	-0.201346	H	-3.203798	-0.447266	-1.446000	H	3.839517	-2.736697	-1.671819
C	1.456355	1.667110	-0.271850	H	-0.423055	-3.586852	-0.568385	H	3.479144	-3.391354	-0.072811
O	-1.899048	0.188847	-0.062705	H	5.380021	-1.405203	0.926565	C	-4.734878	-3.999437	0.675948
C	-1.046529	-0.979874	-0.132483	H	1.971693	-3.906362	0.091647	H	-5.252996	-3.942705	1.639353
C	0.276323	-0.588191	-0.216095	H	4.550400	1.204937	1.520108	H	-5.502681	-4.078581	-0.102388
C	-1.486226	-2.281735	-0.115892	H	5.041692	1.128064	-0.162237	H	-4.139584	-4.915887	0.659938
C	-0.471605	-3.249418	-0.192214	H	-0.049784	2.745580	-0.739203	B	5.356581	0.362345	0.746417
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C	1.267217	-1.565229	-0.290430	H	3.125886	5.524533	-0.034443	F	5.311020	-1.046521	0.841361
C	-2.939442	-2.610550	-0.025977	H	4.636439	3.624725	0.478356	F	6.562325	0.836722	1.309640
C	-3.800977	-1.380452	0.089330	C	-1.806958	1.666106	-1.154082	F	4.259721	0.919103	1.442723
C	-3.352643	-0.056446	0.068593	H	-2.861333	1.592742	-1.418328	47			
C	-4.207331	1.023981	0.157716	H	-1.753691	2.260556	-0.239073	10-BF4-TS_38		Eopt	
C	-5.578278	0.804619	0.283693	H	-1.303963	2.192490	-1.969906	-1349.626993			
C	-6.074779	-0.497350	0.317480	C	-3.063539	-3.130734	-1.273682	C	3.858156	1.227666	-0.548131
C	-5.186927	-1.562707	0.219392	H	-2.664104	-4.136867	-1.426687	C	2.961274	2.290922	-0.701359
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 C 2.877808 -2.803261 0.095364
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 H -2.286582 -4.461794 -0.435833
 H -3.462039 -3.375960 0.333276
 C 5.226365 -3.698369 0.380517
 H 5.688300 -3.699101 1.374622
 H 4.732808 -4.662727 0.235703
 H 6.034662 -3.611712 -0.353590
 B -5.780136 0.313905 0.351133
 F -7.128443 0.272993 0.766487
 F -5.514025 -0.785010 -0.500348
 F -5.536327 1.517599 -0.350463
 F -4.933546 0.248181 1.481161
 47
 10-BF4-TS_41 Eopt
 -1349.622666
 C -1.696560 -2.388933 -0.390702
 C -2.074728 -1.042939 -0.461036

C	-1.204093	0.068222	-0.394318	C	2.884839	4.553357	0.036107	C	2.928365	-3.188515	0.172673
C	0.136964	-0.303070	-0.244758	C	3.790158	3.498470	0.017121	H	3.661174	-3.002830	-0.619081
C	0.571109	-1.632606	-0.173228	H	-3.154504	-0.508381	0.086112	H	3.465016	-3.129276	1.126112
C	-0.344378	-2.681832	-0.246013	H	-0.188034	-3.597705	0.032632	H	2.540786	-4.204215	0.058959
O	1.449499	0.521628	-0.125389	H	5.764052	-1.322831	-0.039447	C	-5.043664	-3.938355	-0.077647
C	2.520157	-0.438789	0.013897	H	2.292889	-3.876133	0.013044	H	-4.469240	-4.867693	-0.047566
C	2.005531	-1.719453	-0.019326	H	5.127864	1.234321	0.809043	H	-5.724483	-3.928548	0.780825
C	3.852419	-0.125738	0.166748	H	5.067302	1.245834	-0.943779	H	-5.661488	-3.947398	-0.982621
C	4.710355	-1.227432	0.285143	H	0.027554	2.756035	0.000413	B	5.930952	0.312461	-0.096575
C	4.250072	-2.555914	0.252095	H	0.783444	5.071897	0.038170	F	7.330958	0.488909	-0.123633
C	2.879560	-2.801806	0.100960	H	3.241157	5.577886	0.053203	F	5.579168	-0.530182	0.983468
C	4.315765	1.292751	0.207822	H	4.858142	3.696549	0.016576	F	5.298359	1.568046	0.064637
C	3.181431	2.274329	0.072516	C	-1.769100	1.632501	0.055804	F	5.502955	-0.275660	-1.308876
C	1.830700	1.953993	-0.089766	H	-2.855072	1.541515	0.081290	47			
C	0.845596	2.910648	-0.226968	H	-1.474877	2.202305	0.941000	10-BF4-TS_45		Eopt	
C	1.193146	4.260349	-0.195494	H	-1.518600	2.196633	-0.846598	-1349.623733			
C	2.525969	4.632494	-0.029305	C	-2.931702	-3.185893	0.092788	C	5.298349	0.527243	0.189970
C	3.493907	3.642856	0.099817	H	-3.662023	-2.989753	-0.698612	C	5.024121	-0.845184	0.181811
H	-3.130166	-0.818341	-0.567716	H	-2.544630	-4.200490	-0.032010	C	3.743145	-1.435554	0.095766
H	0.011346	-3.705098	-0.185691	H	-3.471011	-3.138210	1.045441	C	2.709975	-0.493030	0.014461
H	5.772703	-1.035143	0.410220	C	5.041840	-3.941054	-0.037166	C	2.931698	0.891118	0.017372
H	2.497888	-3.816991	0.079833	H	4.486165	-4.857511	0.177586	C	4.223852	1.406452	0.105281
H	4.845992	1.483410	1.148094	H	5.515674	-4.056152	-1.019312	O	1.177660	-0.627587	-0.098773
H	5.040801	1.470899	-0.594865	H	5.843589	-3.841464	0.701801	C	0.652320	0.722086	-0.135180
H	-0.179311	2.639616	-0.360151	B	-5.931669	0.312655	-0.046101	C	1.691967	1.627279	-0.073958
H	0.411177	5.004341	-0.303042	F	-5.331029	1.587410	0.080919	C	-0.682422	1.052186	-0.210631
H	2.809323	5.679383	-0.002613	F	-5.497368	-0.516897	1.013785	C	-0.950076	2.427247	-0.231404
H	4.537831	3.915066	0.225772	F	-7.336146	0.444413	0.001604	C	0.064197	3.400673	-0.179170
C	-1.887343	1.409722	-0.494031	F	-5.549382	-0.263721	-1.279332	C	1.401545	2.993499	-0.098866
H	-2.958975	1.247800	-0.603711	47				C	-1.740464	0.003191	-0.261582
H	-1.749325	2.010219	0.408727	10-BF4-TS_43		Eopt		C	-1.174788	-1.389879	-0.205023
H	-1.556676	1.975768	-1.368807	-1349.622520				C	0.177830	-1.731613	-0.137012
C	-2.740527	-3.471702	-0.466210	C	1.816501	-2.174054	0.124449	C	0.622811	-3.037776	-0.111716
H	-3.460672	-3.372719	0.353130	C	2.110494	-0.805461	0.136378	C	-0.307699	-4.075768	-0.143292
H	-3.306941	-3.402808	-1.401195	C	1.167924	0.247040	0.100512	C	-1.670344	-3.787862	-0.200599
H	-2.285827	-4.464012	-0.409190	C	-0.153484	-0.210956	0.052405	C	-2.083357	-2.460945	-0.231777
C	5.229609	-3.696899	0.363984	C	-0.504226	-1.566498	0.040815	H	5.862356	-1.531630	0.248081
H	4.714588	-4.644022	0.544391	C	0.479124	-2.554062	0.074924	H	4.369854	2.481363	0.106750
H	5.811283	-3.800207	-0.559881	O	-1.522108	0.525982	-0.010519	H	-1.988773	2.741140	-0.288789
H	5.940381	-3.528605	1.179471	C	-2.535180	-0.504979	-0.031278	H	2.202226	3.724180	-0.053479
B	-5.780572	0.313566	0.348486	C	-1.936678	-1.748441	-0.005982	H	-2.446056	0.141389	0.563618
F	-7.129130	0.272542	0.763004	C	-3.894080	-0.282980	-0.064651	H	-2.329782	0.112702	-1.178790
F	-5.512636	-0.787931	-0.499096	C	-4.683297	-1.440352	-0.078415	H	1.663469	-3.273196	-0.067929
F	-5.537538	1.515173	-0.356925	C	-4.134606	-2.735433	-0.058768	H	0.049758	-5.099717	-0.121745
F	-4.934754	0.252559	1.479346	C	-2.743287	-2.888340	-0.020517	H	-2.404619	-4.586384	-0.222722
47				C	-4.453215	1.100864	-0.081579	H	-3.139403	-2.212865	-0.278790
10-BF4-TS_42		Eopt		C	-3.380826	2.156288	-0.017403	C	3.743309	-2.944562	0.112149
-1349.622513				C	-2.001777	1.929140	0.007447	H	4.773795	-3.289881	0.203927
C	-1.818682	-2.172013	0.061177	C	-1.075627	2.952089	0.037321	H	3.193148	-3.347368	0.965835
C	-2.112041	-0.803270	0.064611	C	-1.516585	4.274504	0.056951	H	3.347196	-3.367426	-0.814926
C	-1.168381	0.248740	0.044515	C	-2.881924	4.553814	0.044160	C	6.717240	1.020175	0.300936
C	0.153339	-0.210117	0.020283	C	-3.787601	3.499744	0.005633	H	6.772925	2.099569	0.139064
C	0.503449	-1.565950	0.017738	H	3.152644	-0.511145	0.176470	H	7.125897	0.803841	1.294930
C	-0.480841	-2.552928	0.037020	H	0.185778	-3.598590	0.062839	H	7.363680	0.526027	-0.431792
O	1.523098	0.525916	-0.020290	H	-5.763124	-1.320482	-0.104208	C	-0.298489	4.863960	-0.204450
C	2.535960	-0.505547	-0.024798	H	-2.294816	-3.875827	-0.000513	H	-0.867413	5.110305	-1.107783
C	1.936397	-1.748869	-0.006243	H	-5.046799	1.250614	-0.991267	H	-0.926271	5.124984	0.654913
C	3.895098	-0.284352	-0.036110	H	-5.142377	1.234509	0.759924	H	0.594720	5.493514	-0.179460
C	4.683965	-1.442347	-0.033386	H	-0.025611	2.754358	0.044859	B	-5.446201	0.268494	0.238977
C	4.134515	-2.736854	-0.020231	H	-0.780493	5.070874	0.081648	F	-6.821723	0.404494	0.523832
C	2.742329	-2.889014	-0.003966	H	-3.237767	5.578516	0.060905	F	-5.200425	-1.015133	-0.304242
C	4.455559	1.098977	-0.045775	H	-4.855321	3.698625	-0.010713	F	-5.054561	1.256292	-0.693468
C	3.382819	2.155192	-0.005371	C	1.768560	1.630577	0.123236	F	-4.698325	0.424353	1.430085
C	2.003392	1.928938	-0.001505	H	2.854058	1.539555	0.162754	47			
C	1.077765	2.952758	0.008962	H	1.530560	2.196130	-0.781642	10-BF4-TS_46		Eopt	
C	1.519292	4.274973	0.029007	H	1.461179	2.198832	1.004982	-1349.623827			

C	-1.526110	3.891111	-0.004783	C	1.421669	-1.009676	0.009699	H	2.120970	1.415328	0.696253
C	-0.195107	3.457443	-0.009183	C	2.407597	-1.995991	0.014121	H	2.051895	1.418274	-1.086136
C	0.240819	2.113033	-0.010024	C	2.043180	-3.341080	0.015501	C	-1.859820	5.360595	-0.061976
C	-0.818698	1.198200	-0.006307	C	0.694917	-3.679337	0.012299	H	-2.937957	5.525927	0.006720
C	-2.166885	1.578176	-0.001717	H	0.216970	4.321544	0.005881	H	-1.379239	5.866234	0.782731
C	-2.526714	2.924767	-0.001009	H	-3.875814	3.053907	-0.009087	H	-1.496396	5.840644	-0.977449
O	-0.866183	-0.349072	-0.005227	H	-4.499519	-3.292061	-0.007577	C	-6.480834	-1.180401	0.223914
C	-2.265452	-0.710829	0.000515	H	-5.238302	0.953492	-0.012802	H	-7.002064	-0.219757	0.232543
C	-3.042965	0.429761	0.002460	H	-1.914235	-3.836334	0.883530	H	-6.846487	-1.760709	-0.630545
C	-2.754346	-1.998632	0.003687	H	-1.908335	-3.841503	-0.870415	H	-6.758430	-1.728247	1.131449
C	-4.151437	-2.101975	0.009170	H	1.719872	0.016126	0.008019	B	5.389892	0.216383	0.164858
C	-4.998144	-0.978644	0.011333	H	3.448046	-1.692388	0.016923	F	5.709621	-1.156922	0.050063
C	-4.433768	0.302620	0.007954	H	2.800989	-4.117601	0.018890	F	4.517209	0.403290	1.261651
C	-1.837737	-3.175978	0.001131	H	0.394248	-4.723065	0.012856	F	6.570721	0.962942	0.368626
C	-0.385601	-2.777468	-0.006261	C	1.506009	2.114312	0.011587	F	4.755352	0.648916	-1.022272
C	0.113389	-1.472025	-0.009436	H	1.917017	3.124328	0.014273	47			
C	1.462765	-1.183785	-0.015708	H	1.887192	1.614574	0.904544	10-BF4-TS_51		Eopt	
C	2.385041	-2.229706	-0.018764	H	1.891791	1.617465	-0.881040	-1349.621643			
C	1.938651	-3.549729	-0.016260	C	-2.281821	5.321852	0.009912	C	-3.803125	3.252903	0.060848
C	0.571927	-3.804214	-0.010225	H	-2.007626	5.796428	0.959213	C	-2.440027	3.558140	-0.029622
H	0.586234	4.211123	-0.012079	H	-1.779052	5.877395	-0.788641	C	-1.380548	2.624855	-0.091725
H	-3.577409	3.195390	0.002801	H	-3.361580	5.426412	-0.123138	C	-1.821648	1.295969	-0.051343
H	-4.588601	-3.097035	0.011802	C	-6.520967	-1.481454	-0.017847	C	-3.173457	0.937364	0.035159
H	-5.063152	1.186311	0.009442	H	-7.098303	-0.553512	-0.016246	C	-4.168711	1.911477	0.093018
H	-2.034328	-3.800972	0.879982	H	-6.806059	-2.060151	-0.903600	O	-1.077756	-0.058088	-0.091115
H	-2.042586	-3.803654	-0.873899	H	-6.812487	-2.067462	0.860931	C	-2.095334	-1.082886	-0.020283
H	1.822688	-0.178044	-0.017711	B	5.808860	0.227862	-0.011041	C	-3.342793	-0.496887	0.052280
H	3.442468	-1.992229	-0.022528	F	6.504833	0.751610	1.100861	C	-1.859816	-2.440057	-0.023387
H	2.646966	-4.371602	-0.018727	F	6.462505	0.608396	-1.204021	C	-3.007857	-3.239842	0.048715
H	0.207208	-4.827382	-0.008046	F	5.772100	-1.184272	0.077321	C	-4.306438	-2.703886	0.121389
C	1.736702	1.928621	-0.014662	F	4.486605	0.729192	-0.017834	C	-4.473155	-1.313775	0.123378
H	2.209874	2.911029	-0.014785	47				C	-0.473423	-2.986965	-0.096194
H	2.093350	1.405869	0.874711	10-BF4-TS_50		Eopt		C	0.571650	-1.904370	-0.151686
H	2.086568	1.408629	-0.908570	-1349.623806				C	0.335833	-0.527430	-0.154738
C	-1.847430	5.362723	-0.003308	C	-1.534436	3.889887	-0.062817	C	1.348704	0.407655	-0.215849
H	-1.425805	5.852916	0.881229	C	-0.203441	3.459803	-0.117461	C	2.673381	-0.022880	-0.272669
H	-1.419978	5.856314	-0.883071	C	0.236203	2.116644	-0.124282	C	2.963757	-1.386017	-0.268515
H	-2.927355	5.530613	-0.006352	C	-0.819684	1.198940	-0.074398	C	1.917954	-2.299621	-0.209402
C	-6.494645	-1.164319	0.017046	C	-2.167675	1.575293	-0.014789	H	-2.154234	4.604850	-0.057320
H	-7.012753	-0.201928	0.019107	C	-2.531116	2.920991	-0.008890	H	-5.208141	1.608074	0.161200
H	-6.822145	-1.727369	-0.864096	O	-0.862042	-0.347915	-0.060126	H	-2.877251	-4.318712	0.048555
H	-6.815426	-1.727613	0.900488	C	-2.258580	-0.714032	0.009404	H	-5.463399	-0.874497	0.179814
B	5.404649	0.214340	0.013183	C	-3.038938	0.424262	0.038421	H	-0.280804	-3.627667	0.772032
F	5.776800	-1.149808	0.053646	C	-2.742575	-2.003406	0.039360	H	-0.373010	-3.628730	-0.979231
F	6.562498	1.022230	0.026017	C	-4.137569	-2.111088	0.110447	H	1.144148	1.455841	-0.220045
F	4.667619	0.463194	-1.167740	C	-4.986900	-0.990264	0.146296	H	3.467265	0.713437	-0.319979
F	4.605847	0.515005	1.140557	C	-4.427637	0.292699	0.108213	H	3.992653	-1.725232	-0.308450
47				C	-1.823412	-3.177956	-0.007167	H	2.125126	-3.366013	-0.206323
10-BF4-TS_47		Eopt		C	-0.374902	-2.774503	-0.089690	C	-0.005830	3.238713	-0.189190
-1349.622722				C	0.119486	-1.467588	-0.112073	H	-0.110413	4.324280	-0.201312
C	-1.871093	3.872708	0.000674	C	1.466416	-1.174846	-0.173916	H	0.619619	2.989838	0.671808
C	-0.516329	3.521061	0.005056	C	2.391037	-2.217631	-0.222299	H	0.508731	2.957250	-1.111213
C	0.000821	2.205741	0.007685	C	1.948840	-3.539063	-0.210427	C	-4.828747	4.354718	0.115056
C	-1.000774	1.227308	0.004915	C	0.584579	-3.797934	-0.143971	H	-4.801512	4.957327	-0.799774
C	-2.370007	1.524506	-0.000736	H	0.574838	4.215657	-0.156381	H	-5.837285	3.949113	0.227246
C	-2.810815	2.847018	-0.003255	H	-3.581210	3.189438	0.040441	H	-4.633045	5.029854	0.955215
O	-0.953719	-0.319416	0.004752	H	-4.570559	-3.107611	0.137326	C	-5.497639	-3.624868	0.202176
C	-2.328383	-0.766618	-0.000737	H	-5.059571	1.174259	0.130510	H	-5.515385	-4.318443	-0.645662
C	-3.174415	0.324203	-0.004564	H	-1.971697	-3.801250	0.882355	H	-5.462833	-4.229047	1.115864
C	-2.736726	-2.082379	-0.001126	H	-2.071086	-3.808639	-0.868798	H	-6.433689	-3.060546	0.202747
C	-4.124732	-2.271917	-0.006869	H	1.822738	-0.167933	-0.180783	B	6.516483	0.285646	0.166281
C	-5.038989	-1.202914	-0.011427	H	3.447044	-1.976967	-0.263029	F	7.886540	0.607314	0.282465
C	-4.554887	0.110789	-0.009951	H	2.658749	-4.358672	-0.248510	F	5.891565	0.410392	1.428045
C	-1.749618	-3.201436	0.005204	H	0.223186	-4.822144	-0.128990	F	5.899855	1.168567	-0.751960
C	-0.324698	-2.713960	0.008430	C	1.731727	1.936742	-0.180152	F	6.381676	-1.043869	-0.297679
C	0.092770	-1.380386	0.007714	H	2.201416	2.920678	-0.196087	47			

10-BF4-TS_52	Eopt	C 1.315368	-0.944284	-0.562144	C -3.688356	-2.981006	-0.142137
-1349.622102		C 0.046767	-1.496249	-0.369441	H -4.711347	-3.344323	-0.247241
C 5.496847	-0.737848	-0.058945	C -0.182781	-2.856184	-0.321271	H -3.120387	-3.373944
C 4.785985	-1.943524	-0.045426	C 0.891476	-3.734349	-0.458983	H -3.296901	-3.397066
C 3.379562	-2.079217	-0.017640	C 2.179340	-3.234527	-0.644155	C -6.725379	0.934360
C 2.712239	-0.847376	-0.003220	C 2.372956	-1.859036	-0.694607	H -7.280673	0.705324
C 3.376993	0.386696	-0.014106	H -5.538328	-2.203278	0.532330	H -6.773953	2.013648
C 4.769191	0.447429	-0.041622	H -4.715666	1.996109	0.337852	H -7.240515	0.433801
O 1.218266	-0.467576	0.029294	H 1.453541	3.265194	-0.645458	C 0.217476	4.892501
C 1.164351	0.978481	0.030181	H -2.797758	3.567567	-0.000171	H -0.685651	5.507314
C 2.445530	1.490956	0.006477	H 2.125964	0.728609	-1.605040	H 0.772855	5.145004
C 0.010724	1.730904	0.049002	H 2.393175	0.760486	0.123415	H 0.849594	5.167021
C 0.211173	3.117442	0.046128	H -1.165244	-3.251327	-0.182048	B 5.431921	0.263473
C 1.490415	3.702569	0.024566	H 0.703216	-4.801909	-0.418041	F 5.218845	-0.934171
C 2.620815	2.876774	0.003548	H 3.025317	-3.905903	-0.746907	F 5.075489	1.368272
C -1.335652	1.088230	0.068464	H 3.368591	-1.450967	-0.834872	F 6.791970	0.359759
C -1.256794	-0.415160	0.068749	C -3.246305	-3.261975	0.171937	F 4.630156	0.255240
C -0.090059	-1.182514	0.050628	H -4.200309	-3.765869	0.331156	47	-1.475072
C -0.097952	-2.562623	0.055178	H -2.861392	-3.605846	-0.791443	10-BF4-TS_6	Eopt
C -1.318256	-3.237399	0.078668	H -2.577410	-3.586312	0.973297	-1349.623688	
C -2.511507	-2.517245	0.097465	C -6.769069	0.190606	0.741175	C -5.251093	-0.745547
C -2.466088	-1.128147	0.092178	H -6.933740	0.370932	1.810565	C -5.056256	0.640679
H 5.354369	-2.867994	-0.056499	H -7.109467	1.079389	0.201896	C -3.809560	1.304637
H 5.260008	1.414702	-0.048845	H -7.393670	-0.657239	0.447397	C -2.721697	0.423578
H -0.666543	3.758237	0.060562	C -0.534503	5.091593	-0.367402	C -2.862896	-0.970874
H 3.618624	3.302186	-0.014762	H 0.153426	5.445527	0.408427	C -4.125145	-1.560746
H -1.894662	1.417808	0.951547	H -0.137329	5.428737	-1.331428	O -1.196934	0.646386
H -1.918866	1.416531	-0.799357	H -1.503843	5.571862	-0.210408	C -0.593536	-0.670876
H 0.808980	-3.125897	0.042358	B 5.487361	0.191401	0.588942	C -1.580567	-1.634214
H -1.315866	-4.322278	0.082323	F 6.637702	0.958771	0.871635	C 0.759546	-0.923523
H -3.469921	-3.024815	0.116331	F 5.182457	0.286755	-0.789794	C 1.107060	-2.280638
H -3.386055	-0.553403	0.106920	F 5.721438	-1.160488	0.925059	C 0.149229	-3.310707
C 2.884703	-3.505029	-0.008374	F 4.395644	0.682746	1.344824	C -1.211283	-2.981252
H 3.747737	-4.171720	-0.031435	47			C 1.755497	0.185042
H 2.324052	-3.742146	0.899657	10-BF4-TS_54	Eopt		C 1.109559	1.542728
H 2.278851	-3.738830	-0.887476	-1349.623726			C -0.262080	1.805818
C 7.002390	-0.741923	-0.104353	C -5.298352	0.465425	-0.248852	C -0.782265	3.084052
H 7.417409	-1.401065	0.665147	C -5.001972	-0.902387	-0.237339	C 0.087495	4.173944
H 7.359224	-1.107913	-1.074177	C -3.713664	-1.472180	-0.125960	C 1.465705	3.965315
H 7.404166	0.263006	0.047217	C -2.697521	-0.513064	-0.024565	C 1.954958	2.664380
C 1.629491	5.203918	0.024085	C -2.941569	0.867271	-0.031201	H -5.933933	1.278186
H 1.128139	5.642755	-0.845758	C -4.239992	1.361901	-0.143812	H -4.207885	-2.642451
H 1.168820	5.639273	0.917901	O -1.164389	-0.622469	0.110741	H 2.163306	-2.534004
H 2.680200	5.504024	0.000524	C -0.662691	0.735476	0.162541	H -1.968847	-3.757125
B -6.273569	0.064888	-0.067842	C -1.715813	1.623481	0.082465	H 2.456035	0.084878
F -6.734763	0.166884	-1.399029	C 0.664360	1.087561	0.268707	H 2.363153	0.111975
F -5.876754	-1.266634	0.193609	C 0.908477	2.466870	0.298352	H -1.835645	3.258905
F -5.162816	0.926261	0.111281	C -0.120376	3.423457	0.225334	H -0.328668	5.175670
F -7.303617	0.435859	0.823349	C -1.448724	2.994200	0.115772	H 2.152876	4.804949
47			C 1.738610	0.056122	0.338544	H 3.024748	2.479082
10-BF4-TS_53	Eopt		C 1.196925	-1.346280	0.274206	C -3.898589	2.810908
-1349.623212			C -0.147804	-1.710221	0.173411	H -4.949616	3.094013
C -5.312439	-0.082204	0.472186	C -0.570277	-3.023554	0.133576	H -3.394890	3.242044
C -4.828200	-1.392102	0.408391	C 0.375941	-4.046196	0.188793	H -3.506283	3.261988
C -3.481857	-1.771513	0.192944	C 1.731647	-3.735934	0.282145	C -6.643056	-1.319657
C -2.623486	-0.677407	0.038774	C 2.121910	-2.402445	0.323740	H -7.171521	-0.995525
C -3.060361	0.655315	0.087911	H -5.827585	-1.601819	-0.323784	H -7.231251	-0.981478
C -4.401921	0.958012	0.303511	H -4.402489	2.434587	-0.149259	H -6.618919	-2.412224
O -1.106391	-0.564924	-0.215305	H 1.940291	2.797923	0.379046	C 0.595917	-4.750761
C -0.807312	0.850630	-0.279250	H -2.260299	3.711641	0.054937	H -0.260095	-5.430509
C -1.966229	1.579084	-0.105571	H 2.453399	0.203486	-0.477028	H 1.205290	-4.971387
C 0.445143	1.388704	-0.474981	H 2.312565	0.176784	1.264071	H 1.211427	-4.967980
C 0.488039	2.788887	-0.497096	H -1.605438	-3.275561	0.060491	B 5.398915	-0.292684
C -0.657197	3.589082	-0.332089	H 0.036064	-5.075820	0.156183	F 5.142552	1.010566
C -1.899255	2.974056	-0.133383	H 2.478284	-4.522171	0.322681	F 4.776607	-0.453556
C 1.646839	0.521623	-0.641175	H 3.172421	-2.137478	0.395100	F 4.877025	-1.244713

F 6.791590 -0.481231 0.245536
 47
 10-BF4-TS_7 Eopt
 -1349.623793
 C -5.069194 -1.265556 0.174802
 C -5.068500 0.134054 0.197645
 C -3.927438 0.964793 0.135041
 C -2.729894 0.243684 0.042672
 C -2.675968 -1.156708 0.016446
 C -3.843349 -1.915963 0.081984
 O -1.252370 0.677424 -0.041093
 C -0.473602 -0.542171 -0.124192
 C -1.316001 -1.634227 -0.084924
 C 0.897962 -0.601388 -0.230488
 C 1.430377 -1.895794 -0.293757
 C 0.626601 -3.049770 -0.252358
 C -0.763328 -2.915850 -0.147823
 C 1.728058 0.636943 -0.272079
 C 0.897172 1.890066 -0.216988
 C -0.493685 1.955830 -0.102543
 C -1.187227 3.147086 -0.035845
 C -0.484754 4.350054 -0.092774
 C 0.903846 4.339984 -0.214076
 C 1.570351 3.121461 -0.272179
 H -6.025109 0.641813 0.269417
 H -3.777374 -2.998586 0.058417
 H 2.508737 -1.995043 -0.376631
 H -1.403762 -3.790822 -0.115603
 H 2.436131 0.635937 0.562917
 H 2.338324 0.647475 -1.181529
 H -2.250268 3.167711 0.062250
 H -1.037289 5.282050 -0.040088
 H 1.462705 5.268793 -0.259179
 H 2.652302 3.093753 -0.360532
 C -4.222073 2.444183 0.177042
 H -5.301360 2.581212 0.255386
 H -3.775933 2.929427 1.048965
 H -3.901109 2.956326 -0.733674
 C -6.366784 -2.027291 0.248055
 H -7.016470 -1.772916 -0.596810
 H -6.191954 -3.105980 0.232904
 H -6.913340 -1.780252 1.164900
 C 1.269880 -4.411612 -0.324425
 H 2.003856 -4.539164 0.478697
 H 0.525045 -5.207242 -0.239374
 H 1.803404 -4.541038 -1.272847
 B 5.310987 -0.335770 0.266655
 F 4.765159 -1.189577 -0.720880
 F 5.317346 0.993752 -0.214505
 F 4.521160 -0.407837 1.438205
 F 6.631090 -0.739099 0.561900
 47
 10-BF4-TS_9 Eopt
 -1349.623619
 C -5.176302 -1.030154 0.001815
 C -5.088166 0.363891 0.003257
 C -3.892023 1.122040 0.004090
 C -2.741742 0.327779 0.002176
 C -2.775344 -1.076094 -0.001094
 C -3.987908 -1.758319 -0.001836
 O -1.237030 0.666434 0.003729
 C -0.533648 -0.601043 -0.000290
 C -1.443645 -1.638100 -0.003327
 C 0.835254 -0.747688 -0.003469
 C 1.288318 -2.073576 -0.010121
 C 0.412858 -3.174780 -0.012123

C -0.969719 -2.952449 -0.009232
 C 1.742620 0.435328 -0.002001
 C 0.992110 1.739227 -0.004088
 C -0.396167 1.894453 -0.001948
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 C -0.233661 4.283153 -0.008000
 C 1.156774 4.183291 -0.010334
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 H -6.011669 0.933256 0.003386
 H -3.988312 -2.843621 -0.005089
 H 2.361699 -2.239921 -0.015419
 H -1.666128 -3.784529 -0.012733
 H 2.402529 0.400774 0.871083
 H 2.404719 0.399906 -0.873301
 H -2.078777 3.218502 -0.001495
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 H 1.775930 5.074205 -0.013620
 H 2.827470 2.825918 -0.009848
 C -4.098837 2.616795 0.005693
 H -5.170993 2.817417 0.009512
 H -3.683401 3.091308 0.898435
 H -3.689698 3.092095 -0.889636
 C -6.513121 -1.723974 0.013768
 H -6.580468 -2.456442 -0.797669
 H -6.658669 -2.266478 0.955076
 H -7.333047 -1.010011 -0.096845
 C 0.971152 -4.575415 -0.009795
 H 1.683781 -4.714187 -0.829763
 H 1.509158 -4.777559 0.923570
 H 0.176927 -5.319385 -0.113126
 B 5.383679 -0.317708 0.007902
 F 4.971654 0.284386 1.219615
 F 6.779595 -0.525399 0.034785
 F 4.723664 -1.559526 -0.147611
 F 5.052150 0.529956 -1.074629
 47
 6-A-2Me-1 Eopt
 -891.105543
 C 4.431022 -0.763033 -0.218367
 C 4.022320 -2.077327 0.039748
 C 2.677108 -2.392936 0.265605
 C 1.730772 -1.364193 0.226237
 C 2.107723 -0.036506 -0.026231
 C 3.464458 0.247005 -0.244607
 H 4.766640 -2.870705 0.064985
 H 0.686867 -1.592968 0.420759
 H 3.766337 1.266611 -0.466854
 C 5.881314 -0.451569 -0.503257
 H 6.548460 -1.050869 0.124558
 H 6.132469 -0.670547 -1.548491
 H 6.104427 0.604499 -0.325541
 C 2.261380 -3.809306 0.585599
 H 2.868959 -4.536502 0.037773
 H 2.382018 -4.021873 1.655166
 H 1.211329 -3.982457 0.332499
 C 1.089497 1.042019 -0.060766
 C -0.171438 0.812784 -0.623262
 C 1.363734 2.309734 0.482204
 C -1.147718 1.815347 -0.646005
 H -0.397107 -0.157305 -1.054425
 C 0.408435 3.327540 0.470435
 H 2.327532 2.490293 0.949408
 C -0.848309 3.063117 -0.095151
 H -1.605687 3.844427 -0.100881
 C 0.709951 4.684964 1.060003
 H 1.677323 4.690870 1.569852

H 0.737648 5.456233 0.281049
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 H -2.409385 1.567474 -2.367945
 H -3.185055 2.363247 -1.009506
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 C -3.369897 -0.038162 0.494027
 C -3.389916 -0.774114 -1.799395
 C -3.907825 -1.254761 0.921037
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 C -3.926035 -2.000222 -1.390847
 H -3.185415 -0.593623 -2.851351
 C -4.182047 -2.239281 -0.042551
 H -4.138190 -2.769661 -2.127617
 H -4.594908 -3.195154 0.269958
 C -4.202001 -1.505732 2.380771
 H -5.281965 -1.500455 2.571882
 H -3.820656 -2.481118 2.701571
 H -3.748054 -0.739439 3.015254
 47
 6-A-2Me-10 Eopt
 -891.104883
 C 5.166860 0.335442 0.163073
 C 5.326207 -1.040063 -0.030808
 C 4.221635 -1.890181 -0.182996
 C 2.940041 -1.337454 -0.137183
 C 2.744693 0.040041 0.059031
 C 3.869959 0.861466 0.209309
 H 6.329353 -1.460314 -0.063098
 H 2.077254 -1.981883 -0.278581
 H 3.732729 1.923680 0.391495
 C 6.366540 1.242499 0.302429
 H 7.246188 0.691070 0.647171
 H 6.622957 1.704593 -0.659038
 H 6.172737 2.052814 1.012226
 C 4.421832 -3.372955 -0.389422
 H 5.091913 -3.570371 -1.233508
 H 4.870523 -3.837684 0.496514
 H 3.472613 -3.878562 -0.587239
 C 1.376152 0.610981 0.107561
 C 0.333475 -0.078181 0.750329
 C 1.091409 1.845103 -0.491737
 C -0.958914 0.445279 0.795307
 H 0.542312 -1.025841 1.238406
 C -0.197502 2.393026 -0.459017
 H 1.880184 2.373551 -1.019862
 C -1.213284 1.679350 0.182686
 H -2.224200 2.079667 0.195512
 C -0.477853 3.733330 -1.096147
 H -0.259619 4.552430 -0.399555
 H 0.139776 3.888275 -1.986232
 H -1.527837 3.822372 -1.389915
 C -2.079111 -0.305424 1.489763
 H -2.438999 0.278733 2.345093
 H -1.678320 -1.239890 1.900478
 C -3.251437 -0.614308 0.577650
 C -4.546432 -0.209745 0.910901
 C -3.050360 -1.308879 -0.624176
 C -5.645332 -0.486098 0.082512
 H -4.707084 0.336883 1.838205
 C -4.128747 -1.591925 -1.458914
 H -2.045784 -1.610199 -0.907146
 C -5.419705 -1.182382 -1.109123
 H -3.966288 -2.127336 -2.389980
 H -6.254851 -1.402004 -1.768988
 C -7.035617 -0.056955 0.486667

H	-7.720839	-0.073285	-0.365693
H	-7.446193	-0.724295	1.254455
H	-7.035580	0.955793	0.903113
47			
6-A-2Me-11			Eopt
-891.104877			
C	4.071059	-1.024967	0.930858
C	3.951235	-2.150887	0.103480
C	2.930999	-2.252148	-0.846835
C	2.019332	-1.196225	-0.968866
C	2.110126	-0.057761	-0.157480
C	3.145359	0.010749	0.790312
H	4.668402	-2.963098	0.203128
H	1.240555	-1.250294	-1.724388
H	3.212414	0.876406	1.442800
C	5.180026	-0.943539	1.953072
H	5.148461	-1.794897	2.642363
H	6.164234	-0.953507	1.470276
H	5.107215	-0.027852	2.546351
C	2.798732	-3.480450	-1.715831
H	3.738685	-4.037762	-1.765172
H	2.032086	-4.159041	-1.321737
H	2.505726	-3.216047	-2.736942
C	1.133625	1.050843	-0.294859
C	-0.219799	0.783802	-0.534469
C	1.545633	2.390264	-0.180558
C	-1.150559	1.821413	-0.662740
H	-0.561788	-0.245111	-0.581547
C	0.636794	3.443008	-0.299029
H	2.596385	2.610811	-0.016375
C	-0.712477	3.141635	-0.538140
H	-1.432251	3.952898	-0.626958
C	1.089821	4.879451	-0.187144
H	2.147543	4.942791	0.082940
H	0.953906	5.412511	-1.135508
H	0.514113	5.418997	0.573288
C	-2.612614	1.513253	-0.940457
H	-2.732065	1.252908	-1.999647
H	-3.201390	2.423891	-0.779531
C	-3.168946	0.389274	-0.091533
C	-3.572975	-0.816800	-0.669807
C	-3.258427	0.532798	1.300428
C	-4.067365	-1.879488	0.102013
H	-3.498677	-0.935990	-1.749011
C	-3.745822	-0.511256	2.083126
H	-2.929860	1.458094	1.765626
C	-4.146597	-1.711926	1.488347
H	-3.809022	-0.395781	3.161329
H	-4.520215	-2.523844	2.106708
C	-4.523760	-3.159019	-0.557264
H	-4.524929	-3.993181	0.150370
H	-5.543295	-3.057518	-0.949613
H	-3.876643	-3.427529	-1.398490
47			
6-A-2Me-12			Eopt
-891.105029			
C	4.064420	-0.705434	1.107420
C	4.238033	-1.719320	0.156646
C	3.381012	-1.843638	-0.942820
C	2.335389	-0.925487	-1.085738
C	2.131479	0.099147	-0.150080
C	3.006479	0.193241	0.943534
H	5.056871	-2.425888	0.275761
H	1.680978	-0.994413	-1.949986
H	2.843776	0.965131	1.690240
C	5.014001	-0.576846	2.274960

H	5.292286	-1.557707	2.673572
H	5.940476	-0.072246	1.973884
H	4.569767	0.006384	3.086755
C	3.565823	-2.960449	-1.942704
H	4.619137	-3.241178	-2.038447
H	3.013749	-3.857186	-1.634693
H	3.198202	-2.673545	-2.932503
C	1.012621	1.060242	-0.311105
C	-0.235875	0.631882	-0.777313
C	1.181500	2.419375	0.008596
C	-1.299516	1.529850	-0.927892
H	-0.397026	-0.421016	-0.986857
C	0.136550	3.334083	-0.128738
H	2.151878	2.767815	0.350181
C	-1.103187	2.871935	-0.596723
H	-1.928347	3.573303	-0.702487
C	0.332407	4.795282	0.199098
H	1.302175	4.969955	0.673275
H	0.286921	5.412990	-0.705741
H	-0.446902	5.157933	0.878504
C	-2.643626	1.043049	-1.439061
H	-2.566392	0.817896	-2.509899
H	-3.372039	1.857852	-1.348495
C	-3.161122	-0.184881	-0.716460
C	-3.337748	-0.159382	0.674962
C	-3.460154	-1.359832	-1.409728
C	-3.808382	-1.271022	1.377551
H	-3.087389	0.747625	1.220229
C	-3.932080	-2.484108	-0.723136
H	-3.323342	-1.398693	-2.487212
C	-4.104983	-2.440522	0.658114
H	-4.160737	-3.394568	-1.269665
H	-4.469142	-3.317707	1.187063
C	-3.992717	-1.225456	2.875603
H	-5.038427	-1.403509	3.152002
H	-3.390411	-1.995029	3.371759
H	-3.698017	-0.254441	3.282842
47			
6-A-2Me-13			Eopt
-891.105442			
C	-2.475950	-2.485601	-0.530696
C	-3.799913	-2.350211	-0.094952
C	-4.288565	-1.130610	0.388782
C	-3.425759	-0.030648	0.428826
C	-2.092927	-0.134006	0.003553
C	-1.633281	-1.371536	-0.472642
H	-4.463605	-3.211691	-0.133324
H	-3.787044	0.914834	0.823453
H	-0.610625	-1.458000	-0.828368
C	-1.980331	-3.798312	-1.089742
H	-2.407788	-4.648670	-0.548872
H	-2.261531	-3.907264	-2.144567
H	-0.890404	-3.869508	-1.030843
C	-5.706665	-1.017419	0.896465
H	-6.391619	-1.635062	0.306986
H	-5.778898	-1.352597	1.938619
H	-6.062282	0.016463	0.858544
C	-1.184231	1.037698	0.054436
C	0.158714	0.880851	0.416761
C	-1.647696	2.324454	-0.271060
C	1.031390	1.974139	0.454003
H	0.530055	-0.104200	0.679941
C	-0.797982	3.431770	-0.241483
H	-2.679900	2.454289	-0.583246
C	0.543864	3.239797	0.120890
H	1.218615	4.093352	0.139373

C	-1.299936	4.808487	-0.607490
H	-2.354522	4.783316	-0.895421
H	-1.197779	5.503582	0.233982
H	-0.732170	5.228568	-1.445565
C	2.480133	1.784814	0.872981
H	2.534680	1.709294	1.966241
H	3.047229	2.681665	0.597586
C	3.128013	0.560768	0.260347
C	3.506219	-0.526058	1.052373
C	3.322980	0.484499	-1.126503
C	4.076195	-1.683385	0.499146
H	3.349548	-0.475308	2.128092
C	3.886757	-0.655748	-1.693877
H	3.016550	1.314820	-1.756796
C	4.259826	-1.735412	-0.886315
H	4.032927	-0.710149	-2.768865
H	4.694756	-2.623507	-1.337201
C	4.498273	-2.828960	1.387735
H	4.626829	-3.751349	0.814116
H	5.452587	-2.611672	1.883213
H	3.759630	-3.017443	2.173702
47			
6-A-2Me-14			Eopt
-891.105032			
C	4.064336	-0.702390	1.109597
C	4.242122	-1.714354	0.155467
C	3.387434	-1.838414	-0.944046
C	2.338456	-0.921876	-1.086213
C	2.131818	0.099902	-0.150070
C	3.006592	0.194336	0.945420
H	5.063358	-2.418335	0.273373
H	1.685793	-0.990305	-1.951975
H	2.842344	0.965844	1.692049
C	5.004831	-0.587697	2.285896
H	5.103258	-1.543618	2.811907
H	6.009213	-0.291423	1.960375
H	4.653680	0.158293	3.004291
C	3.575246	-2.948099	-1.951323
H	4.597605	-3.336690	-1.931419
H	2.898857	-3.786139	-1.742201
H	3.361733	-2.603197	-2.968032
C	1.012248	1.060270	-0.310556
C	-0.235651	0.631258	-0.777730
C	1.179869	2.419259	0.010370
C	-1.299847	1.528527	-0.928466
H	-0.395806	-0.421661	-0.987970
C	0.134336	3.333295	-0.127127
H	2.149703	2.768187	0.353006
C	-1.104726	2.870548	-0.596301
H	-1.930361	3.571353	-0.702079
C	0.328901	4.794412	0.201839
H	1.297980	4.969401	0.677307
H	0.284177	5.412628	-0.702696
H	-0.451467	5.156200	0.880484
C	-2.643295	1.040966	-1.440599
H	-2.565073	0.815269	-2.511249
H	-3.372107	1.855534	-1.351102
C	-3.160968	-0.186790	-0.717785
C	-3.337370	-0.161139	0.673641
C	-3.460112	-1.361839	-1.410881
C	-3.808103	-1.272647	1.376417
H	-3.086513	0.745789	1.218810
C	-3.931723	-2.486091	-0.724068
H	-3.323153	-1.400927	-2.488339
C	-4.104385	-2.442358	0.657230
H	-4.159912	-3.396801	-1.270378

H -4.467863 -3.319677 1.186417
 C -3.995802 -1.225514 2.873999
 H -5.048664 -1.365153 3.145817
 H -3.424802 -2.018667 3.369726
 H -3.667224 -0.267295 3.285622
 47
 6-A-2Me-2 Eopt
 -891.104877
 C 4.071361 -1.023443 0.932360
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 C 2.933972 -2.250619 -0.847044
 C 2.021683 -1.195320 -0.969512
 C 2.110776 -0.057181 -0.157434
 C 3.144929 0.011606 0.791470
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 C 5.179932 -0.941076 1.954925
 H 5.157021 -1.799168 2.636093
 H 6.163948 -0.936886 1.471569
 H 5.098705 -0.031699 2.556767
 C 2.803410 -3.478735 -1.716561
 H 3.744932 -4.033175 -1.768484
 H 2.039800 -4.159935 -1.321069
 H 2.507196 -3.214537 -2.736784
 C 1.133480 1.050675 -0.295189
 C -0.219488 0.782666 -0.536245
 C 1.544290 2.390379 -0.179804
 C -1.150947 1.819594 -0.664946
 H -0.560623 -0.246503 -0.584101
 C 0.634737 3.442454 -0.298667
 H 2.594702 2.611683 -0.014465
 C -0.714059 3.140105 -0.539282
 H -1.434407 3.950816 -0.628459
 C 1.086499 4.879201 -0.185638
 H 2.144018 4.943259 0.085072
 H 0.950657 5.412750 -1.133739
 H 0.509908 5.417789 0.574807
 C -2.612481 1.510253 -0.944012
 H -2.730457 1.247674 -2.002803
 H -3.201904 2.420921 -0.785657
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 C -3.572782 -0.819410 -0.669821
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 H -2.931718 1.459978 1.761927
 C -4.148082 -1.710628 1.489509
 H -3.811919 -0.391343 3.160352
 H -4.522190 -2.521400 2.109065
 C -4.523000 -3.161583 -0.553911
 H -4.535855 -3.991951 0.158022
 H -5.537604 -3.057326 -0.958110
 H -3.867949 -3.437628 -1.386561
 47
 6-A-2Me-3 Eopt
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 C 4.430378 -0.769364 0.220729
 C 4.019741 -2.081933 -0.030104
 C 2.671781 -2.396510 -0.256002
 C 1.729316 -1.367121 -0.223159
 C 2.108496 -0.037729 0.029820
 C 3.463104 0.243145 0.250387
 H 4.761984 -2.877374 -0.048327
 H 0.684990 -1.594200 -0.416377

H 3.766088 1.261538 0.477519
 C 5.888032 -0.441253 0.442525
 H 6.455198 -1.326959 0.743188
 H 6.346807 -0.050687 -0.474322
 H 6.011055 0.321192 1.218376
 C 2.256615 -3.820553 -0.540618
 H 2.686034 -4.177274 -1.484229
 H 2.600047 -4.498692 0.248675
 H 1.169238 -3.910214 -0.612563
 C 1.090298 1.040774 0.065977
 C -0.171590 0.810462 0.625896
 C 1.365823 2.310126 -0.472638
 C -1.147229 1.813629 0.650916
 H -0.398666 -0.160823 1.053577
 C 0.411251 3.328530 -0.458560
 H 2.330272 2.491579 -0.938142
 C -0.846321 3.063062 0.104757
 H -1.603177 3.844868 0.112246
 C 0.713918 4.687419 -1.044148
 H 0.729852 5.458514 -0.264751
 H 1.686774 4.697307 -1.543380
 H -0.044961 4.983194 -1.777050
 C -2.504176 1.543030 1.277431
 H -3.184488 2.361854 1.014438
 H -2.411039 1.559747 2.370413
 C -3.109083 0.219230 0.855681
 C -3.369171 -0.033357 -0.499383
 C -3.393403 -0.778397 1.791065
 C -3.907624 -1.247703 -0.932045
 H -3.129981 0.733666 -1.232476
 C -3.930117 -2.002347 1.376820
 H -3.190341 -0.602313 2.844046
 C -4.184310 -2.235781 0.027216
 H -4.144146 -2.774496 2.110204
 H -4.597672 -3.189986 -0.289711
 C -4.199503 -1.492800 -2.393236
 H -3.814098 -2.465182 -2.718335
 H -5.279284 -1.490812 -2.585360
 H -3.747847 -0.721802 -3.023626
 47
 6-A-2Me-4 Eopt
 -891.105430
 C 4.287010 -1.137021 0.390861
 C 3.793811 -2.357879 -0.080758
 C 2.467958 -2.492079 -0.515872
 C 1.630163 -1.375714 -0.466255
 C 2.093015 -0.136307 0.006025
 C 3.424616 -0.034922 0.431269
 H 4.453003 -3.223202 -0.108125
 H 0.606152 -1.461890 -0.817737
 H 3.786623 0.909351 0.828341
 C 5.724724 -1.002811 0.834200
 H 6.127343 -1.959965 1.178859
 H 6.359383 -0.657253 0.008585
 H 5.824710 -0.278224 1.648261
 C 1.966336 -3.814434 -1.046114
 H 2.410449 -4.042336 -2.022620
 H 2.226356 -4.637347 -0.371454
 H 0.879730 -3.806850 -1.168631
 C 1.184926 1.035806 0.057891
 C -0.158221 0.879929 0.419927
 C 1.649498 2.322543 -0.266321
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 C 0.800946 3.430683 -0.235276
 H 2.681777 2.451715 -0.578532

C -0.541110 3.239587 0.126832
 H -1.215064 4.093753 0.146149
 C 1.304460 4.807455 -0.598906
 H 1.209388 5.499409 0.246011
 H 2.357240 4.780566 -0.893235
 H 0.732779 5.232511 -1.431761
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 H -3.044747 2.683867 0.604226
 H -2.533780 1.705791 1.969450
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 C -3.506198 -0.525777 1.046747
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 C -3.888874 -0.643409 -1.699763
 H -3.017859 1.327021 -1.754813
 C -4.261772 -1.726419 -0.896589
 H -4.035938 -0.693070 -2.774859
 H -4.697457 -2.612359 -1.350964
 C -4.498483 -2.829851 1.372911
 H -5.449692 -2.612466 1.874260
 H -4.632592 -3.748506 0.794608
 H -3.756647 -3.025176 2.154212
 47
 6-A-2Me-5 Eopt
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 C -2.780021 -2.322168 -0.821797
 C -3.843887 -2.240419 0.081929
 C -4.046002 -1.100132 0.872217
 C -3.158920 -0.029300 0.742155
 C -2.078392 -0.080310 -0.154307
 C -1.903425 -1.235686 -0.927519
 H -4.528690 -3.080743 0.175328
 H -3.289156 0.848483 1.368329
 H -1.084574 -1.280322 -1.639956
 C -2.596669 -3.540793 -1.695238
 H -3.085297 -4.418660 -1.262068
 H -3.028825 -3.379643 -2.690738
 H -1.536315 -3.775017 -1.833884
 C -5.184615 -1.049317 1.863382
 H -6.132672 -1.335417 1.394736
 H -5.012948 -1.740287 2.697588
 H -5.303264 -0.045777 2.281732
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 C 0.235916 0.837385 -0.444329
 C -1.602502 2.384327 -0.214618
 C 1.133232 1.902211 -0.553428
 H 0.613101 -0.179703 -0.450266
 C -0.724463 3.468475 -0.317618
 H -2.667018 2.571032 -0.103606
 C 0.641543 3.211045 -0.482798
 H 1.335950 4.045292 -0.555049
 C -1.248015 4.884864 -0.280579
 H -1.694276 5.164205 -1.243014
 H -2.022578 5.003988 0.484120
 H -0.447729 5.599791 -0.067890
 C 2.620096 1.653146 -0.755697
 H 3.169283 2.555032 -0.460494
 H 2.816965 1.511020 -1.825914
 C 3.154877 0.459593 0.006300
 C 3.568943 -0.694683 -0.666113
 C 3.212526 0.480417 1.405978
 C 4.039383 -1.823076 0.020409
 H 3.519933 -0.717853 -1.752878
 C 3.676803 -0.632148 2.106158
 H 2.878342 1.363523 1.943434

C	4.085406	-1.778124	1.418860
H	3.714591	-0.610861	3.191442
H	4.439864	-2.643908	1.972045
C	4.508981	-3.044441	-0.733188
H	5.585797	-2.990413	-0.937023
H	4.329798	-3.959350	-0.160054
H	3.998153	-3.140427	-1.696348
47			
6-A-2Me-6		Eopt	
-891.105033			
C	-3.385541	-1.833585	-0.946596
C	-4.235134	-1.717378	0.157761
C	-4.056563	-0.708511	1.114944
C	-3.003876	0.193793	0.948399
C	-2.130195	0.102940	-0.148221
C	-2.335414	-0.917993	-1.085571
H	-5.051800	-2.426302	0.277958
H	-2.838684	0.962705	1.697526
H	-1.680809	-0.986336	-1.949899
C	-3.613761	-2.900081	-1.991520
H	-4.194673	-3.734883	-1.588571
H	-4.165761	-2.497350	-2.849808
H	-2.666119	-3.295988	-2.370154
C	-4.971784	-0.622046	2.313399
H	-6.024506	-0.618278	2.009929
H	-4.829762	-1.479609	2.981798
H	-4.783951	0.286389	2.892492
C	-1.010520	1.063645	-0.306149
C	0.237943	0.635722	-0.772770
C	-1.178976	2.422003	0.016832
C	1.301964	1.533605	-0.921025
H	0.398591	-0.416811	-0.984512
C	-0.133590	3.336604	-0.118146
H	-2.149276	2.769965	0.359173
C	1.106076	2.875037	-0.586837
H	1.931588	3.576284	-0.690650
C	-0.328882	4.797091	0.213204
H	-0.281680	5.417103	-0.689968
H	-1.299187	4.971234	0.686473
H	0.449725	5.157441	0.894642
C	2.645941	1.047730	-1.433535
H	3.375564	1.860750	-1.336887
H	2.569641	0.829675	-2.505923
C	3.160603	-0.185684	-0.718359
C	3.336545	-0.169233	0.673252
C	3.457020	-1.357122	-1.418717
C	3.804204	-1.286331	1.369200
H	3.087681	0.734855	1.224031
C	3.925393	-2.486900	-0.738809
H	3.320291	-1.389090	-2.496442
C	4.097595	-2.452299	0.642810
H	4.151255	-3.394816	-1.290707
H	4.458355	-3.333940	1.166640
C	3.992737	-1.248596	2.866942
H	3.431343	-2.051902	3.357140
H	5.047462	-1.378331	3.136637
H	3.654016	-0.297220	3.286157
47			
6-A-2Me-7		Eopt	
-891.104970			
C	4.590113	-1.502054	0.485400
C	5.343491	-0.793876	-0.456464
C	4.822982	0.328938	-1.114574
C	3.522515	0.739616	-0.812108
C	2.738205	0.048949	0.126327
C	3.287560	-1.071741	0.764196

H	6.355563	-1.122299	-0.684134
H	3.098356	1.592555	-1.334012
H	2.700509	-1.600811	1.509727
C	5.181367	-2.682637	1.218903
H	5.965349	-3.166592	0.628799
H	5.630904	-2.369080	2.169297
H	4.417680	-3.431545	1.450368
C	5.644889	1.056350	-2.152213
H	6.656750	1.260919	-1.786158
H	5.744656	0.458686	-3.066318
H	5.185054	2.009655	-2.427391
C	1.356887	0.494913	0.433610
C	0.327670	-0.442049	0.628721
C	1.046593	1.857900	0.529491
C	-0.976731	-0.034723	0.910369
H	0.545411	-1.501414	0.527268
C	-0.254605	2.292490	0.812819
H	1.836485	2.592872	0.401940
C	-1.256514	1.335413	0.995308
H	-2.276243	1.657517	1.192271
C	-0.558979	3.765343	0.950752
H	-0.374497	4.110030	1.975854
H	0.068969	4.366571	0.286054
H	-1.606080	3.978067	0.715772
C	-2.086720	-1.051409	1.096622
H	-2.474949	-0.987671	2.120213
H	-1.667003	-2.058649	0.987351
C	-3.236883	-0.873583	0.123310
C	-4.547454	-0.717758	0.581689
C	-2.999210	-0.856514	-1.258805
C	-5.626393	-0.553441	-0.300785
H	-4.736466	-0.721767	1.653497
C	-4.057612	-0.694097	-2.149602
H	-1.982732	-0.955122	-1.629039
C	-5.364357	-0.542023	-1.674530
H	-3.866968	-0.678510	-3.218879
H	-6.183618	-0.409602	-2.376284
C	-7.034227	-0.415659	0.227842
H	-7.701278	0.016346	-0.523716
H	-7.445165	-1.392212	0.512474
H	-7.066214	0.221983	1.117379
47			
6-A-2Me-8		Eopt	
-891.105175			
C	4.420727	-1.264743	0.887115
C	5.099784	-0.976440	-0.300922
C	4.535834	-0.151335	-1.284017
C	3.267693	0.388734	-1.058289
C	2.557504	0.116643	0.122832
C	3.148581	-0.714333	1.084142
H	6.087125	-1.402763	-0.466416
H	2.808627	1.008136	-1.823393
H	2.620443	-0.913838	2.012404
C	5.060145	-2.118849	1.956226
H	5.805365	-2.797815	1.531263
H	5.569034	-1.496870	2.703081
H	4.314278	-2.719746	2.485752
C	5.277961	0.120540	-2.571140
H	6.303906	0.451291	-2.375937
H	5.340228	-0.782880	-3.189553
H	4.779805	0.894435	-3.161731
C	1.209297	0.694581	0.345648
C	0.192372	-0.067895	0.945696
C	0.918104	2.008964	-0.042376
C	-1.081575	0.461829	1.152800
H	0.393038	-1.098498	1.224185

C	-0.352199	2.565062	0.156996
H	1.700542	2.617221	-0.487608
C	-1.342928	1.778192	0.750344
H	-2.340565	2.187550	0.890635
C	-0.632193	3.997330	-0.231789
H	-0.345097	4.685725	0.572773
H	-0.068941	4.285853	-1.124676
H	-1.695935	4.153228	-0.434102
C	-2.183133	-0.377102	1.770043
H	-2.525302	0.091134	2.700548
H	-1.770962	-1.354454	2.049357
C	-3.377132	-0.574875	0.853812
C	-3.192096	-1.041422	-0.455973
C	-4.675039	-0.301708	1.292398
C	-4.268505	-1.246396	-1.322744
H	-2.181780	-1.235808	-0.807650
C	-5.765055	-0.498187	0.437653
H	-4.835862	0.066810	2.302145
C	-5.564265	-0.966862	-0.858699
H	-6.770727	-0.280183	0.785607
H	-6.414506	-1.114519	-1.519886
C	-4.050527	-1.758596	-2.726548
H	-4.498635	-2.750382	-2.859653
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H	-2.985165	-1.838649	-2.959273
47			
6-A-2Me-9		Eopt	
-891.105123			
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C	5.061721	-1.207032	0.001616
C	3.898757	-1.989739	0.043560
C	2.660114	-1.346623	0.079817
C	2.563729	0.055452	0.076259
C	3.744893	0.807677	0.035110
H	6.032502	-1.697741	-0.024237
H	1.751657	-1.941877	0.088430
H	3.686324	1.892208	0.062651
C	6.260321	1.021037	-0.070757
H	7.135929	0.444277	0.240809
H	6.444425	1.375992	-1.092325
H	6.187883	1.903952	0.572409
C	3.992957	-3.497158	0.047228
H	4.545467	-3.863019	-0.825565
H	4.519136	-3.857977	0.938699
H	3.001153	-3.957510	0.034606
C	1.239240	0.722792	0.117405
C	0.200733	0.208095	0.912511
C	0.991964	1.875579	-0.639610
C	-1.051092	0.822391	0.952947
H	0.382136	-0.672512	1.521985
C	-0.255454	2.512913	-0.614203
H	1.775090	2.266408	-1.283283
C	-1.268528	1.971787	0.181760
H	-2.249534	2.440881	0.193857
C	-0.493185	3.765744	-1.423418
H	-0.171369	4.657038	-0.870446
H	0.066803	3.744921	-2.363499
H	-1.553665	3.891061	-1.660727
C	-2.170438	0.253933	1.802398
H	-2.482384	0.995279	2.547434
H	-1.787537	-0.606450	2.364822
C	-3.384643	-0.169591	0.995421
C	-3.234009	-0.997376	-0.126704
C	-4.668682	0.249091	1.353206
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H	-2.234481	-1.307334	-0.421674

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 44
 6-A-Me-1 Eopt
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 H 4.569026 -3.564561 -0.941514
 H 4.130055 -1.648826 -2.468858
 44
 6-A-Me-2 Eopt
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H 1.410294 -1.110699 -1.843613
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 H 4.692150 0.577102 2.746347
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 H 2.789774 -3.815904 -1.550177
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 H -3.922713 -1.226783 3.021557
 44
 6-A-Me-3 Eopt
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 H -6.293901 1.221351 1.335551
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 C 1.326250 0.528140 0.854217
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 C 0.552935 2.440825 -0.445940
 H -1.512429 2.371693 -1.047117
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 H 2.571077 2.179002 0.255672

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 H 0.233988 3.895226 -2.015779
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 C 2.448002 -0.192196 1.575476
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 H 7.013449 -0.385763 0.507008
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 C 3.111190 0.709746 0.861996
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 H 5.527084 0.289195 3.015118
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 H 1.446268 2.620441 -0.286682
 C -1.632352 1.395838 -1.008163
 H -2.647677 1.727985 -1.211527
 C -0.937089 3.820317 -0.824525
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 H -2.872923 -0.830266 -2.243879
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 C -4.923358 -0.824036 -0.645464
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 C -5.964499 -0.768051 0.286403
 H -5.149786 -0.803916 -1.708575
 C -4.351877 -0.868445 2.079698
 H -2.284914 -0.964373 1.483292
 C -5.681672 -0.791237 1.652817
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 H -6.992925 -0.703446 -0.056910
 44

6-A-Me-5			Eopt	C	-0.801761	1.020741	0.040930	C	-4.353216	-0.868568	2.079254
-851.778796				C	0.471354	0.666197	0.501698	H	-2.285962	-0.966516	1.484200
C	4.781650	0.287079	-0.102687	C	-1.012438	2.336523	-0.408111	C	-5.964568	-0.766548	0.284906
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C	3.785886	-1.922662	0.200856	H	0.648647	-0.342546	0.860841	C	-5.682657	-0.790064	1.651501
C	2.516412	-1.344534	0.129052	C	0.016306	3.279927	-0.403086	H	-6.992709	-0.700984	-0.059076
C	2.352699	0.038851	-0.051935	H	-1.987764	2.615295	-0.796378	H	-6.488767	-0.744398	2.377538
C	3.497040	0.840023	-0.164905	C	1.282417	2.890999	0.060714	H	-4.123669	-0.883517	3.140775
H	5.903573	-1.532837	0.137232	H	2.095288	3.614406	0.062161	44			
H	1.638312	-1.973194	0.245278	C	-0.215426	4.687702	-0.898598	6-A-Me-Cl-1		Eopt	
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H	6.875944	0.726222	0.219346	H	0.474074	4.941422	-1.711770	C	4.145918	-2.198107	0.005693
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H	5.837940	2.160367	0.140008	H	2.860047	1.138143	2.134176	C	1.876772	-1.401518	0.104072
C	3.951813	-3.406586	0.428273	H	3.609484	1.975413	0.786014	C	2.319631	-0.078890	-0.046798
H	4.634579	-3.847146	-0.306467	C	3.371885	-0.140674	0.496695	C	3.696611	0.160179	-0.169705
H	4.369005	-3.609666	1.421798	C	3.558639	-0.315466	-0.882456	H	4.856255	-3.022136	0.026216
H	2.994233	-3.929701	0.355938	C	3.619622	-1.222913	1.347517	H	0.815357	-1.596657	0.227641
C	0.996972	0.637846	-0.118441	C	3.988223	-1.538684	-1.395412	H	4.050107	1.177560	-0.311759
C	-0.045820	-0.020955	-0.792307	H	3.352833	0.512603	-1.555504	C	6.095695	-0.623698	-0.331455
C	0.724239	1.868329	0.493485	C	4.048406	-2.453128	0.838269	H	6.700432	-1.288202	0.293848
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H	-2.825320	0.433705	-2.392648	C	2.344862	0.066384	-0.121949	H	2.567884	2.365260	1.112033
C	-3.608467	-0.565548	-0.669957	C	3.109099	0.707297	0.862362	C	-0.505779	3.141486	-0.093997
C	-3.379418	-1.224727	0.546454	H	5.943919	-1.150471	0.702400	H	-1.231076	3.952536	-0.094499
C	-4.927289	-0.270562	-1.032763	H	2.334129	-1.515754	-1.586031	C	1.030516	4.614447	1.270874
C	-4.442892	-1.587894	1.372429	H	2.675385	1.533473	1.418810	H	1.964020	4.547322	1.836218
H	-2.359021	-1.441390	0.849882	C	5.224516	1.003301	2.213178	H	1.132784	5.435871	0.551811
C	-5.996847	-0.630412	-0.207006	H	5.997305	0.353472	2.634220	H	0.232207	4.891389	1.968231
H	-5.119791	0.246157	-1.969670	H	5.727850	1.878682	1.784139	C	-2.132227	1.775305	-1.477853
C	-5.757748	-1.291773	0.998478	H	4.594314	1.359263	3.034169	H	-1.960952	1.798544	-2.560844
H	-7.013238	-0.390479	-0.505450	C	4.793397	-2.650963	-1.254145	H	-2.778759	2.631602	-1.250935
H	-6.585599	-1.570955	1.643252	H	5.761377	-2.394740	-1.698884	C	-2.856177	0.489820	-1.127283
H	-4.246521	-2.098090	2.310987	H	4.961475	-3.495778	-0.575754	C	-3.098443	0.170050	0.216226
44				H	4.133761	-2.992916	-2.056443	C	-3.287284	-0.394018	-2.121522
6-A-Me-6		Eopt		C	0.969845	0.527104	-0.435507	C	-3.764449	-1.008630	0.536054
-851.779186				C	-0.054036	-0.398996	-0.699748	H	-2.754502	0.830204	1.005194
C	-4.255094	-0.540646	0.331047	C	0.659666	1.892952	-0.468566	C	-3.954677	-1.575328	-1.785219
C	-3.967474	-1.862664	-0.030018	C	-1.352782	0.021968	-0.986701	H	-3.097122	-0.159190	-3.164857
C	-2.668736	-2.261521	-0.368526	H	0.162836	-1.462146	-0.648836	C	-4.200474	-1.895130	-0.450359
C	-1.645015	-1.309493	-0.337639	C	-0.635995	2.341463	-0.756385	H	-4.282220	-2.254429	-2.566458
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H	-0.637361	-1.601609	-0.619070	C	-0.938000	3.819552	-0.826276	6-A-Me-Cl-10		Eopt	
H	-3.420087	1.415476	0.646910	H	-0.345626	4.382651	-0.098412	-1311.377387			
C	-5.654499	-0.141761	0.736074	H	-0.703533	4.221477	-1.819803	C	-5.489690	0.202433	-0.178638
H	-6.407030	-0.662708	0.135598	H	-1.996012	4.018399	-0.631992	C	-5.583083	-1.180988	0.001304
H	-5.845510	-0.391040	1.787242	C	-2.459091	-0.983181	-1.238739	C	-4.439499	-1.979005	0.147271
H	-5.811594	0.934560	0.619615	H	-2.030711	-1.992907	-1.229076	C	-3.185778	-1.365156	0.109262
C	-2.386519	-3.681809	-0.797954	H	-2.871546	-0.832845	-2.243452	C	-3.056554	0.022004	-0.072812
C	-3.009315	-4.395347	-0.249239	C	-3.589918	-0.905584	-0.228943	C	-4.219370	0.790365	-0.217070
H	-2.596514	-3.818104	-1.866120	C	-3.317683	-0.922420	1.146689	H	-6.564985	-1.649029	0.027301
H	-1.338059	-3.946543	-0.632879	C	-4.922869	-0.823499	-0.646282	H	-2.293586	-1.969402	0.245703

H	-4.133051	1.859627	-0.388847	H	2.889569	4.759251	0.188361	6-A-Me-Cl-13	Eopt		
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H	-6.575326	1.877700	-1.013402	H	-2.264293	1.476225	-2.093199	C	4.450871	-1.463964	-0.345520
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H	-5.001685	-3.947349	-0.548695	C	-3.490786	-0.257004	-0.609532	C	1.765385	-1.459638	0.453781
H	-3.596204	-3.934438	0.525962	C	-2.862629	1.133554	1.258836	H	4.425743	-3.548348	0.191230
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C	-0.641048	0.025269	-0.759588	H	-3.491855	-0.473969	-1.672608	H	0.731103	-1.451943	0.785561
C	-1.492449	1.900134	0.495216	C	-3.508009	0.258720	2.130198	C	1.878395	-3.903401	1.091173
C	0.623885	0.612099	-0.798000	H	-2.351122	2.009245	1.647065	H	2.248506	-4.793109	0.572010
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C	-0.232407	2.511970	0.467414	H	-3.511480	0.459816	3.197144	H	0.788900	-3.882267	0.996507
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C	0.817624	1.853487	-0.178258	Cl	-4.925218	-2.561529	-0.361493	H	6.497300	-2.154916	-0.211319
H	1.806625	2.305672	-0.190975	44				H	5.950343	-1.830135	-1.858328
C	-0.020263	3.861151	1.111706	6-A-Me-Cl-12			Eopt	H	6.331060	-0.484413	-0.778791
H	-0.288960	4.671186	0.422335	-1311.377387				C	1.547268	0.975907	-0.098733
H	-0.638293	3.976138	2.007480	C	4.209369	-0.696180	1.342661	C	0.205990	0.939699	-0.495930
H	1.025520	4.006039	1.397792	C	4.587173	-1.612576	0.352854	C	2.117167	2.218830	0.230653
C	1.783107	-0.084432	-1.481173	C	3.908913	-1.689701	-0.868878	C	-0.560463	2.108964	-0.564089
H	2.196810	0.561678	-2.263761	C	2.834184	-0.823218	-1.095139	H	-0.246326	-0.009909	-0.764612
H	1.411925	-0.983875	-1.987326	C	2.428574	0.103544	-0.124012	C	1.375088	3.399214	0.169547
C	2.898109	-0.474722	-0.526750	C	3.127638	0.152812	1.092058	H	3.148752	2.256359	0.568341
C	4.231282	-0.198357	-0.847116	H	5.426477	-2.279700	0.538276	C	0.030773	3.327955	-0.228166
C	2.611893	-1.127388	0.680517	H	2.318094	-0.852997	-2.050600	H	-0.561364	4.239646	-0.273970
C	5.249200	-0.579447	0.027701	H	2.805966	0.846940	1.863122	C	1.992565	4.727849	0.535784
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H	1.578549	-1.326400	0.946873	H	5.897704	-0.046676	2.524998	H	1.441256	5.211181	1.350367
C	4.973964	-1.233641	1.225558	H	4.376571	-0.123495	3.421889	C	-2.011974	2.040246	-1.004493
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H	5.779923	-1.518538	1.891958	H	5.387805	-2.907206	-1.877015	H	-2.469016	3.029145	-0.883884
Cl	6.919057	-0.216358	-0.394232	H	3.793048	-3.656261	-1.756229	C	-2.814655	1.012772	-0.231631
44				H	4.066074	-2.356733	-2.921093	C	-3.394203	-0.078870	-0.885031
6-A-Me-Cl-11			Eopt	C	1.281930	1.010741	-0.375420	C	-2.963731	1.130043	1.157763
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C	4.178163	-1.383785	0.983369	C	1.317507	2.349574	0.054553	H	-3.289093	-0.195581	-1.958538
C	3.972535	-2.486576	0.141492	C	-0.948248	1.401795	-1.279107	C	-3.684097	0.178261	1.876297
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C	2.757161	-3.678188	-1.732406	H	-2.878965	1.697850	-2.155846	C	2.831529	-0.814557	-1.098433
H	3.616337	-4.354732	-1.714020	C	-2.908559	-0.208088	-1.171956	C	2.426129	0.105229	-0.121912
H	1.878979	-4.248199	-1.405241	C	-3.123365	-0.042080	0.202922	C	3.127591	0.148881	1.094004
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 H -2.265852 -4.179605 2.034321
 H -2.064684 -4.765468 0.381878
 H -0.781227 -3.813328 1.145398
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 C -0.206226 0.938642 -0.497780
 C -2.119132 2.216802 0.225797
 C 0.559135 2.108570 -0.566798
 H 0.247409 -0.010722 -0.765017
 C -1.378252 3.397866 0.163603
 H -3.150960 2.253747 0.562804
 C -0.033553 3.327418 -0.232952
 H 0.557773 4.239607 -0.279325
 C -1.997485 4.726423 0.527141
 H -1.990443 5.412833 -0.327508
 H -3.034622 4.605837 0.851658
 H -1.445073 5.213597 1.338663
 C 2.011138 2.040583 -1.005688
 H 2.467011 3.030201 -0.886567
 H 2.062570 1.801676 -2.074551
 C 2.814101 1.015451 -0.229994
 C 3.395416 -0.076888 -0.880655
 C 2.961600 1.155594 1.159322
 C 4.111281 -1.022735 -0.144713
 H 3.291539 -0.195821 -1.954035
 C 3.682157 0.185942 1.880469
 H 2.496630 1.971352 1.673752
 C 4.265941 -0.908213 1.233905
 H 3.791804 0.289280 2.955740
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 Cl 4.829785 -2.392598 -0.983796
 44
 6-A-Me-Cl-5 Eopt
 -1311.377352
 C -2.991970 -2.472480 -0.844358
 C -3.975510 -2.483207 0.149414
 C -4.176896 -1.380746 0.991890
 C -3.371035 -0.252843 0.822672
 C -2.371660 -0.210952 -0.163845
 C -2.195192 -1.330176 -0.988000
 H -4.597393 -3.367455 0.272819
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 H -1.441378 -1.302552 -1.769849
 C -2.813214 -3.651499 -1.771195
 H -3.209283 -4.569978 -1.328336
 H -3.339561 -3.488459 -2.719815
 H -1.757306 -3.815586 -2.008093
 C -5.226685 -1.429943 2.076640
 H -6.195668 -1.749157 1.677568
 H -4.948853 -2.142016 2.862866
 H -5.360125 -0.451232 2.545897
 C -1.516435 0.990815 -0.324132
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 C -2.057041 2.281602 -0.185618
 C 0.664029 1.991857 -0.756851
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 C -1.264681 3.421991 -0.325287
 H -3.118800 2.393214 0.014040
 C 0.100355 3.260473 -0.608328
 H 0.731163 4.140701 -0.713707
 C -1.859947 4.804008 -0.197815

C	-4.048239	1.203019	0.518314
H	-1.947090	0.842419	0.239834
C	-5.548659	0.023350	-0.930069
H	-4.622148	-1.271267	-2.380679
C	-5.355053	0.920467	0.121122
H	-6.558562	-0.214627	-1.250017
H	-6.193543	1.386467	0.625620
Cl	-3.779071	2.326426	1.846635
46			
6-B-2Me-1			Eopt
-965.126357			
C	-4.171773	-1.112229	0.530843
C	-3.435770	-2.193317	-0.003262
C	-2.133621	-2.063757	-0.496371
C	-1.602285	-0.778050	-0.428043
C	-2.287907	0.328704	0.098138
C	-3.591248	0.156584	0.582244
H	-3.900819	-3.176242	-0.031532
H	-4.143993	0.995837	0.994303
C	-5.575014	-1.344520	1.041671
H	-6.230808	-1.721697	0.248424
H	-5.587342	-2.082881	1.851738
H	-6.013969	-0.419712	1.426148
C	-1.340401	-3.213671	-1.055916
H	-0.416015	-3.365301	-0.487162
H	-1.920321	-4.139519	-1.024156
H	-1.048810	-3.024838	-2.095194
C	-1.364700	1.445869	-0.010875
C	-0.201366	0.917653	-0.594541
C	-1.403852	2.805509	0.324647
C	0.939806	1.669239	-0.865131
C	-0.285611	3.601530	0.068610
H	-2.291196	3.237618	0.778088
C	0.860137	3.021140	-0.518719
H	1.724160	3.653178	-0.711693
C	-0.285659	5.073510	0.410612
H	-1.233441	5.373641	0.865996
H	0.516973	5.318943	1.115606
H	-0.133423	5.690337	-0.482671
C	2.182772	1.040848	-1.454275
H	1.914659	0.464735	-2.346520
H	2.860946	1.838369	-1.775298
C	2.890693	0.130032	-0.465679
C	2.765512	-1.258965	-0.558123
C	3.646223	0.672828	0.581129
C	3.374022	-2.116721	0.367576
H	2.162989	-1.680712	-1.358154
C	4.260367	-0.165601	1.511042
H	3.742476	1.751459	0.672304
C	4.123614	-1.552181	1.406729
H	4.843557	0.260513	2.322328
H	4.599651	-2.199546	2.138663
C	3.239644	-3.614408	0.228228
H	4.020569	-4.021690	-0.426091
H	3.329292	-4.114909	1.197065
H	2.273728	-3.887603	-0.208221
O	-0.336294	-0.431267	-0.858397
46			
6-B-2Me-2			Eopt
-965.126236			
C	-4.235221	-0.923918	0.647919
C	-3.607819	-2.056322	0.082147
C	-2.327855	-2.022757	-0.479972
C	-1.701894	-0.778691	-0.445818
C	-2.278638	0.376144	0.107533
C	-3.563760	0.300038	0.660368

H	-4.143347	-3.003137	0.084166
H	-4.032680	1.178255	1.094637
C	-5.622567	-1.053764	1.233082
H	-6.344897	-1.383294	0.477256
H	-5.645277	-1.788729	2.046023
H	-5.972835	-0.099337	1.635864
C	-1.652830	-3.226727	-1.079120
H	-0.691065	-3.420899	-0.592071
H	-2.280240	-4.115850	-0.976766
H	-1.444369	-3.072824	-2.143957
C	-1.285167	1.423763	-0.057575
C	-0.195310	0.810784	-0.697337
C	-1.207910	2.783821	0.270935
C	0.982368	1.476802	-1.029546
C	-0.049477	3.495722	-0.046003
H	-2.036902	3.280305	0.766996
C	1.020552	2.830998	-0.685715
H	1.919859	3.395845	-0.921504
C	0.074057	4.965179	0.284503
H	-0.811191	5.326967	0.814804
H	0.947093	5.160073	0.917855
H	0.190147	5.569213	-0.622978
C	2.137973	0.756229	-1.680333
H	1.802975	0.287692	-2.612555
H	2.900499	1.495122	-1.954858
C	2.757208	-0.312055	-0.793026
C	3.075390	-0.028466	0.541678
C	3.022029	-1.589775	-1.291522
C	3.654329	-0.986834	1.379262
H	2.851325	0.958194	0.939687
C	3.599844	-2.560822	-0.468985
H	2.764022	-1.830394	-2.319223
C	3.913161	-2.262951	0.856329
H	3.796963	-3.554161	-0.862029
H	4.355928	-3.024579	1.493306
C	4.004339	-0.656749	2.810759
H	3.646342	-1.432007	3.496707
H	5.090326	-0.580828	2.944447
H	3.563854	0.295950	3.117799
O	-0.437917	-0.524933	-0.942622
46			
6-B-2Me-3			Eopt
-965.125936			
C	5.205299	0.219175	0.225470
C	4.994612	-1.175408	0.150475
C	3.727461	-1.753768	0.023524
C	2.668245	-0.849905	-0.024811
C	2.823359	0.544175	0.045304
C	4.110079	1.083356	0.172140
H	5.858209	-1.835395	0.193194
H	4.256333	2.158138	0.228268
C	6.611370	0.755947	0.362577
H	7.092682	0.384705	1.274781
H	7.238902	0.450940	-0.482825
H	6.615136	1.848681	0.404129
C	3.502932	-3.239593	-0.056710
H	3.003274	-3.513592	-0.992568
H	4.451629	-3.779589	-0.002235
H	2.860920	-3.586866	0.760482
C	1.480235	1.091477	-0.041288
C	0.627736	-0.017844	-0.155755
C	0.927322	2.378951	-0.032965
C	-0.758685	0.073927	-0.262930
C	-0.456968	2.521709	-0.138603
H	1.564475	3.254217	0.054865
C	-1.272540	1.373300	-0.250786

H	-2.347285	1.504082	-0.329313
C	-1.099520	3.889543	-0.133193
H	-0.348941	4.679640	-0.041843
H	-1.663971	4.067590	-1.055733
H	-1.802035	3.995573	0.701490
C	-1.601656	-1.182661	-0.388956
H	-1.316842	-1.701869	-1.312527
H	-1.331276	-1.863207	0.427537
C	-3.091510	-0.939078	-0.380670
C	-3.783861	-0.828683	0.831789
C	-3.798750	-0.776014	-1.576488
C	-5.156910	-0.561560	0.876273
H	-3.235027	-0.947116	1.763694
C	-5.169007	-0.505738	-1.552761
H	-3.274133	-0.853036	-2.525018
C	-5.842807	-0.397485	-0.335919
H	-5.711557	-0.377798	-2.484979
H	-6.908908	-0.185689	-0.324204
C	-5.888215	-0.481151	2.194896
H	-6.660807	0.294074	2.175627
H	-6.385043	-1.431340	2.426912
H	-5.202873	-0.258356	3.017809
O	1.337226	-1.204978	-0.147651
46			
6-B-2Me-4			Eopt
-965.126074			
C	-4.619649	-0.424124	0.720400
C	-4.206749	-1.643730	0.139788
C	-2.946161	-1.830404	-0.436521
C	-2.110540	-0.716349	-0.401072
C	-2.471191	0.517253	0.164249
C	-3.743547	0.662864	0.731878
H	-4.900736	-2.481318	0.139374
H	-4.046562	1.606658	1.175819
C	-6.002017	-0.313031	1.320890
H	-6.778674	-0.506904	0.572052
H	-6.144078	-1.037365	2.131237
H	-6.175740	0.685529	1.731333
C	-2.503317	-3.130397	-1.051797
H	-1.626031	-3.533952	-0.533589
H	-3.301648	-3.875300	-1.004165
H	-2.219739	-2.995041	-2.101387
C	-1.315383	1.380130	-0.011695
C	-0.353708	0.594796	-0.669577
C	-1.007766	2.706513	0.315114
C	0.909382	1.057736	-1.026782
C	0.247373	3.216936	-0.024570
H	-1.734233	3.332914	0.824566
C	1.177015	2.387366	-0.686935
H	2.150583	2.797682	-0.945673
C	0.621187	4.643007	0.307467
H	-0.202276	5.162064	0.805706
H	1.492007	4.681629	0.972101
H	0.876139	5.209041	-0.595864
C	1.931352	0.163908	-1.695913
H	1.420796	-0.515695	-2.385823
H	2.609428	0.784265	-2.290199
C	2.733419	-0.642413	-0.689272
C	3.977622	-0.182684	-0.244571
C	2.223894	-1.834521	-0.159161
C	4.723655	-0.881251	0.713376
H	4.375976	0.744067	-0.652617
C	2.952431	-2.541005	0.798331
H	1.253624	-2.193601	-0.487053
C	4.192335	-2.068393	1.233458
H	2.551355	-3.462812	1.210013

H	4.752030	-2.624088	1.981393
C	6.080565	-0.381832	1.149094
H	6.294138	-0.662032	2.185116
H	6.875792	-0.806960	0.523978
H	6.149046	0.707478	1.070417
O	-0.826553	-0.682313	-0.912976
46			
6-B-2Me-5		Eopt	
-965.126357			
C	-4.419415	-0.623288	0.562149
C	-3.911322	-1.759846	-0.104996
C	-2.630718	-1.811151	-0.665017
C	-1.876909	-0.648619	-0.520725
C	-2.333309	0.506579	0.133926
C	-3.622561	0.516963	0.681601
H	-4.544243	-2.640497	-0.188875
H	-3.999108	1.397831	1.193371
C	-5.816682	-0.657133	1.136917
H	-6.564609	-0.837048	0.356025
H	-5.923242	-1.456618	1.879161
H	-6.065894	0.288409	1.626398
C	-2.086196	-3.022437	-1.372897
H	-1.188749	-3.403014	-0.872091
H	-2.828822	-3.823834	-1.400078
H	-1.798854	-2.782972	-2.402676
C	-1.237366	1.457767	0.057212
C	-0.210683	0.797151	-0.638448
C	-1.028448	2.769308	0.500734
C	1.025334	1.370983	0.921200
C	0.195864	3.388862	0.238399
H	-1.806376	3.300458	1.041445
C	1.194230	2.681724	-0.464498
H	2.143964	3.174809	-0.659451
C	0.464068	4.803352	0.697616
H	-0.400602	5.219893	1.221629
H	1.320860	4.844182	1.380006
H	0.691187	5.461058	-0.149296
C	2.121928	0.607001	-1.632143
H	1.672610	-0.064001	-2.371626
H	2.753635	1.315812	-2.176252
C	2.979037	-0.196168	-0.669082
C	2.503020	-1.400060	-0.131999
C	4.236251	0.269512	-0.272469
C	3.253153	-2.140090	0.787712
H	1.521716	-1.757146	-0.431536
C	4.998071	-0.456793	0.646666
H	4.618910	1.201590	-0.679745
C	4.509944	-1.651574	1.174650
H	5.973171	-0.088066	0.951907
H	5.105785	-2.210534	1.891726
C	2.732003	-3.448336	1.333244
H	3.179903	-4.300817	0.807588
H	2.969485	-3.559962	2.396126
H	1.646756	-3.522048	1.218126
O	-0.589157	-0.484965	-0.997000
43			
6-B-Me-1		Eopt	
-925.799939			
C	-4.147252	-0.681298	0.492859
C	-3.557225	-1.868522	0.004740
C	-2.238783	-1.935729	-0.456423
C	-1.533904	-0.735421	-0.402951
C	-2.070963	0.470371	0.076502
C	-3.396658	0.495324	0.528975
H	-4.154534	-2.777444	-0.012641
H	-3.836251	1.414726	0.904683

C	-5.580922	-0.701916	0.970477
H	-6.264447	-1.000917	0.167346
H	-5.716732	-1.412632	1.793849
H	-5.893735	0.284032	1.325259
C	-1.603871	-3.198736	-0.972169
H	-0.700630	-3.444759	-0.403236
H	-2.298043	-4.040072	-0.902254
H	-1.300649	-3.088660	-2.019563
C	-0.999140	1.445220	-0.035889
C	0.091992	0.743835	-0.574448
C	-0.855603	2.806523	0.263459
C	1.332504	1.322182	-0.833596
C	0.368109	3.432146	0.017490
H	-1.684181	3.370573	0.681845
C	1.435409	2.681157	-0.523324
H	2.383957	3.180618	-0.708274
C	0.564722	4.899682	0.319856
H	-0.336409	5.337178	0.758361
H	1.389512	5.054975	1.024834
H	0.803079	5.465207	-0.588496
C	2.483170	0.508626	-1.377071
H	2.175237	0.004729	-2.299805
H	3.299325	1.190201	-1.642978
C	2.985524	-0.533490	-0.391570
C	2.985747	-1.892815	-0.719821
C	3.449586	-0.146583	0.872783
C	3.446066	-2.848441	0.190066
H	2.612357	-2.206015	-1.690915
C	3.911012	-1.096445	1.784509
H	3.437359	0.905068	1.146385
C	3.911047	-2.453037	1.445653
H	4.267544	-0.779343	2.760227
H	4.267490	-3.193564	2.155316
O	-0.221322	-0.579950	-0.806147
H	3.436915	-3.900112	-0.081406
43			
6-B-Me-2		Eopt	
-925.799929			
C	-4.373470	-0.338687	0.575414
C	-3.966386	-1.573288	0.023162
C	-2.684963	-1.798312	-0.490133
C	-1.821962	-0.706973	-0.420773
C	-2.175897	0.540345	0.117992
C	-3.469764	0.724512	0.622201
H	-4.682209	-2.391758	-0.006013
H	-3.768171	1.679614	1.044511
C	-5.779598	-0.186034	1.107680
H	-6.524286	-0.367896	0.324192
H	-5.978958	-0.898024	1.916890
H	-5.946745	0.820838	1.500108
C	-2.249395	-3.114008	-1.076593
H	-1.407319	-3.537030	-0.517187
H	-3.068649	-3.837205	-1.060657
H	-1.915296	-2.993763	-2.113068
C	-0.990119	1.370897	-0.007490
C	-0.019219	0.555324	-0.613107
C	-0.662646	2.690745	0.325702
C	1.271449	0.981574	-0.911201
C	0.621359	3.164620	0.045179
H	-1.395573	3.340245	0.795390
C	1.559140	2.305678	-0.565809
H	2.555677	2.686801	-0.777523
C	1.017694	4.581882	0.388553
H	0.183598	5.128219	0.837465
H	1.851414	4.600283	1.099948
H	1.338429	5.133275	-0.502730

C	2.300128	0.056827	-1.526245
H	1.796857	-0.643994	-2.200305
H	2.994324	0.648631	-2.130782
C	3.079024	-0.716529	-0.476699
C	2.496477	-1.807504	0.184034
C	4.378884	-0.334252	-0.126195
C	3.199295	-2.497037	1.172841
H	1.485868	-2.107068	-0.076046
C	5.085657	-1.022721	0.863465
H	4.842648	0.508373	-0.632710
C	4.496973	-2.106924	1.517066
H	6.094423	-0.713004	1.120665
H	5.043814	-2.644554	2.285788
O	-0.513759	-0.711537	-0.869650
H	2.734260	-3.340489	1.675004
43			
6-B-Me-Cl-1		Eopt	
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C	-3.915610	-1.896171	0.508436
C	-2.934663	-2.764660	-0.020524
C	-1.700943	-2.321855	-0.507788
C	-1.502996	-0.944960	-0.438569
C	-2.439203	-0.038778	0.084476
C	-3.663696	-0.523932	0.562188
H	-3.144775	-3.831509	-0.048157
H	-4.406518	0.154294	0.971864
C	-5.222043	-2.465030	1.011929
H	-5.764934	-2.983607	0.213241
H	-5.056863	-3.190764	1.816545
H	-5.872833	-1.677046	1.400932
C	-0.646298	-3.242287	-1.060396
H	0.289391	-3.156266	-0.496970
H	-0.977926	-4.282822	-1.019492
H	-0.414826	-2.996646	-2.103065
C	-1.812862	1.269375	-0.014815
C	-0.552347	1.039970	-0.590508
C	-2.177837	2.577888	0.327398
C	0.379718	2.044342	-0.840691
C	-1.279521	3.620370	0.089002
H	-3.146370	2.782275	0.774384
C	-0.021410	3.335557	-0.486024
H	0.669887	4.156755	-0.662077
C	-1.636088	5.047032	0.437144
H	-2.623685	5.105270	0.902830
H	-0.910682	5.480668	1.135004
H	-1.649245	5.683489	-0.455286
C	1.742502	1.732282	-1.418949
H	1.627213	1.170135	-2.352083
H	2.245088	2.672505	-1.667094
C	2.598970	0.929952	-0.454765
C	2.732920	-0.453103	-0.612772
C	3.222534	1.554398	0.632575
C	3.471767	-1.185147	0.313778
H	2.243090	-0.958467	-1.436513
C	3.967369	0.809194	1.546859
H	3.115805	2.627058	0.766583
C	4.097907	-0.573915	1.397832
H	4.449725	1.302813	2.384964
H	4.669229	-1.164170	2.104972
O	-0.356346	-0.298664	-0.861477
Cl	3.603586	-2.929870	0.109785
43			
6-B-Me-Cl-2		Eopt	
-1385.398792			
C	-4.326563	-1.068537	0.790259
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 6-B-Me-Cl-3 Eopt
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 H 4.704133 -3.798381 0.053656
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 6-B-Me-Cl-5 Eopt
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 H -3.118047 2.626223 -0.765246
 C -4.098142 -0.575146 -1.397563
 H -4.451671 1.301810 -2.383663
 H -4.669341 -1.165497 -2.104702
 O 0.356679 -0.298663 0.861871
 Cl -3.601661 -2.931348 -0.110771
 41
 7-A-Me-1 Eopt
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H	0.607023	-0.382826	-0.693593	H	-5.638321	-3.119795	0.667820	H	0.551076	0.117861	-1.277902
C	0.967994	3.295517	0.434015	H	-7.579869	-1.563490	0.672502	C	0.151926	3.283119	0.898673
H	3.067326	2.871563	0.651668	41				H	-1.813515	2.539407	1.365535
C	-0.290308	2.788241	0.104562	7-A-Me-11			Eopt	C	1.350624	3.050239	0.220727
H	-1.165290	3.431435	0.152089	-812.454213				H	2.168632	3.761560	0.303403
C	-1.795393	0.881398	-0.610934	C	-4.314931	0.951309	-0.267037	C	2.824380	1.590606	-1.233846
H	-1.712774	0.123707	-1.398495	C	-4.335857	-0.443632	-0.262731	H	3.344955	2.519326	-1.493636
H	-2.454649	1.667034	-0.996829	C	-3.140190	-1.172095	-0.177018	H	2.648382	1.045808	-2.168189
H	6.448139	0.291002	-1.048760	C	-1.934296	-0.470222	-0.098639	H	-2.362167	-3.158482	-0.154146
H	1.069554	4.330738	0.746517	C	-1.894041	0.934891	-0.104248	H	0.039740	4.174235	1.509508
C	-2.460836	0.237642	0.630037	C	-3.103454	1.640183	-0.188268	C	3.757244	0.738811	-0.329038
H	-1.800923	-0.548549	1.014414	H	-5.284034	-0.971592	-0.326852	H	4.704171	0.581674	-0.858796
H	-2.541948	0.994363	1.418582	H	-1.006203	-1.025189	-0.005078	H	3.984302	1.309623	0.578037
C	-3.822150	-0.334396	0.316631	H	-3.093700	2.725205	-0.219369	C	3.148566	-0.591565	0.044516
C	-3.956704	-1.647050	-0.156102	C	-3.155927	-2.682193	-0.149974	C	3.193005	-1.671638	-0.847687
C	-4.976890	0.449588	0.443429	H	-3.629590	-3.056823	0.765347	C	2.459118	-0.753925	-1.253338
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C	-6.232264	-0.061251	0.106846	C	-0.593329	1.641308	-0.016591	C	1.830788	-1.961396	1.564697
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H	-7.115669	0.561041	0.216452	H	0.433463	0.234202	-1.278295	H	1.295132	-2.063779	2.503712
H	-7.327652	-1.771391	-0.624080	C	0.791615	3.444222	0.838060	H	1.388886	-3.968178	0.904574
41				H	-1.303309	3.215817	1.278350	41			
7-A-Me-10			Eopt	C	1.906866	2.909314	0.189145	7-A-Me-13			Eopt
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C	5.358963	-0.672980	0.295657	H	2.707451	0.604623	-2.145217	C	-3.543682	-0.639852	-0.843524
C	4.272686	0.206057	0.330484	H	-5.245812	1.505882	-0.343186	C	-2.338277	0.060223	-0.945131
C	3.003029	-0.163525	-0.144886	H	0.892556	4.348761	1.430845	C	-1.830207	0.822820	0.119718
C	2.834827	-1.454879	-0.666499	C	3.671409	0.056409	-0.280635	C	-2.564890	0.873950	1.313964
H	5.995983	-2.655272	-0.270744	H	4.561890	-0.334468	-0.786911	H	-5.194325	-1.114226	0.462861
H	4.407581	1.195226	0.759101	H	4.012583	0.564457	0.628015	H	-1.787451	0.028792	-1.880923
H	1.869762	-1.752305	-1.064283	C	2.749259	-1.081398	0.087943	H	-2.177316	1.432323	2.160122
C	6.709078	-0.260876	0.832291	C	2.548010	-2.150975	-0.795341	C	-4.081447	-1.430928	-2.012103
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H	6.724783	0.799464	1.098997	H	3.103519	-2.182735	-1.729677	H	-3.326443	-1.547981	-2.794502
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C	2.058985	2.153198	-0.385759	C	0.926688	-3.140017	0.705180	C	-0.345495	2.800426	0.577793
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H	0.425969	-0.688492	0.503072	H	0.559596	-2.040933	2.524414	H	0.412092	-0.039852	-1.119260
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H	3.043094	2.507794	-0.675261	41				H	-1.170152	3.286147	1.089818
C	-0.288892	2.589505	0.010698	7-A-Me-12			Eopt	C	1.947860	2.836442	-0.197285
H	-1.120351	3.288254	0.055260	-812.453528				H	2.909851	3.338642	-0.262641
C	-1.888692	0.727230	0.631840	C	-2.597425	-2.097947	-0.152116	C	2.947986	0.863891	-1.429188
H	-2.476860	1.515328	1.115327	C	-3.927697	-1.680936	-0.207364	H	3.656219	1.593126	-1.838786
H	-1.825804	-0.102351	1.345253	C	-4.245821	-0.315012	-0.193301	H	2.597177	0.247876	-2.264865
H	3.771937	-3.337232	-1.124067	C	-3.201780	0.611935	-0.118116	H	-4.324592	0.217079	2.363796
H	1.144569	4.092434	-0.561055	C	-1.856926	0.210310	-0.060869	H	1.020812	4.425962	0.923884
C	-2.646220	0.242428	-0.628478	C	-1.564784	-1.162633	-0.078698	C	3.703865	-0.049109	-0.423347
H	-2.709009	1.071487	-1.342448	H	-4.725610	-2.417295	-0.261154	H	4.562613	-0.494902	-0.938857
H	-2.056843	-0.545405	-1.111396	H	-3.436380	1.672900	-0.127382	H	4.098714	0.572584	0.387766
C	-4.028586	-0.269118	-0.302825	H	-0.535341	-1.496239	-0.004803	C	2.820103	-1.133770	0.143503
C	-5.131415	0.595698	-0.297758	C	-5.682459	0.141353	-0.287073	C	2.588230	-2.312364	-0.578696
C	-4.231885	-1.610115	0.050717	H	-6.073983	0.005409	-1.302529	C	2.138159	-0.947819	1.353028
C	-6.402940	0.135933	0.051581	H	-6.326486	-0.431297	0.388733	C	1.691161	-3.275384	-0.112075
H	-4.991784	1.637851	-0.574777	H	-5.781389	1.200502	-0.033011	H	3.110862	-2.473157	-1.518857
C	-5.500752	-2.075951	0.401100	C	-0.765161	1.210110	0.026105	C	1.239270	-1.906432	1.824319
H	-3.387684	-2.295464	0.046945	C	0.440477	1.002910	-0.659542	H	2.295170	-0.032035	1.915637
C	-6.591697	-1.202948	0.403360	C	-0.897806	2.369129	0.808134	C	1.009484	-3.072532	1.090994

H	1.524201	-4.182127	-0.686335
H	0.710156	-1.736998	2.757297
H	0.305930	-3.816113	1.452819
41			
7-A-Me-14			Eopt
-812.451712			
C	3.182546	-0.773658	1.908026
C	4.111179	-0.946764	0.881892
C	3.905911	-0.349593	-0.370648
C	2.754377	0.419129	-0.561777
C	1.808056	0.606496	0.460123
C	2.037563	-0.003047	1.702270
H	5.000506	-1.548633	1.050972
H	2.572565	0.863502	-1.536394
H	1.330639	0.144934	2.512293
C	4.902341	-0.547804	-1.488140
H	5.901302	-0.207181	-1.193035
H	4.987864	-1.606284	-1.759920
H	4.609966	0.005718	-2.384751
C	0.589104	1.416052	0.219709
C	-0.646293	1.012749	0.747386
C	0.634429	2.584507	-0.558177
C	-1.821774	1.730909	0.504522
H	-0.702096	0.089950	1.316019
C	-0.527507	3.317534	-0.798945
H	1.584536	2.930508	-0.952857
C	-1.750130	2.892482	-0.275071
H	2.654066	3.462935	-0.473636
C	-3.152051	1.200967	0.981888
H	-3.844526	2.031493	1.160660
H	-3.024028	0.674499	1.934348
H	3.354481	-1.234417	2.876493
H	-0.478388	4.227342	-1.390219
C	-3.801239	0.226785	-0.040649
H	-4.778539	-0.082515	0.348058
H	-3.980374	0.767611	-0.976482
C	-2.941514	-0.985768	-0.304383
C	-2.968374	-2.081197	0.569419
C	-2.032674	-1.005215	-1.370390
C	-2.104647	-3.163689	0.390277
H	-3.668840	-2.082595	1.401421
C	-1.166309	-2.084332	-1.554474
H	-1.988658	-0.155863	-2.046070
C	-1.196719	-3.166457	-0.672120
H	-2.139911	-4.003212	1.078558
H	-0.460642	-2.074531	-2.379808
H	-0.519449	-4.003779	-0.810072
41			
7-A-Me-2			Eopt
-812.451027			
C	-4.357689	-1.796139	0.820748
C	-5.187020	-0.677494	0.898621
C	-4.742029	0.570924	0.439063
C	-3.452315	0.665029	-0.091465
C	-2.601041	-0.449863	-0.176640
C	-3.072550	-1.686918	0.287577
H	-6.185714	-0.770759	1.317574
H	-3.106245	1.622167	-0.471686
H	-2.423261	-2.556089	0.255127
C	-5.648447	1.777518	0.495559
H	-6.479940	1.679733	-0.212541
H	-6.084277	1.900153	1.493016
H	-5.106811	2.694681	0.247981
C	-1.235372	-0.318641	-0.741000
C	-0.448625	0.809489	-0.462833
C	-0.697166	-1.319668	-1.566960

C	0.842195	0.955614	-0.982266
H	-0.842920	1.578892	0.196274
C	0.586913	-1.185766	-2.092952
H	-1.298089	-2.188312	-1.816945
C	1.354534	-0.056687	-1.802594
H	2.361381	0.033991	-2.199178
C	1.692092	2.138667	-0.585133
H	1.074740	3.043290	-0.533823
H	2.460949	2.314427	-1.345598
H	-4.708764	-2.756413	1.187338
H	0.990581	-1.963020	-2.735120
C	2.384100	1.937429	0.789673
H	2.941193	2.849198	1.034884
H	1.612073	1.814091	1.557254
C	3.312916	0.747438	0.802670
C	4.631190	0.866982	0.342345
C	2.859955	-0.514260	1.210187
C	5.476477	-0.243272	0.288348
H	4.998581	1.839964	0.024303
C	3.700668	-1.627671	1.159587
H	1.836164	-0.624952	1.555734
C	5.012277	-1.496465	0.697001
H	6.496343	-0.129623	-0.067689
H	3.329896	-2.597587	1.477873
H	5.667744	-2.361306	0.658017
41			
7-A-Me-3			Eopt
-812.451793			
C	3.774244	0.190742	1.424969
C	4.260744	-0.563324	0.357452
C	3.543499	-0.636720	-0.845962
C	2.337316	0.061602	-0.946984
C	1.829675	0.825594	0.117456
C	2.566564	0.880741	1.309860
H	5.201800	-1.098562	0.455698
H	1.786017	0.029191	-1.882404
H	2.180738	1.441831	2.155017
C	4.068658	-1.451087	-2.004252
H	5.078080	-1.133218	-2.288363
H	4.123869	-2.514958	-1.745466
H	3.425146	-1.353687	-2.882913
C	0.536555	1.540136	-0.010325
C	-0.535850	0.951533	-0.696409
C	0.343869	2.803117	0.573259
C	-1.783014	1.577849	-0.792879
H	-0.412569	-0.040558	-1.118605
C	-0.890014	3.445593	0.474175
H	1.168500	3.290464	1.083764
C	-1.950141	2.835840	-0.200066
H	-2.912618	3.337097	-0.265498
C	-2.949426	0.860432	-1.428114
H	-2.598748	0.243821	-2.263408
H	-3.658862	1.588394	-1.837887
H	4.332802	0.234383	2.355551
H	-1.023588	4.428020	0.917729
C	-3.703359	-0.052209	-0.420485
H	-4.098000	0.569997	0.390337
H	-4.562202	-0.499404	-0.934624
C	-2.818024	-1.135412	0.146700
C	-2.135182	-0.947537	1.355430
C	-2.585727	-2.314581	-0.574414
C	-1.235098	-1.904866	1.827028
H	-2.292507	-0.031266	1.917156
C	-1.687445	-3.276332	-0.107494
H	-3.109004	-2.476862	-1.513959
C	-1.004956	-3.071591	1.094791

H	-0.705369	-1.733979	2.759392
H	-1.520233	-4.183567	-0.680906
H	-0.300591	-3.814252	1.456948
41			
7-A-Me-4			Eopt
-812.451004			
C	5.026653	1.019583	-0.353280
C	5.318929	-0.342435	-0.420146
C	4.298577	-1.295910	-0.287422
C	2.990055	-0.847833	-0.086243
C	2.675501	0.520049	-0.014127
C	3.715016	1.451858	-0.151381
H	6.343497	-0.670262	-0.576492
H	2.189089	-1.577702	-0.007232
H	3.499537	2.512750	-0.073597
C	4.609759	-2.770968	-0.377253
H	5.001182	-3.033471	-1.366935
H	5.367801	-3.061354	0.358829
H	3.717628	-3.377627	-0.198815
C	1.276257	0.963958	0.199891
C	0.432907	0.277857	1.087076
C	0.762731	2.082330	-0.477872
C	-0.890875	0.675589	1.304031
H	0.825789	-0.573173	1.637625
C	-0.553018	2.492173	-0.267570
H	1.389780	2.613836	-1.186724
C	-1.377749	1.792918	0.615293
H	-2.407936	2.104217	0.760432
C	-1.788340	-0.131654	2.210805
H	-2.606447	0.496949	2.579200
H	-1.224515	-0.475237	3.086084
H	5.825376	1.749456	-0.448634
H	-0.943039	3.350983	-0.805908
C	-2.391740	-1.370913	1.497287
H	-1.573017	-2.022643	1.172234
H	-2.985105	-1.936542	2.225099
C	-3.249840	-0.997926	0.312552
C	-2.702258	-0.911710	-0.974263
C	-4.599819	-0.664343	0.487161
C	-3.481247	-0.503312	-2.058448
H	-1.653627	-1.152679	-1.122898
C	-5.383863	-0.254284	-0.593198
H	-5.040404	-0.727924	1.479447
C	-4.825338	-0.171746	-1.871556
H	-3.037086	-0.440466	-3.047518
H	-6.429383	-0.003895	-0.438292
H	-5.432892	0.145097	-2.713927
41			
7-A-Me-5			Eopt
-812.450989			
C	-3.999705	-1.764071	1.124055
C	-5.128325	-0.978681	0.889915
C	-5.013080	0.251532	0.226076
C	-3.745240	0.668926	-0.189334
C	-2.596135	-0.106980	0.038650
C	-2.740578	-1.334209	0.703140
H	-6.105029	-1.319620	1.223689
H	-3.648244	1.609369	-0.724616
H	-1.863516	-1.937847	0.914077
C	-6.236711	1.091539	-0.052810
H	-6.881521	0.613753	-0.799992
H	-6.837177	1.230821	0.852703
H	-5.963182	2.079856	-0.432530
C	-1.263132	0.364128	-0.410706
C	-0.332537	-0.532832	-0.957287
C	-0.900976	1.717250	-0.303001

C	0.931676	-0.114489	-1.386582
H	-0.610081	-1.577757	-1.070464
C	0.353699	2.148374	-0.731309
H	-1.595629	2.424579	0.138921
C	1.267314	1.239536	-1.267646
H	2.250770	1.576785	-1.581189
C	1.931952	-1.121420	-1.901364
H	2.659954	-0.623145	-2.550937
H	1.421934	-1.879040	-2.507883
H	-4.098522	-2.710639	1.647550
H	0.627285	3.194714	-0.632211
C	2.693377	-1.839825	-0.755428
H	1.968325	-2.378493	-0.135132
H	3.359966	-2.589470	-1.197529
C	3.489195	-0.884432	0.100640
C	2.932901	-0.317814	1.254993
C	4.779752	-0.492305	-0.280033
C	3.645554	0.615749	2.009766
H	1.927850	-0.600647	1.554463
C	5.497194	0.441733	0.470212
H	5.226582	-0.924393	-1.172475
C	4.930534	1.000098	1.619193
H	3.195412	1.045244	2.899935
H	6.497839	0.729780	0.161094
H	5.486603	1.725312	2.205681

41

7-A-Me-6		Eopt
-812.451022		

C	4.615025	-1.404547	-0.693795
C	5.257752	-0.171149	-0.798107
C	4.604846	1.006318	-0.404501
C	3.302278	0.911659	0.093804
C	2.638330	-0.321690	0.207883
C	3.314156	-1.483343	-0.194587
H	6.271943	-0.119162	-1.185829
H	2.779543	1.820038	0.380268
H	2.831155	-2.449622	-0.089559
C	5.289750	2.345630	-0.538173
H	6.277046	2.335163	-0.063515
H	5.438809	2.609887	-1.591791
H	4.700847	3.142063	-0.074854
C	1.255303	-0.389212	0.740146
C	0.313210	-1.264611	0.178575
C	0.855316	0.418770	1.817615
C	-0.997122	-1.347732	0.661584
H	0.602427	-1.876148	-0.672420
C	-0.446865	0.344667	2.310000
H	1.574879	1.083499	2.285042
C	-1.369779	-0.531288	1.736310
H	-2.388097	-0.571684	2.111289
C	-2.006705	-2.234104	-0.027379
H	-2.809993	-2.493061	0.671208
H	-1.531964	-3.172576	-0.337089
H	5.133184	-2.311412	-0.991955
H	-0.743279	0.969609	3.147294
C	-2.629816	-1.561810	-1.279959
H	-1.831141	-1.350333	-1.999539
H	-3.311824	-2.276764	-1.754874
C	-3.368743	-0.288267	-0.947050
C	-2.724219	0.954264	-1.006859
C	-4.698082	-0.330215	-0.505018
C	-3.388788	2.124517	-0.635243
H	-1.689415	1.000571	-1.333806
C	-5.367621	0.836633	-0.130761
H	-5.213165	-1.286772	-0.454827
C	-4.713106	2.069805	-0.194184

H	-2.870839	3.077739	-0.686709
H	-6.399136	0.784043	0.205444
H	-5.231704	2.979144	0.094406

41

7-A-Me-7		Eopt
-812.451028		

C	-4.359803	-1.795013	-0.821826
C	-5.189010	-0.676004	-0.898281
C	-4.743522	0.571700	-0.437783
C	-3.453338	0.664964	0.092227
C	-2.602347	-0.450065	0.175949
C	-3.074514	-1.686695	-0.289219
H	-6.187893	-0.768772	-1.316874
H	-3.107057	1.621720	0.473209
H	-2.425355	-2.556006	-0.258062
C	-5.649425	1.778806	-0.491845
H	-6.095042	1.896537	-1.485524
H	-6.473896	1.685692	0.225086
H	-5.104523	2.696737	-0.254489
C	-1.236332	-0.319906	0.739620
C	-0.449474	0.808437	0.462365
C	-0.697752	-1.322067	1.563895
C	0.841642	0.953727	0.981166
H	-0.844021	1.578679	-0.195585
C	0.586788	-1.189115	2.089098
H	-1.298602	-2.190918	1.813331
C	1.354440	-0.059837	1.799768
H	2.361589	0.030123	2.195720
C	1.691416	2.137332	0.585474
H	2.459691	2.312676	1.346631
H	1.073881	3.041843	0.534463
H	-4.711375	-2.754777	-1.189282
H	0.990685	-1.967368	2.729920
C	2.384552	1.937446	-0.788891
H	1.613158	1.813925	-1.557090
H	2.940928	2.849886	-1.033286
C	3.314311	0.748280	-0.801740
C	2.863067	-0.513460	-1.210826
C	4.631939	0.868608	-0.339550
C	3.704695	-1.626221	-1.159936
H	1.839864	-0.624822	-1.557962
C	5.478092	-0.240909	-0.285264
H	4.998076	1.841684	-0.020326
C	5.015517	-1.494248	-0.695465
H	3.335155	-2.596195	-1.479500
H	6.497396	-0.126659	0.072214
H	5.671693	-2.358550	-0.656217

41

7-A-Me-8		Eopt
-812.449135		

C	-5.214121	-0.158039	1.338876
C	-5.397797	-1.343247	0.626825
C	-4.461368	-1.746774	-0.336335
C	-3.343826	-0.937239	-0.559699
C	-3.140356	0.259150	0.148589
C	-4.094101	0.640650	1.104083
H	-6.272001	-1.960467	0.817627
H	-2.624374	-1.228552	-1.319961
H	-3.943614	1.547358	1.681366
C	-4.672081	-3.014905	-1.128841
H	-4.893717	-3.862004	-0.470660
H	-5.516102	-2.911847	-1.821180
H	-3.786789	-3.267615	-1.718930
C	-1.943011	1.096597	-0.107839
C	-0.688997	0.507124	-0.331463
C	-2.036038	2.497724	-0.134681

C	0.454160	1.274686	-0.578412
H	-0.598643	-0.575249	-0.290595
C	-0.904983	3.275891	-0.379604
H	-3.001080	2.973564	0.007797
C	0.333239	2.670344	-0.600567
H	1.210585	3.281868	-0.795321
C	1.799880	0.611675	-0.748003
H	2.433549	1.209299	-1.413135
H	1.680464	-0.368906	-1.222649
H	-5.940820	0.140519	2.088877
H	-0.991943	4.358049	-0.411718
C	2.533239	0.423919	0.602662
H	2.656185	1.404924	1.075533
H	1.896568	-0.169608	1.268554
C	3.876194	-0.244717	0.435299
C	5.030965	0.513470	0.198589
C	3.990248	-1.641399	0.462742
C	6.266354	-0.104524	-0.006207
H	4.960688	1.598393	0.179493
C	5.222724	-2.265383	0.258641
H	3.104919	-2.244024	0.650858
C	6.366097	-1.497863	0.022422
H	7.150427	0.501005	-0.183508
H	5.291073	-3.348952	0.288512
H	7.326095	-1.980605	-0.133413

41

7-A-Me-9		Eopt
-812.449125		

C	-4.201127	-2.026231	-1.179495
C	-5.229740	-1.835165	-0.257240
C	-5.178091	-0.771342	0.655668
C	-4.076563	0.088214	0.615810
C	-3.030934	-0.087171	-0.306530
C	-3.107276	-1.159917	-1.207216
H	-6.078905	-2.513670	-0.243847
H	-4.015018	0.901167	1.333941
H	-2.324444	-1.298122	-1.946204
C	-6.280697	-0.574808	1.668714
H	-7.260700	-0.519271	1.181939
H	-6.317997	-1.408746	2.379367
H	-6.135931	0.345483	2.241248
C	-1.874856	0.842273	-0.323817
C	-0.572511	0.362064	-0.532182
C	-2.054998	2.222322	-0.135328
C	0.534387	1.217063	-0.557775
H	-0.416779	-0.706363	-0.656928
C	-0.960935	3.086827	-0.158161
H	-3.056339	2.618875	-0.000868
C	0.326441	2.589592	-0.368085
H	1.174880	3.268800	-0.389363
C	1.928560	0.660541	-0.718659
H	2.569635	1.390636	-1.225671
H	1.907186	-0.233979	-1.351449
H	-4.255809	-2.847364	-1.888368
H	-1.114291	4.153848	-0.025426
C	2.571611	0.292323	0.640783
H	2.596323	1.187758	1.272243
H	1.927449	-0.434239	1.148875
C	3.963407	-0.269716	0.480607
C	5.080452	0.576486	0.455210
C	4.165473	-1.645229	0.303042
C	6.364563	0.064907	0.257011
H	4.941605	1.645616	0.596856
C	5.447109	-2.163014	0.104480
H	3.310037	-2.316090	0.325617
C	6.552092	-1.308311	0.079953

H	7.217817	0.736849	0.245142
H	5.583169	-3.232591	-0.026561
H	7.549904	-1.708838	-0.071282
40			
7-B-Me-1			Eopt
-886.472193			
C	-4.988772	-1.360927	0.363786
C	-4.089914	-2.426234	0.176970
C	-2.723456	-2.220474	-0.052595
C	-2.327821	-0.885324	-0.081569
C	-3.195964	0.206438	0.101205
C	-4.555821	-0.036208	0.328640
H	-4.462074	-3.446414	0.210690
H	-5.252966	0.782852	0.473475
C	-1.739146	-3.340506	-0.254825
H	-0.955586	-3.321200	0.510941
H	-2.240040	-4.310719	-0.208491
H	-1.239130	-3.256645	-1.226111
C	-2.361615	1.391730	-0.006642
C	-1.058999	0.917622	-0.246672
C	-2.578734	2.772488	0.072196
C	0.056976	1.733771	-0.417943
C	-1.484230	3.620621	-0.093069
H	-3.570976	3.172041	0.255816
C	-0.196781	3.108808	-0.332240
H	0.633882	3.797629	-0.460026
C	1.430188	1.157314	-0.639046
H	1.386545	0.374899	-1.405241
H	2.100991	1.936662	-1.015605
O	-1.028380	-0.464173	-0.293581
C	2.030100	0.547730	0.651905
H	1.337106	-0.207155	1.037395
H	2.105671	1.333484	1.411708
C	3.384035	-0.072439	0.406765
C	4.561060	0.662158	0.601544
C	3.488753	-1.387003	-0.069512
C	5.810899	0.101019	0.328905
H	4.496860	1.681286	0.975105
C	4.734982	-1.953015	-0.344139
H	2.583813	-1.970086	-0.222197
C	5.901728	-1.209493	-0.146044
H	6.712137	0.685190	0.490846
H	4.796039	-2.974457	-0.708410
H	6.872197	-1.648875	-0.356067
H	-1.624556	4.695622	-0.039071
H	-6.037658	-1.579190	0.538174
40			
7-B-Me-2			Eopt
-886.473973			
C	-4.664707	0.724644	1.149169
C	-4.633848	-0.661125	0.912125
C	-3.544410	-1.290594	0.296104
C	-2.500575	-0.440519	-0.061512
C	-2.494461	0.948966	0.159081
C	-3.600172	1.544608	0.777437
H	-5.481164	-1.270202	1.214623
H	-3.628187	2.613729	0.962068
C	-3.484505	-2.770579	0.031048
H	-2.633961	-3.230719	0.546340
H	-4.398931	-3.263120	0.371101
H	-3.358963	-2.976034	-1.037775
C	-1.223059	1.422423	-0.362568
C	-0.567587	0.280763	-0.859020
C	-0.584500	2.665096	-0.450301
C	0.695946	0.291444	-1.443987
C	0.682687	2.713123	-1.030101

H	-1.061008	3.565202	-0.075119
C	1.306346	1.549795	-1.512054
H	2.302115	1.618061	-1.939956
C	1.375186	-0.976203	-1.890295
H	0.685809	-1.578333	-2.493350
H	2.229669	-0.720148	-2.525340
O	-1.335364	-0.856326	-0.678518
C	1.866872	-1.838520	-0.697376
H	2.335644	-2.744772	-1.097684
H	0.998411	-2.154929	-0.111285
C	2.842566	-1.095717	0.182642
C	2.396746	-0.370666	1.295781
C	4.207125	-1.059261	-0.134489
C	3.288742	0.372565	2.071009
H	1.340476	-0.381645	1.549229
C	5.104372	-0.318000	0.637311
H	4.569611	-1.618968	-0.993682
C	4.646493	0.402519	1.743648
H	2.922678	0.929518	2.928509
H	6.159102	-0.305971	0.377972
H	5.341932	0.978871	2.346385
H	1.203513	3.662363	-1.106070
H	-5.535370	1.159118	1.630260
40			
7-B-Me-3			Eopt
-886.476271			
C	4.029366	0.566647	0.486198
C	3.770860	-0.601016	-0.254681
C	2.516330	-0.868607	-0.816609
C	1.549556	0.106926	-0.584472
C	1.768784	1.285378	0.152067
C	3.036226	1.521663	0.698168
H	4.567890	-1.325485	-0.397894
H	3.239147	2.420279	1.272081
C	2.206021	-2.110290	-1.606119
H	1.900380	-1.862226	-2.628899
H	3.078897	-2.766267	-1.657760
H	1.378073	-2.661637	-1.149164
C	0.495741	1.986092	0.152591
C	-0.387316	1.166430	-0.577439
C	0.017502	3.178398	0.706648
C	-1.737597	1.445976	-0.768380
C	-1.325711	3.502892	0.512346
H	0.671753	3.831620	1.275282
C	-2.181354	2.650499	-0.205540
H	-3.226649	2.924141	-0.323780
C	-2.672223	0.465919	-1.428690
H	-3.474161	1.011126	-1.938730
H	-2.133264	-0.112998	-2.185169
O	0.249939	0.034699	-1.041542
C	-3.312816	-0.514373	-0.405366
H	-4.025441	-1.152348	-0.940394
H	-3.884290	0.069744	0.324797
C	-2.289775	-1.368369	0.304392
C	-1.645764	-0.905560	1.460452
C	-1.903524	-2.606250	-0.224605
C	-0.621950	-1.645467	2.054055
H	-1.933657	0.052348	1.883784
C	-0.889689	-3.357192	0.373218
H	-2.396029	-2.980743	-1.118769
C	-0.238027	-2.873709	1.510468
H	-0.121957	-1.261279	2.938120
H	-0.607284	-4.317137	-0.049781
H	0.559383	-3.449298	1.970721
H	-1.721474	4.424882	0.926700
H	5.021326	0.721760	0.898971

12			
C6H6			Eopt -
232.287286			
C	-1.342699	-0.388464	0.000003
C	-0.334817	-1.357035	0.000069
C	1.007752	-0.968574	-0.000059
C	1.342667	0.388576	0.000007
C	0.334929	1.357005	0.000062
C	-1.007832	0.968493	-0.000058
H	-2.385679	-0.690347	-0.000062
H	-0.595094	-2.411179	0.000080
H	1.790716	-1.720834	-0.000135
H	2.385717	0.690193	0.000015
H	0.594957	2.411204	0.000010
H	-1.790617	1.720950	-0.000048
24			
E			Eopt -
576.702089			
O	0.050470	-1.192775	0.940672
C	1.217515	-0.512176	0.398677
C	1.227560	0.853734	0.279940
C	2.409737	1.357627	-0.281421
C	3.444243	0.489035	-0.670029
C	3.348610	-0.902324	-0.535193
C	2.176885	-1.431690	0.016376
C	-0.017939	1.591126	0.711703
C	-1.233398	0.762974	0.331834
C	-1.204944	-0.629368	0.377420
C	-2.192939	-1.470127	-0.091328
C	-3.352893	-0.866371	-0.588300
C	-3.464808	0.524462	-0.613863
C	-2.409687	1.326345	-0.174945
H	2.522206	2.427577	-0.421755
H	4.160515	-1.545328	-0.854777
H	-0.075380	2.575432	0.243288
H	0.008139	1.753413	1.798631
H	-2.075209	-2.544934	-0.092963
H	-4.156120	-1.491949	-0.962263
H	-4.366176	0.987201	-0.999711
H	-2.484850	2.406566	-0.239588
H	4.345565	0.913636	-1.098307
H	2.029900	-2.498901	0.136834
24			
F			Eopt -
576.706658			
O	1.256089	0.654889	0.000000
C	0.000000	1.378139	0.000000
C	0.248684	2.737723	0.000000
C	-1.246765	0.794078	0.000000
C	-2.321763	1.697404	0.000000
C	-2.120745	3.081194	0.000000
C	-0.833622	3.620298	0.000000
C	-1.415315	-0.690201	0.000000
C	-0.097982	-1.420174	0.000000
C	1.169414	-0.831716	0.000000
C	2.336094	-1.568011	0.000000
C	2.267767	-2.960358	0.000000
C	1.028362	-3.595779	0.000000
C	-0.126641	-2.823309	0.000000
H	-3.331362	1.299118	0.000000
H	-2.979680	3.743050	0.000000
H	-0.676421	4.692981	0.000000
H	-1.997361	-0.997317	0.877000
H	-1.997361	-0.997317	-0.877000
H	3.292275	-1.092604	0.000000
H	3.189262	-3.531863	0.000000

H 0.961141 -4.677882 0.000000
H -1.100012 -3.305384 0.000000
H 1.265884 3.112370 0.000000
27
G Eopt -
616.021128
O 0.049858 -0.791654 1.203491
C -1.226721 -0.600546 0.481591
C -1.637067 0.721049 0.389366
C -1.879179 -1.694442 -0.054559
C -2.851360 0.928407 -0.279938
C -3.085773 -1.446192 -0.714186
H -1.477598 -2.696177 0.036640
C -3.571322 -0.140894 -0.815576
H -3.224803 1.942362 -0.381084
C -3.636150 -2.274603 -1.146155
H -4.511633 0.047052 -1.324029
C 1.251166 -0.382910 0.449604
C 1.427690 0.864001 -0.114633
C 2.156413 -1.442491 0.467342
C 2.665570 0.988680 -0.780256
C 3.371400 -1.271789 -0.194840
C 3.603415 -0.046436 -0.827239
H 2.895436 1.936399 -1.257934
H 4.116474 -2.059072 -0.207226
H 4.539536 0.114718 -1.350628
C -0.756408 1.842690 0.875268
H -1.330404 2.771479 0.891961
H -0.422328 1.655720 1.902234
C 0.463796 2.031465 -0.047120
H 0.112188 2.250674 -1.062756
H 1.026883 2.910843 0.282351
H 1.923816 -2.369720 0.979758
27
H Eopt -
616.008193
O 0.000294 -1.374999 0.344731
C -1.313946 -0.669976 0.105813
C -1.422432 0.631488 -0.404650
C -2.412321 -1.401016 0.518821
C -2.740052 1.048769 -0.672933
C -3.699536 -0.939493 0.257120
H -2.275450 -2.306385 1.070674
C -3.863587 0.279793 -0.394345
H -2.868099 2.047167 -1.081044
H -4.552785 -1.526898 0.578441
H -4.853190 0.657687 -0.626398
C 1.284274 -0.661418 0.182000
C 1.566446 0.636379 0.579628
C 2.183089 -1.497904 -0.462814
C 2.907894 1.017063 0.406176
C 3.504425 -1.081723 -0.642935
C 3.865091 0.176829 -0.169852
H 3.188274 2.023921 0.700316
H 4.225471 -1.728943 -1.128273
H 4.886350 0.525271 -0.278036
C -0.352039 1.697822 -0.459838
H -0.858727 2.660865 -0.551381
H 0.300110 1.599639 -1.333560
C 0.506300 1.666717 0.827256
H -0.121448 1.447515 1.696502
H 0.978679 2.636117 0.998715
H 1.866822 -2.455955 -0.820482
32
N-phenyl-carbazole Eopt
-748.642493

N 0.238928 0.000002 -0.000009
C -0.576724 1.135081 -0.047636
C -0.217511 2.482324 -0.137156
C -1.245889 3.423185 -0.191842
C -2.598055 3.035157 -0.162737
C -2.948438 1.688419 -0.086709
C -1.935836 0.723843 -0.030716
C -1.935830 -0.723855 0.030710
C -0.576717 -1.135082 0.047626
C -0.217485 -2.482320 0.137154
C -1.245852 -3.423193 0.191849
C -2.598023 -3.035176 0.162744
C -2.948421 -1.688443 0.086712
C 2.356009 0.716898 0.977859
C 1.656869 0.000006 -0.000006
C 2.356021 -0.716884 -0.977861
C 3.751419 -0.722486 -0.968902
C 4.452981 0.000015 0.000004
C 3.751405 0.722510 0.968909
H -0.994450 4.477122 -0.260945
H -3.992412 1.389630 -0.074693
H -0.994405 -4.477127 0.260958
H -3.992399 -1.389668 0.074696
H 1.802637 -1.255191 -1.739904
H 4.290062 -1.281427 -1.727947
H 5.538410 0.000020 0.000011
H 4.290041 1.281452 1.727957
H -3.373447 3.793383 -0.205174
H -3.373407 -3.793410 0.205188
H 0.822382 -2.787307 0.169001
H 0.822351 2.787329 -0.169004
H 1.802617 1.255196 1.739903
32
O-phenyl-benzoduranium-ts
Eopt -768.798989
O -0.233440 0.000003 -0.000349
C 0.618701 -1.174216 -0.000210
C 0.183194 -2.477896 -0.000290
C 1.210575 -3.433374 -0.000157
C 2.560194 -3.051727 0.000040
C 2.940357 -1.707288 0.000118
C 1.939652 -0.729939 -0.000006
C 1.939652 0.729936 0.000040
C 0.618700 1.174213 -0.000133
C 0.183200 2.477897 -0.000158
C 1.210582 3.433373 0.000028
C 2.560201 3.051723 0.000205
C 2.940359 1.707283 0.000212
C -2.315812 -0.000287 1.229955
C -1.679817 0.000004 -0.000111
C -2.316198 0.000292 -1.229977
C -3.713724 0.000292 -1.216124
C -4.403990 0.000001 0.000316
C -3.713341 -0.000289 1.216540
H 0.947980 -4.485340 -0.000209
H 3.987532 -1.426073 0.000276
H 0.947990 4.485340 0.000031
H 3.987534 1.426065 0.000347
H -1.748773 0.000504 -2.153925
H -4.257326 0.000514 -2.154422
H -5.488704 -0.000002 0.000487
H -4.256650 -0.000512 2.155009
H 3.325725 -3.819742 0.000137
H 3.325734 3.819735 0.000342
H -0.865164 2.750241 -0.000298
H -0.865172 -2.750236 -0.000443

H -1.748101 -0.000499 2.153727
32
O-phenyl-benzoduranium
Eopt -768.800035
O 0.229900 0.000073 -0.525193
C -0.607521 1.171363 -0.273769
C -0.182333 2.475248 -0.364853
C -1.177867 3.431895 -0.115941
C -2.491830 3.050705 0.192397
C -2.864735 1.706207 0.269474
C -1.891769 0.729972 0.032736
C -1.891633 -0.730248 0.032751
C -0.607309 -1.171417 -0.273756
C -0.181848 -2.475215 -0.364758
C -1.177200 -3.432040 -0.115789
C -2.491239 -3.051090 0.192517
C -2.864408 -1.706664 0.269535
C 1.969405 0.000407 1.188048
C 1.642190 0.000162 -0.157493
C 2.547394 -0.000051 -1.202085
C 3.904327 -0.000015 -0.860010
C 4.288712 0.000233 0.483311
C 3.329819 0.000447 1.503032
H -0.919436 4.483662 -0.166727
H -3.884077 1.425010 0.509291
H -0.918561 -4.483758 -0.166513
H -3.883798 -1.425657 0.509367
H 2.211101 -0.000216 -2.232752
H 4.652676 -0.000175 -1.644759
H 5.342643 0.000253 0.739667
H 3.637041 0.000646 2.543029
H -3.234948 3.818881 0.375913
H -3.234210 -3.819403 0.376065
H 0.839037 -2.747380 -0.603604
H 0.838497 2.747591 -0.603737
H 1.201910 0.000564 1.954219
23
Ph2O Eopt -
538.594283
C -2.616870 1.240678 -0.867188
C -1.363116 0.629032 -0.819730
C -1.195222 -0.519784 -0.041309
C -2.263929 -1.062420 0.672998
C -3.514519 -0.444874 0.610769
C -3.696164 0.710045 -0.154588
H -2.749920 2.133047 -1.471441
H -0.525459 1.034006 -1.376416
H -2.101098 -1.957814 1.263161
H -4.346281 -0.866639 1.166828
H -4.668280 1.190493 -0.197875
O 0.000054 -1.213124 -0.000355
C 1.195253 -0.519692 0.041004
C 2.264350 -1.062596 -0.672534
C 1.362725 0.629466 0.819011
C 3.514882 -0.444985 -0.609947
H 2.101844 -1.958249 -1.262395
C 2.616444 1.241167 0.866830
H 0.524797 1.034670 1.375116
C 3.696113 0.710273 0.155005
H 4.346931 -0.866963 -1.165414
H 2.749154 2.133799 1.470768
H 4.668191 1.190773 0.198568
34
Ph3O+ Eopt -
770.000999
C -0.239618 -1.430839 -0.126708

C 0.326234 -2.267678 -1.072176
 C -0.996954 -1.850364 0.952661
 C 0.113807 -3.639693 -0.913487
 H 0.913773 -1.869594 -1.891600
 C -1.201396 -3.227221 1.084916
 H -1.422119 -1.141885 1.653865
 C -0.647275 -4.115059 0.158643
 H 0.539224 -4.331002 -1.632644
 H -1.792051 -3.599484 1.914793
 H -0.810685 -5.181302 0.271408
 C -1.119692 0.923626 -0.126978
 C -1.103319 1.791828 0.950133
 C -2.128776 0.849087 -1.070856
 C -2.193966 2.657068 1.081717
 H -0.276512 1.808211 1.650453
 C -3.211034 1.718606 -0.912775
 H -2.078395 0.139207 -1.888579
 C -3.241220 2.618143 0.157243
 H -2.220102 3.356618 1.910031
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 45
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 C 0.168343 3.094139 -0.462438
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 42
 SM-6-Cl-Me Eopt
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 39
 SM-7-Me Eopt
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 C 3.033365 -2.265307 -0.418482
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 C 1.415406 1.546807 0.332633
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C	0.773959	3.835271	0.603020
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H	2.749197	3.077868	1.077055
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H	-3.480236	0.570350	-1.943013
H	-1.764774	0.413658	-2.296153
C	-2.255554	2.003798	-0.896557
H	-3.005810	2.188469	-0.118407
H	-2.427529	2.753706	-1.676011
H	4.947906	-1.621040	0.308379
C	0.740674	-2.957109	-1.309146
H	0.179759	-3.515444	-0.552319
H	0.013313	-2.465039	-1.960044
H	1.303866	-3.675682	-1.907762
36			
n6-a-Me-TS			Eopt
-826.069407			
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C	-1.585018	-2.211885	0.000003
C	-1.154824	-0.851685	-0.000036
C	-2.168603	0.164156	-0.000034
C	-3.535549	-0.110949	-0.000008
N	0.113482	-0.163907	-0.000107
C	-0.155606	1.217511	-0.000081
C	-1.535890	1.456005	-0.000056
C	0.771464	2.257187	-0.000066
C	0.269611	3.559548	-0.000039
C	-1.111696	3.816961	-0.000030
C	-2.026344	2.766619	-0.000036
C	2.233509	1.933278	-0.000082
C	2.499921	0.442494	0.000041
C	1.488220	-0.553149	-0.000019
C	1.899679	-1.890134	-0.000022
C	3.242227	-2.257866	0.000087
C	4.236977	-1.283778	0.000195
C	3.842817	0.050395	0.000160
H	-4.998783	-1.694995	0.000046
H	-3.307871	-3.467404	0.000066
H	-4.249236	0.706808	-0.000011
H	0.969460	4.391281	-0.000022
H	-1.464260	4.843499	-0.000011
H	-3.094390	2.959993	-0.000019
H	2.719118	2.385487	-0.875758
H	2.719182	2.385659	0.875468
H	1.169141	-2.667256	-0.000126
H	3.497655	-3.313185	0.000083
H	5.288325	-1.551840	0.000288
H	4.597469	0.833263	0.000215
C	-0.772461	-3.492480	0.000033
H	-1.457404	-4.342673	0.000096
H	-0.146416	-3.597222	-0.890319
H	-0.146349	-3.597139	0.890347
36			
n6-a-Me			Eopt
-826.083509			
N	-0.061274	-0.153759	0.336087
C	0.084312	1.233418	0.184922
C	-0.946251	2.144979	0.365836
C	-0.632402	3.483955	0.129927
C	0.671257	3.859767	-0.253335
C	1.690868	2.917377	-0.413756
C	1.392245	1.565765	-0.195717
C	2.125322	0.309179	-0.238160
C	1.216364	-0.729389	0.129752

C	1.665334	-2.034062	0.390505
C	3.015576	-2.291138	0.108383
C	3.898343	-1.302001	-0.344763
C	3.466345	0.015420	-0.488681
C	-2.251800	1.565517	0.856968
C	-2.458965	0.174737	0.279388
C	-1.349103	-0.665754	0.027984
C	-1.535132	-1.895435	-0.612052
C	-2.821138	-2.339498	-0.920204
C	-3.929396	-1.544527	-0.628117
C	-3.733447	-0.286840	-0.052547
H	-1.395483	4.247239	0.255450
H	2.688467	3.231462	-0.704709
H	3.395425	-3.292544	0.293775
H	4.159269	0.802169	-0.770382
H	-3.099318	2.089031	0.602312
H	-2.219676	1.505930	1.956556
H	-0.676803	-2.485493	-0.899584
H	-2.948586	-3.299813	-1.410317
H	-4.931296	-1.884422	-0.869445
H	-4.586729	0.359102	0.136905
H	0.887121	4.910238	-0.421761
H	4.935560	-1.558114	-0.536594
C	0.826967	-3.100467	1.056746
H	-0.016718	-2.670319	1.600004
H	0.422480	-3.829597	0.345779
H	1.443418	-3.654441	1.770918
39			
n7-a-Me-1			Eopt
-865.409317			
N	-0.030394	-0.094775	-0.234212
C	-1.347653	-0.504886	0.122640
C	-2.453343	0.141267	-0.455096
C	-1.536680	-1.510926	1.077942
C	-3.736296	-0.278769	-0.088133
C	-2.823503	-1.919830	1.423944
H	-0.670945	-1.959790	1.551781
C	-3.931252	-1.310689	0.831574
H	-4.594468	0.216783	-0.534384
H	-2.957045	-2.703613	2.163175
H	-4.936821	-1.624766	1.093039
C	1.093017	-0.948234	-0.165915
C	2.234879	-0.181337	0.174822
C	1.189090	-2.311799	-0.497686
C	3.487824	-0.789401	0.290618
C	2.458524	-2.888481	-0.358524
C	3.586123	-2.156358	0.044788
H	4.364940	-0.204403	0.549552
H	2.573857	-3.939906	-0.608122
C	0.420835	1.231933	-0.021685
C	-0.289996	2.437570	-0.116922
C	1.808563	1.201810	0.266116
C	0.439599	3.604389	0.148989
C	2.503169	2.386048	0.524106
C	1.802503	3.589100	0.478423
H	-0.073697	4.559519	0.071441
H	3.566057	2.367183	0.744305
H	2.316317	4.525739	0.670621
C	-2.247728	1.328702	-1.355745
H	-3.195631	1.588334	-1.836709
H	-1.529482	1.090938	-2.149757
C	-1.736846	2.543662	-0.554128
H	-2.388918	2.682194	0.318263
H	-1.838910	3.449437	-1.162953
H	4.546137	-2.656358	0.126440
C	0.044888	-3.119267	-1.057999

H	-0.612701	-3.517742	-0.278372
H	-0.583294	-2.513420	-1.717666
H	0.433069	-3.963726	-1.633963
39			
n7-a-Me-TS			Eopt
-865.372893			
N	-0.080911	-0.124615	0.314888
C	-1.451864	-0.500195	0.069983
C	-2.455002	0.361396	-0.459339
C	-1.838531	-1.814512	0.357609
C	-3.717867	-0.181490	-0.746786
C	-3.093911	-2.331132	0.057630
H	-1.146327	-2.453520	0.853734
C	-4.052352	-1.513665	-0.530212
H	-4.467716	0.490924	-1.153636
H	-3.312221	-3.366232	0.302717
H	-5.039905	-1.885554	-0.782658
C	1.075674	-0.977468	0.085612
C	2.156615	-0.131128	-0.295441
C	1.367120	-2.359274	0.277266
C	3.392672	-0.610736	-0.727351
C	2.606184	-2.810091	-0.216580
C	3.595137	-1.981772	-0.749662
H	4.170063	0.083770	-1.029170
H	2.824964	-3.868623	-0.108916
C	0.388537	1.220884	0.262925
C	-0.271814	2.433703	0.531187
C	1.748868	1.234356	-0.100637
C	0.487231	3.606855	0.474843
C	2.486941	2.420248	-0.163282
C	1.850481	3.614739	0.147408
H	-0.016806	4.548035	0.676277
H	3.537923	2.398808	-0.433400
H	2.396244	4.552577	0.125314
C	-2.341578	1.857250	-0.626989
H	-3.341529	2.248542	-0.835322
H	-1.711478	2.129858	-1.481604
C	-1.762285	2.513328	0.642530
H	-2.150263	1.998196	1.529102
H	-2.067307	3.561619	0.712477
H	4.530138	-2.405929	-1.100910
C	0.646116	-3.401768	1.119379
H	0.176183	-2.961955	2.002686
H	-0.102633	-3.981637	0.571110
H	1.388813	-4.113737	1.487433
33			
ox6-H-TS			Eopt
-806.908696			
C	-3.686012	-2.133820	-0.000166
C	-1.136761	-1.128379	0.000110
C	-2.213663	-0.234350	0.000057
C	-3.511384	-0.750955	-0.000072
O	0.092720	-0.306777	0.000236
C	-0.328833	1.078619	0.000140
C	-1.715083	1.129941	0.000078
C	0.541912	2.139709	0.000049
C	-0.086893	3.395613	-0.000056
C	-1.482206	3.515437	-0.000080
C	-2.314303	2.391805	-0.000023
C	2.025032	1.922355	0.000060
C	2.416366	0.460352	-0.000052
C	1.534314	-0.620711	0.000111
C	1.936849	-1.947020	0.000189
C	3.303693	-2.224562	0.000024
C	4.229504	-1.182533	-0.000203
C	3.780817	0.133958	-0.000222

H	-4.686818	-2.550861	-0.000273
H	-4.363022	-0.079836	-0.000108
H	0.530055	4.288794	-0.000132
H	-1.925568	4.505068	-0.000161
H	-3.393157	2.496773	-0.000072
H	2.468735	2.408878	-0.876777
H	2.468686	2.408702	0.877024
H	1.238411	-2.762711	0.000391
H	3.629840	-3.258457	0.000081
H	5.292993	-1.393515	-0.000343
H	4.497455	0.949878	-0.000358
C	-2.581171	-2.990469	-0.000126
C	-1.265696	-2.503218	0.000013
H	-0.449794	-3.204408	0.000050
H	-2.728461	-4.064729	-0.000204
33			
ox6-H		Eopt	-
806.915549			
O	-0.037812	-0.282446	0.540006
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C	-0.786331	2.048273	0.344567
C	-0.385167	3.344245	-0.014104
C	0.926657	3.595098	-0.449086
C	1.888121	2.582156	-0.556823
C	1.512238	1.278267	-0.215274
C	2.160465	-0.030456	-0.156765
C	1.234048	-0.971026	0.304514
C	1.504996	-2.282793	0.625548
C	2.822240	-2.695489	0.376233
C	3.779434	-1.807072	-0.131348
C	3.466805	-0.469767	-0.387532
C	-2.135878	1.578979	0.827134
C	-2.405750	0.173099	0.321522
C	-1.385314	-0.756158	0.129466
C	-1.536625	-2.015131	-0.417287
C	-2.835334	-2.405852	-0.758602
C	-3.906237	-1.534412	-0.559076
C	-3.687993	-0.257616	-0.039481
H	-1.098560	4.159697	0.046768
H	2.892595	2.805901	-0.897422
H	3.099526	-3.720391	0.596131
H	4.224340	0.220277	-0.741999
H	-2.927048	2.251631	0.488731
H	-2.155604	1.591409	1.925945
H	-0.696400	-2.670169	-0.597300
H	-2.995423	-3.388455	-1.187969
H	-4.911482	-1.840952	-0.826230
H	-4.519901	0.429037	0.081788
H	1.202214	4.609975	-0.714061
H	4.789226	-2.160736	-0.307711
H	0.772026	-2.951391	1.057659
36			
ox6-a-Cl-b-Me-TS		Eopt	
-1305.784390			
C	-4.528312	0.005597	-0.166695
C	-4.166889	1.347369	-0.101683
C	-2.803320	1.773532	0.025615
C	-2.075063	0.643231	0.082698
C	-2.169873	-0.705361	0.053526
C	-3.570394	-0.993272	-0.095427
O	0.451500	-0.060025	-0.339048
C	0.199295	-1.395298	-0.128083
C	-1.145777	-1.746694	0.075202
C	1.212812	-2.358070	-0.120081
C	0.859755	-3.686656	0.120589
C	-0.468882	-4.057121	0.337913

C	-1.467638	-3.092246	0.310489
C	2.629925	-1.947901	-0.417181
C	2.847326	-0.482274	-0.144324
C	1.757037	0.393159	-0.150885
C	1.955858	1.765325	0.016604
C	3.233338	2.280893	0.216983
C	4.322299	1.410813	0.243332
C	4.125366	0.042821	0.061822
H	-5.572791	-0.262399	-0.281303
H	-4.907974	2.141368	-0.087345
H	-3.834564	-2.036679	-0.226263
H	1.640656	-4.441061	0.133528
H	-0.721618	-5.092101	0.537655
H	-2.491563	-3.384482	0.509112
H	3.327041	-2.549708	0.173772
H	2.856788	-2.159037	-1.472365
H	3.362490	3.348769	0.348325
H	5.320862	1.803573	0.399123
H	4.974130	-0.634014	0.068153
C	-2.475061	3.234011	0.168902
H	-1.939229	3.587540	-0.715036
H	-3.402007	3.799934	0.262239
H	-1.860623	3.408740	1.053099
Cl	0.588565	2.844624	-0.019188
36			
ox6-a-Cl-b-Me		Eopt	
-1305.824625			
O	-0.015643	0.126332	0.539952
C	0.157024	1.516244	0.154488
C	-0.844682	2.414920	0.405192
C	-0.540980	3.719107	-0.012809
C	0.703725	4.002149	-0.602635
C	1.694626	3.027191	-0.785828
C	1.413256	1.715486	-0.383675
C	2.147914	0.454574	-0.252654
C	1.323743	-0.492843	0.367392
C	1.700324	-1.696565	0.923109
C	3.049451	-2.015811	0.666850
C	3.905178	-1.157880	-0.030750
C	3.477833	0.097802	-0.474805
C	-2.069355	1.875531	1.107942
C	-2.381466	0.482966	0.580374
C	-1.353803	-0.376958	0.175383
C	-1.572218	-1.526942	-0.580911
C	-2.899994	-1.931405	-0.765568
C	-3.948657	-1.159479	-0.275640
C	-3.691971	0.059098	0.353406
H	-1.264568	4.514759	0.130886
H	2.654656	3.289995	-1.215158
H	3.431937	-2.956804	1.049894
H	4.166153	0.789350	-0.947167
H	-2.935100	2.523453	0.957946
H	-1.875100	1.842978	2.189113
H	-3.088721	-2.836424	-1.331365
H	-4.970760	-1.484663	-0.434772
H	-4.511466	0.703348	0.654136
C	0.806719	-2.590701	1.739403
H	-0.100519	-2.079085	2.066796
H	0.510367	-3.475221	1.168462
H	1.340723	-2.931434	2.630011
H	0.910565	5.020624	-0.912954
H	4.935105	-1.457229	-0.191777
Cl	-0.325772	-2.410189	-1.410780
36			
ox6-a-Me-TS		Eopt	
-846.221794			

C	-3.973829	-1.366455	-0.000085
C	-3.035077	-2.393576	-0.000037
C	-1.630782	-2.212259	0.000025
C	-1.259530	-0.862535	0.000027
C	-2.175060	0.200801	-0.000022
C	-3.546733	-0.047355	-0.000078
O	0.122557	-0.159867	0.000122
C	-0.141817	1.264998	0.000042
C	-1.507166	1.481773	-0.000016
C	0.823154	2.247470	0.000013
C	0.327725	3.560714	-0.000055
C	-1.044379	3.831015	-0.000094
C	-1.980104	2.795601	-0.000081
C	2.278654	1.913178	0.000043
C	2.529854	0.427689	-0.000006
C	1.554059	-0.571716	0.000062
C	1.861084	-1.917110	0.000123
C	3.197116	-2.314873	0.000062
C	4.208242	-1.356868	-0.000049
C	3.863332	-0.010884	-0.000074
H	-5.031235	-1.606058	-0.000128
H	-3.389304	-3.418187	-0.000048
H	-4.246426	0.780406	-0.000115
H	1.038853	4.381035	-0.000081
H	-1.383243	4.861049	-0.000146
H	-3.043783	3.003892	-0.000125
H	2.762376	2.359788	-0.877020
H	2.762319	2.359705	0.877183
H	1.095461	-2.660636	0.000226
H	3.430399	-3.373788	0.000106
H	5.251242	-1.652988	-0.000103
H	4.640901	0.747308	-0.000135
C	-0.833555	-3.496272	0.000065
H	-1.528376	-4.336131	0.000025
H	-0.215331	-3.603238	-0.894755
H	-0.215433	-3.603243	0.894956
39			
ox6-a-Me-b-Me-TS		Eopt	
-885.507343			
C	3.744425	-1.470034	0.939263
C	2.896631	-2.440322	0.420120
C	1.645912	-2.183500	-0.198103
C	1.259981	-0.843171	-0.105964
C	2.152136	0.170532	0.266811
C	3.397821	-0.132527	0.811022
O	-0.057124	-0.084353	-0.589963
C	0.310730	1.334750	-0.448545
C	1.616176	1.475161	-0.020192
C	-0.570627	2.391348	-0.550529
C	-0.014284	3.671275	-0.419594
C	1.341436	3.852737	-0.130359
C	2.162931	2.753586	0.115132
C	-2.030825	2.107932	-0.559622
C	-2.282466	0.803065	0.156937
C	-1.512019	-0.344768	-0.092492
C	-2.076526	-1.618488	-0.046863
C	-3.231729	-1.732340	0.754890
C	-3.874404	-0.629361	1.296067
C	-3.450114	0.639288	0.904247
H	4.691480	-1.759869	1.380513
H	3.220574	-3.475479	0.430920
H	4.067701	0.665466	1.109438
H	-0.671765	4.530852	-0.503109
H	1.740340	4.856911	-0.038810
H	3.193947	2.883292	0.423323
H	-2.578850	2.920095	-0.077338

H	-2.427659	2.015291	-1.580322	C	1.884443	-1.812187	0.518285	H	4.681264	2.262985	0.748839
H	-3.667873	-2.721706	0.858381	C	3.237921	-1.934245	0.137858	H	4.530408	0.722865	1.602654
H	-4.759389	-0.751938	1.910359	C	3.954892	-0.883936	-0.440986	C	2.904154	1.730551	-1.314105
H	-4.042963	1.518488	1.134590	C	3.372586	0.371542	-0.642968	H	3.230737	2.774908	-1.303571
C	1.072051	-3.370297	-0.925874	C	-2.409609	1.229426	1.006225	H	3.574231	1.174507	-1.976659
H	0.686631	-3.102640	-1.907837	C	-2.439759	-0.130928	0.330377	H	1.902826	1.687480	-1.749917
H	1.878218	-4.086834	-1.086269	C	-1.264688	-0.815147	0.025142	42			
H	0.296947	-3.880287	-0.357750	C	-1.177994	-1.972130	-0.721426	ox6-a-iPr		Eopt	-
C	-1.839478	-2.744289	-1.019197	C	-2.382730	-2.543156	-1.144267	924.890632			
H	-1.612875	-3.695805	-0.538905	C	-3.597517	-1.934471	-0.826898	O	0.237275	0.021074	0.393110
H	-2.780286	-2.877951	-1.562492	C	-3.621711	-0.734022	-0.113667	C	1.375342	-0.881219	0.303263
H	-1.083738	-2.506525	-1.757926	H	-1.936202	4.015486	0.335473	C	2.624224	-0.456444	0.677633
39				H	2.154225	3.486897	-0.948959	C	3.621558	-1.427980	0.507230
ox6-a-Me-b-Me			Eopt	H	3.739050	-2.876518	0.336660	C	3.303643	-2.694503	-0.012131
-885.563552				H	3.951584	1.202178	-1.030210	C	2.002841	-3.045124	-0.396470
O	-0.026665	-0.025574	0.498746	H	-3.334821	1.770288	0.797535	C	0.989843	-2.091410	-0.241893
C	0.038940	1.386338	0.184496	H	-2.344885	1.110773	2.096727	C	-0.451365	-2.025047	-0.481757
C	-1.030752	2.191466	0.471442	H	-0.226475	-2.412338	-0.983807	C	-0.926243	-0.773582	-0.064345
C	-0.831190	3.533108	0.114611	H	-2.359410	-3.455910	-1.728973	C	-2.245432	-0.389918	0.083166
C	0.385104	3.940570	-0.462344	H	-4.528898	-2.380786	-1.157474	C	-3.150467	-1.358466	-0.402681
C	1.446781	3.055275	-0.696195	H	-4.567268	-0.241593	0.090298	C	-2.736193	-2.593376	-0.908060
C	1.269776	1.708571	-0.354602	H	0.177300	4.926081	-0.548102	C	-1.386143	-2.957405	-0.928154
C	2.092988	0.497299	-0.300416	H	4.996602	-1.036874	-0.701339	C	2.750997	0.971972	1.151181
C	1.338243	-0.532486	0.279388	C	1.171108	-2.918317	1.252250	C	1.825665	1.842989	0.318679
C	1.806576	-1.738991	0.757754	H	0.257846	-2.571099	1.737959	C	0.593352	1.369121	-0.126509
C	3.164137	-1.962277	0.449905	H	0.905535	-3.742136	0.581771	C	-0.246027	2.016520	-1.009166
C	3.949690	-1.012964	-0.211589	H	1.830505	-3.326080	2.022587	C	0.145204	3.289466	-1.436094
C	3.436995	0.238505	-0.568929	42				C	1.345236	3.842140	-0.986952
C	-2.212406	1.517583	1.129672	ox6-a-iPr-TS			Eopt	C	2.181409	3.118416	-0.134009
C	-2.415590	0.144203	0.507443	-924.862654				H	4.647611	-1.195143	0.772680
C	-1.334016	-0.621644	0.060269	C	2.960641	-2.699450	0.043179	H	1.792509	-4.026537	-0.805934
C	-1.408265	-1.731694	-0.776801	C	3.295238	-1.349594	0.081302	H	-4.211582	-1.141663	-0.350220
C	-2.720394	-2.191188	-1.003526	C	2.373688	-0.276215	0.104518	H	-1.074853	-3.941648	-1.259064
C	-3.838123	-1.541163	-0.490718	C	1.044616	-0.721212	0.069148	H	3.779505	1.327414	1.062454
C	-3.688512	-0.354052	0.226162	C	0.662510	-2.068485	0.037286	H	2.478480	1.035039	2.213794
H	-1.615046	4.261858	0.293099	C	1.627778	-3.074736	0.025667	H	-1.158888	1.560856	-1.365982
H	2.379424	3.411313	-1.118732	O	-0.350387	0.040688	0.051109	H	-0.489765	3.834991	-2.125165
H	3.612230	-2.899324	0.765521	C	-1.366188	-0.990733	0.011109	H	1.644685	4.829457	-1.320888
H	4.070609	0.996925	-1.014508	C	-0.769999	-2.237640	0.009825	H	3.134503	3.535239	0.175896
H	-3.123524	2.108325	1.017368	C	-2.726278	-0.768921	-0.028386	H	4.098556	-3.423085	-0.128936
H	-2.017279	1.428687	2.207557	C	-3.519731	-1.925941	-0.061265	H	-3.483596	-3.298096	-1.256237
H	-2.847314	-3.065827	-1.633248	C	-2.958773	-3.206072	-0.058250	C	-2.720592	0.862126	0.803009
H	-4.829618	-1.928605	-0.697865	C	-1.574946	-3.377838	-0.024794	H	-1.856574	1.508829	0.978460
H	-4.558263	0.208012	0.550466	C	-3.294461	0.610467	-0.042679	C	-3.286537	0.471952	2.183599
H	0.510065	4.985595	-0.724513	C	-2.228199	1.669669	0.031655	H	-3.578119	1.371373	2.733752
H	4.990738	-1.239624	-0.414616	C	-0.848769	1.447678	0.077401	H	-4.171449	-0.163487	2.080182
C	1.009604	-2.702209	1.597705	C	0.062022	2.482033	0.144308	H	-2.547417	-0.071108	2.780031
H	-0.067923	-2.584964	1.474551	C	-0.387171	3.800969	0.169401	C	-3.751016	1.658011	-0.013768
H	1.275426	-3.735475	1.361553	C	-1.752272	4.071465	0.126665	H	-4.006989	2.581443	0.512765
H	1.239635	-2.538410	2.656309	C	-2.645331	3.009675	0.059335	H	-3.374162	1.926786	-1.005336
C	-0.268585	-2.400486	-1.508912	H	3.747007	-3.445883	0.030514	H	-4.676441	1.091310	-0.151763
H	0.456790	-1.680645	-1.891138	H	4.344033	-1.089835	0.097501	36			
H	0.268815	-3.120977	-0.888702	H	1.323991	-4.114804	0.001483	ox6-b-Me-TS		Eopt	
H	-0.677455	-2.944864	-2.361976	H	-4.598763	-1.809685	-0.091170	-846.214393			
36				H	-3.608864	-4.073511	-0.084487	C	-3.579280	-2.295678	0.360117
ox6-a-Me			Eopt	H	-1.134923	-4.368342	-0.026288	C	-2.462579	-3.063130	0.022852
-846.243659				H	-3.887020	0.758237	-0.953917	C	-1.218726	-2.479257	-0.259325
O	-0.030562	-0.156512	0.529798	H	-3.987732	0.737172	0.797326	C	-1.142504	-1.107226	-0.154741
C	-0.061567	1.276211	0.275653	H	1.111040	2.291702	0.174896	C	-2.249727	-0.306729	0.138368
C	-1.206642	1.993787	0.506929	H	0.341192	4.602463	0.221646	C	-3.481484	-0.907802	0.406940
C	-1.087195	3.355362	0.190983	H	-2.116736	5.092411	0.146116	O	0.021707	-0.190502	-0.461527
C	0.118685	3.868056	-0.316841	H	-3.713734	3.201844	0.026132	C	-0.533533	1.156842	-0.257326
C	1.241786	3.062438	-0.546027	C	2.974493	1.127401	0.105303	C	-1.877983	1.086837	0.066771
C	1.147152	1.698607	-0.245245	H	2.408762	1.723716	0.821817	C	0.204216	2.312577	-0.335909
C	2.031314	0.534615	-0.300727	C	4.418789	1.208254	0.629218	C	-0.512049	3.499858	-0.125913
C	1.344492	-0.580882	0.198930	H	5.144523	0.778323	-0.066834	C	-1.882979	3.483002	0.153264

C	-2.579570	2.278409	0.265129
C	1.672887	2.213418	-0.552836
C	2.203871	0.901509	-0.026001
C	1.531307	-0.326464	-0.132964
C	2.184776	-1.561101	-0.047030
C	3.493742	-1.505298	0.474720
C	4.138678	-0.318109	0.783103
C	3.509439	0.880105	0.471627
H	-4.526250	-2.781054	0.568195
H	-2.542952	-4.142835	-0.038647
H	-4.343689	-0.291667	0.636541
H	0.021437	4.443989	-0.170185
H	-2.405831	4.420662	0.306044
H	-3.635547	2.263981	0.509579
H	1.909000	2.275851	-1.624884
H	2.189837	3.044896	-0.069025
H	4.020118	-2.447289	0.588888
H	5.143641	-0.327683	1.189863
H	4.031323	1.824602	0.584549
H	-0.406517	-3.111708	-0.545326
C	1.784199	-2.914632	-0.588899
H	1.288611	-3.542120	0.155539
H	1.170869	-2.831924	-1.486563
H	2.696083	-3.436477	-0.884029
36			
ox6-b-Me			Eopt
-846.234364			
O	0.012378	-0.133906	-0.503326
C	-0.306336	1.222698	-0.113229
C	0.607551	2.222936	-0.311717
C	0.152044	3.485085	0.097393
C	-1.143403	3.639283	0.621681
C	-2.041666	2.570073	0.741817
C	-1.607747	1.297890	0.349470
C	-2.203722	-0.027237	0.167328
C	-1.242603	-0.876263	-0.393133
C	-1.473456	-2.125271	-0.920138
C	-2.782036	-2.603123	-0.764071
C	-3.769584	-1.825011	-0.143882
C	-3.500303	-0.530515	0.308323
C	1.902693	1.832544	-0.981598
C	2.337576	0.452685	-0.514440
C	1.415061	-0.538037	-0.160272
C	1.705218	-1.719057	0.518213
C	3.082635	-1.969413	0.673311
C	4.056954	-1.074056	0.246706
C	3.684127	0.150167	-0.306947
H	0.798158	4.350516	-0.007616
H	-3.046966	2.732124	1.113556
H	-3.030614	-3.587380	-1.145037
H	-4.285698	0.083926	0.734131
H	2.694045	2.553892	-0.767755
H	1.751642	1.838254	-2.070384
H	3.375164	-2.883553	1.179734
H	5.105872	-1.306273	0.394598
H	4.434790	0.890608	-0.563532
H	-1.466296	4.629371	0.924681
H	-4.772256	-2.225517	-0.042434
H	-0.706120	-2.700050	-1.422458
C	0.725944	-2.671869	1.162944
H	-0.137301	-2.160264	1.590311
H	0.356570	-3.430690	0.468361
H	1.236314	-3.194775	1.973891
39			
ox7-a-Me-1			Eopt
-885.575527			

O	-0.006096	-0.107978	-0.470299
C	-1.166928	-0.788134	0.144121
C	-2.387042	-0.463379	-0.430315
C	-0.972724	-1.637381	1.216647
C	-3.502621	-1.103975	0.125735
C	-2.109873	-2.256237	1.743398
H	0.013067	-1.818421	1.627292
C	-3.366474	-1.996470	1.191223
H	-4.485051	-0.891350	-0.284153
H	-2.005962	-2.935256	2.582335
H	-4.245778	-2.483161	1.599052
C	1.332111	-0.684690	-0.293936
C	2.169004	0.299753	0.227348
C	1.680221	-1.967125	-0.675204
C	3.504031	-0.036119	0.457624
C	3.033365	-2.265307	-0.418482
C	3.915554	-1.333624	0.140908
H	4.202351	0.692318	0.853667
H	3.398357	-3.251903	-0.685791
C	0.119888	1.323257	-0.130777
C	-0.882125	2.255330	-0.308949
C	1.415406	1.546807	0.332633
C	-0.497915	3.550470	0.098656
C	1.754320	2.843936	0.715638
C	0.773959	3.835271	0.603020
H	-1.222384	4.352866	-0.002496
H	2.749197	3.077868	1.077055
H	1.009193	4.853250	0.893960
C	-2.485730	0.600698	-1.492453
H	-3.480236	0.570350	-1.943013
H	-1.764774	0.413658	-2.296153
C	-2.255554	2.003798	-0.896557
H	-3.005810	2.188469	-0.118407
H	-2.427529	2.753706	-1.676011
H	4.947906	-1.621040	0.308379
C	0.740674	-2.957109	-1.309146
H	0.179759	-3.515444	-0.552319
H	0.013313	-2.465039	-1.960044
H	1.303866	-3.675682	-1.907762
39			
ox7-a-Me-2			Eopt
-885.562895			
O	-0.000867	-0.087248	0.567573
C	-1.047051	-0.949965	-0.096982
C	-2.389932	-0.682383	0.156514
C	-0.581294	-1.940109	-0.951195
C	-3.284905	-1.569034	-0.476281
C	-1.508328	-2.783747	-1.557687
H	0.474195	-2.056233	-1.152419
C	-2.868530	-2.605624	-1.302912
H	-4.346793	-1.411289	-0.311638
H	-1.161823	-3.564794	-2.225054
H	-3.602967	-3.258018	-1.762288
C	1.413263	-0.447199	0.339944
C	2.024216	0.574059	-0.391472
C	2.008167	-1.582671	0.852245
C	3.373127	0.422842	-0.711837
C	3.370097	-1.695513	0.503822
C	4.027513	-0.731345	-0.267421
H	3.903726	1.188601	-1.266164
H	3.921386	-2.557553	0.865812
C	-0.087008	1.316099	0.140985
C	-1.134797	2.115326	0.528733
C	1.074188	1.681173	-0.522721
C	-1.042668	3.428397	0.034482
C	1.141720	2.996413	-0.992173

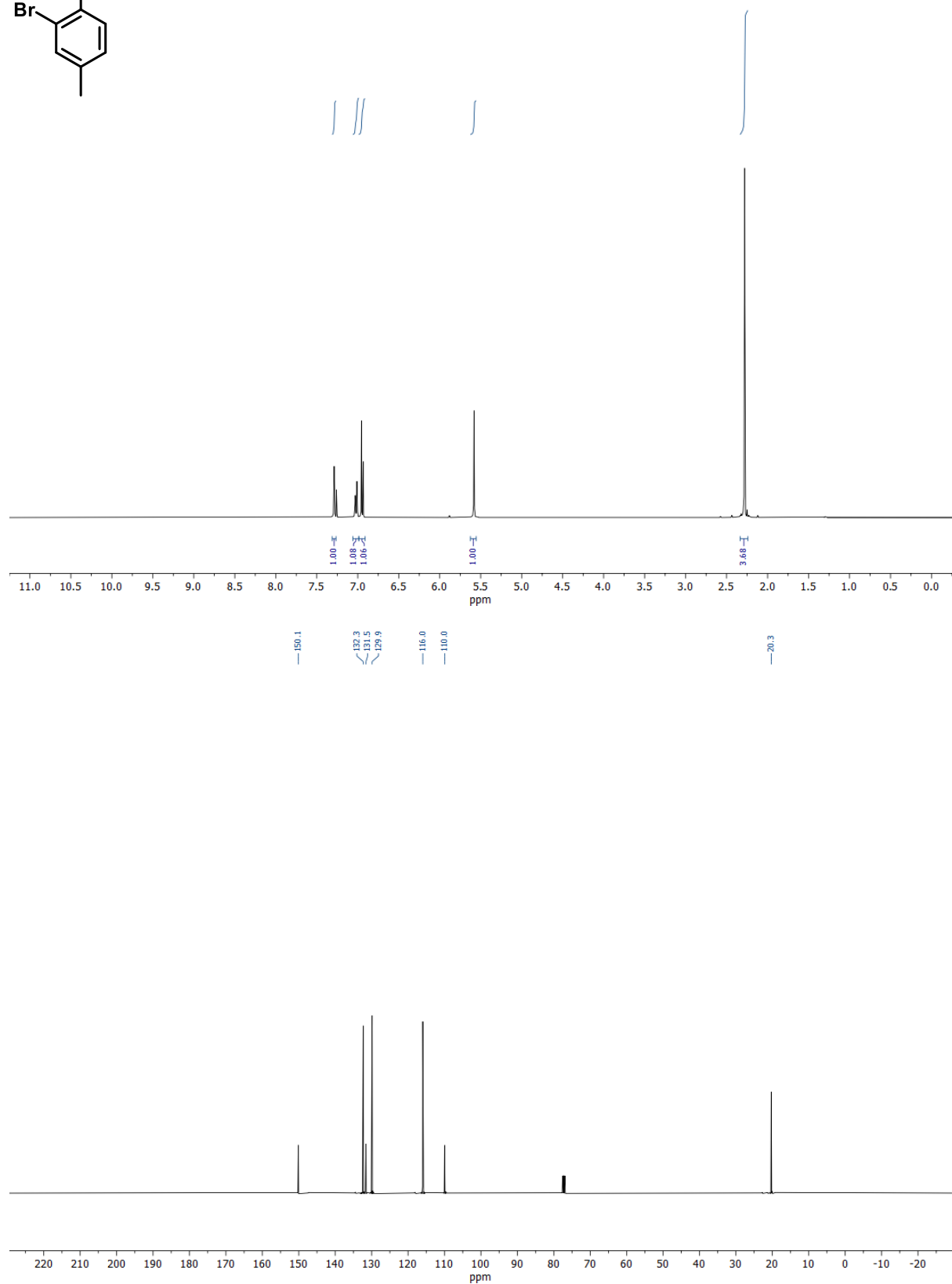
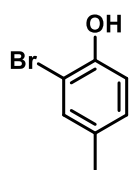
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H	0.092749	4.868464	-1.084057
C	-3.031004	0.452324	0.942412
H	-3.595752	0.014829	1.773256
H	-3.776182	0.892897	0.271123
C	-2.157067	1.585997	1.496909
H	-1.623985	1.240507	2.391103
H	-2.812369	2.398052	1.820825
H	5.077736	-0.870225	-0.500310
C	1.295504	-2.605874	1.693543
H	0.501881	-2.152431	2.292605
H	0.836444	-3.380543	1.069842
H	2.000374	-3.094539	2.369192
39			
ox7-a-Me-TS			Eopt
-885.532520			
O	-0.067975	-0.123534	0.507839
C	-1.457420	-0.550194	0.094977
C	-2.369506	0.288005	-0.561243
C	-1.782230	-1.830539	0.500794
C	-3.558478	-0.345846	-0.972190
C	-2.980474	-2.411789	0.094307
H	-1.129269	-2.366302	1.156706
C	-3.857368	-1.675385	-0.696561
H	-4.287684	0.264702	-1.495122
H	-3.219076	-3.420711	0.412021
H	-4.790155	-2.106036	-1.043327
C	1.166861	-0.967501	0.119302
C	2.116926	-0.054403	-0.346315
C	1.443222	-2.320050	0.341314
C	3.336519	-0.499028	-0.851464
C	2.674089	-2.725934	-0.228817
C	3.584598	-1.866624	-0.837443
H	4.067880	0.209979	-1.221902
H	2.932170	-3.775162	-0.130553
C	0.368386	1.280864	0.366367
C	-0.384353	2.412715	0.640068
C	1.668580	1.300366	-0.113587
C	0.324789	3.621202	0.528401
C	2.340114	2.519029	-0.238358
C	1.661065	3.679752	0.121098
H	-0.213334	4.541532	0.731399
H	3.363452	2.551973	-0.593900
H	2.157345	4.641591	0.053294
C	-2.343920	1.797401	-0.650792
H	-3.359035	2.125476	-0.884510
H	-1.699913	2.162804	-1.457436
C	-1.881653	2.408609	0.692845
H	-2.287660	1.833525	1.531024
H	-2.241555	3.434599	0.793157
H	4.511098	-2.263029	-1.237692
C	0.752214	-3.372325	1.181027
H	0.329229	-2.956377	2.098533
H	-0.022289	-3.916105	0.634475
H	1.500827	-4.104133	1.488744
39			
ox7-a-Me-flip-TS			Eopt
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O	-0.016661	-0.103593	0.611117
C	0.954465	-1.010723	-0.096365
C	2.302130	-0.870205	0.218888
C	0.439706	-1.864567	-1.059109
C	3.156408	-1.729119	-0.498637
C	1.326985	-2.699566	-1.736740

H	-0.617030	-1.883979	-1.287950	H	-1.185974	1.387579	2.286847	O	0.283229	0.067235	0.421113
C	2.689711	-2.635354	-1.446481	C	-3.020289	1.090909	1.156735	C	0.303918	1.524601	0.048360
H	4.221549	-1.668051	-0.297789	H	-3.636704	1.668373	0.457456	C	1.376604	2.137467	-0.616428
H	0.948047	-3.381079	-2.490035	H	-3.636140	0.924789	2.047152	C	-0.791463	2.236916	0.497094
H	3.391002	-3.276970	-1.968618	H	3.161209	-3.810916	-0.902941	C	1.158079	3.476937	-0.987232
C	-1.450467	-0.356232	0.375825	C	2.759089	0.538568	0.864609	C	-0.957576	3.571607	0.133448
C	-1.983563	0.712641	-0.346794	H	1.933756	1.237352	1.031979	H	-1.507190	1.770414	1.143820
C	-2.118828	-1.465710	0.852735	C	3.377580	0.215897	2.238378	C	0.004683	4.183939	-0.662457
C	-3.338253	0.658679	-0.675521	H	4.233448	-0.458642	2.137993	H	1.961649	3.982965	-1.512633
C	-3.483227	-1.479633	0.497900	H	3.729821	1.136041	2.713665	H	-1.828826	4.113842	0.483083
C	-4.071201	-0.455638	-0.253071	H	2.649823	-0.258285	2.903614	H	-0.107571	5.215638	-0.976971
H	-3.811928	1.465061	-1.223749	C	3.775124	1.227707	-0.060947	C	-0.837293	-0.888554	-0.080265
H	-4.091978	-2.312561	0.834971	H	3.333080	1.480221	-1.028643	C	-0.176925	-2.061329	-0.457636
C	0.183590	1.287764	0.173805	H	4.131187	2.152737	0.401208	C	-2.227859	-0.765133	-0.032045
C	1.315780	1.991019	0.510230	H	4.645807	0.589871	-0.240969	C	-0.876244	-3.093483	-1.077422
C	-0.948286	1.738919	-0.487927	45				C	-2.877644	-1.801263	-0.747384
C	1.334469	3.290021	-0.029133	ox7-a-iPr-2			Eopt	C	-2.240409	-2.915929	-1.282542
C	-0.903698	3.040474	-0.996420	-964.210020				H	-0.364396	-3.999041	-1.381966
C	0.260071	3.787956	-0.781475	O	0.215383	-0.010145	0.398372	H	-3.956656	-1.741582	-0.821503
H	2.186973	3.929312	0.176964	C	0.361316	1.317340	-0.306436	C	1.517031	-0.745247	0.410416
H	-1.750601	3.466839	-1.521935	C	1.380964	2.175682	0.097258	C	2.799460	-0.325154	0.738441
H	0.317929	4.798561	-1.171009	C	-0.527661	1.571438	-1.341436	C	1.210244	-2.014742	-0.054580
C	2.938898	0.069908	1.225705	C	1.407773	3.405464	-0.591457	C	3.757229	-1.353784	0.759640
H	3.046463	-0.467128	2.175325	C	-0.453843	2.798969	-1.994203	C	2.191164	-3.009785	-0.051757
H	3.956941	0.239992	0.867403	H	-1.263192	0.838795	-1.640341	C	3.461927	-2.673538	0.404590
C	2.289572	1.447853	1.522066	C	0.511191	3.727704	-1.603285	H	4.777148	-1.085186	1.015442
H	1.744865	1.388413	2.471786	H	2.180195	4.117549	-0.315935	H	1.960273	-4.012922	-0.391061
H	3.084856	2.180149	1.677679	H	-1.143963	3.015750	-2.801858	H	4.243413	-3.424569	0.439556
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C	-1.470384	-2.557832	1.658070	C	-0.926806	-0.864594	-0.001852	H	3.427116	2.466823	-1.014554
H	-0.987246	-3.294217	1.006530	C	-0.426267	-2.008669	-0.630230	H	2.929151	0.839839	-1.450403
H	-0.704994	-2.160540	2.330112	C	-2.243930	-0.568099	0.279256	C	3.236248	1.109289	0.687626
H	-2.217622	-3.079926	2.258612	C	-1.347263	-2.946459	-1.094166	H	2.804082	1.731886	1.476965
45				C	-3.139931	-1.541778	-0.212113	H	4.322270	1.154143	0.792056
ox7-a-iPr-1			Eopt	C	-2.707189	-2.685329	-0.889644	H	-2.823160	-3.670934	-1.798517
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O	-0.226212	-0.013571	0.348325	H	-4.201598	-1.399517	-0.042696	H	-2.551785	0.651456	1.533091
C	-0.219497	1.307813	-0.318282	C	1.390864	-0.866285	0.195484	C	-3.842007	1.202264	-0.125900
C	-0.959943	2.278495	0.340538	C	2.594921	-0.573340	0.788364	H	-4.444064	1.882030	0.484581
C	0.460289	1.471786	-1.509632	C	1.033386	-2.004731	-0.509963	H	-3.130184	1.791659	-0.707248
C	-0.962822	3.544007	-0.261214	C	3.602878	-1.506387	0.488186	H	-4.515299	0.705434	-0.831245
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H	0.995282	0.653914	-1.975676	C	3.337896	-2.636088	-0.300739	H	-4.704114	0.025627	2.257636
C	-0.267576	3.779729	-1.449448	H	4.593756	-1.362988	0.907134	H	-4.948968	-1.105687	0.931398
H	-1.522143	4.345836	0.210658	H	1.855267	-3.836466	-1.327096	H	-3.713345	-1.440204	2.157721
H	0.957256	2.926440	-3.010907	H	4.143189	-3.334117	-0.502579	48			
H	-0.281299	4.770037	-1.891573	C	2.498247	1.959923	1.107858	ox7-a-tBu-1			Eopt
C	0.847866	-0.970873	0.036863	H	2.382226	2.699610	1.907956	-1003.539358			
C	0.259134	-2.153675	-0.410267	H	3.424385	2.224043	0.585907	O	-0.282419	-0.033025	0.356530
C	2.191087	-0.724227	0.240171	C	2.688402	0.578669	1.750901	C	-0.429244	1.217854	-0.429570
C	1.102833	-3.207460	-0.760688	H	1.932691	0.425646	2.530952	C	-1.198861	2.189298	0.196198
C	3.006111	-1.811228	-0.139886	H	3.659372	0.562980	2.251661	C	0.135847	1.312846	-1.685402
C	2.481444	-3.009523	-0.634170	H	-3.444083	-3.399477	-1.241229	C	-1.363333	3.380939	-0.521094
H	0.701409	-4.153292	-1.106246	C	-2.698586	0.637839	1.081947	C	-0.054747	2.516527	-2.371561
H	4.080193	-1.715289	-0.024060	H	-1.829781	1.284886	1.240616	H	0.707052	0.500054	-2.115472
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C	-2.730652	-0.260072	0.535187	H	-3.410150	1.794106	-0.639075	H	-1.948515	4.180864	-0.078255
C	-1.192713	-2.021177	-0.316425	H	-4.682054	0.880932	0.189141	H	0.376256	2.639493	-3.358897
C	-3.774442	-1.172793	0.273404	H	-4.025732	2.344228	0.926009	H	-0.931752	4.481258	-2.318570
C	-2.254366	-2.893806	-0.552016	C	-3.201631	0.184462	2.466260	C	0.821212	-0.952375	-0.011391
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H	-2.082050	-3.892462	-0.936906	H	-2.434429	-0.378103	3.006585	C	1.060698	-3.148180	-0.954397
H	-4.391547	-3.101384	-0.434255	45				C	2.964860	-1.737102	-0.408394
C	-1.788239	1.930510	1.549930	ox7-a-iPr-TS			Eopt	C	2.436349	-2.911397	-0.947145
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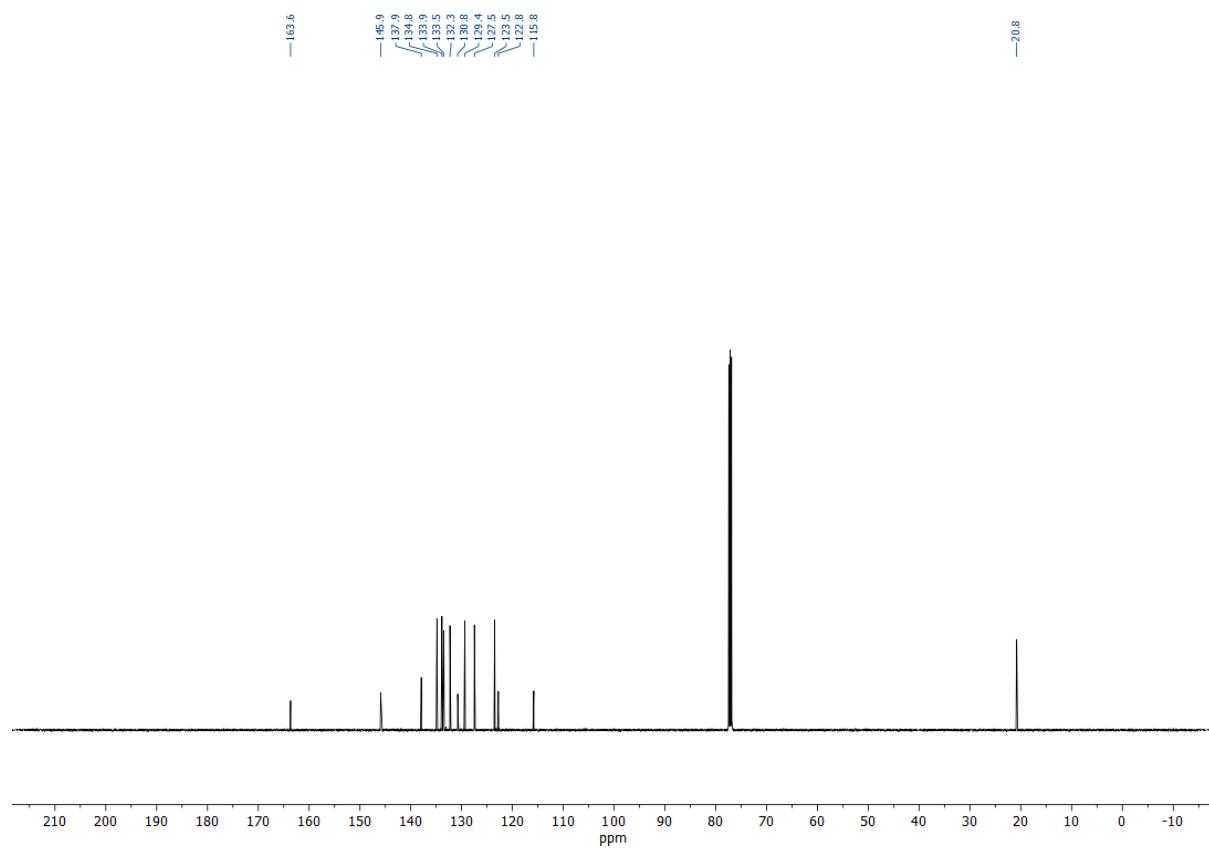
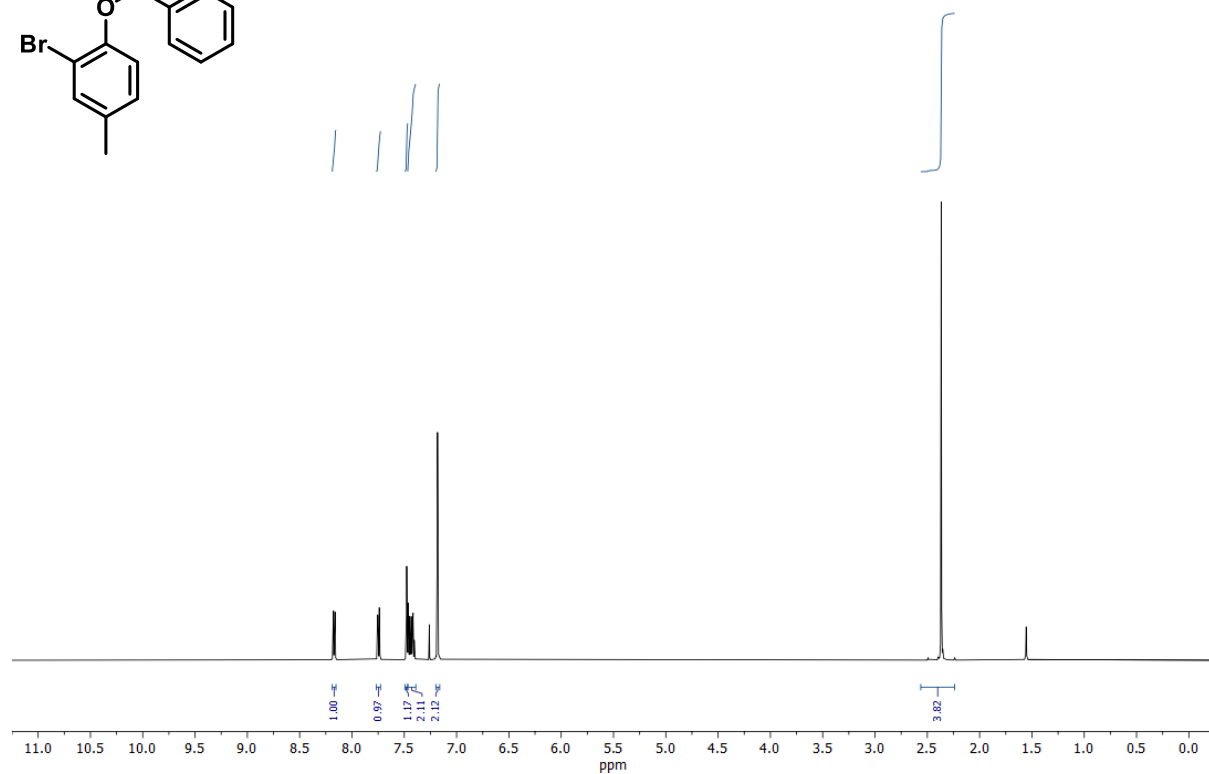
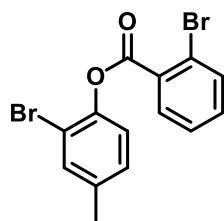
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C	-2.755986	-0.393101	0.718455	C	-1.163299	-2.951375	-1.241421	H	2.248816	3.868975	-1.634329
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C	-3.774642	-1.349306	0.520334	C	-2.534690	-2.688541	-1.162019	H	0.261252	5.226500	-1.084414
C	-2.243778	-2.989971	-0.437229	H	-0.786631	-3.849354	-1.717795	C	-0.754732	-0.905330	-0.210432
C	-3.529625	-2.604168	-0.043701	H	-4.093599	-1.448425	-0.401310	C	-0.073981	-2.083208	-0.525509
H	-4.783465	-1.091580	0.828296	C	1.461264	-0.894594	0.279728	C	-2.155371	-0.795628	-0.216087
H	-2.057002	-3.972338	-0.855835	C	2.630405	-0.583989	0.929410	C	-0.726901	-3.125051	-1.180636
H	-4.355314	-3.296484	-0.167226	C	1.148930	-2.031651	-0.443682	C	-2.744267	-1.837745	-0.974191
C	-1.871692	1.908427	1.514238	C	3.655006	-1.519081	0.701657	C	-2.071290	-2.948528	-1.476266
H	-2.232092	2.844869	1.945816	C	2.185412	-2.947925	-0.648024	H	-0.193070	-4.031761	-1.440443
H	-1.153218	1.484275	2.223699	C	3.436219	-2.658997	-0.087675	H	-3.815258	-1.796355	-1.112196
C	-3.067388	0.951271	1.342185	H	4.621244	-1.367484	1.172090	C	1.585456	-0.769377	0.410702
H	-3.831114	1.440593	0.726532	H	2.022640	-3.867657	-1.198390	C	2.864837	-0.363598	0.775591
H	-3.526037	0.775531	2.321612	H	4.252387	-3.358357	-0.233522	C	1.282685	-2.047015	-0.031087
H	3.114629	-3.665445	-1.331668	C	2.502574	1.959919	1.150624	C	3.793247	-1.412227	0.894697
C	2.859405	0.502179	0.827704	H	2.258914	2.713291	1.908512	C	2.236767	-3.063630	0.063392
C	3.358614	1.507294	-0.233634	H	3.474888	2.250461	0.739890	C	3.485999	-2.739854	0.582309
H	2.531273	1.953563	-0.789973	C	2.663675	0.600902	1.854989	H	4.806006	-1.153994	1.187089
H	3.908322	2.315820	0.258109	H	1.862270	0.470939	2.591773	H	2.001452	-4.072488	-0.255136
H	4.033839	1.025666	-0.947314	H	3.602199	0.610303	2.414085	H	4.245598	-3.505913	0.692386
C	1.926176	1.218327	1.824016	H	-3.240149	-3.379523	-1.610842	C	2.952890	1.490816	-0.789684
H	1.463169	0.513194	2.521573	C	-2.823230	0.515603	0.982923	H	3.621796	2.274725	-1.150247
H	2.513283	1.928151	2.412317	C	-1.810554	1.277444	1.859465	H	3.052745	0.644618	-1.475870
H	1.147336	1.794573	1.325700	H	-1.234297	0.599912	2.496812	C	3.353237	1.049856	0.644629
C	4.074656	-0.010285	1.638158	H	-1.122738	1.887629	1.272467	H	2.931350	1.739497	1.381714
H	3.781290	-0.787152	2.350674	H	-2.359090	1.959271	2.514441	H	4.438312	1.062191	0.766496
H	4.870486	-0.406135	1.003796	C	-3.526852	1.512747	0.035999	H	-2.621675	-3.702661	-2.027803
H	4.502077	0.823921	2.200929	H	-4.037249	2.280025	0.626009	C	-3.115652	0.116128	0.577366
48				H	-2.810948	2.015057	-0.620110	C	-2.547848	0.318716	2.014382
ox7-a-tBu-2			Eopt	H	-4.275434	1.015502	-0.587519	H	-3.015217	1.185111	2.492524
-1003.528463				C	-3.870535	-0.109676	1.936726	H	-2.792685	-0.558419	2.619681
O	0.282742	-0.028791	0.385018	H	-3.411679	-0.854742	2.593815	H	-1.465942	0.428807	2.080488
C	0.510079	1.230626	-0.416420	H	-4.300893	0.677588	2.562020	C	-3.456395	1.399840	-0.226950
C	1.513266	2.100885	0.002932	H	-4.695268	-0.586431	1.402913	H	-3.928693	2.142828	0.424126
C	-0.277754	1.407349	-1.544070	48				H	-2.602718	1.857928	-0.718305
C	1.641194	3.259688	-0.788118	ox7-a-tBu-TS			Eopt	H	-4.172726	1.147141	-1.013494
C	-0.108133	2.568802	-2.294402	-1003.481295				C	-4.480041	-0.582587	0.824209
H	-1.009986	0.669458	-1.838066	O	0.368770	0.061212	0.329574	H	-4.359089	-1.571388	1.274854
C	0.847915	3.506255	-1.903338	C	0.454826	1.513899	-0.057680	H	-5.050593	0.037112	1.522599
H	2.405582	3.978259	-0.507363	C	1.557842	2.065108	-0.730108	H	-5.086700	-0.675764	-0.079140
H	-0.718517	2.727361	-3.176385	C	-0.594363	2.291708	0.393247				
H	0.988483	4.417334	-2.474529	C	1.418403	3.412954	-1.105028				
C	-0.848324	-0.890395	-0.051797	C	-0.677236	3.635696	0.030995				

7 NMR Spectra

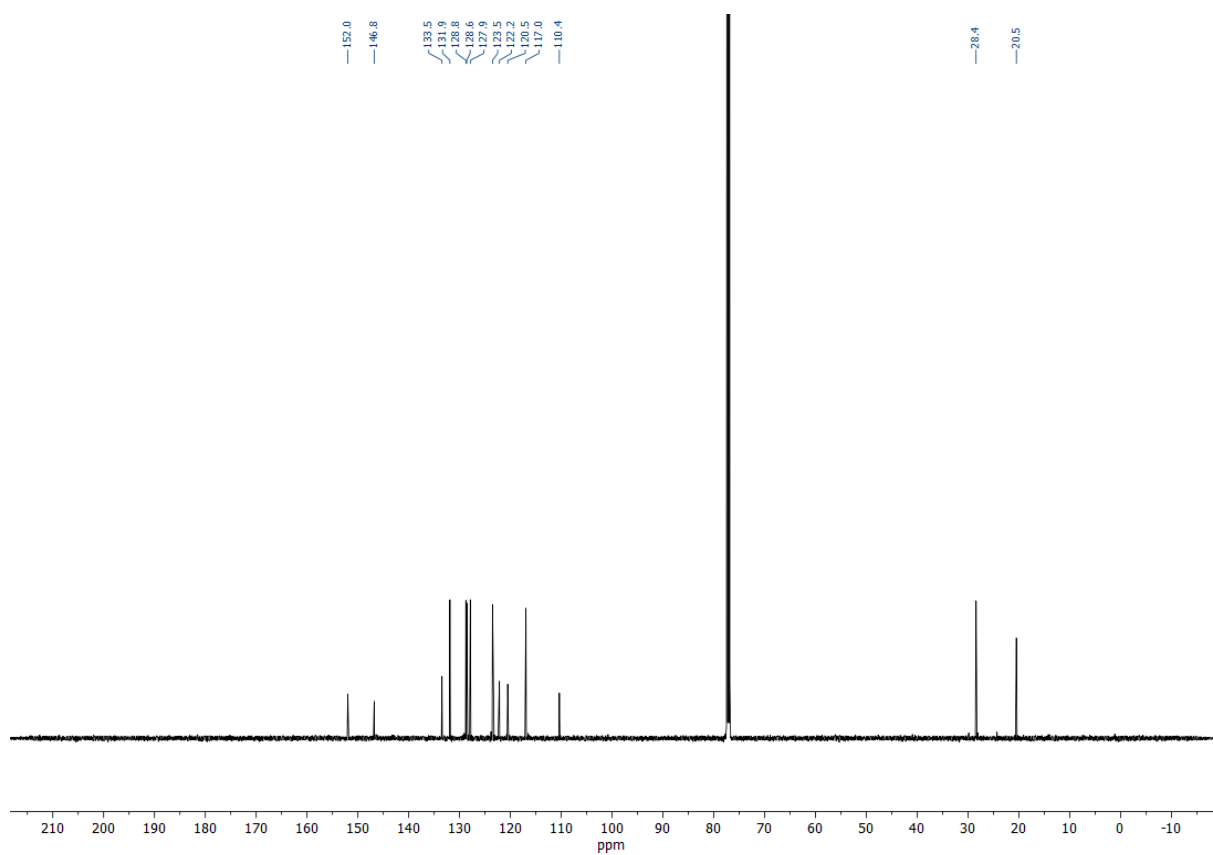
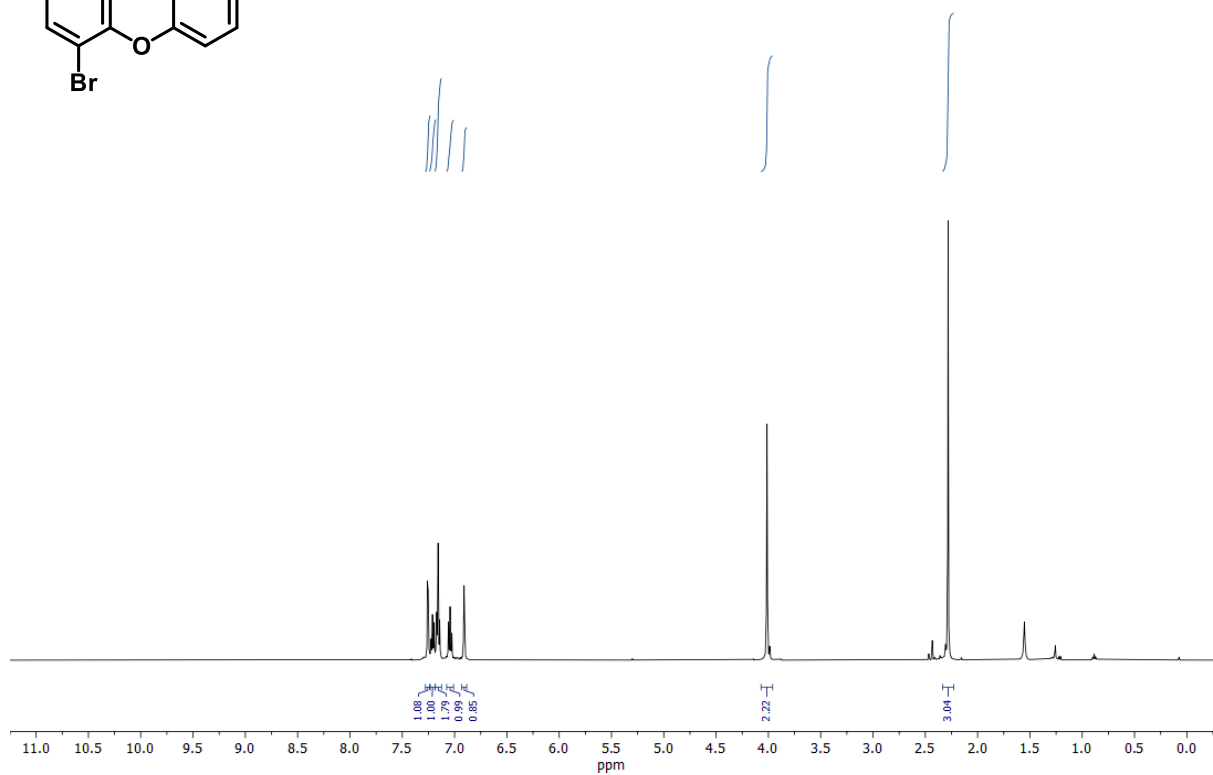
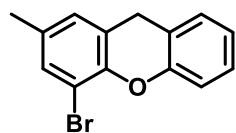
2-Bromo-4-methylphenol, S1:



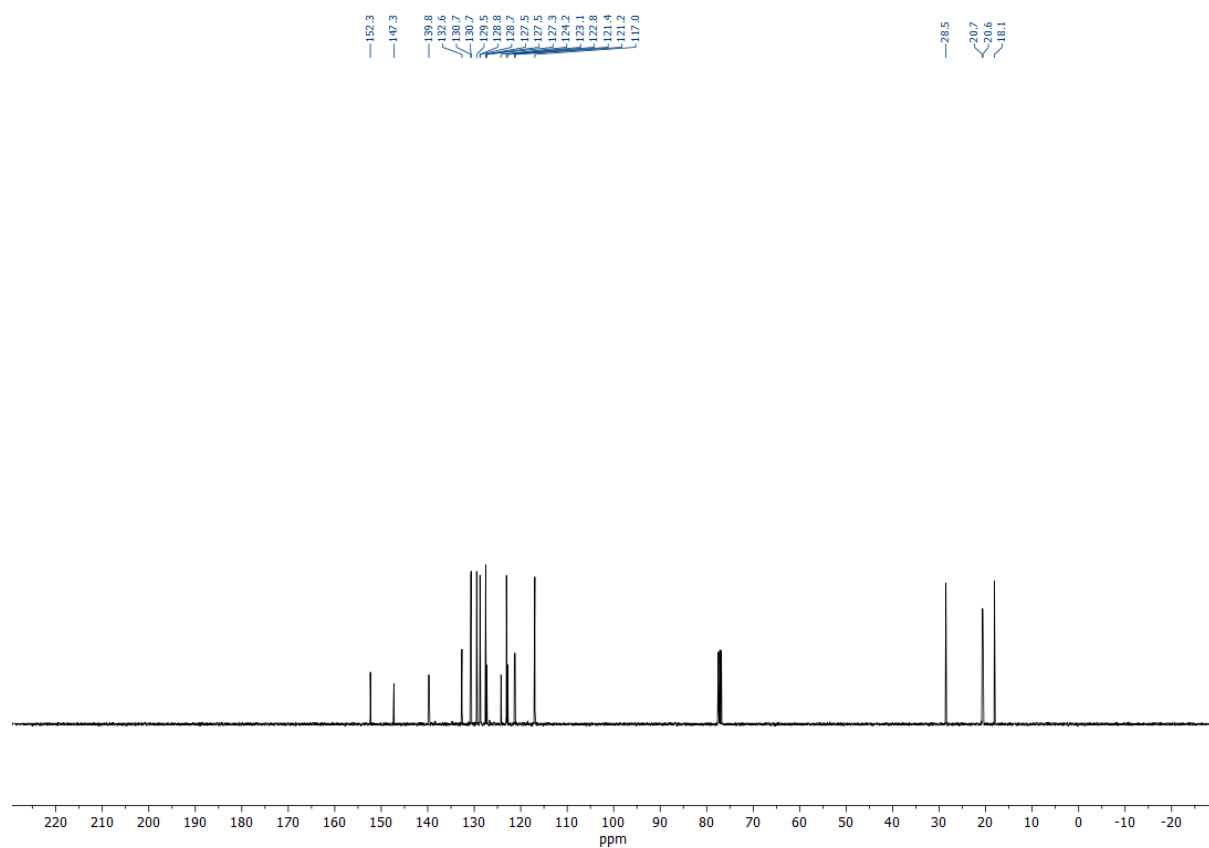
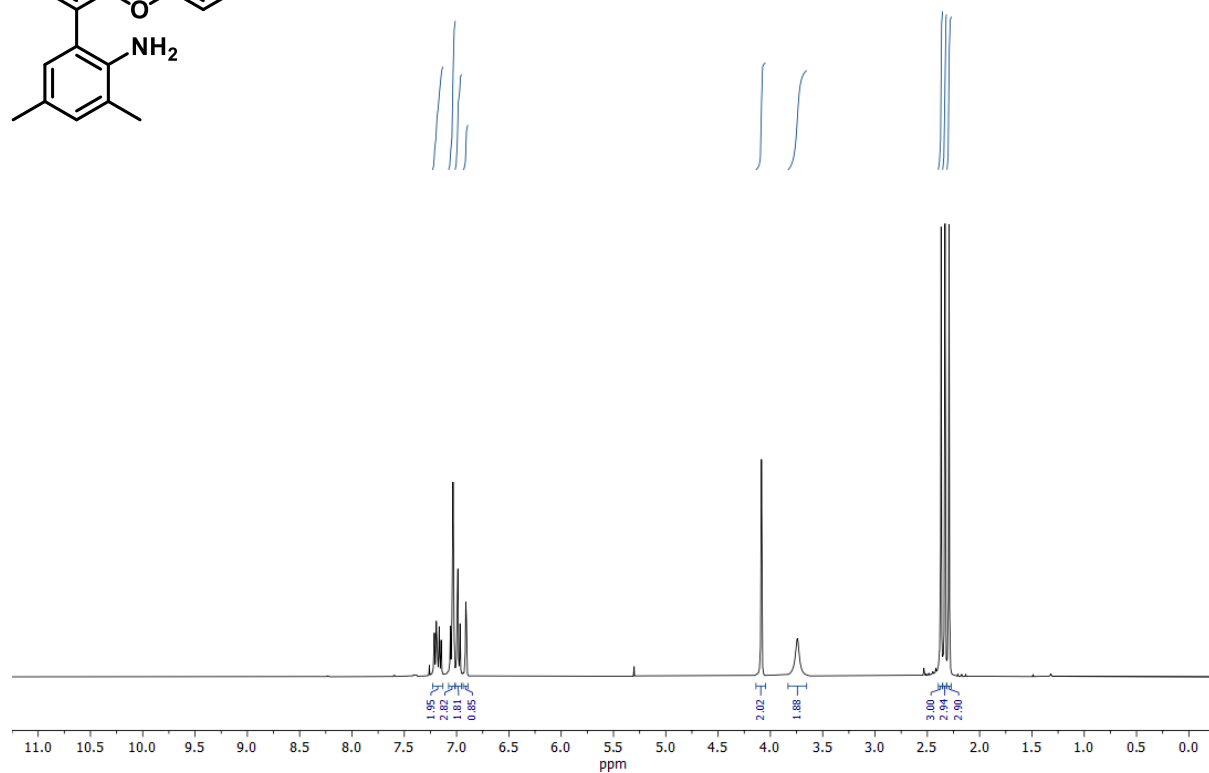
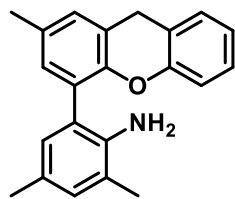
2-Bromo-4-methylphenyl 2-bromobenzoate, S2:



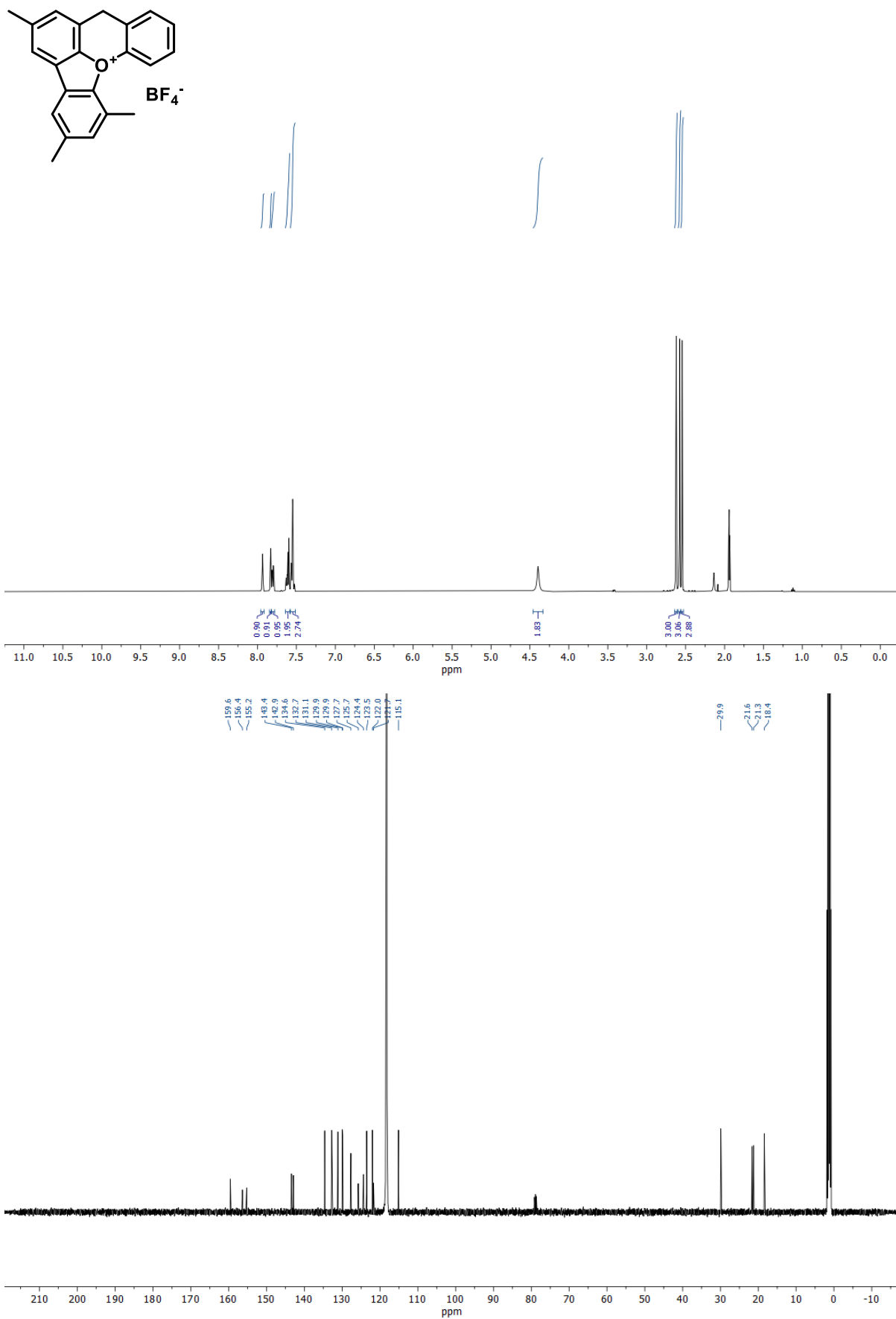
4-Bromo-2-methyl-9H-xanthene, S3:

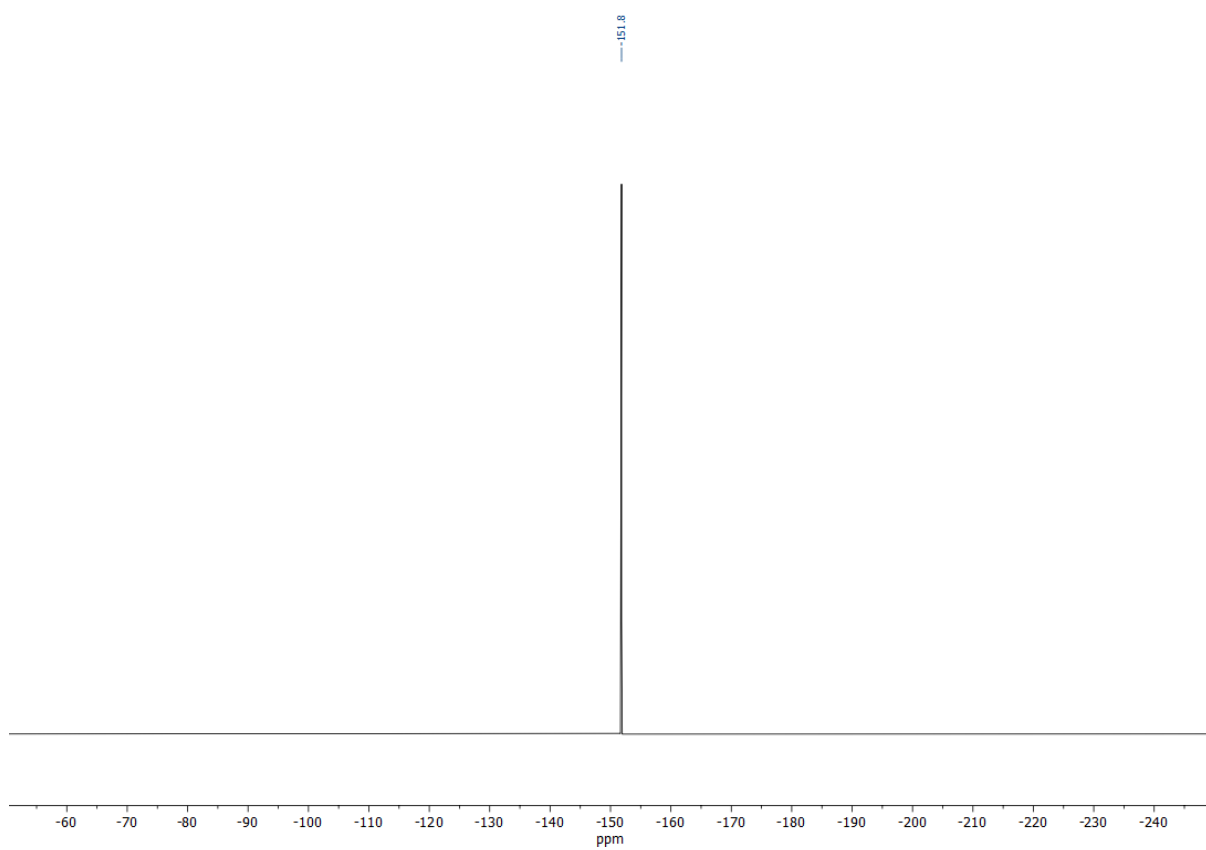


2,4-Dimethyl-6-(2-methyl-9H-xanthen-4-yl)aniline, 8:

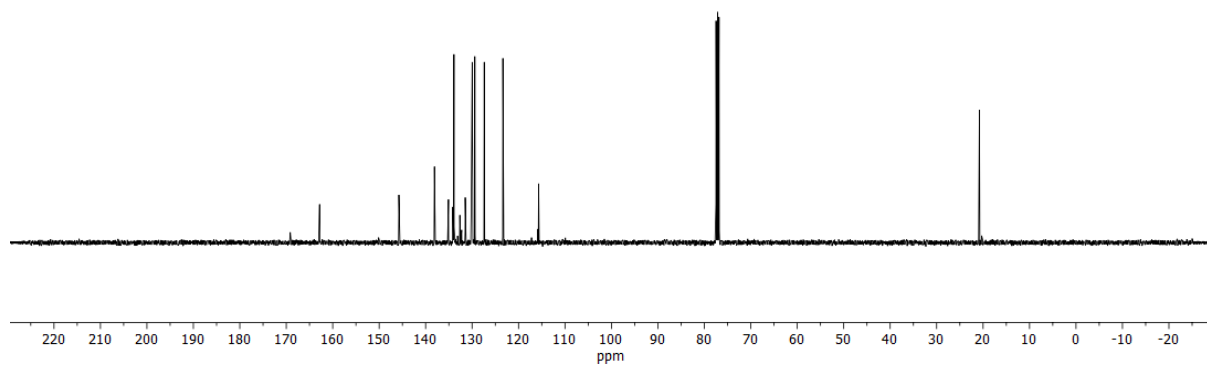
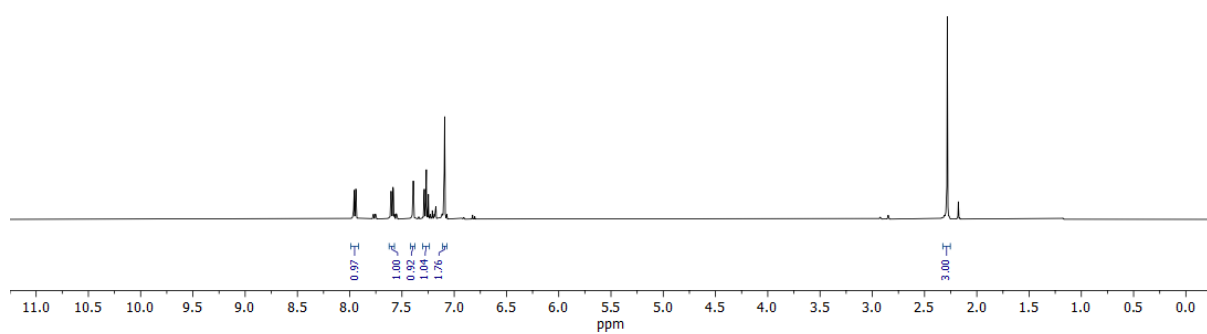
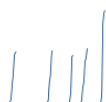
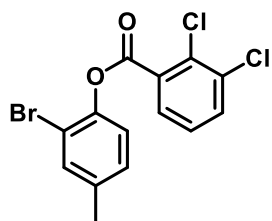


1,3,6-Trimethyl-8*H*-benzofuro[3,2,1-*de*]xanthen-13-ium tetrafluoroborate, 10:

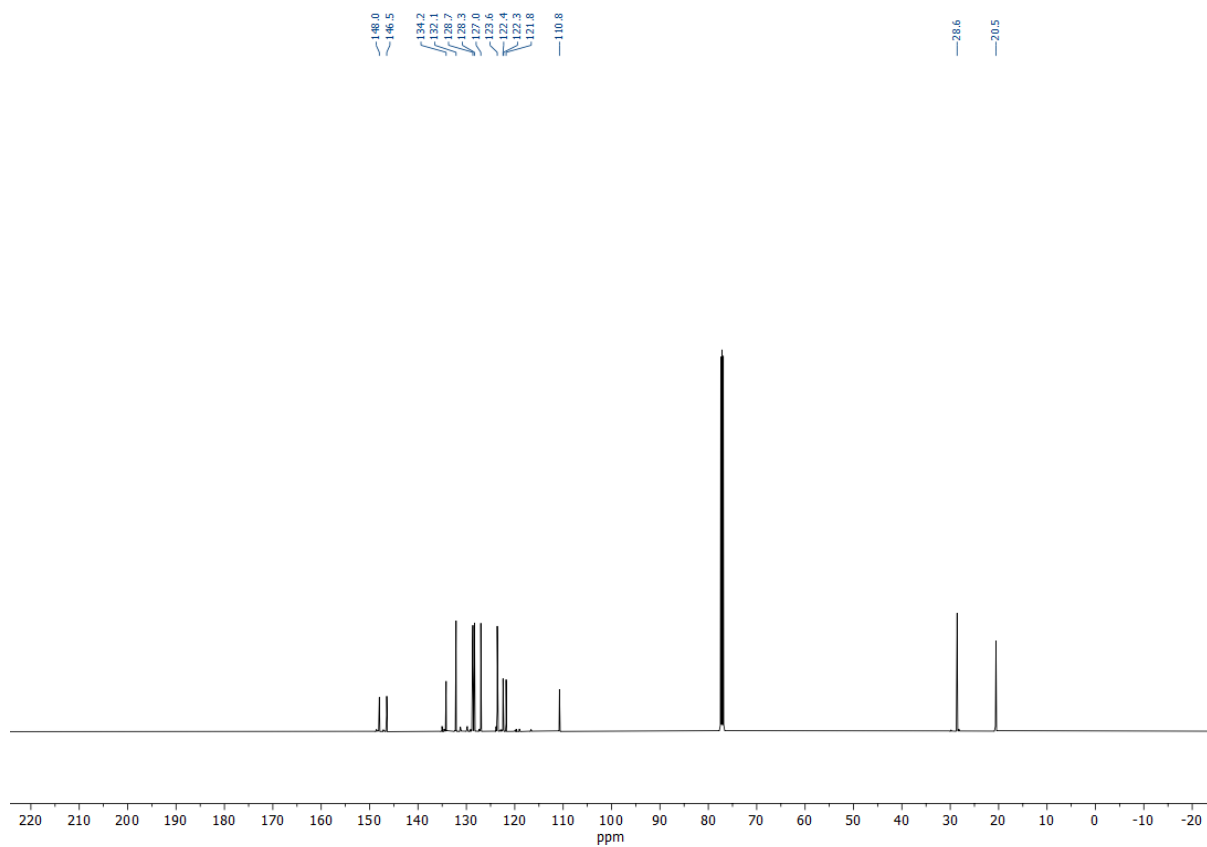
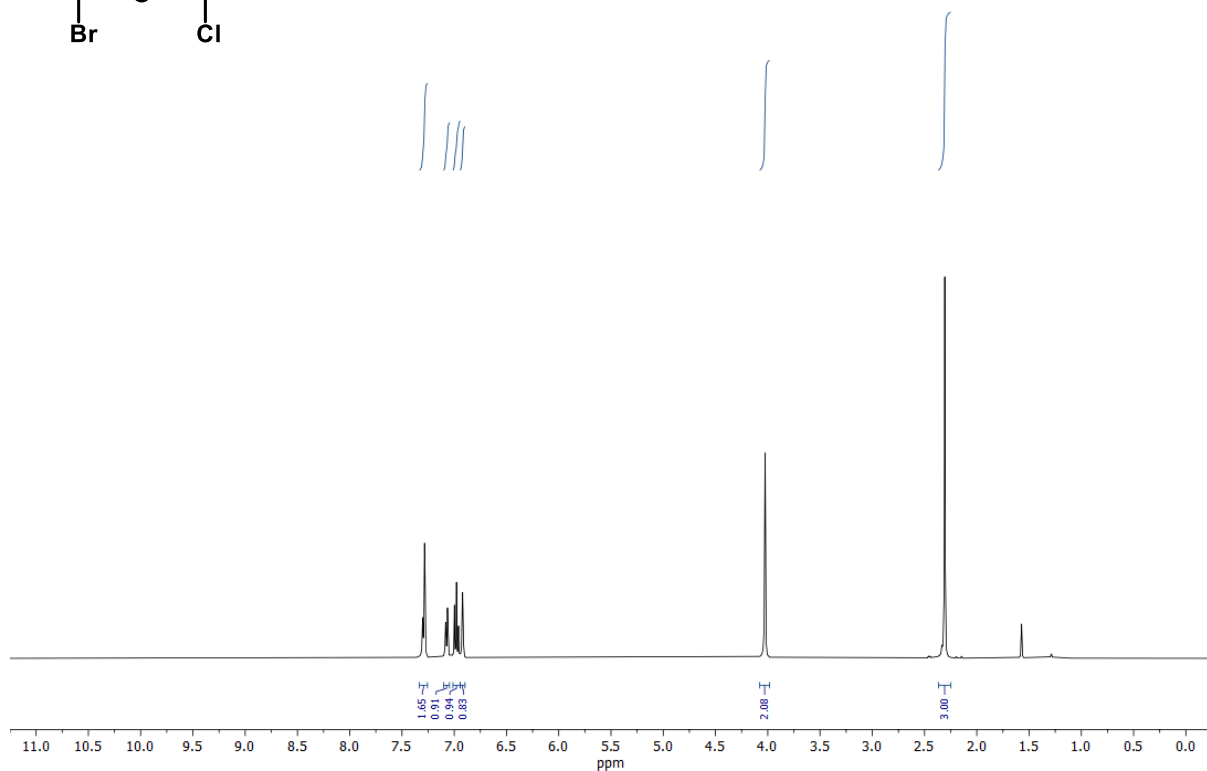
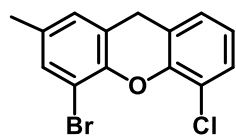




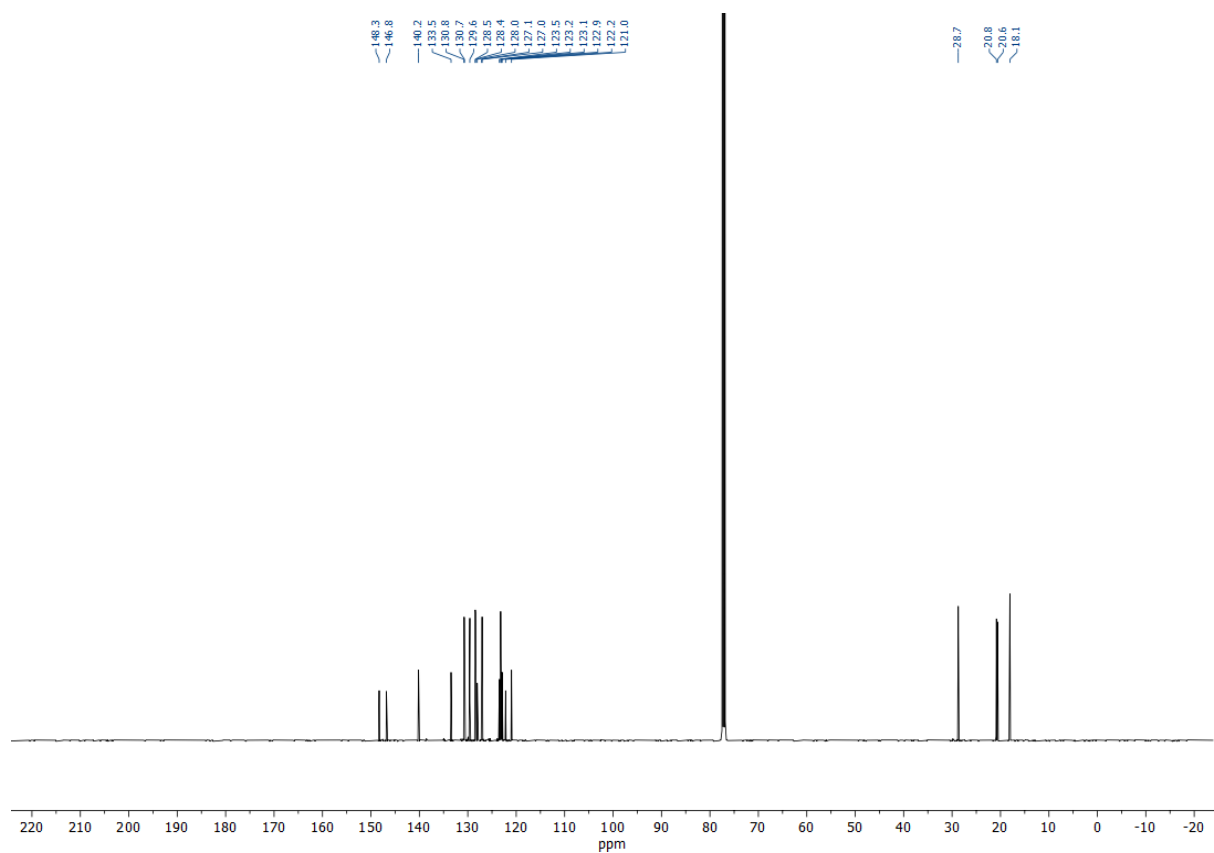
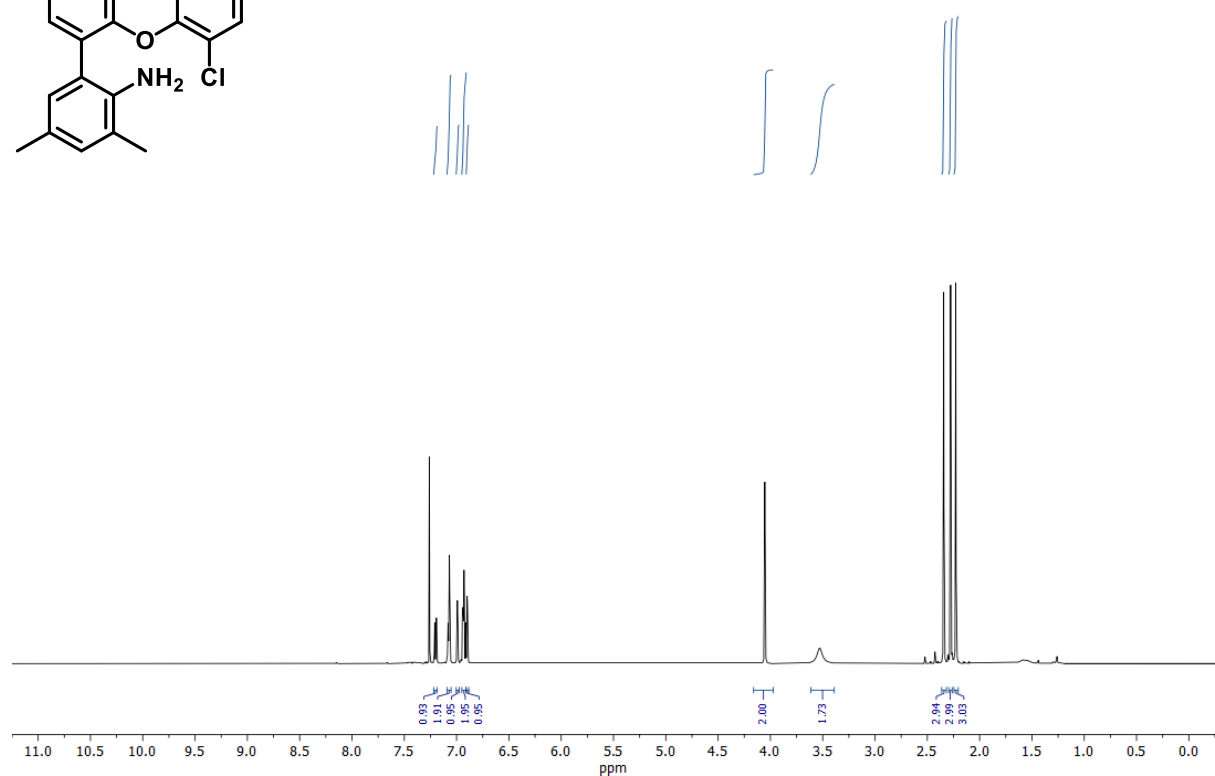
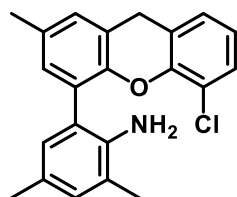
2-Bromo-4-methylphenyl 2,3-dichlorobenzoate, S4:



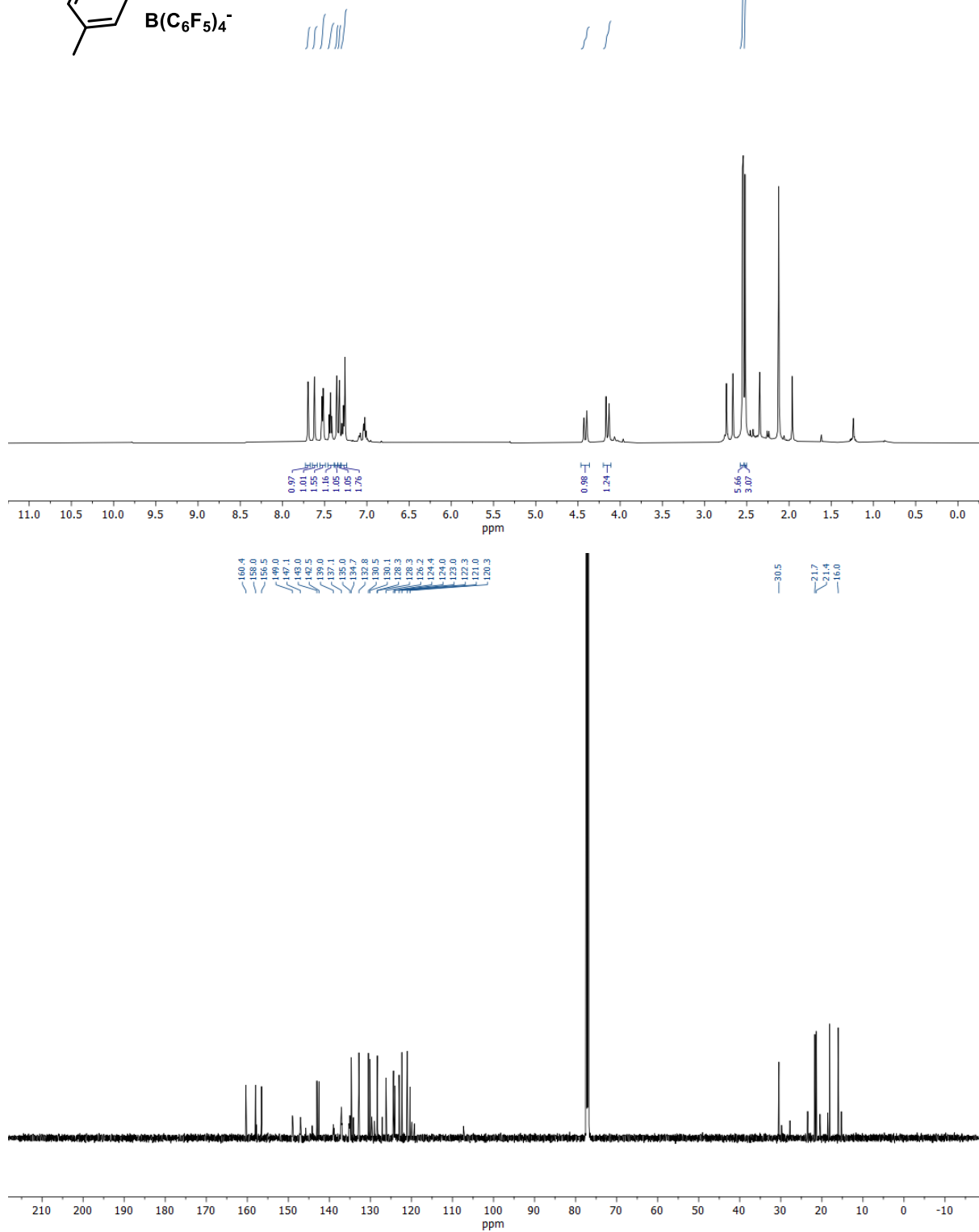
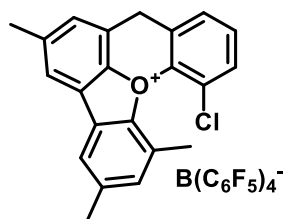
4-Bromo-5-chloro-2-methyl-9H-xanthene, S5:



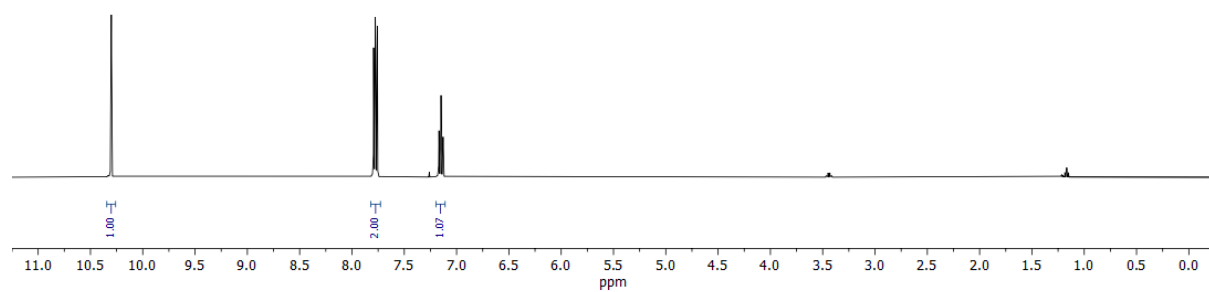
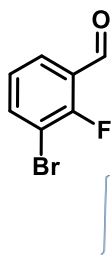
2-(5-Chloro-2-methyl-9H-xanthen-4-yl)-4,6-dimethylaniline, 9:



**12-Chloro-1,3,6-trimethyl-8*H*-benzofuro[3,2,1-*de*]xanthen-13-ium
tetrakis(perfluorophenyl)borate, 12:**



3-bromo-2-fluorobenzaldehyde, S6:



186.3
186.2

162.3
159.7

139.5

127.8

125.7

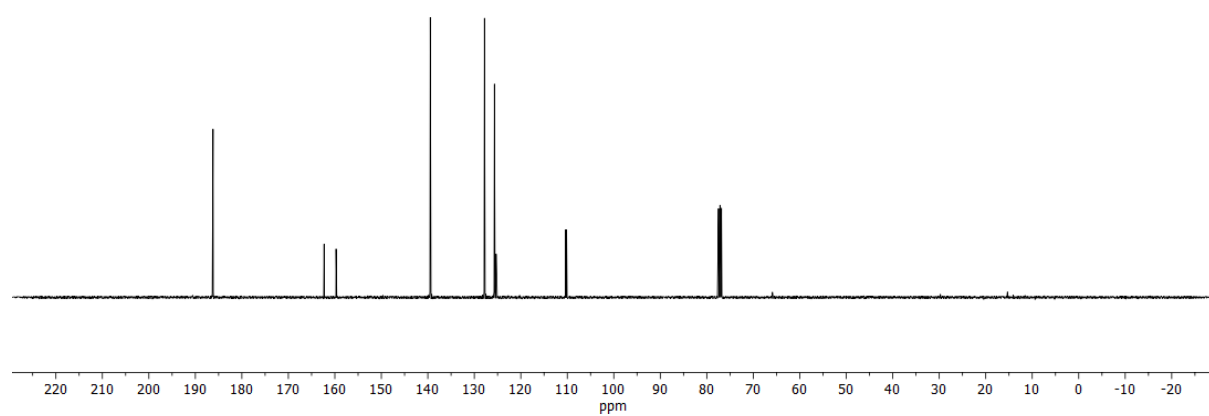
125.6

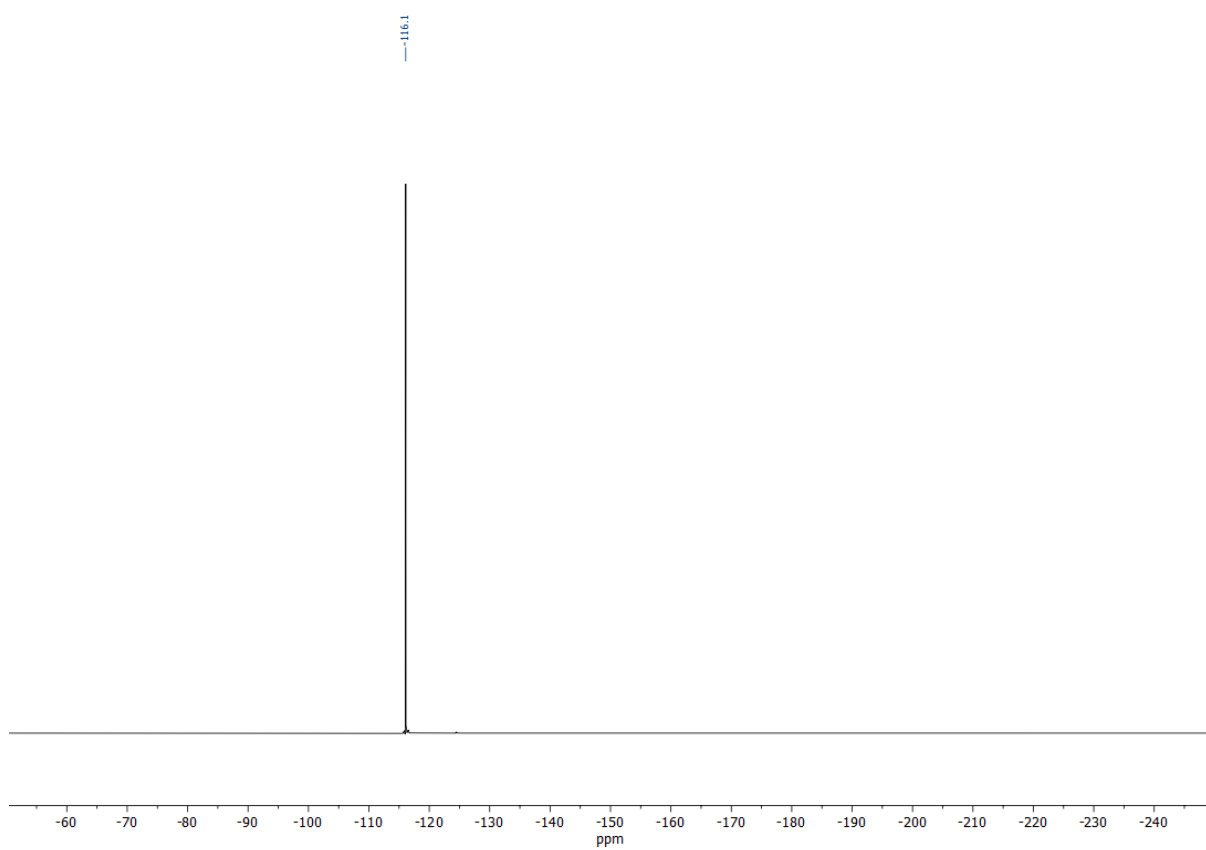
125.4

125.3

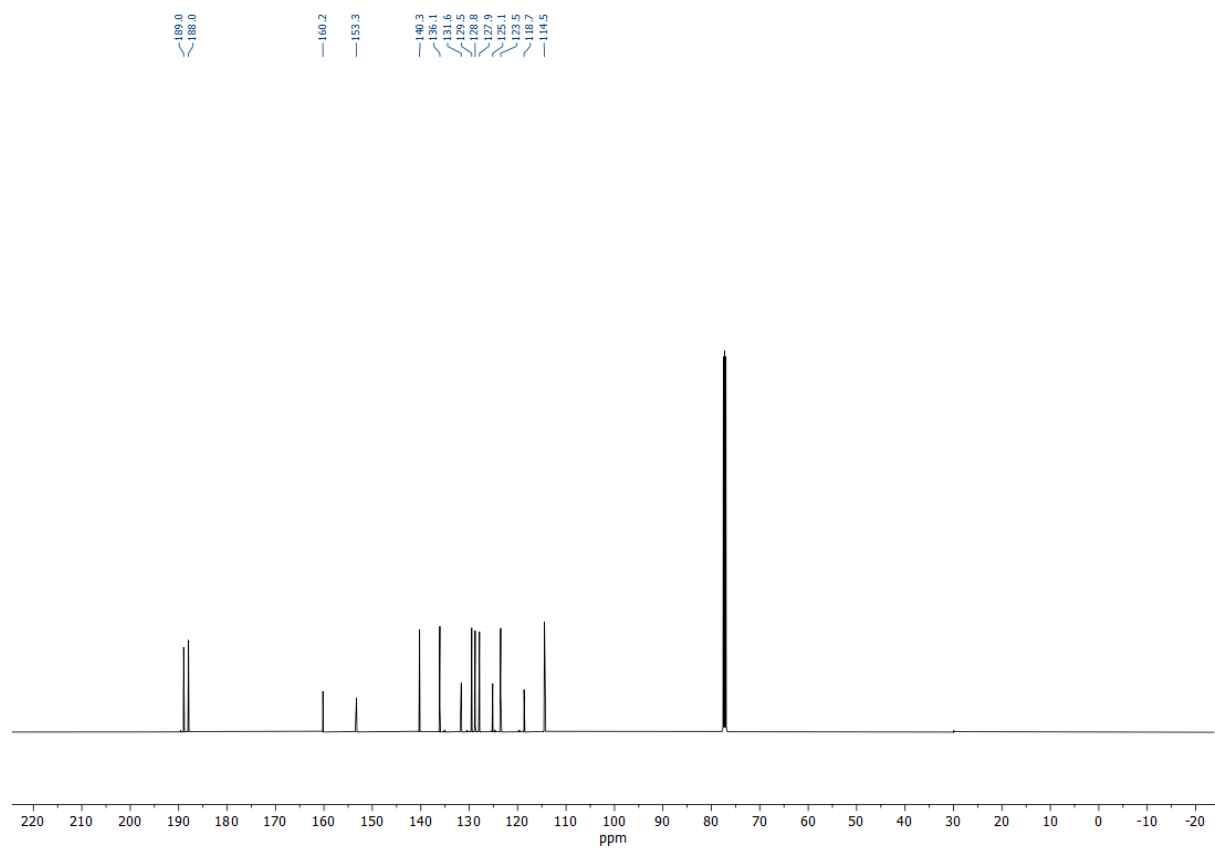
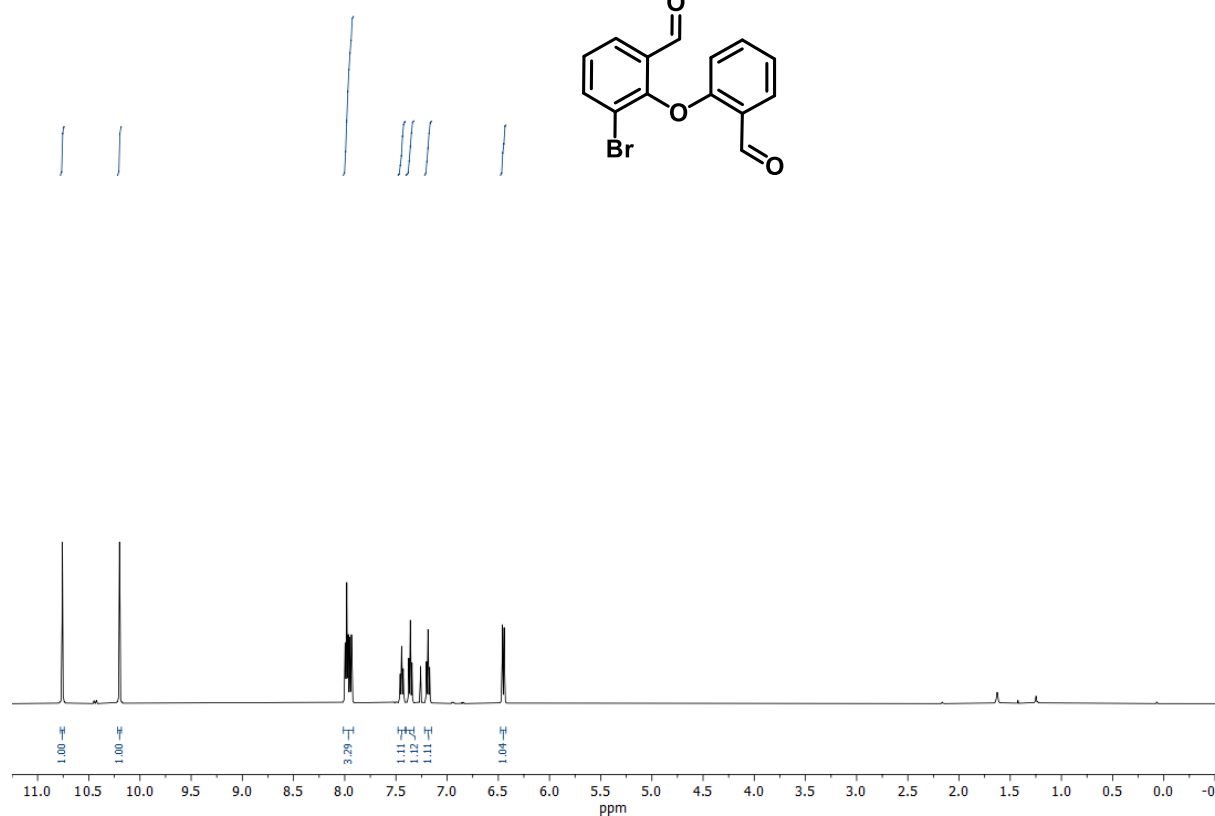
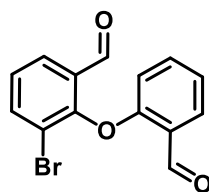
110.4

110.2

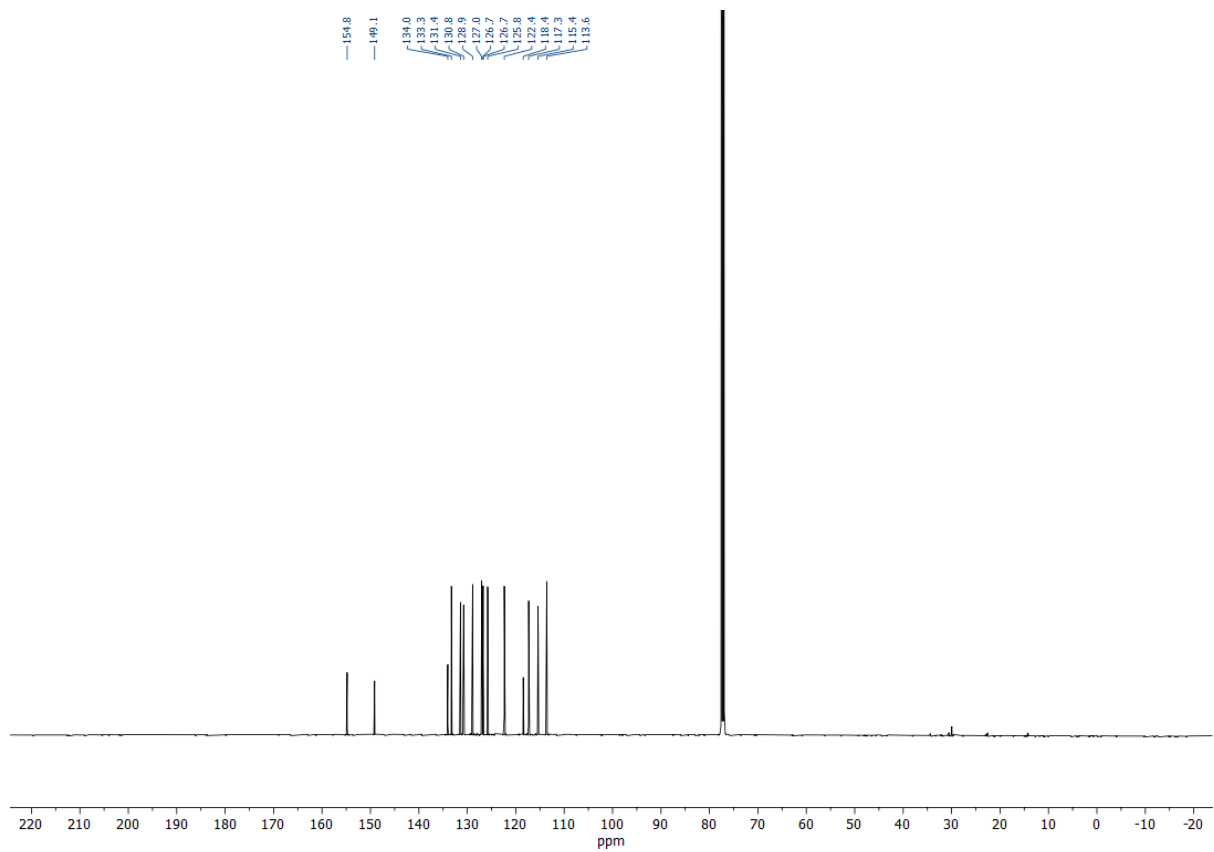
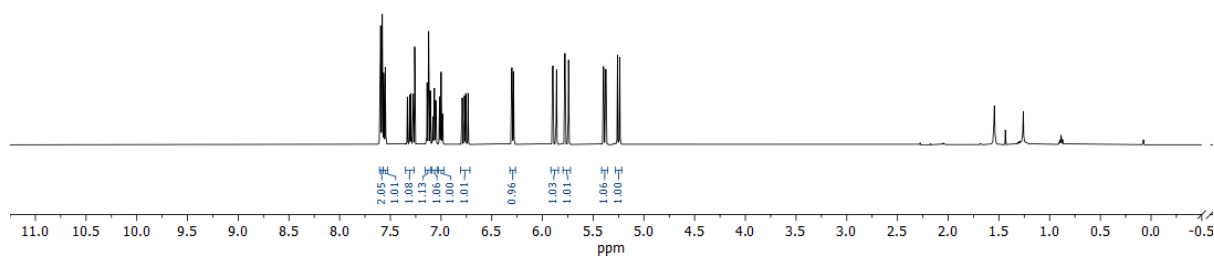
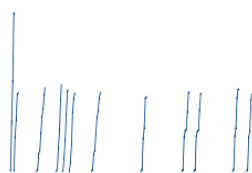
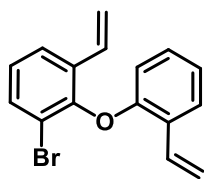




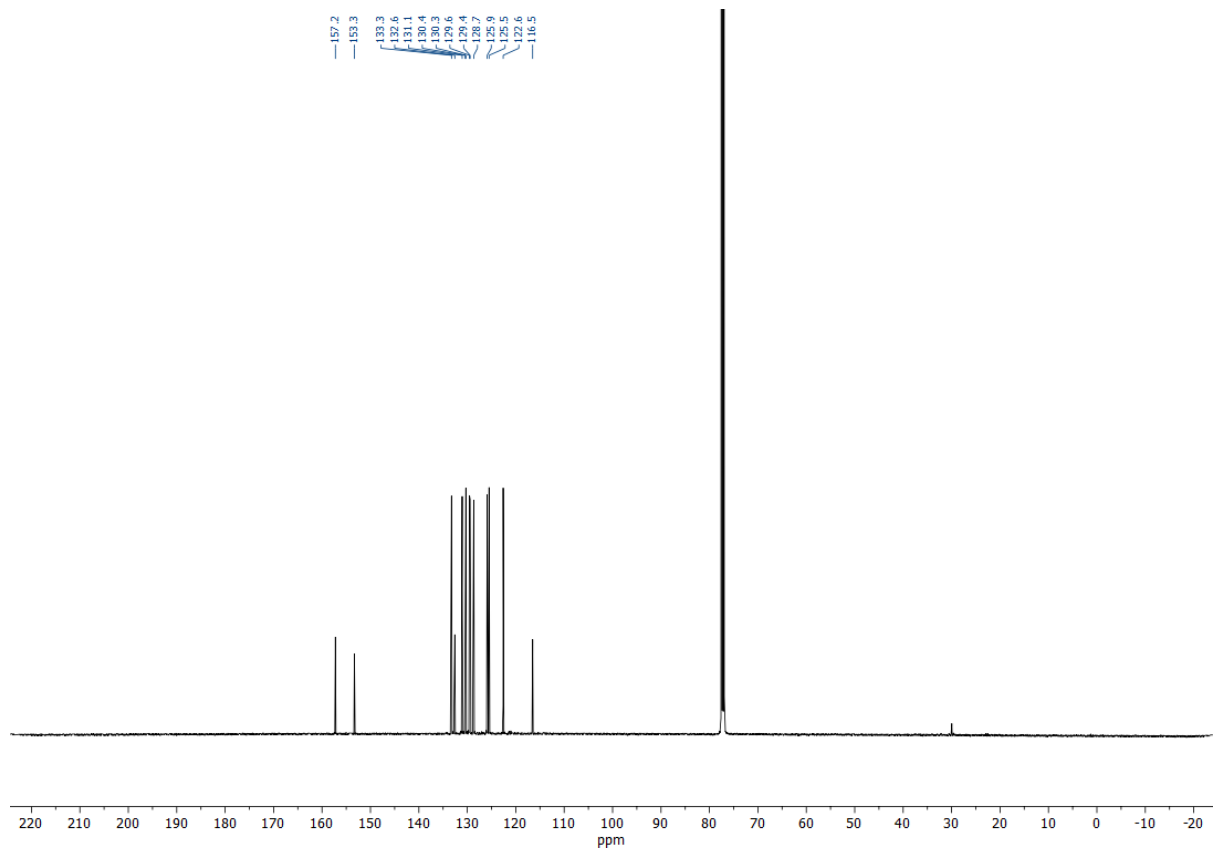
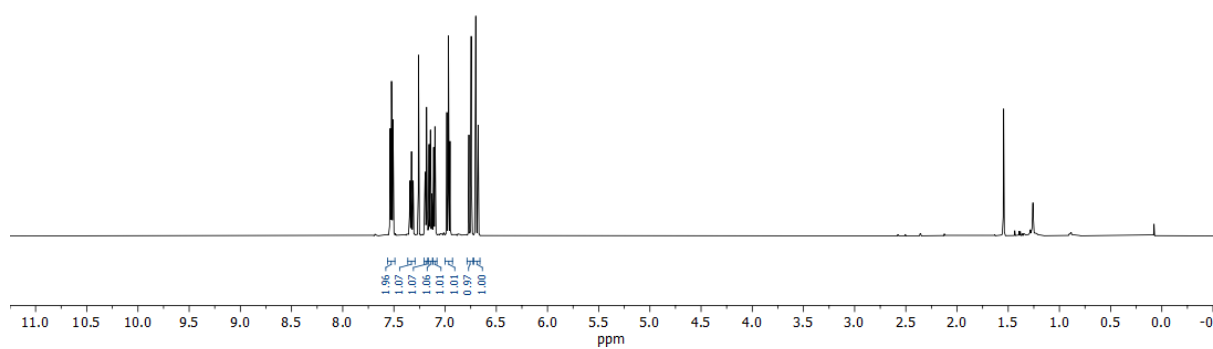
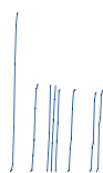
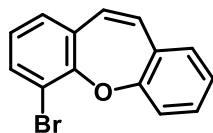
3-Bromo-2-(2-formylphenoxy)benzaldehyde, S7:



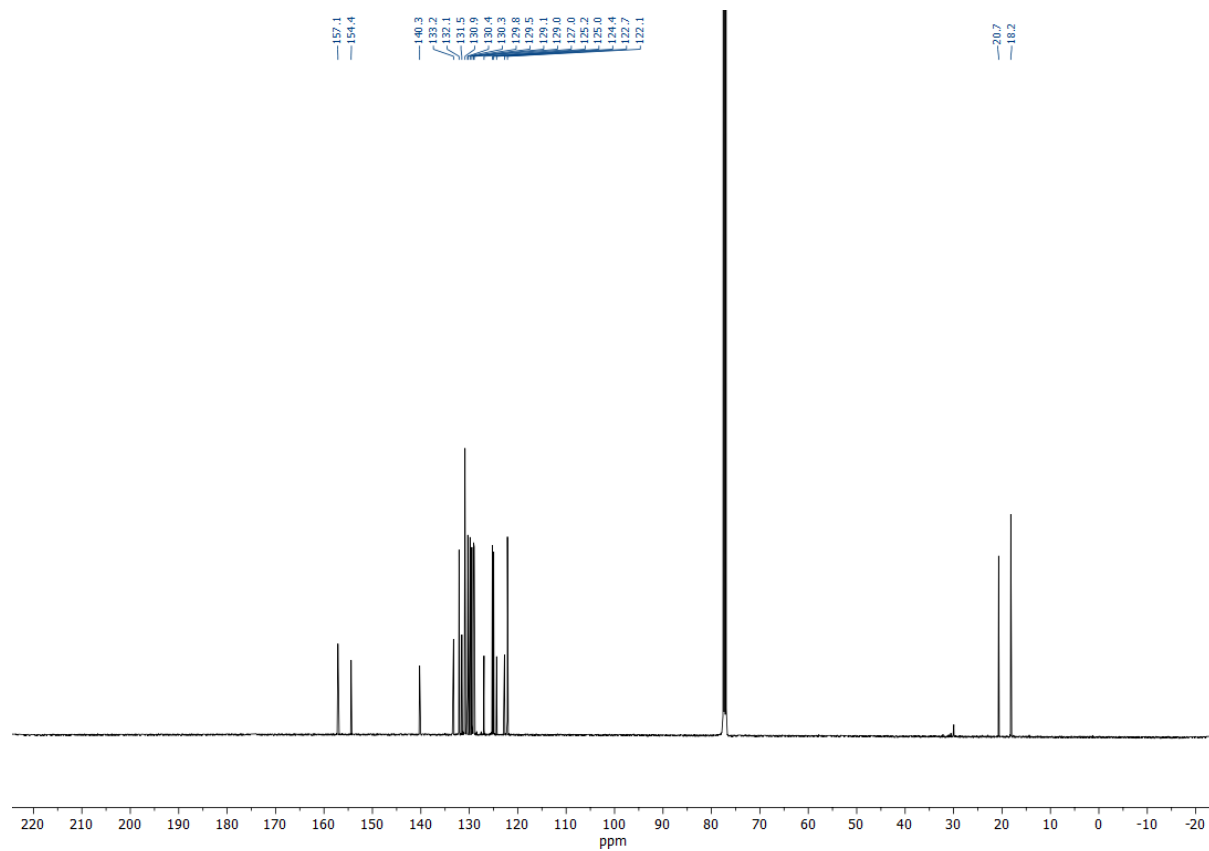
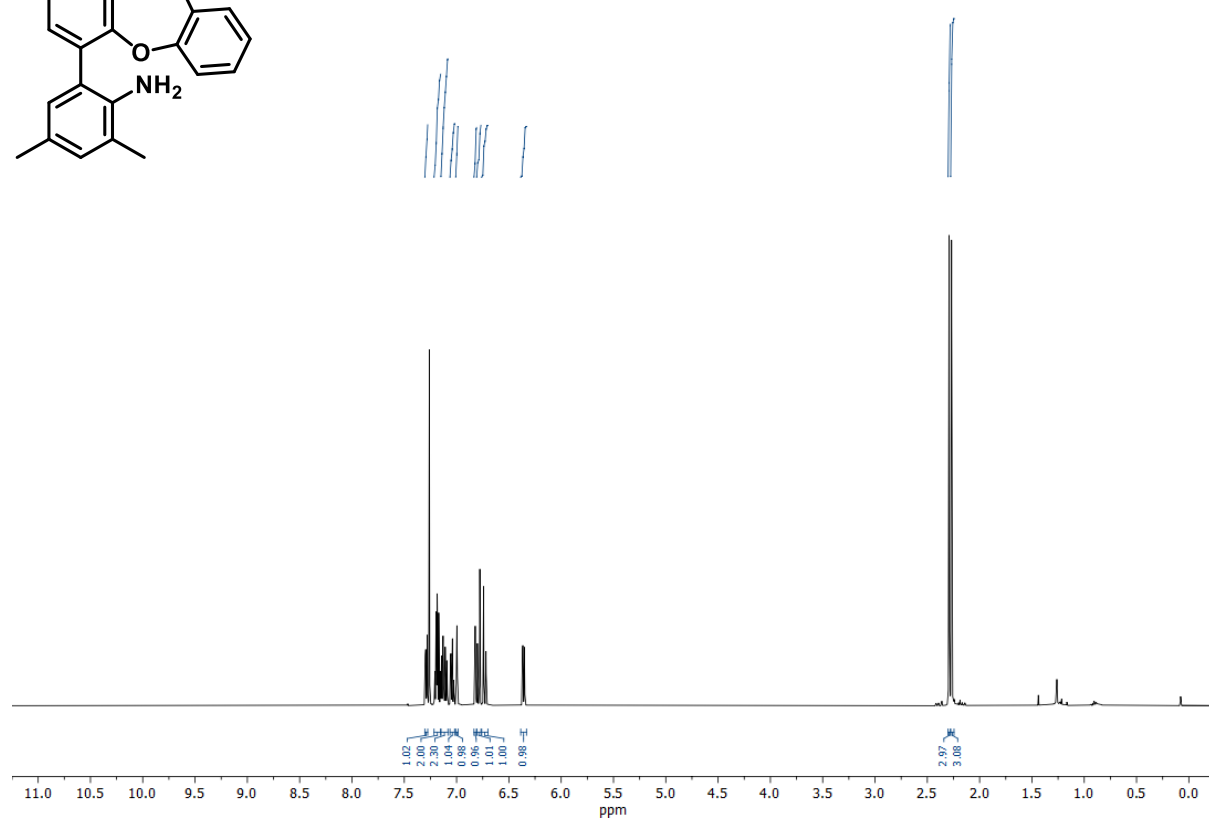
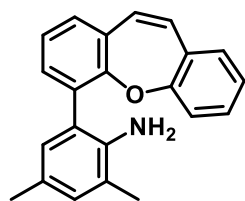
1-Bromo-3-vinyl-2-(2-vinylphenoxy)benzene, S8:



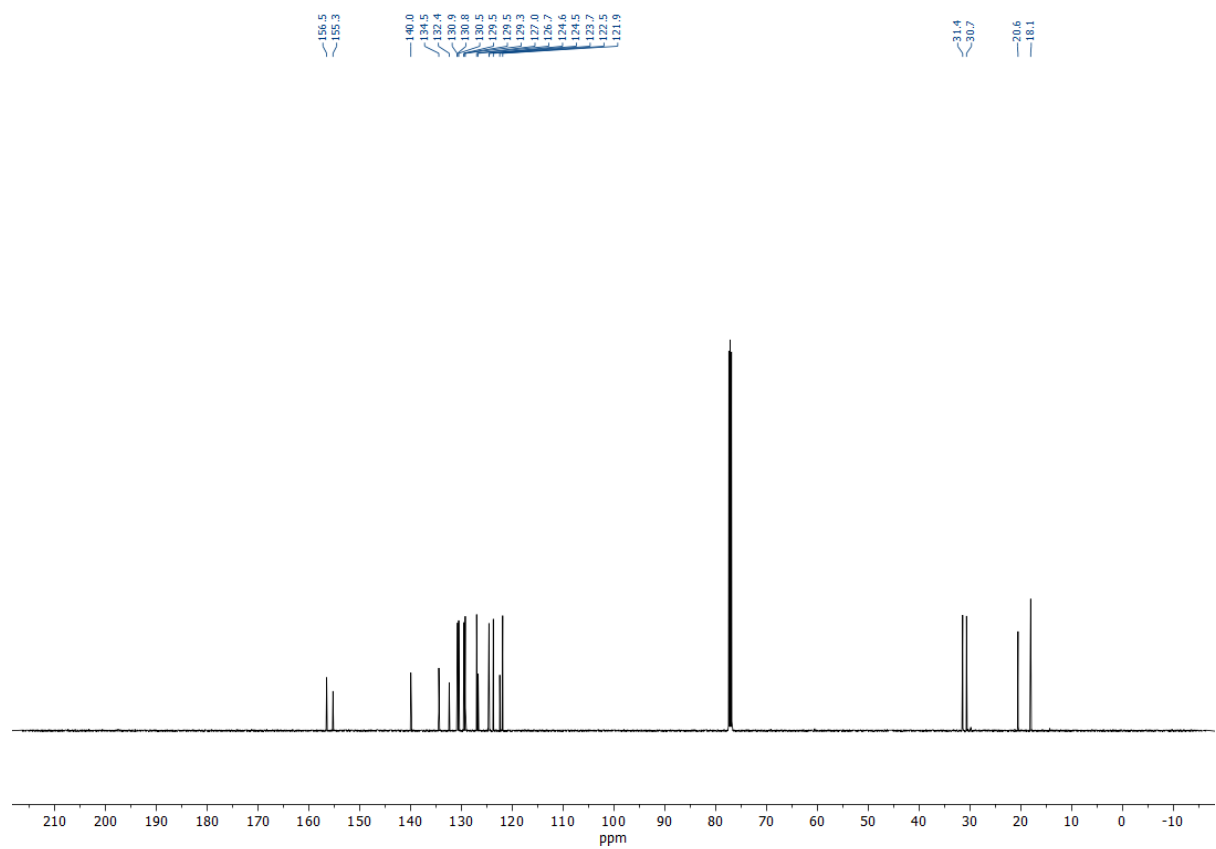
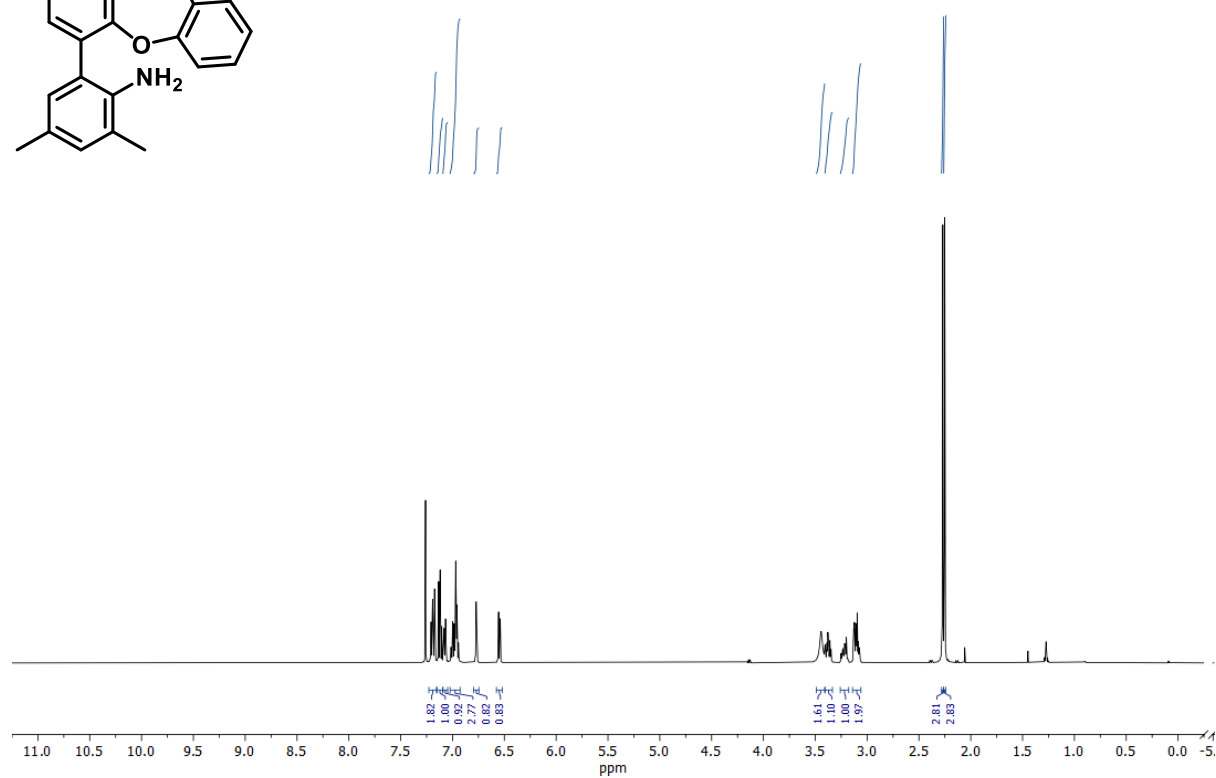
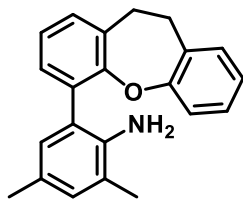
4-Bromodibenzo[*b,f*]oxepine, 13:



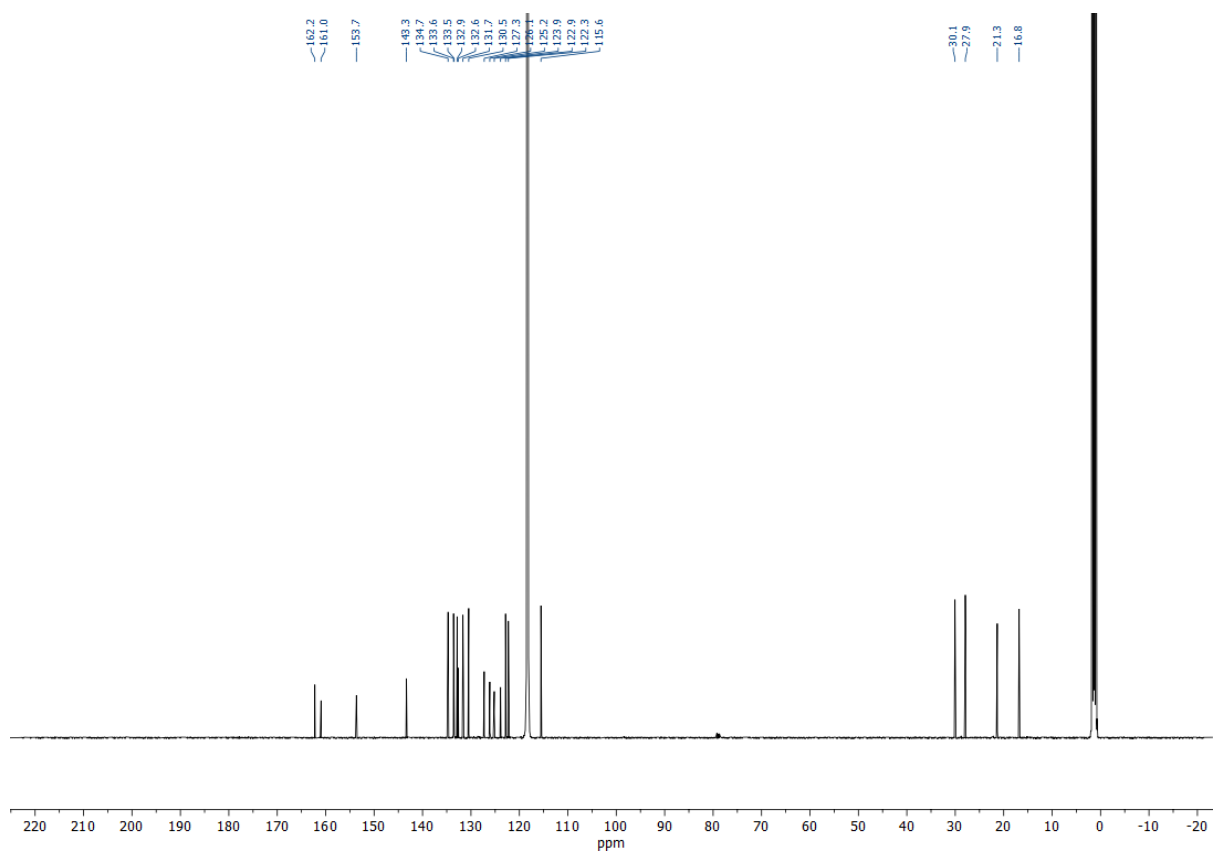
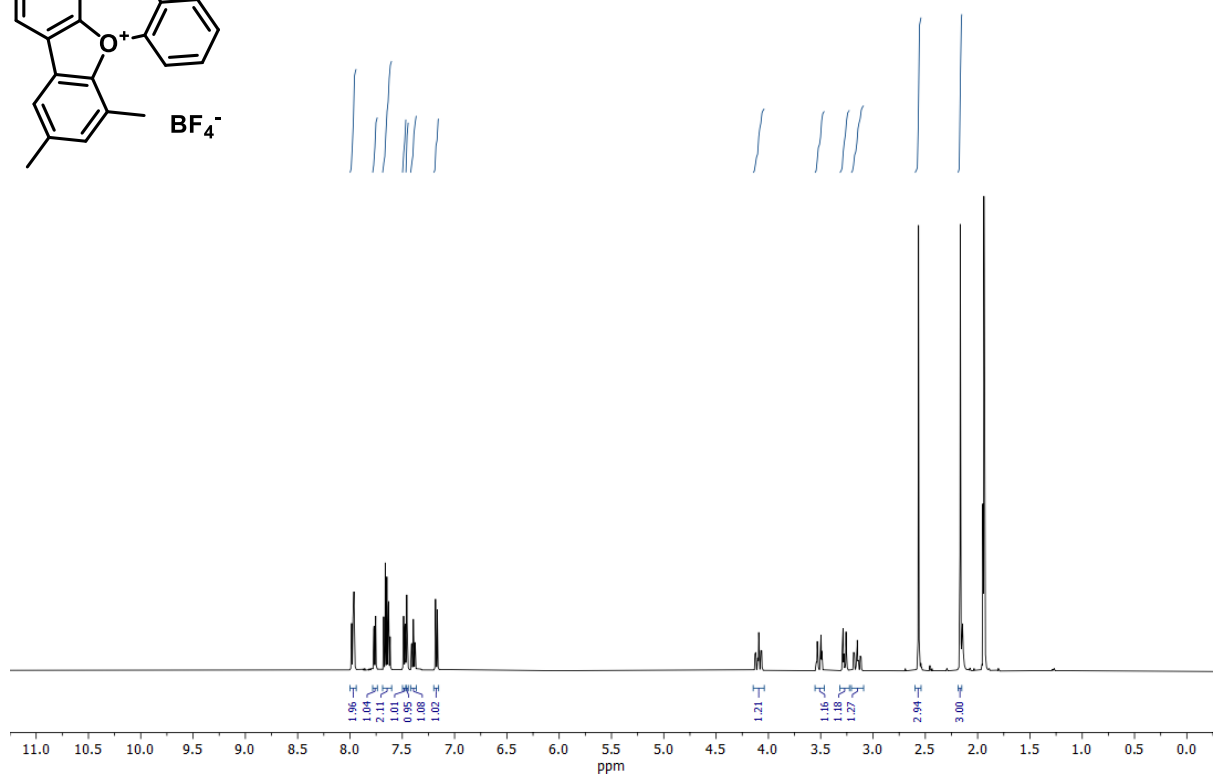
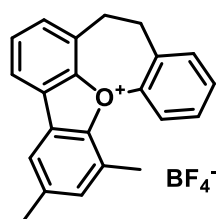
2-(Dibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, S9:

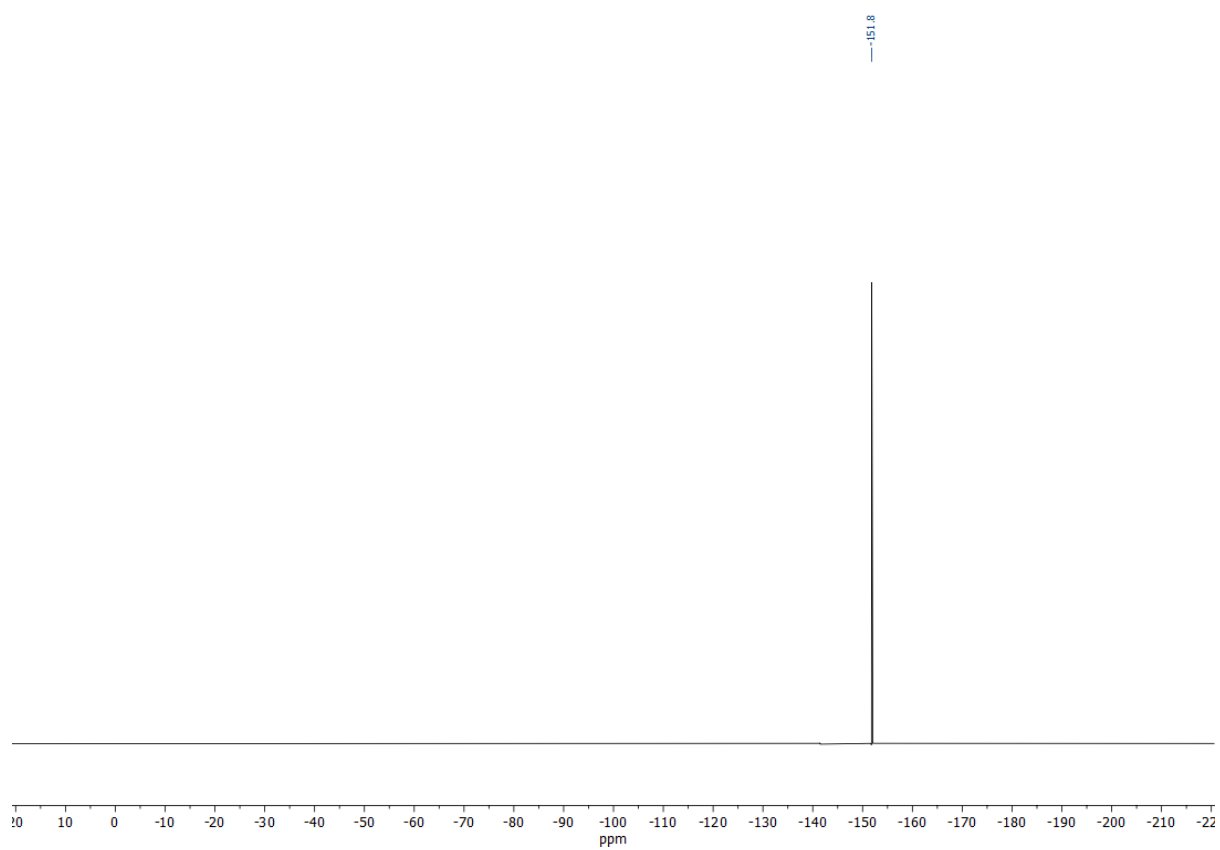


2-(10,11-Dihydrodibenzo[*b,f*]oxepin-4-yl)-4,6-dimethylaniline, 15:

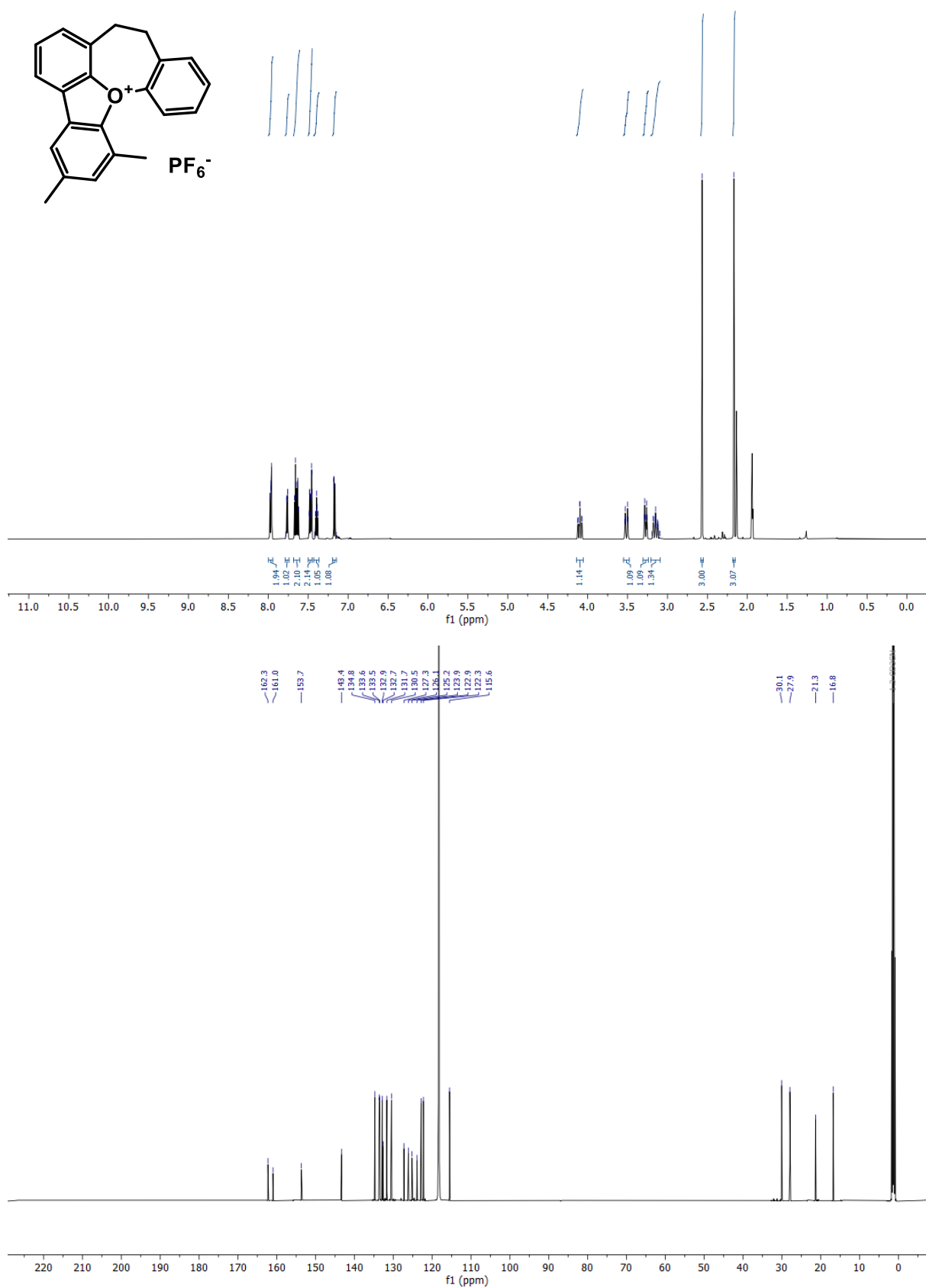


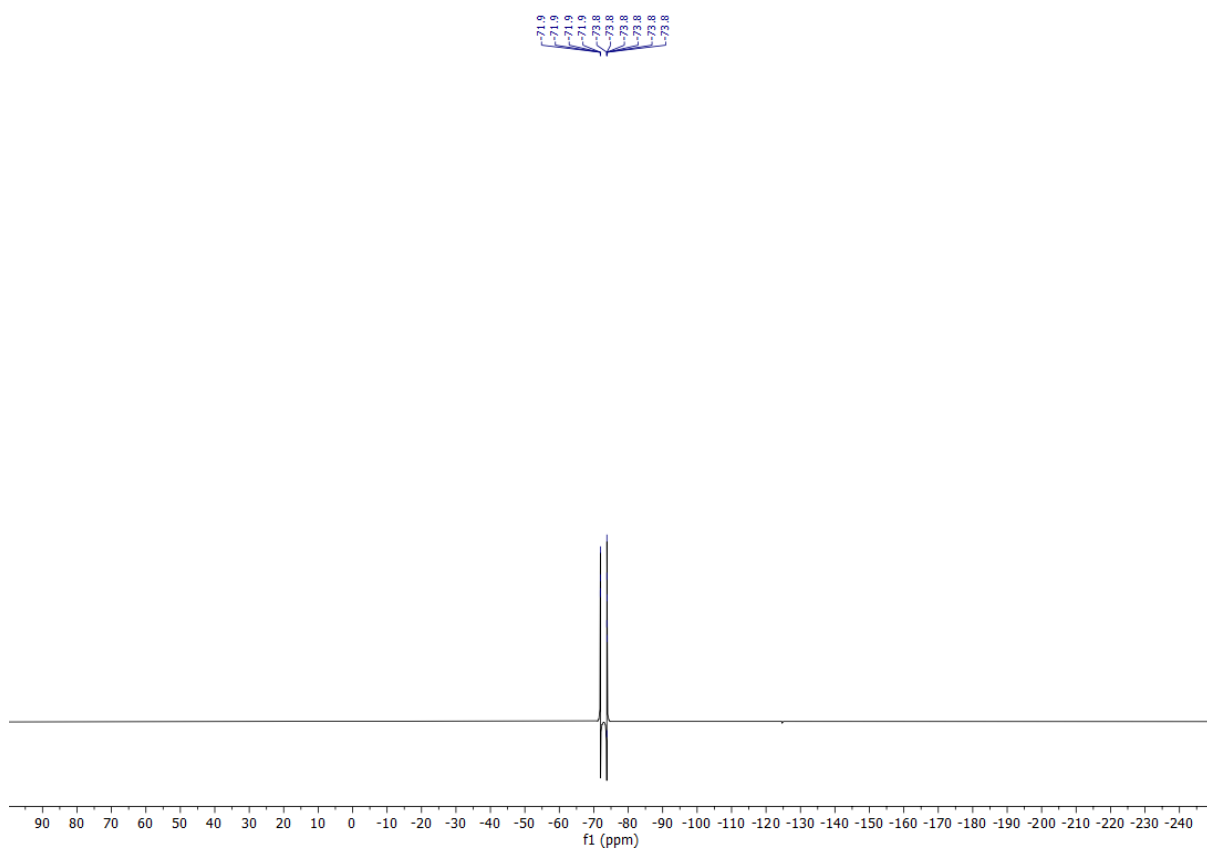
11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium tetrafluoroborate, *rac*-16:



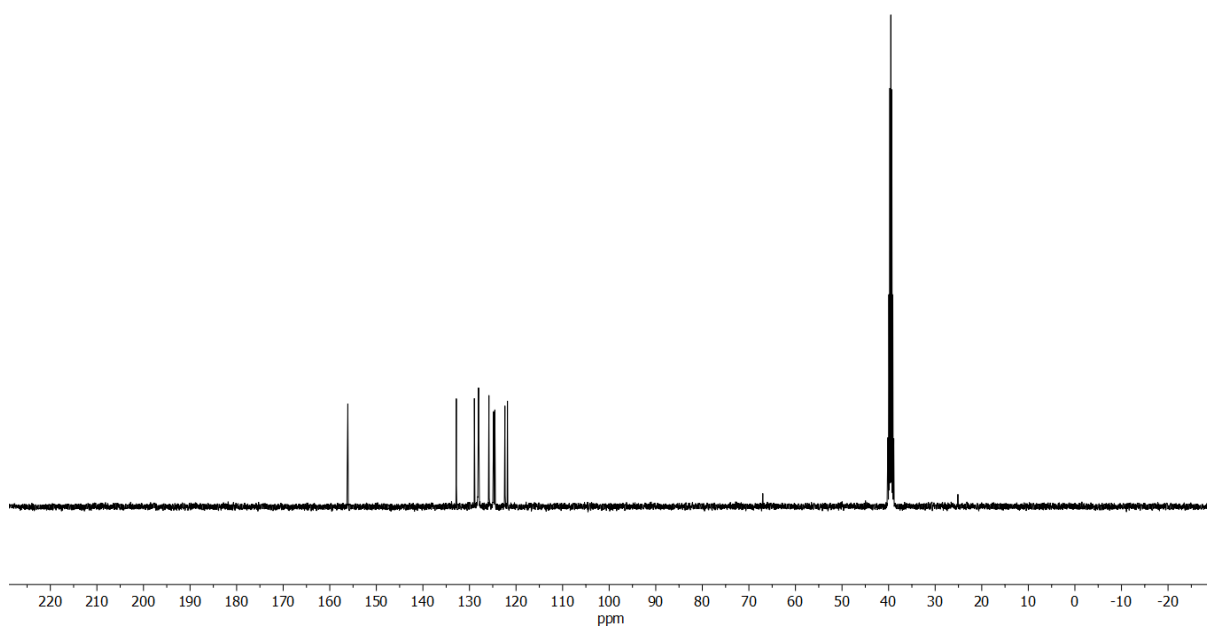
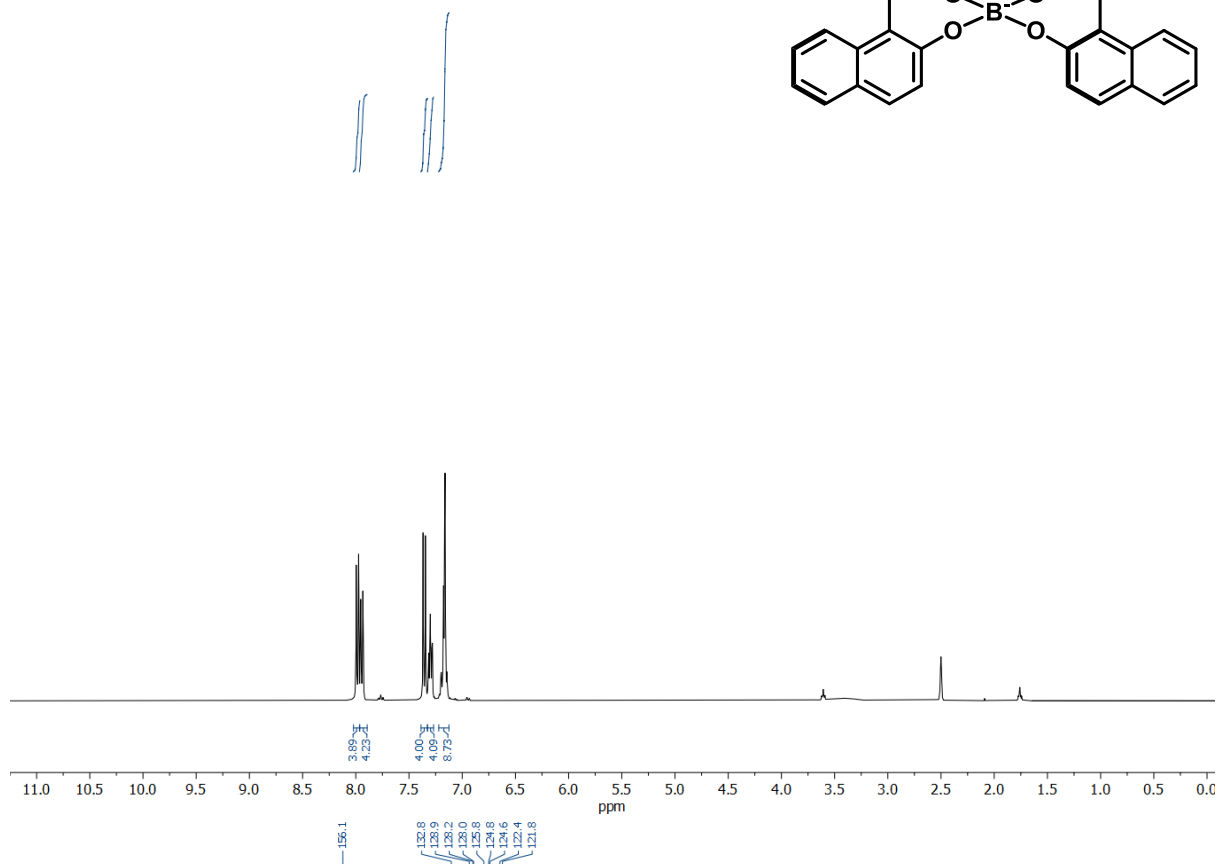
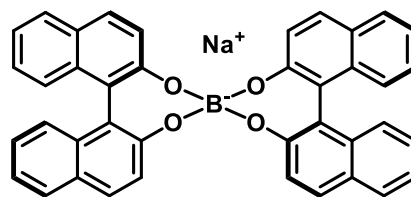


**11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium
hexafluorophosphate, *rac*-17:**

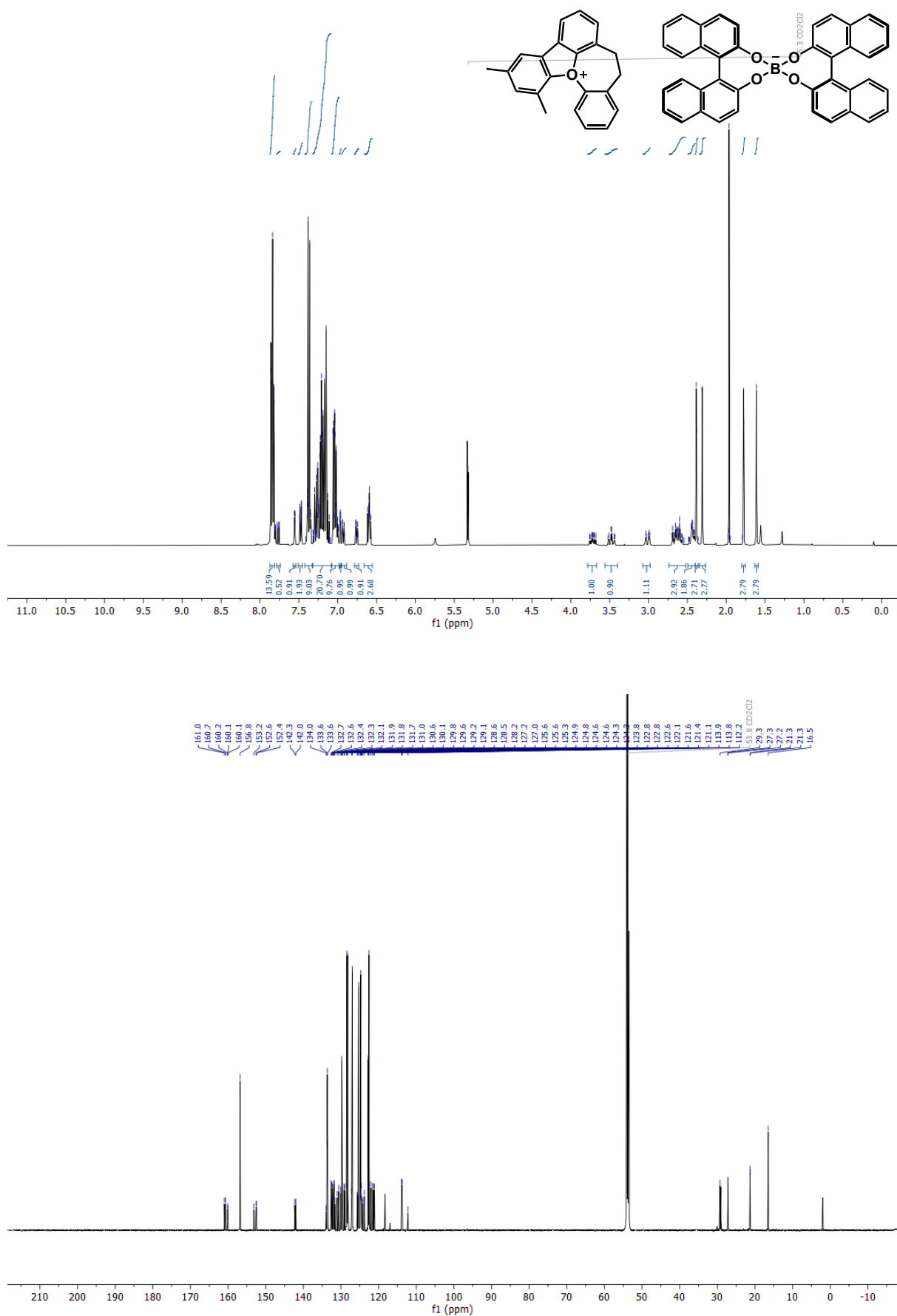




Sodium bis-(*R*)-BINOL borate, S10:



11,13-Dimethyl-4,5-dihydrobenzo[*b*]benzo[6,7]oxepino[3,2,1-*hi*]benzofuran-10-ium, bis-*(R)*-BINOL borate, 18 [(*P*, *R*_O)-(*R*)] and 19 [(*M*, *S*_O)-(*R*)] (1:1 mixture of diastereoisomers):





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