*Supporting Information*

# Regioselective B(3,4)–H Arylation of *o*-Carboranes by Weak Amide Coordination at Room Temperature

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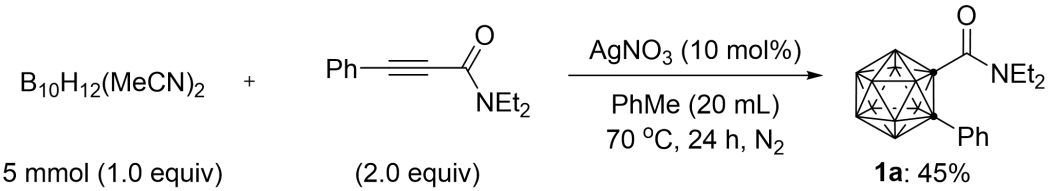
# Table of Contents

## General remarks

Catalytic reactions were carried out in Schlenk flasks under a $N_2$ atmosphere using pre-dried glassware. Chemicals were purchased from commercial sources and used without further purification. Yields refer to isolated compounds estimated to be >95% pure as determined by $^1$H NMR and GC. TLC was performed on Merck TLC Silica Gel 60 $F_{254}$ with detection under UV light at 254 nm. Chromatographic separations were carried out on Merck Geduran SI-60 (0.040–0.063 mm, 230–400 mesh ASTM). IR spectra were recorded on a Bruker FT-IR alpha-P device. EI-MS was recorded on Jeol *AccuTOF* at 70 eV; ESI-MS was recorded on Bruker Daltonik *micrOTOF* and *maXis*. Melting points (M.p.) were measured on Stuart™ melting point apparatus SMP3, and the values are uncorrected. Nuclear magnetic resonance (NMR) spectroscopy was performed at 300, 400, 500 or 600 MHz ($^1$H-NMR), 75, 100 or 125 MHz ($^{13}$C-NMR, APT) and 96, 128 or 160 MHz ($^{11}$B-NMR) on Bruker *Avance III HD 300*, *Avance III 300*, *Avance III 400*, *Avance III HD 500*, Varian *Unity-300, Inova 500* and *Inova 600* instruments. Chemical shifts ($\delta$) are provided in ppm and spectra refer to non-deuterated solvent signal. X-ray structures were measured on Bruker APEX-II CCD diffractometer.

## Preparation of amide *o*-carboranes

The amide *o*-carboranes **1** were synthesized according to a previously described method:[1] $B_{10}H_{12}(CH_3CN)_2$ (1.02 g, 5 mmol) and alkyne (10 mmol) were combined in the presence of $AgNO_3$ (85 mg, 0.5 mmol) in anhydrous toluene (20 mL) and heated at 70 °C for 24 h under $N_2$.




The details for the preparation of **1a**: $B_{10}H_{12}(CH_3CN)_2$ (1.02 g, 5 mmol), *N*,*N*-diethyl-3-phenylpropiolamide (2.01 g, 10 mmol), $AgNO_3$ (85 mg, 0.5 mmol) and anhydrous toluene (20 mL) were placed in a 50 mL Schlenk flask under $N_2$ atmosphere. The mixture was stirred at 70 °C for 24 h. At ambient temperature, the reaction mixture was transferred into a round bottom flask with EtOAc (20 mL) and washed with brine (5.0 mL). The mixture was extracted with EtOAc (3 × 20 mL) and the combined organic layer was dried over $Na_2SO_4$, concentrated under reduced pressure and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (10:1) to afford the amide *o*-carborane **1a** (0.72 g, 45% yield).

# General procedures

**General procedure A for B(3,4)−H diarylation.**

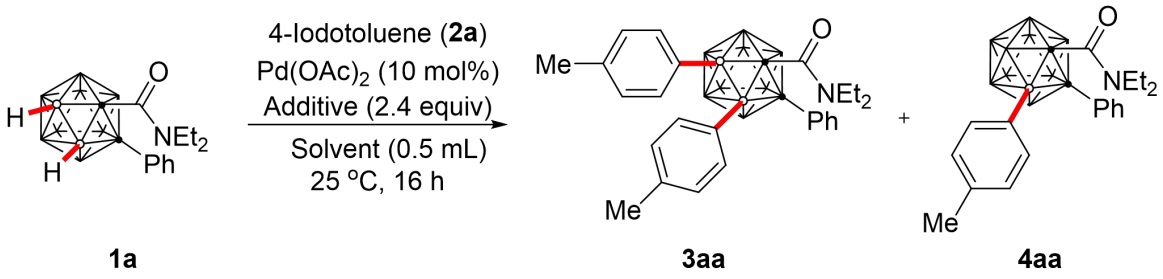
*o*-Carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (0.20 mmol), 4-iodotoluene **2a** (0.48 mmol), $Pd(OAc)_2$ (10 mol %), AgTFA (0.48 mmol), TFA (0.20 mmol) and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) and Gel Permeation Chromatography (GPC) to afford the desired product **3aa**.

**General procedure B for B(3)−H monoarylation.**

*o*-Carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (0.20 mmol), 4-iodotoluene **2a** (0.08 mmol), $Pd(OAc)_2$ (10 mol %), $Ag_2CO_3$ (0.24 mmol) and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 4 h. Then, 4-iodotoluene **2a** (0.08 mmol) was added. And 4 h later, another portion of 4-iodotoluene **2a** (0.08 mmol) was added. The resulting mixture was then stirred for 8 h. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) and Gel Permeation Chromatography (GPC) to afford the desired product **4aa**.

## Optimization studies

**Table S1**. Optimization of reaction conditions.[a]

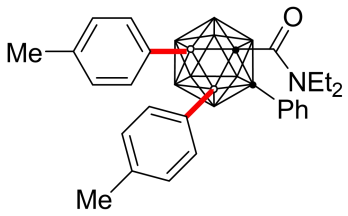



**1a** **3aa** **4aa**

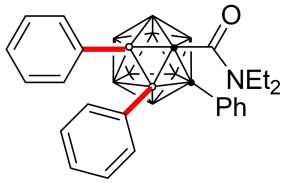
| Entry | Additive | Solvent | Yield of **3aa**/% | Yield of **4aa**/% |
|---|---|---|---|---|
| 1 | AgTFA | PhMe | 0 | 0 |
| 2 | AgTFA | DCE | 0 | 0 |
| 3 | AgTFA | MeCN | 0 | 0 |
| 4 | AgTFA | 1,4-Dioxane | 0 | 0 |
| 5 | AgTFA | $H_2O$ | 0 | 0 |
| 6 | AgTFA | TFE | 21 | 3 |
| 7 | AgTFA | HFIP | 59 | 4 |
| 8 | AgTFA | HFIP | 0 | 0[b] |
| 9 | --- | HFIP | 0 | 0 |
| 10 | AgOAc | HFIP | 5 | <3 |
| 11 | $Ag_2O$ | HFIP | <3 | <3 |
| 12 | $K_2HPO_4$ | HFIP | 0 | 0 |
| 13 | $Na_2CO_3$ | HFIP | 0 | 0 |
| 14 | $K_2CO_3$ | HFIP | 0 | 0 |
| 15 | $NEt_3$ | HFIP | 0 | 0 |
| 16 | AgTFA | HFIP | 53 | 4[c] |
| 17 | AgTFA | HFIP | 42 | 3[d] |
| **18** | **AgTFA** | **HFIP** | **71** | **<3[e]** |
| 19 | $Ag_2CO_3$ | HFIP | 9 | 34[f] |
| **20** | **$Ag_2CO_3$** | **HFIP** | **5** | **55[f,g]** |

[a] Reaction conditions: **1a** (0.20 mmol), **2** (0.48 mmol), $Pd(OAc)_2$ (10 mol %), additive (0.48 mmol), solvent (0.50 mL), 25 °C, 16 h, isolated yield. [b] Without $Pd(OAc)_2$. [c] At 40 °C. [d] At 60 °C. [e] TFA (0.2 mmol) was added. [f] **1a** (0.20 mmol), **2a** (0.24 mmol), $Ag_2CO_3$ (0.24 mmol). [g] **2a** was added in three portions every 4 h. DCE = dichloroethane, TFE = 2,2,2-trifluoroethanol, HFIP = hexafluoroisopropanol, TFA = trifluoroacetic acid.

## Analytical data for products

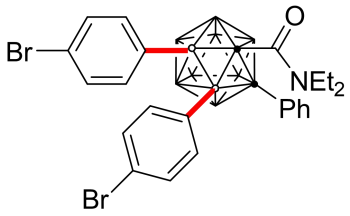



**3aa**. The representative procedure **A** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 4-iodotoluene **2a** (105 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3aa** (71 mg, 71%) as a colorless solid. **M.p.** = 171–172 °C. **$^1$H NMR** (500 MHz, $CDCl_3$): $\delta$ = 7.45 (d, $J$ = 8.5 Hz, 2H), 7.39–7.32 (m, 3H), 7.22 (dd, $J$ = 8.5, 7.3 Hz, 2H), 7.17 (d, $J$ = 8.0 Hz, 2H), 6.94–6.90 (m, 4H), 3.49–3.44 (m, 2H), 3.26–3.22 (m, 2H), 2.28 (s, 3H), 2.24 (s, 3H), 1.00 (t, $J$ = 7.0 Hz, 6H). **$^{13}$C NMR** (125 MHz, $CDCl_3$): $\delta$ = 156.6 ($C_q$), 138.1 ($C_q$), 137.7($C_q$), 136.5 (CH), 133.9 (CH), 133.3($C_q$), 130.0 (CH), 129.3 (CH), 128.1 (CH), 127.6 (CH), 127.5 (CH), 85.5 ($C_q$), 79.3 ($C_q$), 43.7 ($CH_2$), 21.2 ($CH_3$), 21.1 ($CH_3$), 12.9 ($CH_3$). **$^{11}$B NMR** (160 MHz, $CDCl_3$): $\delta$ = 0.65 (2B), -1.38 (1B), -3.61 (1B), -6.20 (1B), -10.54 (5B). **IR** (ATR): 2978, 2566, 1653, 1608, 1415, 1264, 1191, 772 cm$^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 522 (100) $[M+Na]^+$, 500 (40) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{27}H_{38}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 500.3964, found: 500.3951.

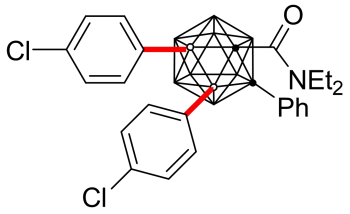



**3ab**. The representative procedure **A** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and iodobenzene **2b** (98 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ab** (64 mg, 68%) as a colorless solid. **M.p.** = 197–198 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.53–7.42 (m, 4H), 7.37–7.32 (m, 1H), 7.29–7.15 (m, 6H), 7.14–7.04 (m, 4H), 3.50–3.41 (m, 2H), 3.26–3.20 (m, 2H), 0.99 (t, $J$ = 7.0 Hz, 6H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 156.6 ($C_q$), 136.6 (CH), 134.0 (CH), 133.2 ($C_q$), 130.1 (CH), 129.4 (CH), 128.4 (CH), 128.0 (CH), 127.6 (CH), 127.2 (CH), 126.6 (CH), 86.0 ($C_q$), 79.7 ($C_q$), 43.8 ($CH_2$), 12.9 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$

= 0.34 (2B), -1.31 (1B), -3.28 (1B), -5.82 (1B), -10.20 (5B). **IR** (ATR): 2973, 2567, 1647, 1430, 1266, 1208, 696 $cm^{-1}$. **MS** (ESI) *m/z* (relative intensity): 494 (100) $[M+Na]^+$, 472 (40) $[M+H]^+$. **HR-MS** (ESI): *m/z* calcd. for $C_{25}H_{34}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 472.3650, found: 472.3631.

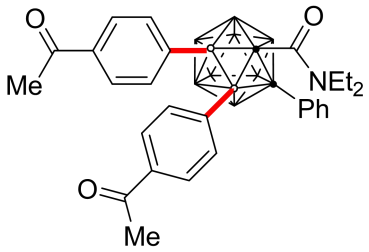



**3ac**. The representative procedure **A** was followed using *o*-carborane **1a** (1-$CONEt_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-bromo-4-iodobenzene **2c** (136 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ac** (76 mg, 61%) as a colorless solid. **M.p.** = 205–206 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 7.50–7.39 (m, 3H), 7.32–7.27 (m, 5H), 7.25–7.22 (m, 3H), 7.21–7.14 (m, 2H), 3.60–3.42 (m, 4H), 1.05 (t, $J$ = 6.9 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 156.2 ($C_q$), 138.0 (CH), 135.6 (CH), 132.0 ($C_q$), 130.5 (CH), 129.8 (CH), 129.7 (CH), 129.6 (CH), 127.9 (CH), 123.6 ($C_q$), 123.2 ($C_q$), 84.6 ($C_q$), 78.5 ($C_q$), 44.0 ($CH_2$), 13.1 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.22 (3B), -3.11 (1B), -6.02 (1B), -9.94 (5B). **IR** (ATR): 2573, 1647, 1578, 1487, 1381, 1205,1010,693 $cm^{-1}$. **MS** (ESI) *m/z* (relative intensity): 652 (100) $[M+Na]^+$, 630 (10) $[M+H]^+$. **HR-MS** (ESI): *m/z* calcd. for $C_{25}H_{31}{}^{11}B_{10}{}^{79}Br_2NONa$ $[M+Na]^+$: 652.1657, found: 652.1642.

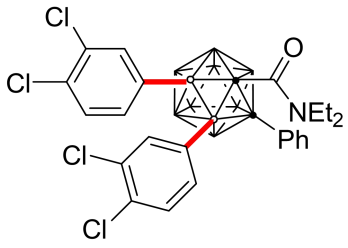



**3ad**. The representative procedure **A** was followed using *o*-carborane **1a** (1-$CONEt_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-chloro-4-iodobenzene **2d** (115 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ad** (73 mg, 68%) as a colorless solid. **M.p.** = 185–186 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 7.48–7.40 (m, 3H), 7.35–7.22 (m, 6H), 7.17–7.08 (m, 4H), 3.54–3.40 (m, 4H), 1.06 (t, $J$ = 7.0 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 156.2 ($C_q$), 137.8 (CH), 135.3 (CH), 135.0 ($C_q$), 134.7 ($C_q$), 132.1 ($C_q$), 129.9 (CH), 129.6 (CH), 128.0 (CH), 127.5 (CH), 126.9 (CH), 84.9 ($C_q$), 78.9 ($C_q$), 44.2 ($CH_2$), 12.9 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.49 (3B),

-3.10 (1B), -6.38 (1B), -10.40 (5B). **IR** (ATR): 2571, 1648, 1584, 1489, 1268, 1205, 1092, 730 $cm^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 564 (100) $[M+Na]^+$, 542 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{25}H_{31}{}^{11}B_{10}{}^{35}Cl_2NONa$ $[M+Na]^+$: 564.2649, found: 564.2640.

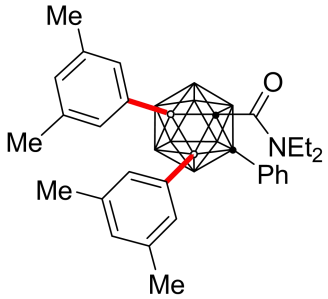



**3ae**. The representative procedure **A** was followed using *o*-carborane **1a** (1-$CONEt_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-(4-iodophenyl)ethanone **2e** (118 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ae** (64 mg, 58%) as a colorless solid. **M.p.** = 244–245 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 7.74 (d, *J* = 8.3 Hz, 2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.51–7.39 (m, 7H), 7.34–7.27 (m, 2H), 3.60–3.45 (m, 4H), 2.56 (s, 3H), 2.55 (s, 3H), 1.09 (t, *J* = 6.9 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 198.3 ($C_q$), 198.1 ($C_q$), 156.0 ($C_q$), 136.6 ($C_q$), 136.5 (CH), 136.4 ($C_q$), 134.2 (CH), 131.8 ($C_q$), 130.1 (CH), 129.7 (CH), 128.0 (CH), 127.0 (CH), 126.0 (CH), 84.9 ($C_q$), 78.5 ($C_q$), 43.9 ($CH_2$), 26.7 ($CH_3$), 26.5 ($CH_3$), 13.0 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.58 (3B), -2.61 (1B), -5.98 (1B), -9.67 (5B). **IR** (ATR): 2572, 1679, 1642, 1357, 1266, 1200, 730, 590 $cm^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 578 (100) $[M+Na]^+$, 556 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{29}H_{37}{}^{10}B_2{}^{11}B_8NO_3Na$ $[M+Na]^+$: 578.3683, found: 578.3676.

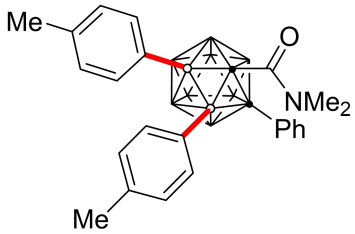



**3af**. The representative procedure **A** was followed using *o*-carborane **1a** (1-$CONEt_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1,2-dichloro-4-iodobenzene **2f** (131 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3af** (78 mg, 64%) as a colorless solid. **M.p.** = 208–209 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 7.48–7.40 (m, 4H), 7.36–7.26 (m, 4H), 7.22–7.11 (m, 3H), 3.60–3.45 (m, 4H), 1.13 (t, *J*

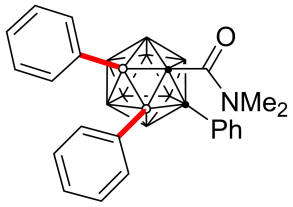
= 6.9 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 155.8 ($C_q$), 138.1 (CH), 135.6 (CH), 135.4 (CH), 133.2 (CH), 133.0 ($C_q$), 132.9 ($C_q$), 132.0 ($C_q$), 131.5 ($C_q$), 130.9 ($C_q$), 130.2 (CH), 129.7 (CH), 129.5 (CH), 128.7 (CH), 128.2 (CH), 85.0 ($C_q$), 78.2 ($C_q$), 44.2 ($CH_2$), 13.0 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.76 (3B), -3.10 (1B), -6.49 (1B), -10.24 (5B). **IR** (ATR): 2578, 1646, 1473, 1424, 1203, 1028, 695 $cm^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 632 (100) $[M+Na]^+$, 610 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{25}H_{29}{}^{11}B_{10}{}^{35}Cl_4NONa$ $[M+Na]^+$: 632.1879, found: 632.1867.



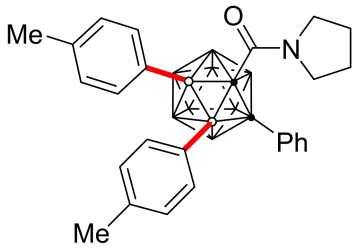

**3ag**. The representative procedure **A** was followed using *o*-carborane **1a** (1-$CONEt_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-iodo-3,5-dimethylbenzene **2g** (112 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ag** (66 mg, 63%) as a colorless solid. **M.p.** = 203–205 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 7.52 (d, *J* = 7.4 Hz, 2H), 7.40–7.32 (m, 1H), 7.29–7.18 (m, 4H), 7.00–6.90 (m, 3H), 6.87 (s, 1H), 3.62 (q, *J* = 7.0 Hz, 2H), 3.09 (q, *J* = 7.0 Hz, 2H), 2.19 (s, 6H), 2.16 (s, 6H), 1.08 (t, *J* = 7.0 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 156.8 ($C_q$), 136.2 ($C_q$), 135.6 ($C_q$), 134.3 (CH), 134.3 ($C_q$), 131.8 (CH), 130.4 (CH), 130.2 (CH), 129.7 (CH), 129.3 (CH), 127.5 (CH), 87.6 ($C_q$), 80.3 ($C_q$), 43.5 ($CH_2$), 21.4 ($CH_3$), 21.2 ($CH_3$), 12.7 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.69 (2B), -1.17 (1B), -3.10 (1B), -5.90 (1B), -10.05 (5B). **IR** (ATR): 2916, 2557, 1646, 1420, 1264, 1183, 855, 689 $cm^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 550 (100) $[M+Na]^+$, 528 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{29}H_{41}{}^{10}B_2{}^{11}B_8NONa$ $[M+Na]^+$: 550.4097, found: 550.4096.



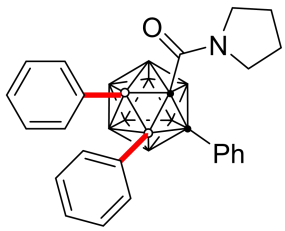

**3ba**. The representative procedure **A** was followed using *o*-carborane **1b** (1-CONMe$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (58 mg, 0.20 mmol) and 4-iodotoluene **2a** (105 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ba** (48 mg, 51%) as a colorless solid. **M.p.** = 158–159 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.45 (d, $J$ = 7.4 Hz, 2H), 7.40–7.36 (m, 1H), 7.34–7.23 (m, 4H), 7.20 (d, $J$ = 7.9 Hz, 2H), 6.99–6.90 (m, 4H), 3.04 (s, 6H), 2.31 (s, 3H), 2.29 (s, 3H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 157.7 ($C_q$), 138.3 ($C_q$), 137.9 ($C_q$), 136.3 (CH), 133.9 (CH), 133.1 ($C_q$), 130.0 (CH), 129.5 (CH), 128.4 (CH), 127.8 (CH), 127.6 (CH), 85.9 ($C_q$), 78.6 ($C_q$), 40.8 ($CH_3$), 21.3 ($CH_3$), 21.2 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = 0.7 (2B), -1.3 (1B), -3.2 (1B), -6.4 (1B), -10.6 (5B). **IR** (ATR): 2921, 2570, 1644, 1393, 1195, 743, 693 cm$^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 473 (100) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{25}H_{34}{}^{10}B_1{}^{11}B_9NO$ $[M+H]^+$: 473.3607, found: 473.3606.




**3bb**. The representative procedure **A** was followed using *o*-carborane **1b** (1-CONMe$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (58 mg, 0.20 mmol) and iodobenzene **2b** (98 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3bb** (47 mg, 53%) as a colorless solid. **M.p.** = 99–100 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.47–7.41 (m, 4H), 7.40–7.35 (m, 1H), 7.32–7.29 (m, 2H), 7.28–7.20 (m, 4H), 7.18–7.10 (m, 4H), 3.03 (s, 6H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 157.7 ($C_q$), 136.4 (CH), 133.9 (CH), 133.0 ($C_q$), 130.0 (CH), 129.6 (CH), 128.6 (CH), 128.2 (CH), 127.9 (CH), 127.5 (CH), 126.8 (CH), 86.4 ($C_q$), 79.0 ($C_q$), 40.8 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = 0.57 (2B), -1.13 (1B), -3.10 (1B), -6.27 (1B), -10.23 (5B). **IR** (ATR): 3053, 2581, 1654, 1493, 1373, 1167, 744 cm$^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 444 (100) $[M+H]^+$, 466 (10) $[M+Na]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{23}H_{30}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 444.3336, found: 444.3328.

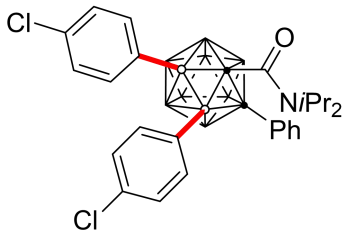



**3ca**. The representative procedure **A** was followed using *o*-carborane **1c** (1-CON$(CH_2)_4$-2-Ph-*o*-$C_2B_{10}H_{10}$) (63 mg, 0.20 mmol) and 4-iodotoluene **2a** (105 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ca** (59 mg, 60%) as a pink solid. **M.p.** = 228–230 °C. **$^1$H NMR (**400 MHz, $CDCl_3$**)**: $\delta$ = 7.44–7.38 (m, 2H), 7.36–7.28 (m, 3H), 7.22–7.16 (m, 2H), 7.16–7.10 (m, 2H), 6.96–6.87 (m, 4H), 3.65–3.28 (m, 4H), 2.25 (s, 3H), 2.23 (s, 3H), 1.80–1.63 (m, 4H). **$^{13}$C NMR (**100 MHz, $CDCl_3$**)**: $\delta$ = 155.7 ($C_q$), 138.1 ($C_q$), 137.7 ($C_q$), 136.6 (CH), 133.6 (CH), 132.9 ($C_q$), 129.9 (CH), 129.4 (CH), 128.3 (CH), 127.7 (CH), 127.5 (CH), 85.0 ($C_q$), 78.7 ($C_q$), 50.5 (overlapped, $CH_2$), 21.2 ($CH_3$), 21.2 ($CH_3$). **$^{11}$B NMR (**128 MHz, $CDCl_3$): $\delta$ = 0.57 (2B), -1.61 (1B), -3.32 (1B), -6.45 (1B), -10.78 (5B). **IR** (ATR): 2975, 2878, 2570, 1639, 1446, 1225, 865, 753, 690 $cm^{-1}$. **MS** (ESI) *m/z* (relative intensity): 498 (20) $[M+H]^+$, 520 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{35}{}^{10}B_2{}^{11}B_8NONa$ $[M+Na]^+$ 520.3627, found 520.3623.

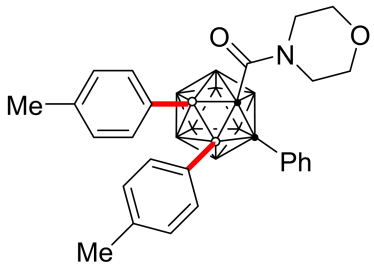



**3cb**. The representative procedure **A** was followed using *o*-carborane **1c** (1-CON$(CH_2)_4$-2-Ph-*o*-$C_2B_{10}H_{10}$) (63 mg, 0.20 mmol) and iodobenzene **2b** (98 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3cb** (50 mg, 53%) as a colorless solid. **M.p.** = 176–177 °C. **$^1$H NMR** (500 MHz, $CDCl_3$): $\delta$ = 7.51–7.44 (m, 2H), 7.43–7.38 (m, 2H), 7.35–7.30 (m, 1H), 7.25–7.24 (m, 1H), 7.24–7.16 (m, 5H), 7.13–7.04 (m, 4H), 3.63–3.41 (m, 4H), 1.83–1.61 (m, 4H). **$^{13}$C NMR** (125 MHz, $CDCl_3$): $\delta$ = 155.7 ($C_q$), 136.7 (CH), 133.6 (CH), 132.8 ($C_q$), 129.9 (CH), 129.5 (CH), 128.4 (CH), 128.1 (CH), 127.7 (CH), 127.4 (CH), 126.6 (CH), 85.5 ($C_q$), 79.1 ($C_q$), 50.5 (overlapped, $CH_2$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = 0.48 (2B), -1.36 (1B), -3.15 (1B), -6.18 (1B), -10.26 (5B). **IR** (ATR): 2921, 2570, 1643, 1389, 1195, 861, 743, 692 $cm^{-1}$. **MS** (ESI) *m/z* (relative

intensity): 471 (100) $[M+H]^+$, 493 (10) $[M+Na]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{25}H_{32}{}^{10}B_1{}^{11}B_9NO$ $[M+H]^+$: 471.3450, found: 471.3448.

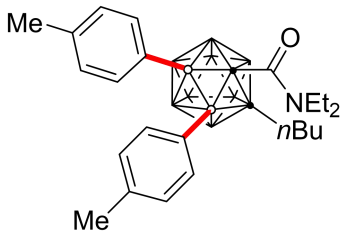



**3dd**. The representative procedure **A** was followed using *o*-carborane **1d** (1-CON$^i$Pr$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (70 mg, 0.20 mmol) and 1-chloro-4-iodobenzene **2d** (114 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3dd** (61 mg, 54%) as a colorless solid. **M.p.** = 232–233 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.52 (d, $J$ = 7.4 Hz, 2H), 7.45–7.41 (m, 1H), 7.35 (d, $J$ = 8.4 Hz, 2H), 7.32–7.27 (m, 2H), 7.19 (d, $J$ = 8.6 Hz, 2H), 7.14 (d, $J$ = 8.4 Hz, 2H), 7.07 (d, $J$ = 8.4 Hz, 2H), 5.24–5.18 (m, 1H), 3.44–3.39 (m, 1H), 1.29 (d, $J$ = 6.7 Hz, 6H), 1.04 (d, $J$ = 6.7 Hz, 6H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 154.5 ($C_q$), 137.9 (CH), 136.1 (CH), 134.7 ($C_q$), 134.5 ($C_q$), 132.0 ($C_q$), 129.9 (CH), 129.5 (CH), 128.0 (CH), 127.5 (CH), 126.5 (CH), 83.9 ($C_q$), 79.1 ($C_q$), 50.3 (CH), 49.4 (CH), 20.5 ($CH_3$), 20.3 ($CH_3$), 19.7 ($CH_3$), 19.6 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = 1.47 (1B), -1.05 (2B), -3.30 (1B), -6.75 (1B), -10.90 (5B). **IR** (ATR): 2968, 2620, 2585, 1657, 1586, 1491, 1369, 1296, 691 $cm^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 569 (100) $[M+H]^+$, 591 (10) $[M+Na]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{27}H_{36}{}^{10}B_1{}^{11}B_9{}^{35}Cl_2NO$ $[M+H]^+$: 569.3141, found: 569.3142.

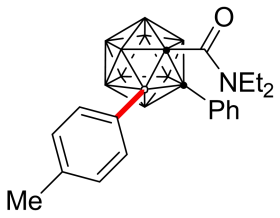



**3ea**. The representative procedure **A** was followed using *o*-carborane **1e** (1-CON$(CH_2)_4$O-2-Ph-*o*-$C_2B_{10}H_{10}$) (67 mg, 0.20 mmol) and 4-iodotoluene **2a** (105 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3ea** (54 mg, 52%) as a colorless solid. **M.p.** = 258–259 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.49–7.41 (m, 2H), 7.40–7.32 (m, 3H), 7.28–7.21 (m, 2H), 7.21–7.14 (m, 2H), 7.01 (d, $J$ = 7.9 Hz, 2H),

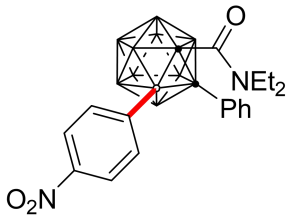
6.96 (d, $J$ = 7.8 Hz, 2H), 3.73–3.58 (m, 4H), 3.48–3.32 (m, 4H), 2.34 (s, 3H), 2.28 (s, 3H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 157.6 ($C_q$), 138.7 ($C_q$), 138.2 ($C_q$), 136.2 (CH), 134.2 (CH), 133.4 ($C_q$), 130.1 (CH), 129.6 (CH), 128.5 (CH), 128.0 (CH), 127.8 (CH), 86.7 ($C_q$), 78.6 ($C_q$), 66.5 ($CH_2$), 47.9 ($CH_2$), 21.3 ($CH_3$), 21.2 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = 0.67 (2B), -0.88 (1B), -3.11 (1B), -6.12 (1B), -10.53 (5B). **IR** (ATR): 2843, 2549, 1660, 1447, 1411, 1264, 1225, 771 cm$^{-1}$. **MS** (ESI) *m/z* (relative intensity): 514 (70) $[M+H]^+$, 536 (100) $[M+Na]^+$. **HR-MS** (ESI): *m/z* calcd. for $C_{27}H_{35}{}^{10}B_2{}^{11}B_8NO_2Na$ $[M+Na]^+$: 536.3576, found: 536.3557.



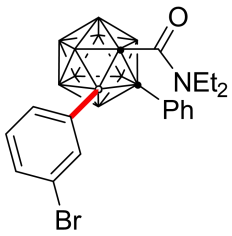

**3fa**. The representative procedure **A** was followed using *o*-carborane **1f** (1-$CONEt_2$-2-$^n$Bu-*o*-$C_2B_{10}H_{10}$) (60 mg, 0.20 mmol) and 4-iodotoluene **2a** (105 mg, 0.48 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **3fa** (45 mg, 47%) as a colorless solid. **M.p.** = 88–89 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.39 (d, $J$ = 7.9 Hz, 2H), 7.17 (d, $J$ = 7.8 Hz, 2H), 7.12 (d, $J$ = 7.9 Hz, 2H), 6.99 (d, $J$ = 7.8 Hz, 2H), 4.15–3.66 (m, 2H), 3.66–3.46 (m, 2H), 2.56–2.46 (m, 1H), 2.38 (s, 3H), 2.30 (s, 3H), 2.29–2.18 (m, 1H), 1.66–1.56 (m, 1H), 1.54–1.42 (m, 1H), 1.35–1.19 (m, 8H), 0.91 (t, $J$ = 7.3 Hz, 3H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 156.3 ($C_q$), 137.9 ($C_q$), 137.8 ($C_q$), 134.8 (CH), 133.3 (CH), 128.6 (CH), 127.7 (CH), 83.6 ($C_q$), 73.6 ($C_q$), 44.2 ($CH_2$), 34.5 ($CH_2$), 32.0 ($CH_2$), 22.4 ($CH_2$), 21.4 ($CH_3$), 21.3 ($CH_3$), 13.8 ($CH_3$), 13.1 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = 2.34 (2B), -1.13 (2B), -2.77 (1B), -7.74 (1B), -10.36 (2B), -12.42 (1B), -13.91 (1B). **IR** (ATR): 2951, 2867, 2568, 1647, 1419, 1265, 809 cm$^{-1}$. **MS** (ESI) *m/z* (relative intensity): 480 (100) $[M+H]^+$, 502 (20) $[M+Na]^+$. **HR-MS** (ESI): *m/z* calcd. for $C_{25}H_{42}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 480.4276, found: 480.4272.



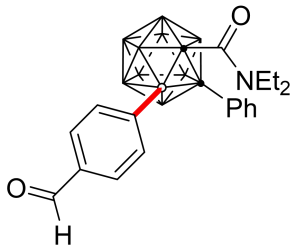

**4aa**. The representative procedure **B** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 4-iodotoluene **2a** (53 mg, 0.24 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **4aa** (45 mg, 55%) as a colorless solid. **M.p.** = 180–181 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.45–7.39 (m, 4H), 7.28–7.22 (m, 1H), 7.16–7.05 (m, 4H), 3.55–3.35 (m, 4H), 2.34 (s, 3H), 1.00 (t, $J$ = 7.1 Hz, 6H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 158.3 ($C_q$), 139.1 ($C_q$), 134.6 (CH), 134.0 ($C_q$), 131.9 (CH), 129.2 (CH), 128.5 (CH), 127.0 (CH), 89.5 ($C_q$), 82.4 ($C_q$), 43.6 ($CH_2$), 21.3 ($CH_3$), 12.2 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = -1.0 (1B), -2.26 (1B), -3.69 (1B), -7.91 (3B), -10.32 (4B). **IR** (ATR): 2635, 2563, 1648, 1476, 1418, 1269, 1208, 1080, 689 cm$^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 432 (100) $[M+Na]^+$, 410 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{20}H_{31}{}^{10}B_2{}^{11}B_8NONa$ $[M+Na]^+$: 432.3311, found: 432.3304.




**4ah**. The representative procedure **B** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-iodo-4-nitrobenzene **2h** (60 mg, 0.24 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **4ah** (54 mg, 61%) as a colorless solid. **M.p.** = 147–148 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 8.14 (d, $J$ = 8.7 Hz, 2H), 7.78 (d, $J$ = 8.7 Hz, 2H), 7.41–7.30 (m, 3H), 7.22–7.16 (m, 2H), 3.43–3.32 (m, 4H), 1.03 (t, $J$ = 7.0 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 158.0 ($C_q$), 148.3 ($C_q$), 135.5 (CH), 133.5 ($C_q$), 131.4 (CH), 129.8 (CH), 127.6 (CH), 122.3 (CH), 90.8 ($C_q$), 83.0 ($C_q$), 43.7 ($CH_2$), 14.0 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = -0.10 (2B), -3.09 (2B), -7.61 (3B), -8.98 (2B), -10.71 (1B). **IR** (ATR): 2980, 2561, 1647, 1513, 1346, 1265, 1208, 843, 687 cm$^{-1}$. **MS** (ESI) *m*/*z* (relative intensity): 463 (100) $[M+Na]^+$, 441 (10) $[M+H]^+$. **HR-MS** (ESI): *m*/*z* calcd. for $C_{19}H_{28}{}^{10}B_2{}^{11}B_8N_2O_3Na$ $[M+Na]^+$: 463.3005, found: 463.2995.

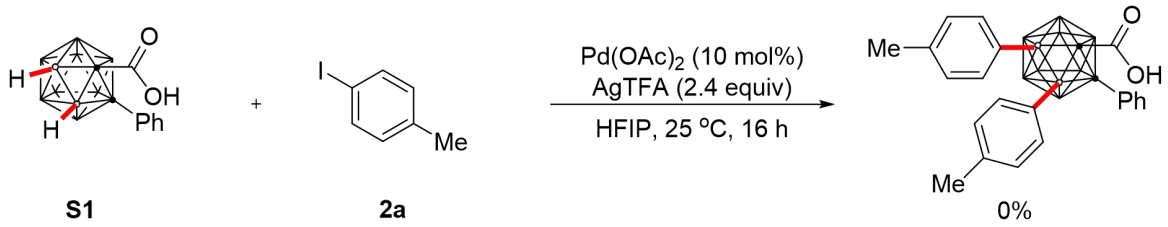



**4ai**. The representative procedure **B** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 1-iodo-3-bromobenzene **2i** (60 mg, 0.24 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **4ai** (47.3 mg, 50%) as a colorless solid**. M.p.** = 168–169 °C. **$^1$H NMR** (400 MHz, $CDCl_3$): $\delta$ = 7.66–7.61 (m, 1H), 7.52–7.45 (m, 2H), 7.40–7.35 (m, 2H), 7.31–7.23 (m, 1H), 7.17–7.09 (m, 3H), 3.36–3.10 (m, 4H), 1.01 (t, $J$ = 7.2 Hz, 6H). **$^{13}$C NMR** (100 MHz, $CDCl_3$): $\delta$ = 158.0 ($C_q$), 137.1 (CH), 133.8 ($C_q$), 133.2 (CH), 132.3 (CH), 131.8 (CH), 129.5 (CH), 129.4 (CH), 127.3(CH), 122.5 ($C_q$), 90.5 ($C_q$), 82.8 ($C_q$), 44.1 ($CH_2$), 43.7 ($CH_2$), 14.0 ($CH_3$), 12.2 ($CH_3$). **$^{11}$B NMR** (128 MHz, $CDCl_3$): $\delta$ = -0.49 (2B), -3.35 (2B), -7.81 (3B), -9.66 (3B). **IR** (ATR): 2976, 2575, 1645, 1420, 1266, 1156, 770, 689 cm$^{-1}$. **MS** (ESI) *m/z* (relative intensity): 497 (100) $[M+Na]^+$, 475 (20) $[M+H]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{19}H_{28}{}^{10}B_1{}^{11}B_9{}^{79}BrNONa$ $[M+Na]^+$: 497.2220, found 497.2229.

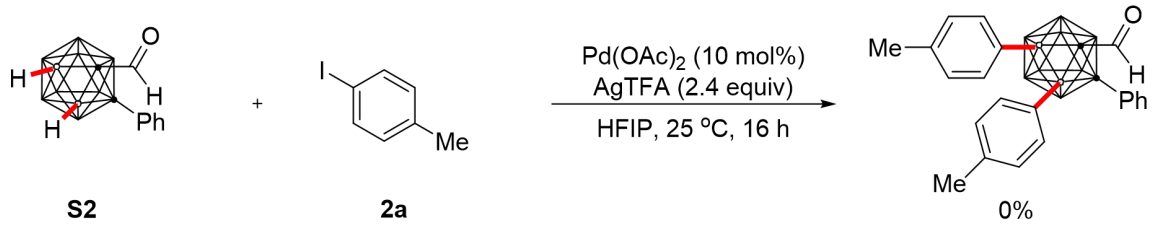



**4aj**. The representative procedure **B** was followed using *o*-carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol) and 4-iodobenzaldehyde **2j** (56 mg, 0.24 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 20/1) yielded **4aj** (43 mg, 51%) as a colorless solid. **M.p.** = 211–212 °C. **$^1$H NMR** (300 MHz, $CDCl_3$): $\delta$ = 10.07 (s, 1H), 7.88–7.70 (m, 4H), 7.44–7.37 (m, 2H), 7.35–7.29 (m, 1H), 7.20–7.11 (m, 2H), 3.43–3.30 (m, 4H), 1.03 (t, $J$ = 7.0 Hz, 6H). **$^{13}$C NMR** (75 MHz, $CDCl_3$): $\delta$ = 192.3 (CH), 158.0 ($C_q$), 136.3 ($C_q$), 135.3 (CH), 133.7 ($C_q$), 131.8 (CH), 129.7 (CH), 128.5 (CH), 127.2 (CH), 90.8 ($C_q$), 83.0 ($C_q$), 43.7 ($CH_2$), 13.2 ($CH_3$). **$^{11}$B NMR** (96 MHz, $CDCl_3$): $\delta$ = -0.28 (2B), -3.35 (2B), -7.51 (3B), -9.39 (2B), -11.02 (1B). **IR** (ATR): 2980, 2560, 1719, 1650, 1627, 1420, 1266, 1181, 761, 688 cm$^{-1}$. **MS** (ESI) *m/z* (relative intensity): 424 (100) $[M+H]^+$. **HR-MS** (ESI): *m/z* calcd. for $C_{20}H_{30}{}^{10}B_2{}^{11}B_8NO_2$ $[M+H]^+$: 424.3284, found: 424.3266.

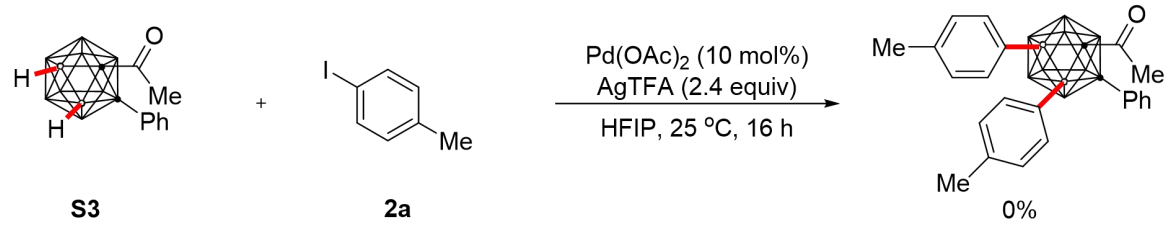
## Attempts with Other Groups



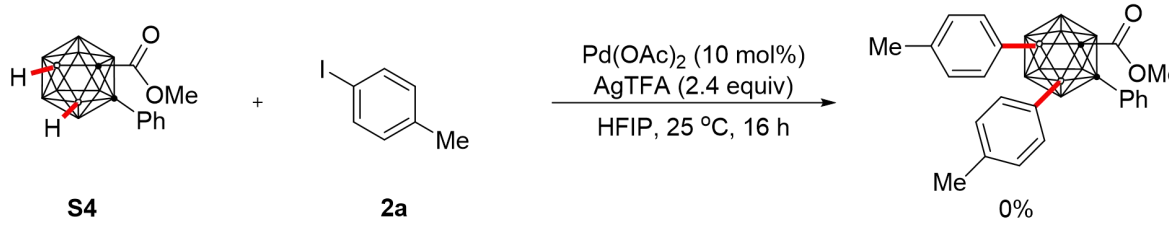

**S1** **2a** 0%




**S2** **2a** 0%




**S3** **2a** 0%

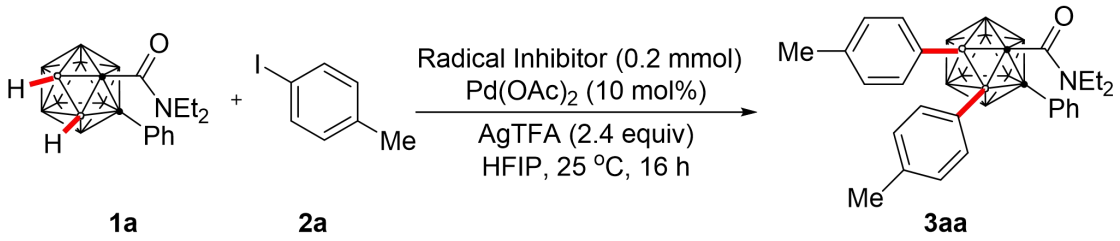



**S4** **2a** 0%

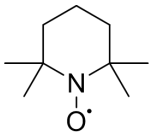
**> 95% carborane starting materials were recovered in all examples!**

*o*-Carborane **S1-S4** (0.20 mmol), 4-iodotoluene **2a** (105 mg, 0.48 mmol), $Pd(OAc)_2$ (4.5 mg, 10 mol %), AgTFA (106 mg, 0.48 mmol), and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h.

## Mechanistic Studies



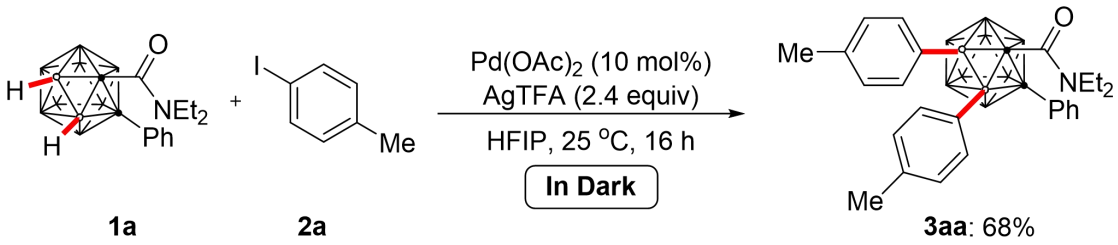

| Radical Inhibitor | Yield of **3aa** |
|---|---|
| TEMPO | 27% |
| 1,4-Cyclohexadiene | 52% |


TEMPO


1,4-Cyclohexadiene

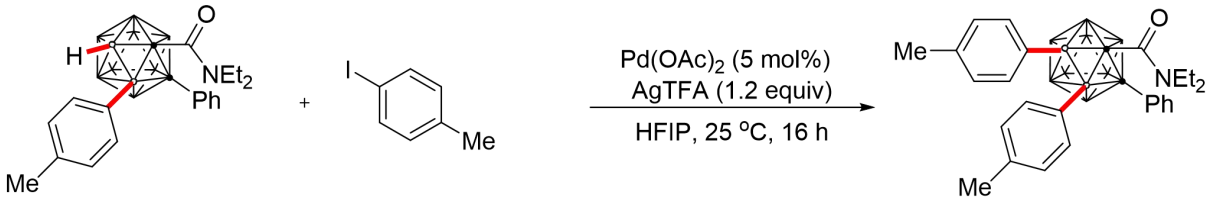
*o*-Carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol), 4-iodotoluene **2a** (105 mg, 0.48 mmol), TEMPO (31 mg, 0.20 mmol), $Pd(OAc)_2$ (4.5 mg, 10 mol %), AgTFA (106 mg, 0.48 mmol), and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) to afford the desired product **3aa** (27 mg, 27%).

*o*-Carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol), 4-iodotoluene **2a** (105 mg, 0.48 mmol), 1,4-cyclohexadiene (16 mg, 0.20 mmol), $Pd(OAc)_2$ (4.5 mg, 10 mol %), AgTFA (106 mg, 0.48 mmol), and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) to afford the desired product **3aa** (52 mg, 52%).




**1a** **2a** **3aa**: 68%

*o*-Carborane **1a** (1-CONEt$_2$-2-Ph-*o*-$C_2B_{10}H_{10}$) (64 mg, 0.20 mmol), 4-iodotoluene **2a** (105 mg, 0.48 mmol), Pd(OAc)$_2$ (4.5 mg, 10 mol %), AgTFA (106 mg, 0.48 mmol), and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h in dark. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) to afford the desired product **3aa** (68 mg, 68%).




**4aa** **2a** **3aa**: 79%

Compound **4aa** (86 mg, 0.20 mmol), 4-iodotoluene **2a** (53 mg, 0.24 mmol), Pd(OAc)$_2$ (2.3 mg, 5 mol %), AgTFA (53 mg, 0.24 mmol), and HFIP (0.50 mL) were placed in a 25 mL Schlenk tube under $N_2$ atmosphere. The mixture was stirred at 25 °C for 16 h. Then, the reaction solution was concentrated to dryness in vacuum and purified by column chromatography on silica gel using a mixture of *n*-hexane and EtOAc (20/1 in v/v) to afford the desired product **3aa** (79 mg, 79%).

## Computational Data

All calculations were carried out with the Gaussian 16, Revision A.03 package.[5] Geometry optimizations of all stationary points were performed at the TPSS[6] level of theory including D3(BJ)[7] dispersion corrections. All atoms were described with a def2-SVP[8] basis set. For palladium, the Stuttgart-Dresden effective core potentials was employed.[9] All stationary points were fully characterized by analytical frequency calculations as either a minimum (no imaginary frequency) or a transition state (only one imaginary frequency) at the same level of theory.

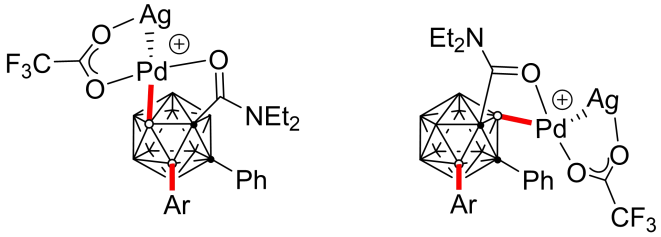
Single point calculations were performed at the PW6B95[10] level of theory including D3(BJ) dispersion corrections with a def2-TZVP[8] basis set for all atoms. For palladium, the same pseudopotential as in the optimization was used. Solvent effects were taken into consideration in the single point calculations through the use of SMD[11] model with a dielectric constant of $\varepsilon = 16.7$, which corresponds to HFIP (Hexafluoro-propan-2-ol).

Unless otherwise stated, all reported energies are Gibbs free energies in kcal $mol^{-1}$, which were calculated by adding the gas-phase thermal correction to Gibbs free energy at 298.15 K to the single-point energies.

The 3D structures of optimized geometries were constructed by using the CYLview software.[12]

**Scheme S1.** Relative Gibbs free energies in kcal $mol^{-1}$ for various Pd(II) cyclometalated complexes at the B4 and B6 position generated after a second B–H activation at the PBE0-D3(BJ)/def2-TZVP+SMD(HFIP)//TPSS-D3(BJ)/def2-SVP level of theory.

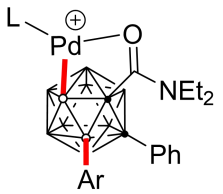
a) Cationic palladacyclic intermediates with AgTFA as a ligand



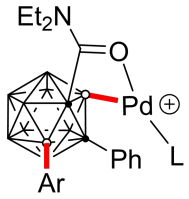

**IMA-B4** **0.0**

**IMA-B6** **1.0**

b) Cationic palladacyclic intermediates with HFIP as a ligand



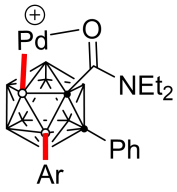

**IMA1-B4**
**0.0**



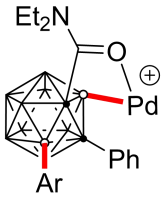

**IMA1-B6**
**-0.6**

L= HFIP

c) Cationic palladacyclic intermediates without any ligand

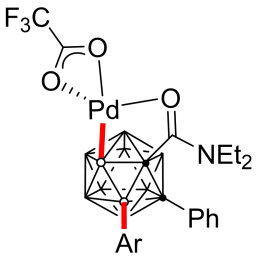



**IMA2-B4**
**0.0**

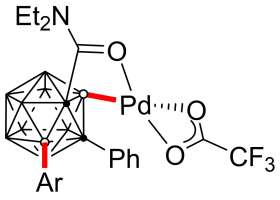



**IMA2-B6**
**1.8**

d) Neutral palladacyclic intermediates with TFA as a ligand



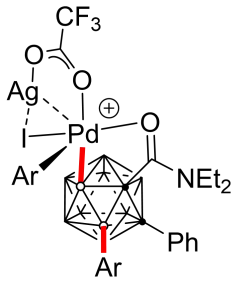

**IMA3-B4**
**0.0**




**IMA3-B6**
**-2.7**

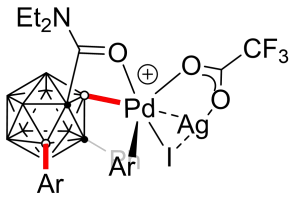
**Scheme S2.** Relative Gibbs free energies in kcal $mol^{-1}$ for various Pd(IV) intermediates at the B4 and B6 position generated after a second oxidative addition at the PBE0-D3(BJ)/def2- TZVP+SMD(HFIP)//TPSS-D3(BJ)/def2- SVP level of theory.

a) Cationic Pd(IV) intermediates with AgTFA as a ligand




**IMB-B4**

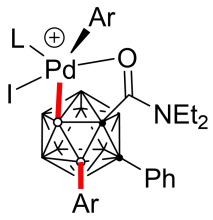
**0.0**




**IMB-B6**

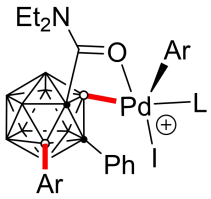
**1.9**

b) Cationic Pd(IV) intermediates with HFIP as a ligand




**IMB1-B4**

**0.0**

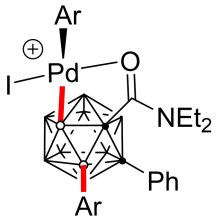



**IMB1-B6**

**0.1**

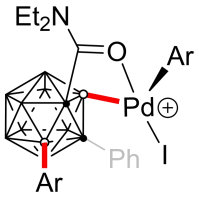
L=HFIP

c) Cationic Pd(IV) intermediates without any ligand




**IMB2-B4**

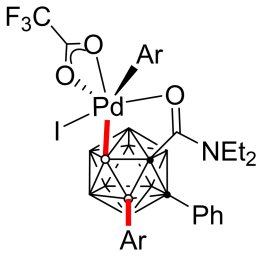
**0.0**



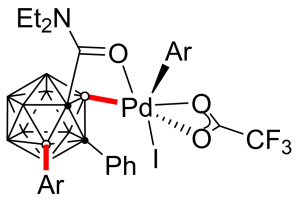

**IMB2-B6**

**-0.02**

d) Neutral Pd(IV) intermediates with TFA as a ligand



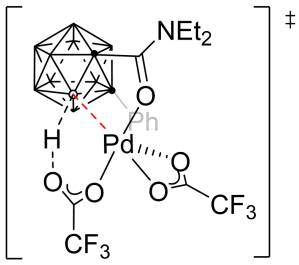

**IMB3-B4**
**0.0**



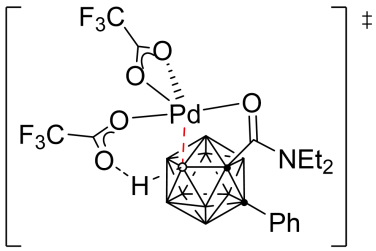

**IMB3-B6**
**-1.5**

**Scheme S3.** Relative Gibbs free energies in kcal $mol^{-1}$ for the first and second B–H activation transition states of neutral Pd(II) complexes at the B3 vs B4 and B4 vs B6 position, respectively, at the PBE0-D3(BJ)/def2- TZVP+SMD(HFIP)//TPSS-D3(BJ)/def2- SVP level of theory.

a) First B–H activation transition states at the B3 and B4 position

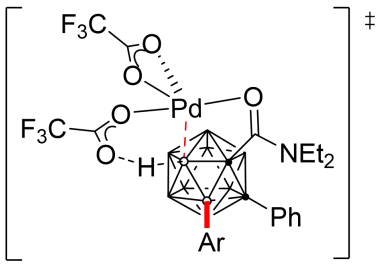



**TS1a-B3**
**0.0**

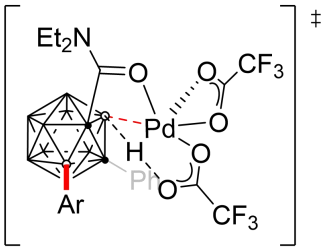



**TS1a-B4**
**1.3**

b) Second B–H activation transition states at the B4 and B6 position



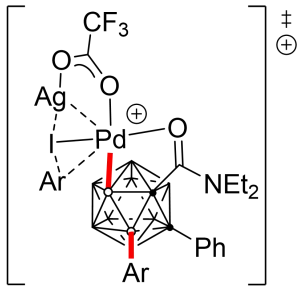

**TS2a-B4**
**0.0**




**TS2a-B6**
**0.7**

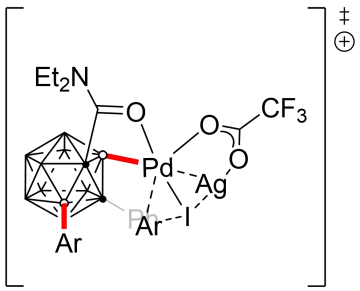
**Scheme S4.** Relative Gibbs free energies in kcal $mol^{-1}$ for various second oxidative addition transition states at the B4 and B6 position at the PBE0-D3(BJ)/def2- TZVP+SMD(HFIP) //TPSS-D3(BJ)/def2- SVP level of theory.

a) Oxidative addition transition states to the cationic palladacyclic intermediate with AgTFA as a ligand.




**TS3-B4**

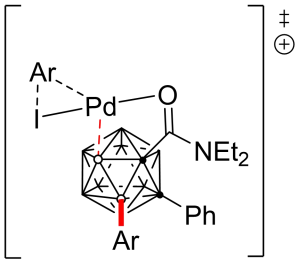
**0.0**




**TS3-B6**

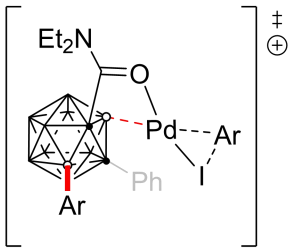
**1.0**

b) Oxidative addition transition states to the cationic palladacyclic intermediate without any ligand.




**TS3a-B4**

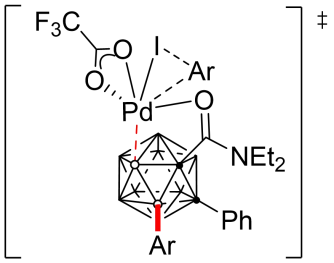
**0.0**




**TS3a-B6**

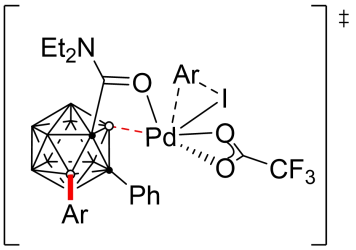
**-1.0**

c) Oxidative addition transition states to the neutral palladacyclic intermediate with TFA as a ligand.




**TS3b-B4**

**0.0**




**TS3b-B6**

**-0.6**

**Table S2.** Calculated electronic energies at the PBE0-D3(BJ)/def2- TZVP+SMD(HFIP) level of theory and total Gibbs free energies for all reported structures (in Hartree).

| Structure | Electronic Energy | Total Gibbs Free Energy |
|---|---|---|
| **IMA-B6** | -1958.72738 | -1958.28092 |
| **IMA-B4** | -1958.73032 | -1958.28255 |
| **IMA1-B6** | -2075.15553 | -2074.67689 |
| **IMA1-B4** | -2075.15294 | -2074.67593 |
| **IMA2-B6** | -1285.71571 | -1285.28436 |
| **IMA2-B4** | -1285.71878 | -1285.28720 |
| **IMA3-B6** | -1811.84673 | -1811.39893 |
| **IMA3-B4** | -1811.84314 | -1811.39462 |
| **IMB-B6** | -2240.83080 | -2240.28129 |
| **IMB-B4** | -2240.83569 | -2240.28436 |
| **IMB1-B6** | -2357.26437 | -2356.68199 |
| **IMB1-B4** | -2357.26806 | -2356.68209 |
| **IMB2-B6** | -1567.84397 | -1567.30874 |
| **IMB2-B4** | -1567.84474 | -1567.30870 |
| **IMB3-B6** | -2093.94339 | -2093.38933 |
| **IMB3-B4** | -2093.94276 | -2093.38689 |
| **TS1-B3** | -2215.06249 | -2214.68844 |
| **TS1-B4** | -2215.05063 | -2214.67925 |
| **TS1a-B3** | -2068.18141 | -2067.80638 |
| **TS1a-B4** | -2068.17822 | -2067.80425 |
| **TS2-B6** | -2485.22152 | -2484.75264 |
| **TS2-B4** | -2485.22716 | -2484.75800 |
| **TS2a-B6** | -2338.34253 | -2337.86967 |
| **TS2a-B4** | -2338.34461 | -2337.87077 |
| **TS3-B6** | -2240.81864 | -2240.26843 |
| **TS3-B4** | -2240.82092 | -2240.26999 |
| **TS3a-B6** | -1567.83254 | -1567.29860 |

| | | |
|---|---|---|
| **TS3a-B4** | -1567.83447 | -1567.29706 |
| **TS3b-B6** | -2093.92642 | -2093.37574 |
| **TS3b-B4** | -2093.92805 | -2093.37477 |

## Cartesian coordinates of the optimized structures

### IMA-B6

Lowest frequency = 8.77 $cm^{-1}$
Charge = 1, Multiplicity = 1
71

| | | | |
|---|---|---|---|
| O | -0.320984 | 1.990162 | 0.899212 |
| N | -2.080945 | 2.887741 | -0.152742 |
| C | -1.307988 | 1.832008 | 0.096827 |
| C | -1.437729 | 0.456173 | -0.540653 |
| C | -1.543458 | -0.861790 | 0.467729 |
| C | -1.827883 | -0.684555 | 1.939649 |
| C | -2.391576 | 0.478763 | 2.485662 |
| H | -2.726303 | 1.287611 | 1.836353 |
| C | -2.575226 | 0.610763 | 3.870760 |
| H | -3.012641 | 1.533149 | 4.264384 |
| C | -2.209692 | -0.419428 | 4.744560 |
| H | -2.343394 | -0.306628 | 5.824126 |
| C | -1.717806 | -1.627337 | 4.217267 |
| H | -1.528462 | -2.483321 | 4.872853 |
| C | -1.539278 | -1.773146 | 2.818622 |
| H | -1.322739 | -2.762148 | 2.401868 |
| C | -1.713693 | 4.173685 | 0.501075 |
| H | -2.142080 | 4.968267 | -0.127741 |
| H | -0.617437 | 4.263583 | 0.476351 |
| C | -2.238830 | 4.265589 | 1.935178 |
| H | -2.006468 | 5.262549 | 2.344558 |
| H | -1.758478 | 3.510973 | 2.578455 |
| H | -3.333630 | 4.130049 | 1.970287 |
| C | -3.281347 | 2.918148 | -1.011008 |
| H | -4.066487 | 3.434089 | -0.431730 |
| H | -3.625403 | 1.890007 | -1.153607 |
| C | -3.034798 | 3.619228 | -2.347237 |
| H | -2.241235 | 3.112955 | -2.920157 |
| H | -2.752019 | 4.676974 | -2.215897 |
| H | -3.963697 | 3.591085 | -2.940424 |
| B | -2.864526 | -0.625279 | -0.683539 |
| B | -2.407038 | -1.673413 | -2.045121 |
| H | -3.298833 | -2.116950 | -2.706049 |
| B | -1.989862 | 0.049861 | -2.102332 |
| H | -2.530184 | 0.885857 | -2.755360 |
| B | -0.836852 | -1.163381 | -2.720412 |
| H | -0.595062 | -1.222783 | -3.889473 |
| B | 0.423334 | -1.424978 | -1.473828 |
| H | 1.568228 | -1.678948 | -1.702059 |
| B | -0.397054 | -2.073039 | -0.030932 |
| H | 0.113710 | -2.745057 | 0.816751 |
| B | -2.128117 | -2.228955 | -0.378893 |

| | | | |
|---|---|---|---|
| H | -2.800850 | -2.985927 | 0.254530 |
| B | -0.923959 | -2.585514 | -1.647914 |
| H | -0.754585 | -3.710950 | -2.012945 |
| B | 0.061858 | -0.382380 | -0.113032 |
| B | -0.243669 | 0.207941 | -1.759903 |
| H | 0.336513 | 1.188303 | -2.121687 |
| Pd | 1.244654 | 0.725481 | 1.025143 |
| O | 2.798899 | -1.601076 | 2.868063 |
| C | 3.379887 | -1.170266 | 1.845749 |
| O | 2.956671 | -0.341651 | 0.975267 |
| C | 4.794304 | -1.729671 | 1.529432 |
| F | 4.683178 | -2.612207 | 0.515314 |
| F | 5.315193 | -2.353325 | 2.590049 |
| F | 5.619807 | -0.740717 | 1.154027 |
| C | -4.348518 | -0.310418 | -0.288929 |
| C | -5.217496 | 0.200050 | -1.284551 |
| C | -4.932250 | -0.657892 | 0.948994 |
| C | -6.576026 | 0.410170 | -1.035227 |
| H | -4.825521 | 0.420193 | -2.283959 |
| C | -6.293293 | -0.447251 | 1.199542 |
| H | -4.329064 | -1.124809 | 1.731715 |
| C | -7.141934 | 0.100068 | 0.218669 |
| H | -7.214494 | 0.806456 | -1.832664 |
| H | -6.709320 | -0.728201 | 2.173445 |
| C | -8.615418 | 0.299472 | 0.475949 |
| H | -9.201463 | -0.510973 | 0.003582 |
| H | -8.843023 | 0.292077 | 1.554007 |
| H | -8.972638 | 1.250872 | 0.046505 |
| Ag | 0.672513 | -1.228754 | 3.020507 |

## IMA-B4

Lowest frequency = 13.92 $cm^{-1}$
Charge = 1, Multiplicity = 1
71

| | | | |
|---|---|---|---|
| O | -0.591613 | 2.137574 | -0.544123 |
| N | -2.809693 | 2.504689 | -0.507127 |
| C | -1.730797 | 1.895952 | -0.011280 |
| C | -1.665147 | 0.960055 | 1.184690 |
| C | -2.651634 | -0.326844 | 1.600219 |
| C | -3.886425 | -0.631729 | 0.788146 |
| C | -3.870029 | -0.613416 | -0.621206 |
| H | -2.956246 | -0.370489 | -1.163817 |
| C | -5.033303 | -0.887835 | -1.349134 |
| H | -4.999438 | -0.868318 | -2.443010 |
| C | -6.229657 | -1.190165 | -0.683655 |
| H | -7.137907 | -1.408876 | -1.253555 |
| C | -6.253549 | -1.210465 | 0.717610 |
| H | -7.180676 | -1.444179 | 1.249677 |
| C | -5.093220 | -0.931473 | 1.450361 |
| H | -5.125975 | -0.945762 | 2.541130 |
| C | -2.620817 | 3.332037 | -1.730294 |
| H | -1.644583 | 3.832511 | -1.658992 |
| H | -3.406998 | 4.101390 | -1.709290 |
| C | -2.719964 | 2.482517 | -2.998809 |
| H | -2.622618 | 3.131168 | -3.884934 |
| H | -3.692278 | 1.964196 | -3.057356 |

| | | | |
|---|---|---|---|
| H | -1.915656 | 1.729741 | -3.034073 |
| C | -4.177897 | 2.518049 | 0.055214 |
| H | -4.305021 | 1.647647 | 0.705126 |
| H | -4.866078 | 2.378785 | -0.795034 |
| C | -4.476322 | 3.814804 | 0.809953 |
| H | -4.392424 | 4.702267 | 0.161014 |
| H | -3.790801 | 3.941792 | 1.663970 |
| H | -5.508438 | 3.774527 | 1.195584 |
| B | -1.072417 | -0.676911 | 0.873972 |
| B | -0.004487 | -1.010775 | 2.267305 |
| H | 0.903646 | -1.773941 | 2.096179 |
| B | -0.010242 | 0.599202 | 1.548377 |
| B | 0.089923 | 0.445210 | 3.307145 |
| H | 1.090571 | 0.748211 | 3.885656 |
| B | -1.552961 | 0.761917 | 3.953558 |
| H | -1.766512 | 1.282794 | 5.007614 |
| B | -2.631974 | -0.501684 | 3.317243 |
| H | -3.619321 | -0.893362 | 3.854620 |
| B | -1.689301 | -1.579617 | 2.282631 |
| H | -2.075964 | -2.691722 | 2.099489 |
| B | -0.961937 | -0.916453 | 3.768624 |
| H | -0.749808 | -1.631767 | 4.702200 |
| B | -2.635420 | 1.110764 | 2.602375 |
| H | -3.588229 | 1.817249 | 2.579164 |
| B | -0.950093 | 1.698967 | 2.575562 |
| H | -0.781230 | 2.879782 | 2.501685 |
| Pd | 1.190667 | 1.582362 | 0.299707 |
| O | 2.928975 | 1.150513 | 1.227368 |
| C | 3.574764 | 0.051800 | 1.202072 |
| O | 3.352554 | -0.985644 | 0.535991 |
| C | 4.760265 | 0.015497 | 2.203569 |
| F | 5.610389 | -0.975006 | 1.916242 |
| F | 4.251413 | -0.193059 | 3.438579 |
| F | 5.427391 | 1.178582 | 2.204191 |
| Ag | 1.502537 | -1.086161 | -0.579578 |
| C | -0.910612 | -1.399285 | -0.539584 |
| C | -1.195552 | -2.789099 | -0.633681 |
| C | -0.473376 | -0.761574 | -1.750298 |
| C | -1.079978 | -3.487331 | -1.837613 |
| H | -1.525355 | -3.326000 | 0.258277 |
| C | -0.345113 | -1.486986 | -2.958119 |
| H | -0.352336 | 0.325703 | -1.782023 |
| C | -0.645392 | -2.857979 | -3.025330 |
| H | -1.325114 | -4.554764 | -1.855783 |
| H | -0.024305 | -0.955124 | -3.860241 |
| C | -0.493618 | -3.638137 | -4.306309 |
| H | 0.399767 | -4.287903 | -4.256430 |
| H | -1.363152 | -4.295624 | -4.475644 |
| H | -0.379045 | -2.972333 | -5.176122 |

**IMA1-B6**

Lowest frequency = 6.86 $cm^{-1}$

Charge = 1, Multiplicity = 1

75

| | | | |
|---|---|---|---|
| O | -0.056387 | 2.227031 | -0.276009 |
| N | -2.161580 | 2.720750 | -0.855498 |

| | | | |
|---|---|---|---|
| C | -1.169675 | 1.835831 | -0.778445 |
| C | -1.201909 | 0.412282 | -1.318990 |
| C | -0.791469 | -0.810332 | -0.247958 |
| C | -0.725266 | -0.479812 | 1.223720 |
| C | -1.568506 | 0.491772 | 1.795405 |
| H | -2.324156 | 0.994052 | 1.188516 |
| C | -1.486580 | 0.793104 | 3.158740 |
| H | -2.152950 | 1.550004 | 3.583593 |
| C | -0.571315 | 0.116618 | 3.976980 |
| H | -0.510038 | 0.349037 | 5.044543 |
| C | 0.253533 | -0.870139 | 3.420544 |
| H | 0.964301 | -1.413803 | 4.050019 |
| C | 0.179887 | -1.166602 | 2.054194 |
| H | 0.828187 | -1.936674 | 1.634403 |
| C | -1.896254 | 4.093366 | -0.348108 |
| H | -2.607116 | 4.754165 | -0.866816 |
| H | -0.876531 | 4.372968 | -0.652365 |
| C | -2.060087 | 4.187445 | 1.170238 |
| H | -1.903232 | 5.231121 | 1.489331 |
| H | -1.321324 | 3.552075 | 1.683983 |
| H | -3.074352 | 3.884364 | 1.482588 |
| C | -3.524075 | 2.461406 | -1.356268 |
| H | -4.218524 | 2.875952 | -0.605114 |
| H | -3.685588 | 1.379390 | -1.363551 |
| C | -3.775458 | 3.076199 | -2.733375 |
| H | -3.077805 | 2.668159 | -3.482493 |
| H | -3.673985 | 4.174297 | -2.721324 |
| H | -4.804259 | 2.836884 | -3.049494 |
| B | -2.370790 | -0.926523 | -1.035478 |
| B | -2.063823 | -1.989853 | -2.426237 |
| H | -2.980945 | -2.647003 | -2.821226 |
| B | -2.029982 | -0.230806 | -2.661611 |
| H | -2.873469 | 0.424776 | -3.188191 |
| B | -0.843494 | -1.266975 | -3.506412 |
| H | -0.884916 | -1.392231 | -4.694790 |
| B | 0.703124 | -1.175017 | -2.610079 |
| H | 1.788525 | -1.236612 | -3.116479 |
| B | 0.406310 | -1.831080 | -0.977540 |
| H | 1.243807 | -2.323634 | -0.280854 |
| B | -1.285336 | -2.334844 | -0.861505 |
| H | -1.616809 | -3.146521 | -0.051996 |
| B | -0.379572 | -2.575815 | -2.383234 |
| H | -0.078711 | -3.678364 | -2.735365 |
| B | 0.456739 | -0.102001 | -1.250361 |
| B | -0.322965 | 0.274172 | -2.796901 |
| H | -0.046131 | 1.303441 | -3.337224 |
| Pd | 1.650008 | 1.167165 | -0.347200 |
| O | 3.391574 | -0.032668 | -0.628611 |
| C | -3.754977 | -0.882698 | -0.299178 |
| C | -4.921716 | -0.576537 | -1.038149 |
| C | -3.937799 | -1.327760 | 1.030172 |
| C | -6.194329 | -0.644714 | -0.461572 |
| H | -4.838527 | -0.305012 | -2.096658 |
| C | -5.209928 | -1.398526 | 1.605803 |
| H | -3.077475 | -1.645294 | 1.625370 |
| C | -6.363974 | -1.043969 | 0.878523 |

| | | | |
|---|---|---|---|
| H | -7.074389 | -0.404711 | -1.068486 |
| H | -5.311532 | -1.752335 | 2.637864 |
| C | -7.731822 | -1.096417 | 1.514091 |
| H | -8.526940 | -1.174594 | 0.755025 |
| H | -7.820194 | -1.951409 | 2.205171 |
| H | -7.921331 | -0.178892 | 2.102930 |
| C | 4.505754 | 0.034649 | 0.263446 |
| H | 5.376282 | -0.478178 | -0.180865 |
| C | 4.171183 | -0.668260 | 1.597237 |
| C | 4.861471 | 1.528524 | 0.395376 |
| F | 3.740220 | 2.252826 | 0.721068 |
| F | 5.769066 | 1.720211 | 1.350338 |
| F | 5.317534 | 2.000273 | -0.766841 |
| F | 3.260409 | 0.014379 | 2.314284 |
| F | 5.267774 | -0.846165 | 2.334913 |
| F | 3.642791 | -1.883532 | 1.298466 |
| H | 3.168588 | -0.964914 | -0.838040 |

**IMA1-B4**

Lowest frequency = 3.90 $cm^{-1}$

Charge = 1, Multiplicity = 1

75

| | | | |
|---|---|---|---|
| O | 0.072841 | 1.863033 | 0.141064 |
| N | 2.098988 | 2.553380 | -0.536011 |
| C | 1.127309 | 1.640952 | -0.553319 |
| C | 1.078885 | 0.357478 | -1.364302 |
| C | 2.228483 | -0.819740 | -1.598237 |
| C | 3.632245 | -0.623187 | -1.077544 |
| C | 4.727044 | -1.019752 | -1.870246 |
| H | 4.555879 | -1.465781 | -2.851407 |
| C | 6.037447 | -0.845623 | -1.407741 |
| H | 6.874926 | -1.162690 | -2.036539 |
| C | 6.274882 | -0.270977 | -0.151777 |
| H | 7.299765 | -0.137318 | 0.208005 |
| C | 5.189792 | 0.128898 | 0.640893 |
| H | 5.359576 | 0.574171 | 1.626250 |
| C | 3.878599 | -0.047797 | 0.186295 |
| H | 3.051724 | 0.265013 | 0.824782 |
| C | 1.947004 | 3.683056 | 0.422080 |
| H | 2.551437 | 4.511781 | 0.024076 |
| H | 0.891837 | 3.993037 | 0.422783 |
| C | 2.410373 | 3.283052 | 1.824528 |
| H | 2.301847 | 4.142160 | 2.507027 |
| H | 1.804456 | 2.449532 | 2.216082 |
| H | 3.470970 | 2.979064 | 1.820744 |
| C | 3.289059 | 2.613242 | -1.411364 |
| H | 4.139793 | 2.885175 | -0.765065 |
| H | 3.499319 | 1.611263 | -1.797390 |
| C | 3.107808 | 3.615407 | -2.552806 |
| H | 2.268152 | 3.322969 | -3.204974 |
| H | 2.921044 | 4.636746 | -2.181384 |
| H | 4.027889 | 3.638474 | -3.159935 |
| B | 1.700324 | 0.159519 | -2.957487 |
| B | 0.490886 | -0.799959 | -3.814599 |
| H | 0.369173 | -0.656268 | -4.994795 |
| B | -0.035589 | 0.453803 | -2.679204 |

| | | | |
|---|---|---|---|
| H | -0.468633 | 1.541389 | -2.917699 |
| B | -0.873782 | -1.118052 | -2.702928 |
| H | -2.005433 | -1.189114 | -3.090733 |
| B | -0.264732 | -2.097442 | -1.330658 |
| H | -0.942317 | -2.877422 | -0.719023 |
| B | 1.473391 | -2.370687 | -1.602704 |
| H | 2.125923 | -3.283030 | -1.201457 |
| B | 1.929666 | -1.582267 | -3.117361 |
| H | 2.855205 | -1.980961 | -3.750670 |
| B | 0.345577 | -2.380900 | -2.983632 |
| H | 0.125047 | -3.395045 | -3.577221 |
| B | 0.938982 | -1.162271 | -0.400860 |
| B | -0.461612 | -0.361335 | -1.162290 |
| Pd | -1.583507 | 0.692324 | 0.077819 |
| H | 2.454663 | 0.964267 | -3.395318 |
| C | 1.269580 | -1.312914 | 1.128667 |
| C | 2.183250 | -2.316055 | 1.535060 |
| C | 0.695360 | -0.528164 | 2.152088 |
| C | 2.510966 | -2.508234 | 2.878974 |
| H | 2.659092 | -2.952678 | 0.784376 |
| C | 1.024193 | -0.718618 | 3.499980 |
| H | -0.029779 | 0.253093 | 1.896282 |
| C | 1.941460 | -1.711041 | 3.892917 |
| H | 3.225522 | -3.294006 | 3.148124 |
| H | 0.555322 | -0.085323 | 4.261473 |
| C | 2.281752 | -1.939254 | 5.345221 |
| H | 1.996930 | -1.076404 | 5.968627 |
| H | 1.744974 | -2.825381 | 5.732614 |
| H | 3.360260 | -2.129874 | 5.478654 |
| O | -3.189056 | -0.669554 | 0.040068 |
| C | -4.201845 | -0.734206 | -0.978257 |
| H | -3.798784 | -1.172582 | -1.907470 |
| C | -5.324513 | -1.655771 | -0.456199 |
| C | -4.645309 | 0.708284 | -1.287471 |
| F | -6.149305 | -2.004816 | -1.445649 |
| F | -6.023858 | -1.098217 | 0.538119 |
| F | -4.722963 | -2.779413 | 0.024603 |
| F | -5.800046 | 0.706312 | -1.959454 |
| F | -4.784327 | 1.428010 | -0.158631 |
| F | -3.705501 | 1.314788 | -2.049157 |
| H | -2.875170 | -1.582913 | 0.216193 |

**IMA2-B6**

Lowest frequency = 20.07 $cm^{-1}$

Charge = 1, Multiplicity = 1

63

| | | | |
|---|---|---|---|
| O | -1.773162 | 0.901077 | 1.386865 |
| N | 0.269333 | 1.095375 | 2.288841 |
| C | -0.580739 | 0.450684 | 1.489718 |
| C | -0.292499 | -0.859741 | 0.763567 |
| C | -0.469629 | -0.891976 | -0.923892 |
| C | -0.779521 | 0.454821 | -1.541938 |
| C | -1.961042 | 0.596033 | -2.327363 |
| H | -2.494528 | -0.292468 | -2.677904 |
| C | -2.358052 | 1.867987 | -2.782677 |
| H | -3.252813 | 1.958871 | -3.406138 |

| | | | |
|---|---|---|---|
| C | -1.601105 | 3.002543 | -2.457980 |
| H | -1.910190 | 3.989893 | -2.813718 |
| C | -0.436238 | 2.861960 | -1.689791 |
| H | 0.165595 | 3.741539 | -1.441888 |
| C | -0.032168 | 1.601390 | -1.226135 |
| H | 0.867212 | 1.516109 | -0.612326 |
| C | -0.238735 | 2.310336 | 2.981077 |
| H | -1.270480 | 2.107321 | 3.304996 |
| H | 0.387348 | 2.438190 | 3.876763 |
| C | -0.178832 | 3.548182 | 2.084651 |
| H | -0.520555 | 4.428386 | 2.653836 |
| H | 0.851545 | 3.743211 | 1.740412 |
| H | -0.833539 | 3.427238 | 1.207009 |
| C | 1.674068 | 0.734979 | 2.554210 |
| H | 2.003698 | 0.046846 | 1.771090 |
| H | 2.264536 | 1.659086 | 2.427365 |
| C | 1.884524 | 0.138846 | 3.946582 |
| H | 1.619283 | 0.849397 | 4.747048 |
| H | 1.287581 | -0.777730 | 4.080614 |
| H | 2.949779 | -0.119135 | 4.066434 |
| B | -1.814772 | -1.337709 | 0.061268 |
| B | -1.886059 | -3.085727 | 0.135904 |
| H | -2.935473 | -3.644568 | 0.262883 |
| B | -1.154000 | -2.161184 | 1.484984 |
| H | -1.625013 | -1.944223 | 2.561077 |
| B | -0.347129 | -3.625540 | 0.883885 |
| H | -0.284510 | -4.597436 | 1.576941 |
| B | 0.997170 | -3.123226 | -0.182360 |
| H | 2.019095 | -3.737135 | -0.269748 |
| B | 0.311019 | -2.268004 | -1.585050 |
| H | 0.797884 | -2.145310 | -2.667202 |
| B | -1.446305 | -2.254403 | -1.385320 |
| H | -2.157048 | -2.152128 | -2.337004 |
| B | -0.540837 | -3.684830 | -0.888726 |
| H | -0.625033 | -4.697611 | -1.517711 |
| B | 1.096063 | -1.348232 | -0.267560 |
| B | 0.628661 | -2.178135 | 1.271108 |
| H | 1.330547 | -2.050597 | 2.224936 |
| Pd | -3.111816 | 0.156739 | -0.038634 |
| C | 2.457520 | -0.617005 | -0.541139 |
| C | 3.561775 | -0.861853 | 0.309868 |
| C | 2.710035 | 0.119309 | -1.720338 |
| C | 4.829470 | -0.342883 | 0.032528 |
| H | 3.433213 | -1.488997 | 1.199383 |
| C | 3.979313 | 0.637964 | -1.999318 |
| H | 1.910453 | 0.278160 | -2.450616 |
| C | 5.063393 | 0.426813 | -1.125272 |
| H | 5.658553 | -0.553017 | 0.717342 |
| H | 4.135617 | 1.206579 | -2.922682 |
| C | 6.440478 | 0.956178 | -1.442241 |
| H | 7.052275 | 0.169842 | -1.923123 |
| H | 6.395456 | 1.811896 | -2.135179 |
| H | 6.971836 | 1.269124 | -0.527868 |

**IMA2-B4**

Lowest frequency = 25.25 $cm^{-1}$

Charge = 1, Multiplicity = 1

63

| | | | |
|---|---|---|---|
| O | 1.416630 | 0.345117 | 1.719532 |
| N | -0.092658 | -1.224183 | 2.269135 |
| C | 0.661041 | -0.626230 | 1.349276 |
| C | 0.793819 | -0.986843 | -0.115759 |
| C | -0.362722 | -1.314367 | -1.256455 |
| C | -1.808683 | -1.457080 | -0.846508 |
| C | -2.590972 | -2.484086 | -1.409922 |
| H | -2.150955 | -3.166540 | -2.139152 |
| C | -3.932973 | -2.636539 | -1.039546 |
| H | -4.526201 | -3.438067 | -1.489955 |
| C | -4.511679 | -1.771113 | -0.101160 |
| H | -5.561070 | -1.891447 | 0.185087 |
| C | -3.737368 | -0.749024 | 0.465928 |
| H | -4.177748 | -0.062351 | 1.195718 |
| C | -2.397669 | -0.589011 | 0.096006 |
| H | -1.817572 | 0.217842 | 0.545425 |
| C | -0.122334 | -0.609464 | 3.625541 |
| H | -0.404380 | -1.411484 | 4.323854 |
| H | 0.896137 | -0.276583 | 3.873830 |
| C | -1.117127 | 0.552044 | 3.682104 |
| H | -1.128979 | 0.976238 | 4.699671 |
| H | -0.831726 | 1.349636 | 2.976452 |
| H | -2.138374 | 0.212207 | 3.439883 |
| C | -0.865622 | -2.476540 | 2.114838 |
| H | -1.837486 | -2.306161 | 2.606347 |
| H | -1.076443 | -2.636535 | 1.053089 |
| C | -0.131356 | -3.675331 | 2.717499 |
| H | 0.829050 | -3.848666 | 2.204228 |
| H | 0.067340 | -3.541497 | 3.793847 |
| H | -0.756781 | -4.575413 | 2.597812 |
| B | 0.761909 | -2.576962 | -0.772373 |
| B | 2.035481 | -2.599458 | -1.998033 |
| H | 2.589301 | -3.632075 | -2.232004 |
| B | 2.307069 | -1.737847 | -0.476647 |
| H | 2.958489 | -2.066291 | 0.470935 |
| B | 2.854215 | -1.002257 | -2.011684 |
| H | 4.023167 | -0.874544 | -2.235536 |
| B | 1.641242 | 0.242125 | -2.495501 |
| H | 1.919466 | 1.254015 | -3.069444 |
| B | 0.091990 | -0.601715 | -2.762695 |
| H | -0.796968 | -0.250561 | -3.474368 |
| B | 0.338938 | -2.326039 | -2.465168 |
| H | -0.347441 | -3.131640 | -3.010321 |
| B | 1.627580 | -1.378025 | -3.247339 |
| H | 1.882852 | -1.540552 | -4.403446 |
| B | 0.343350 | 0.335238 | -1.269805 |
| B | 2.022047 | -0.025256 | -0.808921 |
| Pd | 2.835302 | 1.212548 | 0.508307 |
| H | 0.348086 | -3.472132 | -0.111911 |
| C | -0.504021 | 1.608601 | -0.919208 |
| C | -1.679261 | 1.879404 | -1.661522 |

| | | | |
|---|---|---|---|
| C | -0.138494 | 2.559861 | 0.057221 |
| C | -2.447543 | 3.020966 | -1.424001 |
| H | -2.007014 | 1.178042 | -2.433932 |
| C | -0.906109 | 3.706065 | 0.296487 |
| H | 0.771903 | 2.408088 | 0.653357 |
| C | -2.080233 | 3.959314 | -0.437250 |
| H | -3.351849 | 3.190477 | -2.018809 |
| H | -0.584228 | 4.419352 | 1.063292 |
| C | -2.900030 | 5.204704 | -0.205997 |
| H | -2.658407 | 5.675876 | 0.760290 |
| H | -2.703048 | 5.947915 | -1.001095 |
| H | -3.980537 | 4.982965 | -0.230062 |

**IMA3-B6**

Lowest frequency = 14.66 $cm^{-1}$

Charge = 0, Multiplicity = 1

70

| | | | |
|---|---|---|---|
| O | -0.172404 | -2.148743 | -0.459436 |
| N | 1.896020 | -2.172898 | -1.309512 |
| C | 0.807330 | -1.487546 | -0.922621 |
| C | 0.612546 | 0.018349 | -1.076848 |
| C | 0.221276 | 0.880112 | 0.295575 |
| C | 0.352846 | 0.166224 | 1.620659 |
| C | -0.620777 | 0.362177 | 2.619225 |
| H | -1.462278 | 1.030442 | 2.430332 |
| C | -0.529948 | -0.319011 | 3.838123 |
| H | -1.299446 | -0.157426 | 4.599281 |
| C | 0.523927 | -1.213470 | 4.075929 |
| H | 0.588042 | -1.749970 | 5.028074 |
| C | 1.492944 | -1.416276 | 3.084912 |
| H | 2.324178 | -2.107759 | 3.256285 |
| C | 1.409898 | -0.728487 | 1.868148 |
| H | 2.187234 | -0.884178 | 1.117153 |
| C | 1.855252 | -3.644464 | -1.138786 |
| H | 0.849729 | -3.990597 | -1.421875 |
| H | 2.580593 | -4.061868 | -1.854723 |
| C | 2.189561 | -4.068512 | 0.293345 |
| H | 2.183857 | -5.169356 | 0.365001 |
| H | 3.190532 | -3.710459 | 0.591744 |
| H | 1.444076 | -3.668684 | 0.998816 |
| C | 3.139761 | -1.612772 | -1.852384 |
| H | 3.165171 | -0.545409 | -1.618720 |
| H | 3.973640 | -2.074070 | -1.293629 |
| C | 3.294753 | -1.849588 | -3.355754 |
| H | 3.325546 | -2.924422 | -3.603370 |
| H | 2.463714 | -1.386805 | -3.912267 |
| H | 4.239649 | -1.396050 | -3.699634 |
| B | -1.108199 | 0.289891 | -0.710015 |
| B | -1.574220 | 1.642623 | -1.729525 |
| H | -2.703807 | 1.711779 | -2.109987 |
| B | -0.457286 | 0.404204 | -2.366875 |
| H | -0.694420 | -0.480491 | -3.134787 |
| B | -0.159031 | 2.121128 | -2.714118 |
| H | -0.267082 | 2.538768 | -3.831537 |
| B | 1.120127 | 2.696114 | -1.613427 |
| H | 1.930985 | 3.525415 | -1.911758 |

| | | | |
|---|---|---|---|
| B | 0.507785 | 2.553346 | 0.054072 |
| H | 0.871748 | 3.177707 | 1.005538 |
| B | -1.139765 | 1.910063 | -0.020587 |
| H | -1.909317 | 2.134387 | 0.859454 |
| B | -0.589061 | 3.055248 | -1.258821 |
| H | -1.016939 | 4.173250 | -1.290205 |
| B | 1.673927 | 1.367353 | -0.580074 |
| B | 1.204945 | 1.058164 | -2.285181 |
| H | 2.032576 | 0.653463 | -3.042943 |
| Pd | -1.968288 | -1.309543 | 0.018682 |
| O | -3.626797 | -0.362085 | 0.610518 |
| C | -4.484916 | -0.019319 | -0.313195 |
| O | -4.521017 | -0.345842 | -1.489087 |
| C | -5.507839 | 1.002305 | 0.251035 |
| F | -6.555871 | 1.164906 | -0.573266 |
| F | -5.984255 | 0.642917 | 1.464641 |
| F | -4.901604 | 2.212796 | 0.392306 |
| C | 3.148729 | 1.349013 | -0.019179 |
| C | 4.235607 | 1.396736 | -0.921624 |
| C | 3.454874 | 1.499420 | 1.351741 |
| C | 5.557763 | 1.514117 | -0.478002 |
| H | 4.042668 | 1.367382 | -2.000026 |
| C | 4.775430 | 1.619213 | 1.797460 |
| H | 2.648042 | 1.539640 | 2.088411 |
| C | 5.856025 | 1.612667 | 0.894123 |
| H | 6.371628 | 1.549388 | -1.211525 |
| H | 4.970066 | 1.734314 | 2.870078 |
| C | 7.282324 | 1.709226 | 1.382335 |
| H | 7.950740 | 2.103573 | 0.598905 |
| H | 7.360242 | 2.361308 | 2.268902 |
| H | 7.664775 | 0.712443 | 1.674571 |

**IMA3-B4**

Lowest frequency = 13.79 $cm^{-1}$

Charge = 0, Multiplicity = 1

70

| | | | |
|---|---|---|---|
| O | -0.066648 | -0.085552 | 2.036724 |
| N | -1.978939 | -1.256226 | 2.104785 |
| C | -0.899559 | -0.824134 | 1.427174 |
| C | -0.521440 | -1.157290 | -0.007229 |
| C | -1.467556 | -1.140038 | -1.370103 |
| C | -2.954777 | -0.900207 | -1.253273 |
| C | -3.842971 | -1.639263 | -2.058406 |
| H | -3.447295 | -2.375442 | -2.760178 |
| C | -5.226007 | -1.439225 | -1.964325 |
| H | -5.897483 | -2.023785 | -2.601225 |
| C | -5.746317 | -0.500192 | -1.063441 |
| H | -6.827510 | -0.343897 | -0.991567 |
| C | -4.869200 | 0.239484 | -0.258501 |
| H | -5.257294 | 0.983187 | 0.444962 |
| C | -3.486630 | 0.045969 | -0.353419 |
| H | -2.826153 | 0.640551 | 0.277452 |
| C | -2.164543 | -0.699480 | 3.467348 |
| H | -2.804403 | -1.409864 | 4.013631 |
| H | -1.182969 | -0.664988 | 3.963318 |
| C | -2.802308 | 0.691364 | 3.420187 |

| | | | |
|---|---|---|---|
| H | -2.931166 | 1.078871 | 4.445011 |
| H | -2.161725 | 1.393490 | 2.861623 |
| H | -3.793935 | 0.655751 | 2.937032 |
| C | -2.949515 | -2.284854 | 1.694009 |
| H | -3.947290 | -1.919314 | 1.990618 |
| H | -2.958296 | -2.355072 | 0.602308 |
| C | -2.643747 | -3.646651 | 2.321742 |
| H | -1.656331 | -4.013116 | 1.995279 |
| H | -2.649984 | -3.601791 | 3.424149 |
| H | -3.408266 | -4.376229 | 2.005336 |
| B | -0.824375 | -2.661085 | -0.787771 |
| B | 0.613426 | -2.986245 | -1.750420 |
| H | 0.913786 | -4.125878 | -1.961549 |
| B | 0.789976 | -2.268612 | -0.136856 |
| H | 1.118272 | -2.815516 | 0.873500 |
| B | 1.795883 | -1.668683 | -1.481706 |
| H | 2.973390 | -1.866595 | -1.487667 |
| B | 1.070993 | -0.141423 | -2.072520 |
| H | 1.701804 | 0.773316 | -2.512559 |
| B | -0.554488 | -0.530173 | -2.693888 |
| H | -1.166353 | 0.065811 | -3.527653 |
| B | -0.827438 | -2.266366 | -2.505434 |
| H | -1.584425 | -2.845530 | -3.222294 |
| B | 0.787218 | -1.671377 | -2.947575 |
| H | 1.212726 | -1.865478 | -4.050099 |
| B | -0.364100 | 0.255183 | -1.099839 |
| B | 1.062051 | -0.520155 | -0.343929 |
| Pd | 1.785110 | 0.374413 | 1.260666 |
| O | 3.534003 | 0.831520 | 0.404428 |
| C | 4.411541 | -0.134835 | 0.399490 |
| O | 4.359276 | -1.221142 | 0.958661 |
| C | 5.609702 | 0.211256 | -0.524086 |
| F | 6.664545 | -0.588385 | -0.284790 |
| F | 5.244466 | 0.034899 | -1.821217 |
| F | 6.020142 | 1.491268 | -0.385001 |
| H | -1.579251 | -3.437679 | -0.299416 |
| C | -0.961824 | 1.690444 | -0.833507 |
| C | -1.885827 | 2.249058 | -1.748541 |
| C | -0.591125 | 2.496011 | 0.263310 |
| C | -2.427143 | 3.523465 | -1.559894 |
| H | -2.199615 | 1.670057 | -2.621741 |
| C | -1.134460 | 3.772264 | 0.456013 |
| H | 0.157841 | 2.118924 | 0.971245 |
| C | -2.067309 | 4.311286 | -0.448540 |
| H | -3.143708 | 3.916025 | -2.290806 |
| H | -0.817115 | 4.364505 | 1.322292 |
| C | -2.629886 | 5.700947 | -0.262822 |
| H | -2.579632 | 6.019263 | 0.791878 |
| H | -2.055828 | 6.435834 | -0.858652 |
| H | -3.680023 | 5.758942 | -0.597201 |

**IMB-B6**

Lowest frequency = 15.73 $cm^{-1}$

Charge = 1, Multiplicity = 1

86

| | | | |
|---|---|---|---|
| O | 0.113444 | -1.372279 | 1.828079 |
| N | 2.240699 | -2.021977 | 1.890552 |
| C | 1.191845 | -1.609208 | 1.181213 |
| C | 1.129208 | -1.459764 | -0.332189 |
| C | 0.560392 | -0.027259 | -0.971240 |
| C | 0.358566 | 1.195381 | -0.103287 |
| C | 0.993914 | 1.373774 | 1.140059 |
| H | 1.685501 | 0.623170 | 1.522508 |
| C | 0.803090 | 2.543091 | 1.889557 |
| H | 1.292015 | 2.641235 | 2.862490 |
| C | -0.000114 | 3.577715 | 1.399456 |
| H | -0.148656 | 4.488689 | 1.985323 |
| C | -0.612682 | 3.440548 | 0.138851 |
| H | -1.180251 | 4.271462 | -0.293944 |
| C | -0.439488 | 2.255613 | -0.612784 |
| H | -0.852254 | 2.185668 | -1.621701 |
| C | 2.035974 | -2.202183 | 3.356551 |
| H | 2.805707 | -2.917789 | 3.681867 |
| H | 1.047115 | -2.661599 | 3.502146 |
| C | 2.148218 | -0.884223 | 4.124334 |
| H | 2.070369 | -1.086085 | 5.205326 |
| H | 1.332203 | -0.197261 | 3.854452 |
| H | 3.119314 | -0.394363 | 3.937178 |
| C | 3.604582 | -2.294918 | 1.398886 |
| H | 4.291569 | -1.782455 | 2.094009 |
| H | 3.723732 | -1.807424 | 0.428001 |
| C | 3.915006 | -3.790159 | 1.322743 |
| H | 3.220504 | -4.305023 | 0.639420 |
| H | 3.858271 | -4.275641 | 2.311209 |
| H | 4.940790 | -3.922608 | 0.940874 |
| B | 2.213766 | -0.510047 | -1.406638 |
| B | 1.996899 | -1.325077 | -2.972029 |
| H | 2.923346 | -1.298723 | -3.727119 |
| B | 2.047558 | -2.297581 | -1.494396 |
| H | 2.952824 | -2.978973 | -1.132976 |
| B | 0.907468 | -2.727071 | -2.792798 |
| H | 1.057815 | -3.736494 | -3.415829 |
| B | -0.711246 | -2.123706 | -2.331820 |
| H | -1.734981 | -2.657622 | -2.640894 |
| B | -0.596441 | -0.354124 | -2.217900 |
| H | -1.498943 | 0.408748 | -2.359637 |
| B | 1.059220 | 0.139557 | -2.603155 |
| H | 1.276475 | 1.254869 | -2.970970 |
| B | 0.295475 | -1.206647 | -3.489648 |
| H | -0.016313 | -1.076158 | -4.636259 |
| B | -0.588306 | -1.350931 | -0.763493 |
| B | 0.381303 | -2.807302 | -1.095513 |
| H | 0.222461 | -3.771006 | -0.410871 |
| Pd | -1.683592 | -0.992152 | 0.919241 |
| O | -2.233415 | 1.881808 | 2.893414 |
| C | -2.190646 | 0.761985 | 3.472008 |

| | | | |
|---|---|---|---|
| O | -2.313856 | -0.390246 | 2.980461 |
| C | -1.856129 | 0.827707 | 4.986427 |
| F | -2.064006 | -0.345131 | 5.604104 |
| F | -2.554668 | 1.780216 | 5.614535 |
| F | -0.529075 | 1.128362 | 5.104922 |
| C | 3.509046 | 0.270443 | -0.996162 |
| C | 4.757800 | -0.390702 | -1.094825 |
| C | 3.540724 | 1.650787 | -0.698922 |
| C | 5.961801 | 0.272795 | -0.845129 |
| H | 4.790520 | -1.443718 | -1.397160 |
| C | 4.746434 | 2.315626 | -0.446863 |
| H | 2.616366 | 2.233186 | -0.685124 |
| C | 5.980549 | 1.640741 | -0.503398 |
| H | 6.906735 | -0.275003 | -0.932860 |
| H | 4.729805 | 3.386526 | -0.215852 |
| C | 7.283488 | 2.362934 | -0.262093 |
| H | 7.779154 | 2.594459 | -1.223445 |
| H | 7.126159 | 3.314583 | 0.270565 |
| H | 7.983698 | 1.742967 | 0.323191 |
| Ag | -2.585253 | 1.769141 | 0.720069 |
| I | -3.888664 | -0.433178 | -0.366760 |
| C | -2.234424 | -2.938909 | 1.127853 |
| C | -2.639555 | -3.768248 | 0.086914 |
| C | -2.161855 | -3.337432 | 2.459879 |
| C | -2.957934 | -5.097776 | 0.413230 |
| H | -2.702578 | -3.427210 | -0.946884 |
| C | -2.487321 | -4.676669 | 2.744360 |
| H | -1.883843 | -2.647002 | 3.259538 |
| C | -2.887807 | -5.573591 | 1.736237 |
| H | -3.274098 | -5.766981 | -0.394879 |
| H | -2.427883 | -5.013358 | 3.785540 |
| C | -3.271794 | -6.996565 | 2.068542 |
| H | -4.368668 | -7.082886 | 2.180390 |
| H | -2.966990 | -7.691764 | 1.268898 |
| H | -2.813965 | -7.326859 | 3.014779 |

**IMB-B4**

Lowest frequency = 19.98 $cm^{-1}$

Charge = 1, Multiplicity = 1

86

| | | | |
|---|---|---|---|
| O | 0.384987 | 1.093042 | 1.183958 |
| N | 2.327716 | 1.689126 | 2.093470 |
| C | 1.621962 | 1.352800 | 1.013473 |
| C | 2.085096 | 1.308791 | -0.435187 |
| C | 3.485049 | 0.467682 | -1.167532 |
| C | 4.558084 | -0.216164 | -0.370559 |
| C | 5.753160 | 0.478909 | -0.078878 |
| H | 5.874426 | 1.515317 | -0.405250 |
| C | 6.795145 | -0.154955 | 0.604702 |
| H | 7.715661 | 0.397064 | 0.817867 |
| C | 6.667412 | -1.495777 | 0.998113 |
| H | 7.483709 | -1.992083 | 1.532052 |
| C | 5.501260 | -2.203778 | 0.677769 |
| H | 5.405066 | -3.259164 | 0.950547 |
| C | 4.457075 | -1.574005 | -0.010909 |
| H | 3.573385 | -2.149728 | -0.285124 |

| | | | |
|---|---|---|---|
| C | 1.584408 | 1.770078 | 3.384636 |
| H | 2.185249 | 2.424907 | 4.033477 |
| H | 0.621892 | 2.264596 | 3.185046 |
| C | 1.371298 | 0.401520 | 4.033258 |
| H | 0.923405 | 0.541105 | 5.030997 |
| H | 0.679410 | -0.215852 | 3.441101 |
| H | 2.327960 | -0.133955 | 4.160585 |
| C | 3.768346 | 1.991072 | 2.165589 |
| H | 4.158865 | 1.432081 | 3.033341 |
| H | 4.254855 | 1.568166 | 1.282221 |
| C | 4.054833 | 3.486804 | 2.302627 |
| H | 3.659531 | 4.046923 | 1.439536 |
| H | 3.614736 | 3.908183 | 3.221662 |
| H | 5.145511 | 3.642004 | 2.349591 |
| B | 3.380862 | 2.197945 | -1.103389 |
| B | 2.830404 | 2.723970 | -2.708442 |
| H | 3.213968 | 3.765629 | -3.151643 |
| B | 1.678045 | 2.693333 | -1.355069 |
| H | 1.298920 | 3.638080 | -0.732916 |
| B | 1.179776 | 2.083686 | -2.962361 |
| H | 0.355413 | 2.656448 | -3.612150 |
| B | 1.287091 | 0.299824 | -2.909217 |
| H | 0.549566 | -0.422034 | -3.510084 |
| B | 2.978788 | -0.158822 | -2.656054 |
| H | 3.465828 | -1.200992 | -2.976588 |
| B | 3.935073 | 1.340824 | -2.555771 |
| H | 5.101522 | 1.350978 | -2.804527 |
| B | 2.570976 | 1.248006 | -3.689434 |
| H | 2.764217 | 1.209896 | -4.868416 |
| B | 1.839971 | -0.186504 | -1.270440 |
| B | 0.726602 | 1.204867 | -1.503316 |
| Pd | -0.905795 | 0.699442 | -0.377338 |
| H | 4.104433 | 2.802738 | -0.384268 |
| C | 1.304830 | -1.510113 | -0.585954 |
| C | 0.828498 | -2.547458 | -1.444312 |
| C | 1.280869 | -1.776597 | 0.802506 |
| C | 0.331587 | -3.763713 | -0.916811 |
| H | 0.926297 | -2.434247 | -2.529037 |
| C | 0.784336 | -2.977352 | 1.321357 |
| H | 1.679230 | -1.044544 | 1.507530 |
| C | 0.282200 | -3.988921 | 0.481127 |
| H | 0.027791 | -4.562205 | -1.603869 |
| H | 0.765486 | -3.123944 | 2.405656 |
| C | -0.338797 | -5.233098 | 1.054811 |
| H | 0.244785 | -5.615934 | 1.908505 |
| H | -1.350450 | -4.987017 | 1.428245 |
| H | -0.433750 | -6.029883 | 0.300353 |
| C | -1.606784 | 2.599683 | -0.262641 |
| C | -2.121105 | 2.865810 | 1.005117 |
| C | -1.573139 | 3.533507 | -1.294697 |
| C | -2.592989 | 4.168334 | 1.247316 |
| H | -2.170403 | 2.098068 | 1.781407 |
| C | -2.054169 | 4.824097 | -1.013999 |
| H | -1.186473 | 3.297156 | -2.286881 |
| C | -2.568811 | 5.163403 | 0.251175 |
| H | -2.992384 | 4.398966 | 2.241489 |

| | | | |
|---|---|---|---|
| H | -2.029595 | 5.572280 | -1.814312 |
| C | -3.120123 | 6.544343 | 0.519490 |
| H | -3.050088 | 6.805439 | 1.587981 |
| H | -2.586564 | 7.311268 | -0.065616 |
| H | -4.187771 | 6.594482 | 0.234905 |
| I | -2.447759 | 0.286898 | -2.448016 |
| Ag | -1.577526 | -2.042974 | -1.210008 |
| O | -2.194402 | -0.145159 | 1.251711 |
| C | -2.399887 | -1.347402 | 1.567499 |
| O | -2.334648 | -2.383337 | 0.856679 |
| C | -2.681687 | -1.590086 | 3.074703 |
| F | -1.475090 | -1.763357 | 3.698344 |
| F | -3.290818 | -0.544614 | 3.653990 |
| F | -3.411208 | -2.691583 | 3.286716 |

**IMB1-B6**

Lowest frequency = 10.18 $cm^{-1}$

Charge = 1, Multiplicity = 1

90

| | | | |
|---|---|---|---|
| O | 0.542182 | 0.593065 | 1.035800 |
| N | 2.212832 | 0.541067 | 2.513507 |
| C | 1.568024 | -0.018710 | 1.489965 |
| C | 1.906830 | -1.360412 | 0.853192 |
| C | 1.954930 | -1.383421 | -0.822753 |
| C | 1.777273 | -0.044809 | -1.511285 |
| C | 0.830369 | 0.074931 | -2.555185 |
| H | 0.325064 | -0.812093 | -2.941004 |
| C | 0.570799 | 1.326237 | -3.140143 |
| H | -0.164962 | 1.393624 | -3.944836 |
| C | 1.245325 | 2.468333 | -2.693117 |
| H | 1.041916 | 3.441539 | -3.150010 |
| C | 2.194352 | 2.352411 | -1.663299 |
| H | 2.738050 | 3.236003 | -1.314674 |
| C | 2.455933 | 1.111105 | -1.075066 |
| H | 3.190866 | 1.045120 | -0.270219 |
| C | 1.641817 | 1.798849 | 3.066199 |
| H | 0.547134 | 1.692053 | 3.077222 |
| H | 1.994809 | 1.862525 | 4.106629 |
| C | 2.067881 | 3.029739 | 2.264662 |
| H | 1.667626 | 3.937262 | 2.746317 |
| H | 3.166930 | 3.120755 | 2.224715 |
| H | 1.676176 | 2.979181 | 1.236384 |
| C | 3.448648 | 0.063402 | 3.161457 |
| H | 3.967077 | -0.598845 | 2.463521 |
| H | 4.092265 | 0.950186 | 3.290839 |
| C | 3.181123 | -0.623485 | 4.500949 |
| H | 2.703674 | 0.058103 | 5.224740 |
| H | 2.533070 | -1.505154 | 4.370289 |
| H | 4.139227 | -0.957060 | 4.932686 |
| B | 0.473803 | -1.886611 | -0.037271 |
| B | 0.497059 | -3.632048 | 0.013890 |
| H | -0.533175 | -4.236716 | -0.010539 |
| B | 1.004829 | -2.696246 | 1.454438 |
| H | 0.406024 | -2.512229 | 2.469400 |
| B | 1.932672 | -4.131733 | 0.955773 |
| H | 1.935141 | -5.106511 | 1.648338 |

| | | | |
|---|---|---|---|
| B | 3.392830 | -3.581733 | 0.087971 |
| H | 4.441678 | -4.152994 | 0.138590 |
| B | 2.868420 | -2.723063 | -1.382462 |
| H | 3.483794 | -2.566475 | -2.392710 |
| B | 1.101058 | -2.768265 | -1.426351 |
| H | 0.536969 | -2.679571 | -2.469454 |
| B | 1.984201 | -4.175328 | -0.823327 |
| H | 2.015830 | -5.183489 | -1.464605 |
| B | 3.448299 | -1.808650 | 0.035174 |
| B | 2.794219 | -2.663461 | 1.478536 |
| H | 3.349488 | -2.547741 | 2.523652 |
| Pd | -0.803423 | -0.322653 | -0.259705 |
| O | -1.696200 | 1.843474 | -0.687850 |
| C | 4.794569 | -1.005729 | -0.025566 |
| C | 5.750298 | -1.156138 | 1.005564 |
| C | 5.203669 | -0.290405 | -1.175186 |
| C | 7.015823 | -0.565136 | 0.925781 |
| H | 5.517062 | -1.778112 | 1.877097 |
| C | 6.468177 | 0.299865 | -1.256746 |
| H | 4.531168 | -0.203639 | -2.034016 |
| C | 7.397908 | 0.184831 | -0.203507 |
| H | 7.727945 | -0.704399 | 1.746741 |
| H | 6.746485 | 0.848854 | -2.163257 |
| C | 8.774785 | 0.793360 | -0.310365 |
| H | 9.215312 | 0.974668 | 0.683538 |
| H | 9.454383 | 0.111397 | -0.855405 |
| H | 8.752440 | 1.745493 | -0.866347 |
| C | -1.912807 | -0.871413 | 1.335958 |
| C | -2.171323 | 0.207479 | 2.182427 |
| C | -2.353852 | -2.167262 | 1.614893 |
| C | -2.895394 | -0.034365 | 3.363698 |
| H | -1.830984 | 1.218273 | 1.950176 |
| C | -3.066264 | -2.376942 | 2.804700 |
| H | -2.157698 | -3.002114 | 0.940790 |
| C | -3.352371 | -1.322666 | 3.695266 |
| H | -3.102713 | 0.808519 | 4.032538 |
| H | -3.413361 | -3.391454 | 3.030823 |
| I | -2.498842 | -1.514969 | -1.807734 |
| C | -4.147446 | -1.571866 | 4.955092 |
| H | -3.745898 | -2.433951 | 5.515214 |
| H | -4.140719 | -0.691905 | 5.617691 |
| H | -5.200010 | -1.804332 | 4.710326 |
| C | -2.977398 | 2.289365 | -1.111322 |
| H | -3.657190 | 1.422795 | -1.073890 |
| C | -3.478990 | 3.364195 | -0.122876 |
| C | -2.888870 | 2.784847 | -2.570915 |
| F | -2.622033 | 4.412336 | -0.101223 |
| F | -3.521699 | 2.847059 | 1.122691 |
| F | -4.700312 | 3.806376 | -0.437855 |
| F | -4.009184 | 3.388683 | -2.972640 |
| F | -2.630759 | 1.758468 | -3.400161 |
| F | -1.855146 | 3.666532 | -2.682029 |
| H | -1.032417 | 2.536259 | -0.888386 |

**IMB1-B4**

Lowest frequency = 16.48 $cm^{-1}$

Charge = 1, Multiplicity = 1

90

| | | | |
|---|---|---|---|
| O | 0.111114 | -0.915174 | -0.527259 |
| N | 1.241981 | -2.638961 | -1.376559 |
| C | 1.067793 | -1.744280 | -0.400406 |
| C | 1.844133 | -1.628137 | 0.904883 |
| C | 3.604037 | -1.366959 | 1.129210 |
| C | 4.617577 | -1.437209 | 0.026040 |
| C | 5.242702 | -2.661924 | -0.291944 |
| H | 4.961545 | -3.572805 | 0.243680 |
| C | 6.251920 | -2.713459 | -1.259046 |
| H | 6.729751 | -3.670193 | -1.491078 |
| C | 6.666288 | -1.540827 | -1.908326 |
| H | 7.459033 | -1.581278 | -2.661759 |
| C | 6.085678 | -0.312750 | -1.561960 |
| H | 6.430348 | 0.612429 | -2.033817 |
| C | 5.076299 | -0.257411 | -0.593758 |
| H | 4.664329 | 0.709919 | -0.300966 |
| C | 0.267596 | -2.600159 | -2.502907 |
| H | 0.273538 | -3.609162 | -2.942834 |
| H | -0.728923 | -2.412186 | -2.077606 |
| C | 0.621307 | -1.542765 | -3.549288 |
| H | -0.097336 | -1.603739 | -4.383125 |
| H | 0.559342 | -0.531706 | -3.119640 |
| H | 1.634492 | -1.705085 | -3.955728 |
| C | 2.273841 | -3.686910 | -1.464462 |
| H | 2.622106 | -3.690675 | -2.511297 |
| H | 3.129487 | -3.381548 | -0.856201 |
| C | 1.751647 | -5.064096 | -1.053816 |
| H | 1.406292 | -5.060167 | -0.007029 |
| H | 0.915937 | -5.392016 | -1.694377 |
| H | 2.562657 | -5.804994 | -1.150639 |
| B | 2.799393 | -2.818176 | 1.652097 |
| B | 2.527921 | -2.631320 | 3.398479 |
| H | 2.567768 | -3.593658 | 4.106319 |
| B | 1.167580 | -2.397683 | 2.274700 |
| H | 0.288601 | -3.175428 | 2.057708 |
| B | 1.403106 | -1.260757 | 3.641934 |
| H | 0.617502 | -1.215569 | 4.541474 |
| B | 2.211676 | 0.202804 | 2.990532 |
| H | 2.017976 | 1.300699 | 3.414977 |
| B | 3.809668 | -0.246966 | 2.382853 |
| H | 4.744425 | 0.487893 | 2.283881 |
| B | 4.013924 | -1.997746 | 2.652671 |
| H | 5.095301 | -2.495712 | 2.730212 |
| B | 3.154656 | -1.020151 | 3.862564 |
| H | 3.650353 | -0.800774 | 4.927759 |
| B | 2.455855 | -0.031730 | 1.223655 |
| B | 0.994448 | -0.649890 | 2.045845 |
| Pd | -0.425761 | 0.383856 | 1.019980 |
| H | 3.008464 | -3.846125 | 1.100054 |
| C | 2.167729 | 1.113496 | 0.163031 |
| C | 1.687188 | 2.358154 | 0.640971 |

| | | | |
|---|---|---|---|
| C | 2.255250 | 0.959301 | -1.245110 |
| C | 1.322057 | 3.393930 | -0.240253 |
| H | 1.620058 | 2.535365 | 1.717633 |
| C | 1.901766 | 1.987547 | -2.116330 |
| H | 2.615417 | 0.017089 | -1.669260 |
| C | 1.431990 | 3.235350 | -1.633816 |
| H | 0.956727 | 4.339406 | 0.173964 |
| H | 1.990222 | 1.832466 | -3.197107 |
| C | 1.104845 | 4.356422 | -2.589402 |
| H | 0.461423 | 4.004492 | -3.412906 |
| H | 0.596384 | 5.187560 | -2.077884 |
| H | 2.033298 | 4.749486 | -3.042501 |
| C | -1.890653 | -0.904818 | 1.517365 |
| C | -2.663035 | -1.281428 | 0.414729 |
| C | -2.117682 | -1.427810 | 2.793849 |
| C | -3.697019 | -2.215152 | 0.607318 |
| H | -2.465806 | -0.894546 | -0.587677 |
| C | -3.149949 | -2.364157 | 2.953342 |
| H | -1.519343 | -1.123402 | 3.654029 |
| C | -3.959310 | -2.769526 | 1.873456 |
| H | -4.300670 | -2.517414 | -0.256097 |
| H | -3.329775 | -2.776163 | 3.952764 |
| C | -5.087043 | -3.753042 | 2.079711 |
| H | -5.475443 | -4.129653 | 1.119948 |
| H | -4.759522 | -4.614500 | 2.686565 |
| H | -5.925187 | -3.274358 | 2.618929 |
| I | -1.166909 | 1.919800 | 2.965535 |
| C | -2.962905 | 3.471417 | -1.222013 |
| C | -2.568679 | 1.982743 | -1.326390 |
| C | -2.451089 | 1.448732 | -2.770066 |
| H | -3.339482 | 1.394846 | -0.803726 |
| F | -1.369254 | 1.980845 | -3.388026 |
| F | -2.267623 | 0.104204 | -2.737923 |
| F | -3.536304 | 1.702340 | -3.506795 |
| F | -1.997085 | 4.244534 | -1.784316 |
| F | -3.069439 | 3.819266 | 0.067441 |
| F | -4.124224 | 3.723695 | -1.838769 |
| O | -1.342321 | 1.769481 | -0.662157 |
| H | -0.637966 | 2.352219 | -1.032929 |

**IMB2-B6**

Lowest frequency = 15.23 $cm^{-1}$

Charge = 1, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | -0.236676 | 0.865503 | -1.239357 |
| N | 1.397705 | 2.361180 | -0.952922 |
| C | 0.721085 | 1.301102 | -0.513901 |
| C | 0.941500 | 0.601726 | 0.821814 |
| C | 1.056365 | -1.077853 | 0.757130 |
| C | 1.043219 | -1.671090 | -0.636505 |
| C | 0.083418 | -2.664171 | -0.948437 |
| H | -0.510553 | -3.120186 | -0.154351 |
| C | -0.058861 | -3.126880 | -2.269491 |
| H | -0.809758 | -3.892489 | -2.485653 |
| C | 0.760670 | -2.620303 | -3.284739 |
| H | 0.654574 | -2.982702 | -4.311622 |

| | | | |
|---|---|---|---|
| C | 1.725768 | -1.648901 | -2.974397 |
| H | 2.375996 | -1.251711 | -3.759939 |
| C | 1.858851 | -1.167214 | -1.667475 |
| H | 2.595365 | -0.389555 | -1.455167 |
| C | 0.946797 | 2.972830 | -2.232532 |
| H | -0.153258 | 2.961138 | -2.238753 |
| H | 1.282467 | 4.020525 | -2.203528 |
| C | 1.513655 | 2.246035 | -3.452919 |
| H | 1.200151 | 2.772582 | -4.369529 |
| H | 2.616896 | 2.227909 | -3.430535 |
| H | 1.138476 | 1.211630 | -3.500226 |
| C | 2.567991 | 2.995694 | -0.317934 |
| H | 3.021580 | 2.272210 | 0.364484 |
| H | 3.301018 | 3.169460 | -1.124107 |
| C | 2.215159 | 4.301198 | 0.395500 |
| H | 1.805595 | 5.053005 | -0.299680 |
| H | 1.479087 | 4.128063 | 1.197185 |
| H | 3.128508 | 4.722178 | 0.847383 |
| B | -0.486971 | -0.366851 | 1.128044 |
| B | -0.698765 | -0.420089 | 2.856706 |
| H | -1.795765 | -0.512592 | 3.320768 |
| B | -0.139573 | 1.091854 | 2.071008 |
| H | -0.759625 | 2.090041 | 1.865693 |
| B | 0.629050 | 0.538557 | 3.577942 |
| H | 0.486114 | 1.171358 | 4.582229 |
| B | 2.176683 | -0.246693 | 3.160988 |
| H | 3.145308 | -0.196023 | 3.859508 |
| B | 1.821119 | -1.682706 | 2.167862 |
| H | 2.493375 | -2.659428 | 2.036818 |
| B | 0.063708 | -1.790466 | 1.995228 |
| H | -0.446291 | -2.842399 | 1.776002 |
| B | 0.745609 | -1.238367 | 3.529780 |
| H | 0.682182 | -1.936485 | 4.497686 |
| B | 2.448023 | -0.194135 | 1.407424 |
| B | 1.639405 | 1.176981 | 2.254527 |
| H | 2.164128 | 2.244450 | 2.260592 |
| Pd | -1.618195 | -0.532964 | -0.556198 |
| C | 3.887833 | -0.163882 | 0.785828 |
| C | 4.775179 | 0.886564 | 1.120529 |
| C | 4.431842 | -1.255099 | 0.071000 |
| C | 6.109021 | 0.881210 | 0.702950 |
| H | 4.426910 | 1.712549 | 1.750898 |
| C | 5.767006 | -1.262003 | -0.346780 |
| H | 3.810829 | -2.127770 | -0.153340 |
| C | 6.631021 | -0.190112 | -0.050272 |
| H | 6.763865 | 1.713934 | 0.982980 |
| H | 6.151198 | -2.124805 | -0.901923 |
| C | 8.079134 | -0.206823 | -0.474504 |
| H | 8.730049 | -0.447902 | 0.386562 |
| H | 8.263443 | -0.961588 | -1.255674 |
| H | 8.396639 | 0.779018 | -0.855196 |
| C | -2.894280 | 0.961895 | -0.156449 |
| C | -3.125875 | 1.755077 | -1.283342 |
| C | -3.483681 | 1.220168 | 1.082567 |
| C | -3.979173 | 2.864348 | -1.147018 |
| H | -2.661833 | 1.543331 | -2.252250 |

| | | | |
|---|---|---|---|
| C | -4.318202 | 2.342403 | 1.189315 |
| H | -3.310472 | 0.578496 | 1.948335 |
| C | -4.585145 | 3.176493 | 0.084470 |
| H | -4.166925 | 3.494750 | -2.023254 |
| H | -4.781569 | 2.557956 | 2.158585 |
| I | -3.410131 | -2.208827 | 0.203125 |
| C | -5.520783 | 4.354501 | 0.217086 |
| H | -5.318027 | 4.924027 | 1.139943 |
| H | -5.434985 | 5.037878 | -0.642644 |
| H | -6.569865 | 4.009178 | 0.269957 |

**IMB2-B4**

Lowest frequency = 10.43 $cm^{-1}$

Charge = 1, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | -0.019404 | -0.543358 | 1.898782 |
| N | -2.204427 | -0.466784 | 2.361904 |
| C | -1.222021 | -0.704075 | 1.493958 |
| C | -1.332735 | -1.217966 | 0.062017 |
| C | -2.469394 | -0.896698 | -1.171884 |
| C | -3.721658 | -0.078718 | -0.956729 |
| C | -4.968098 | -0.744720 | -0.990213 |
| H | -5.008071 | -1.821826 | -1.166280 |
| C | -6.158690 | -0.038148 | -0.794368 |
| H | -7.113003 | -0.572608 | -0.828030 |
| C | -6.129015 | 1.344778 | -0.561130 |
| H | -7.060847 | 1.897802 | -0.407295 |
| C | -4.897897 | 2.012839 | -0.538979 |
| H | -4.860327 | 3.093921 | -0.372395 |
| C | -3.701474 | 1.311601 | -0.739759 |
| H | -2.757797 | 1.853340 | -0.727532 |
| C | -1.806539 | 0.027799 | 3.712003 |
| H | -2.657758 | -0.188206 | 4.373688 |
| H | -0.945520 | -0.567163 | 4.052732 |
| C | -1.481277 | 1.522197 | 3.719882 |
| H | -1.316919 | 1.849203 | 4.759888 |
| H | -0.564553 | 1.733053 | 3.146885 |
| H | -2.311805 | 2.113807 | 3.299501 |
| C | -3.647431 | -0.719397 | 2.179268 |
| H | -4.172720 | 0.192256 | 2.511166 |
| H | -3.850022 | -0.824486 | 1.111351 |
| C | -4.130818 | -1.951347 | 2.946372 |
| H | -3.602559 | -2.859117 | 2.610901 |
| H | -3.992837 | -1.850286 | 4.035625 |
| H | -5.208274 | -2.086173 | 2.755220 |
| B | -2.415326 | -2.465907 | -0.425725 |
| B | -1.494255 | -3.511198 | -1.524084 |
| H | -1.759276 | -4.675152 | -1.577308 |
| B | -0.695046 | -2.826385 | -0.098233 |
| H | -0.428286 | -3.372889 | 0.933870 |
| B | 0.167146 | -2.869998 | -1.663666 |
| H | 1.121747 | -3.572060 | -1.796958 |
| B | 0.072988 | -1.211119 | -2.357515 |
| H | 0.938825 | -0.717325 | -3.017954 |
| B | -1.644682 | -0.861974 | -2.668032 |
| H | -2.079368 | -0.104901 | -3.480326 |

| | | | |
|---|---|---|---|
| B | -2.590820 | -2.280866 | -2.178370 |
| H | -3.650167 | -2.490202 | -2.680283 |
| B | -1.009056 | -2.512042 | -2.937431 |
| H | -0.927691 | -2.955170 | -4.044317 |
| B | -0.842462 | -0.137449 | -1.238203 |
| B | 0.235980 | -1.432980 | -0.637953 |
| Pd | 1.652319 | -1.132629 | 0.793259 |
| H | -3.290931 | -2.767418 | 0.318855 |
| C | -0.575665 | 1.403971 | -1.128098 |
| C | -0.382934 | 2.116810 | -2.333867 |
| C | -0.485808 | 2.137513 | 0.073063 |
| C | -0.127369 | 3.491435 | -2.335289 |
| H | -0.434146 | 1.588164 | -3.290369 |
| C | -0.233190 | 3.512236 | 0.071934 |
| H | -0.607526 | 1.639760 | 1.035350 |
| C | -0.050514 | 4.219606 | -1.131978 |
| H | 0.015803 | 4.008900 | -3.290468 |
| H | -0.166246 | 4.046622 | 1.025770 |
| C | 0.224741 | 5.703428 | -1.140435 |
| H | 0.307101 | 6.105803 | -0.118169 |
| H | 1.163490 | 5.927987 | -1.677081 |
| H | -0.581738 | 6.250823 | -1.660831 |
| C | 2.322126 | 0.718781 | 0.475407 |
| C | 2.582245 | 1.278413 | -0.772792 |
| C | 2.493578 | 1.403659 | 1.680404 |
| C | 2.999496 | 2.618555 | -0.801683 |
| H | 2.457377 | 0.715322 | -1.698905 |
| C | 2.922907 | 2.739355 | 1.613422 |
| H | 2.292086 | 0.942575 | 2.652972 |
| C | 3.178883 | 3.365332 | 0.377690 |
| H | 3.195255 | 3.081764 | -1.774425 |
| H | 3.052554 | 3.296238 | 2.548211 |
| C | 3.643785 | 4.801489 | 0.328737 |
| H | 3.711097 | 5.167049 | -0.707808 |
| H | 2.954477 | 5.460895 | 0.884757 |
| H | 4.640934 | 4.906621 | 0.792705 |
| I | 3.718555 | -2.084046 | -0.341922 |

**IMB3-B6**

Lowest frequency = 17.47 $cm^{-1}$

Charge = 0, Multiplicity = 1

85

| | | | |
|---|---|---|---|
| O | -0.198969 | -0.140459 | 1.380639 |
| N | 1.554248 | -1.157624 | 2.291450 |
| C | 0.838955 | -0.846161 | 1.201983 |
| C | 1.122891 | -1.327199 | -0.219757 |
| C | 1.248331 | -0.190626 | -1.420863 |
| C | 1.422384 | 1.266853 | -1.080193 |
| C | 1.108674 | 2.233823 | -2.051062 |
| H | 0.705780 | 1.922405 | -3.015886 |
| C | 1.283869 | 3.593592 | -1.775213 |
| H | 1.018448 | 4.332921 | -2.536880 |
| C | 1.764778 | 4.007853 | -0.527366 |
| H | 1.874469 | 5.073531 | -0.304220 |
| C | 2.096023 | 3.048449 | 0.437641 |
| H | 2.481851 | 3.355977 | 1.414320 |

| | | | |
|---|---|---|---|
| C | 1.938386 | 1.688413 | 0.157873 |
| H | 2.261543 | 0.960969 | 0.904193 |
| C | 1.039769 | -0.647854 | 3.589416 |
| H | -0.049611 | -0.802303 | 3.602281 |
| H | 1.490824 | -1.283946 | 4.366731 |
| C | 1.381118 | 0.826355 | 3.819332 |
| H | 1.045768 | 1.124422 | 4.827061 |
| H | 2.470202 | 0.997202 | 3.756834 |
| H | 0.870853 | 1.470109 | 3.086695 |
| C | 2.814901 | -1.909821 | 2.344785 |
| H | 3.244188 | -1.932885 | 1.340402 |
| H | 3.511952 | -1.322710 | 2.968472 |
| C | 2.637630 | -3.322446 | 2.903776 |
| H | 2.256863 | -3.311718 | 3.939218 |
| H | 1.938757 | -3.904667 | 2.281543 |
| H | 3.613566 | -3.836453 | 2.906796 |
| B | -0.352898 | -0.955705 | -1.164297 |
| B | -0.421127 | -2.245914 | -2.354341 |
| H | -1.485651 | -2.576565 | -2.782598 |
| B | 0.104819 | -2.624960 | -0.692365 |
| H | -0.495322 | -3.166320 | 0.183222 |
| B | 0.922618 | -3.388060 | -2.071485 |
| H | 0.806388 | -4.566002 | -2.255719 |
| B | 2.454531 | -2.528793 | -2.353940 |
| H | 3.453508 | -3.056965 | -2.750126 |
| B | 2.058814 | -0.849164 | -2.783230 |
| H | 2.733019 | -0.087813 | -3.410137 |
| B | 0.296627 | -0.673249 | -2.782195 |
| H | -0.219072 | 0.167421 | -3.447483 |
| B | 1.038032 | -2.178772 | -3.373845 |
| H | 1.012055 | -2.453305 | -4.539156 |
| B | 2.654770 | -1.238407 | -1.155218 |
| B | 1.880486 | -2.783468 | -0.699277 |
| H | 2.394212 | -3.469453 | 0.128972 |
| Pd | -1.646428 | 0.191291 | -0.086186 |
| O | -2.568688 | 1.731624 | 1.411807 |
| C | -1.771785 | 2.576531 | 0.927115 |
| O | -1.034361 | 2.367479 | -0.079302 |
| C | -1.576178 | 3.924618 | 1.656213 |
| F | -0.534591 | 3.801342 | 2.531533 |
| F | -1.269045 | 4.922098 | 0.804899 |
| F | -2.658576 | 4.287844 | 2.362265 |
| C | 4.078332 | -0.755066 | -0.684043 |
| C | 4.984363 | -1.709338 | -0.166170 |
| C | 4.589436 | 0.539291 | -0.928186 |
| C | 6.303301 | -1.374002 | 0.159581 |
| H | 4.658350 | -2.747769 | -0.036737 |
| C | 5.908139 | 0.875591 | -0.604270 |
| H | 3.956540 | 1.297650 | -1.394240 |
| C | 6.787749 | -0.067215 | -0.037799 |
| H | 6.973703 | -2.144671 | 0.557451 |
| H | 6.265189 | 1.891658 | -0.808358 |
| C | 8.199756 | 0.312563 | 0.341295 |
| H | 8.853869 | -0.573214 | 0.400182 |
| H | 8.634065 | 1.020178 | -0.385472 |
| H | 8.219452 | 0.807865 | 1.330913 |

| | | | |
|---|---|---|---|
| C | -2.655041 | -1.462085 | 0.468963 |
| C | -2.849948 | -1.467602 | 1.855544 |
| C | -3.186816 | -2.477867 | -0.332592 |
| C | -3.554808 | -2.531335 | 2.444887 |
| H | -2.482896 | -0.645088 | 2.477101 |
| C | -3.887753 | -3.528547 | 0.274689 |
| H | -3.063116 | -2.462027 | -1.416390 |
| C | -4.079029 | -3.580320 | 1.669528 |
| H | -3.704150 | -2.531673 | 3.531304 |
| H | -4.299274 | -4.322820 | -0.359588 |
| I | -3.251696 | 0.600156 | -2.079955 |
| C | -4.850940 | -4.715995 | 2.302580 |
| H | -4.454135 | -5.696724 | 1.984253 |
| H | -4.806936 | -4.667891 | 3.403179 |
| H | -5.915606 | -4.684559 | 2.005273 |

**IMB3-B4**

Lowest frequency = 15.78 $cm^{-1}$

Charge = 0, Multiplicity = 1

85

| | | | |
|---|---|---|---|
| O | -0.113884 | -0.757698 | -1.109979 |
| N | 1.323477 | -2.446117 | -1.384635 |
| C | 0.791346 | -1.490874 | -0.609514 |
| C | 1.112855 | -1.200375 | 0.855383 |
| C | 2.615346 | -0.957138 | 1.534879 |
| C | 3.858530 | -1.148990 | 0.697835 |
| C | 4.934484 | -1.895465 | 1.219438 |
| H | 4.869043 | -2.304122 | 2.229179 |
| C | 6.082151 | -2.123763 | 0.451017 |
| H | 6.906005 | -2.705306 | 0.876893 |
| C | 6.175391 | -1.616222 | -0.852445 |
| H | 7.072842 | -1.797278 | -1.452751 |
| C | 5.109904 | -0.873106 | -1.377204 |
| H | 5.166080 | -0.463149 | -2.390817 |
| C | 3.962221 | -0.638844 | -0.610216 |
| H | 3.153238 | -0.049421 | -1.038993 |
| C | 0.790612 | -2.538039 | -2.770330 |
| H | 1.000325 | -3.563439 | -3.111464 |
| H | -0.300024 | -2.408743 | -2.727453 |
| C | 1.438217 | -1.511878 | -3.701339 |
| H | 1.053977 | -1.649861 | -4.725908 |
| H | 1.197827 | -0.486383 | -3.379453 |
| H | 2.535685 | -1.629739 | -3.723577 |
| C | 2.340789 | -3.454167 | -1.038301 |
| H | 3.043206 | -3.494855 | -1.888468 |
| H | 2.917682 | -3.103407 | -0.177920 |
| C | 1.720665 | -4.825961 | -0.764140 |
| H | 1.021858 | -4.776307 | 0.086757 |
| H | 1.169746 | -5.209638 | -1.639204 |
| H | 2.520417 | -5.545478 | -0.520461 |
| B | 1.717713 | -2.379829 | 1.967873 |
| B | 0.937077 | -2.032138 | 3.504070 |
| H | 0.736345 | -2.934988 | 4.264045 |
| B | 0.010543 | -1.882720 | 1.998447 |
| H | -0.785368 | -2.654619 | 1.565054 |
| B | -0.179041 | -0.656617 | 3.275559 |

| | | | |
|---|---|---|---|
| H | -1.199336 | -0.568217 | 3.887575 |
| B | 0.788714 | 0.768521 | 2.796025 |
| H | 0.507078 | 1.894473 | 3.082163 |
| B | 2.495254 | 0.256543 | 2.733285 |
| H | 3.461304 | 0.938341 | 2.887817 |
| B | 2.580503 | -1.447483 | 3.185813 |
| H | 3.576978 | -1.895850 | 3.662176 |
| B | 1.420733 | -0.386182 | 3.999304 |
| H | 1.586535 | -0.079390 | 5.145068 |
| B | 1.561050 | 0.476872 | 1.217158 |
| B | -0.098617 | -0.151540 | 1.567626 |
| Pd | -1.606721 | 0.048884 | 0.183618 |
| O | -2.367210 | -2.103899 | -0.054535 |
| C | -3.027320 | -1.745527 | -1.073727 |
| O | -3.132247 | -0.558376 | -1.478858 |
| C | -3.651767 | -2.867233 | -1.933872 |
| F | -4.698444 | -2.437306 | -2.655526 |
| F | -2.704927 | -3.319778 | -2.813125 |
| F | -4.045904 | -3.917950 | -1.194026 |
| H | 2.096661 | -3.429104 | 1.565784 |
| C | 1.994410 | 1.626744 | 0.223865 |
| C | 2.750557 | 2.692710 | 0.763710 |
| C | 1.632790 | 1.738854 | -1.136803 |
| C | 3.130619 | 3.794858 | -0.008884 |
| H | 3.038647 | 2.670541 | 1.817689 |
| C | 2.016404 | 2.837727 | -1.911086 |
| H | 1.008911 | 0.974520 | -1.599771 |
| C | 2.773880 | 3.889944 | -1.366043 |
| H | 3.710339 | 4.600328 | 0.457124 |
| H | 1.697722 | 2.888073 | -2.958048 |
| C | 3.169797 | 5.089844 | -2.193265 |
| H | 2.829257 | 4.989028 | -3.236792 |
| H | 2.729906 | 6.015529 | -1.779996 |
| H | 4.266438 | 5.226810 | -2.199899 |
| C | -1.295137 | 1.983099 | -0.246348 |
| C | -0.811689 | 3.004839 | 0.572309 |
| C | -1.623307 | 2.222849 | -1.588233 |
| C | -0.580665 | 4.270202 | 0.011379 |
| H | -0.595716 | 2.828746 | 1.626927 |
| C | -1.389931 | 3.496484 | -2.126999 |
| H | -2.053034 | 1.429820 | -2.209129 |
| C | -0.855248 | 4.536170 | -1.341527 |
| H | -0.174026 | 5.064281 | 0.648025 |
| H | -1.632501 | 3.678837 | -3.180942 |
| C | -0.603681 | 5.902173 | -1.938277 |
| H | -0.069757 | 6.556553 | -1.229628 |
| H | -0.000021 | 5.830369 | -2.860819 |
| H | -1.553135 | 6.400304 | -2.208950 |
| I | -3.348285 | 0.868894 | 1.907960 |

**TS1-B3**

Lowest frequency = -821.43 $cm^{-1}$

Charge = 1, Multiplicity = 1

66

| | | | |
|---|---|---|---|
| O | 1.042245 | 0.374216 | 0.336472 |
| N | 2.969081 | -0.434921 | -0.452845 |

| | | | |
|---|---|---|---|
| C | 1.643776 | -0.504387 | -0.378265 |
| C | 0.756215 | -1.521656 | -1.056499 |
| C | -0.129319 | -2.500492 | 0.008115 |
| C | 0.158985 | -2.388717 | 1.485535 |
| C | -0.893183 | -2.014308 | 2.367775 |
| H | -1.919970 | -1.943681 | 1.998071 |
| C | -0.641642 | -1.869746 | 3.758792 |
| H | -1.481221 | -1.711605 | 4.445473 |
| C | 0.665151 | -2.089341 | 4.267462 |
| H | 0.856618 | -1.985121 | 5.339383 |
| C | 1.684250 | -2.482212 | 3.395957 |
| H | 2.688453 | -2.678465 | 3.782470 |
| C | 1.431369 | -2.636744 | 2.020383 |
| H | 2.244287 | -2.953436 | 1.364353 |
| C | 3.624568 | 0.682521 | 0.290543 |
| H | 3.021928 | 1.590179 | 0.138731 |
| H | 4.604985 | 0.831995 | -0.184616 |
| C | 3.774515 | 0.377153 | 1.781502 |
| H | 4.270401 | 1.230034 | 2.272947 |
| H | 4.388925 | -0.523755 | 1.949742 |
| H | 2.789893 | 0.236528 | 2.256013 |
| C | 3.874244 | -1.328429 | -1.212213 |
| H | 3.339239 | -2.255916 | -1.442243 |
| H | 4.700001 | -1.583176 | -0.525698 |
| C | 4.404368 | -0.670053 | -2.487544 |
| H | 4.981178 | 0.244122 | -2.271213 |
| H | 3.579395 | -0.411571 | -3.170921 |
| H | 5.073680 | -1.378776 | -3.002156 |
| B | -0.951948 | -1.140429 | -0.734935 |
| B | -1.816138 | -1.814438 | -2.109411 |
| H | -2.835561 | -1.287033 | -2.445634 |
| B | -0.240426 | -1.010894 | -2.365816 |
| H | -0.032939 | 0.083975 | -2.798723 |
| B | -0.623665 | -2.519092 | -3.243193 |
| H | -0.777987 | -2.500949 | -4.427763 |
| B | 0.206512 | -3.871915 | -2.406570 |
| H | 0.646267 | -4.832902 | -2.964112 |
| B | -0.477207 | -3.997931 | -0.762812 |
| H | -0.491679 | -4.956734 | -0.052963 |
| B | -1.718872 | -2.740923 | -0.589685 |
| H | -2.586267 | -2.890159 | 0.210690 |
| B | -1.536086 | -3.584499 | -2.143337 |
| H | -2.376010 | -4.350927 | -2.509811 |
| B | 1.083796 | -3.200141 | -1.027523 |
| H | 2.093780 | -3.576237 | -0.525949 |
| B | 0.997708 | -2.287631 | -2.557358 |
| H | 2.004322 | -2.047058 | -3.145492 |
| H | -1.972446 | -0.551311 | 0.325987 |
| Pd | -0.920559 | 0.806295 | 0.094089 |
| O | 0.224940 | 2.305399 | 2.704391 |
| C | 0.196071 | 3.009843 | 1.660053 |
| O | -0.342826 | 2.765315 | 0.542556 |
| C | 1.020500 | 4.323860 | 1.719665 |
| F | 2.298086 | 4.000596 | 1.367535 |
| F | 1.042399 | 4.836322 | 2.952954 |
| F | 0.567258 | 5.241807 | 0.864363 |

| | | | |
|---|---|---|---|
| O | -2.837268 | 1.425235 | -0.154820 |
| C | -3.675419 | 0.568061 | 0.273794 |
| O | -3.374444 | -0.555473 | 0.748015 |
| C | -5.174607 | 0.933605 | 0.114072 |
| F | -5.892521 | 0.371453 | 1.093345 |
| F | -5.589046 | 0.448635 | -1.070953 |
| F | -5.353472 | 2.255880 | 0.137862 |
| Ag | -0.405733 | 0.272149 | 2.873182 |

**TS1-B4**

Lowest frequency = -669.46 $cm^{-1}$

Charge = 1, Multiplicity = 1

66

| | | | |
|---|---|---|---|
| O | -0.239527 | 1.107893 | 0.519985 |
| N | -2.216283 | 1.133549 | 1.576061 |
| C | -1.291021 | 0.474810 | 0.887460 |
| C | -1.321664 | -0.992649 | 0.478514 |
| C | -2.497633 | -1.664263 | -0.598769 |
| C | -3.734789 | -0.859981 | -0.885678 |
| C | -4.992371 | -1.392839 | -0.533749 |
| H | -5.058409 | -2.387277 | -0.085567 |
| C | -6.158481 | -0.653090 | -0.759644 |
| H | -7.128909 | -1.080952 | -0.490697 |
| C | -6.083483 | 0.627709 | -1.326596 |
| H | -6.996331 | 1.205486 | -1.500970 |
| C | -4.835287 | 1.161762 | -1.677765 |
| H | -4.768686 | 2.156209 | -2.129536 |
| C | -3.665486 | 0.422303 | -1.464455 |
| H | -2.702673 | 0.850552 | -1.751604 |
| C | -1.954780 | 2.574435 | 1.859387 |
| H | -2.534007 | 2.815669 | 2.763824 |
| H | -0.884612 | 2.683680 | 2.088487 |
| C | -2.358473 | 3.464947 | 0.683002 |
| H | -2.188895 | 4.520156 | 0.952931 |
| H | -1.749270 | 3.236830 | -0.206541 |
| H | -3.425654 | 3.339513 | 0.433125 |
| C | -3.493535 | 0.597470 | 2.091941 |
| H | -4.237708 | 1.397411 | 1.946252 |
| H | -3.807340 | -0.237972 | 1.457335 |
| C | -3.396340 | 0.187350 | 3.561346 |
| H | -2.665784 | -0.627246 | 3.698213 |
| H | -3.098059 | 1.033687 | 4.202206 |
| H | -4.381772 | -0.168562 | 3.904486 |
| B | -2.315146 | -2.279469 | 1.024863 |
| B | -1.318322 | -3.736078 | 0.875302 |
| H | -1.481044 | -4.644856 | 1.632602 |
| B | -0.578675 | -2.217176 | 1.433726 |
| H | -0.275829 | -1.922079 | 2.549743 |
| B | 0.289248 | -3.257120 | 0.253126 |
| H | 1.296873 | -3.821167 | 0.552263 |
| B | 0.033804 | -2.551238 | -1.368784 |
| H | 0.864856 | -2.757598 | -2.281104 |
| B | -1.700013 | -2.630685 | -1.768967 |
| H | -2.165931 | -2.639612 | -2.866118 |
| B | -2.528558 | -3.354742 | -0.375878 |
| H | -3.571317 | -3.914029 | -0.511345 |

| | | | |
|---|---|---|---|
| B | -0.922580 | -3.960498 | -0.859314 |
| H | -0.794895 | -5.040329 | -1.352831 |
| B | -0.982941 | -1.112109 | -1.205681 |
| H | -0.966087 | -0.106708 | -1.840666 |
| B | 0.265310 | -1.496143 | 0.052612 |
| H | 1.638944 | -1.076973 | 0.958722 |
| Pd | 1.444177 | 0.178279 | -0.155799 |
| O | 2.146606 | 0.897825 | -3.248852 |
| C | 2.279772 | 1.859852 | -2.445380 |
| O | 2.054733 | 1.904969 | -1.199578 |
| C | 2.716773 | 3.215804 | -3.067457 |
| F | 1.609976 | 3.974746 | -3.242358 |
| F | 3.556759 | 3.867449 | -2.251112 |
| F | 3.307645 | 3.041047 | -4.253462 |
| O | 3.192349 | -0.781259 | -0.627295 |
| C | 3.534620 | -1.585277 | 0.318430 |
| O | 2.887001 | -1.791605 | 1.363253 |
| C | 4.810282 | -2.413634 | 0.023506 |
| F | 5.314172 | -2.937837 | 1.138388 |
| F | 4.439428 | -3.417726 | -0.808040 |
| F | 5.738986 | -1.669706 | -0.584439 |
| H | -3.182415 | -2.083106 | 1.809419 |
| Ag | 1.509698 | -1.081025 | -2.737373 |

**TS1a-B3**

Lowest frequency = -817.84 $cm^{-1}$

Charge = 0, Multiplicity = 1

65

| | | | |
|---|---|---|---|
| O | 1.253467 | 0.131692 | 0.574072 |
| N | 3.100041 | -0.603965 | -0.459908 |
| C | 1.780723 | -0.647540 | -0.284371 |
| C | 0.826519 | -1.584283 | -1.006845 |
| C | -0.062067 | -2.545033 | 0.072939 |
| C | 0.305035 | -2.507893 | 1.535656 |
| C | -0.662524 | -2.109763 | 2.477554 |
| H | -1.674662 | -1.861116 | 2.152732 |
| C | -0.340138 | -2.039374 | 3.837444 |
| H | -1.105346 | -1.726244 | 4.554357 |
| C | 0.951741 | -2.360709 | 4.276298 |
| H | 1.204372 | -2.298203 | 5.339544 |
| C | 1.916467 | -2.766787 | 3.344770 |
| H | 2.927383 | -3.026183 | 3.674931 |
| C | 1.595312 | -2.844698 | 1.984173 |
| H | 2.358048 | -3.164546 | 1.271400 |
| C | 3.844576 | 0.441443 | 0.293567 |
| H | 3.265592 | 1.372447 | 0.220333 |
| H | 4.792223 | 0.588151 | -0.246962 |
| C | 4.095099 | 0.043061 | 1.747808 |
| H | 4.664668 | 0.844100 | 2.248133 |
| H | 4.680435 | -0.891054 | 1.815281 |
| H | 3.142584 | -0.093254 | 2.283266 |
| C | 3.895485 | -1.441248 | -1.375193 |
| H | 3.328205 | -2.350441 | -1.604980 |
| H | 4.796290 | -1.748885 | -0.815775 |
| C | 4.272689 | -0.691128 | -2.655099 |
| H | 4.882734 | 0.201234 | -2.437996 |

| | | | |
|---|---|---|---|
| H | 3.369452 | -0.365045 | -3.194849 |
| H | 4.857147 | -1.358029 | -3.310797 |
| B | -0.824298 | -1.104571 | -0.588244 |
| B | -1.794587 | -1.687143 | -1.939509 |
| H | -2.796624 | -1.094451 | -2.220743 |
| B | -0.184994 | -0.978796 | -2.257226 |
| H | 0.068981 | 0.110701 | -2.674362 |
| B | -0.708298 | -2.432439 | -3.149371 |
| H | -0.920511 | -2.374030 | -4.326113 |
| B | 0.070968 | -3.857246 | -2.391380 |
| H | 0.420143 | -4.828350 | -2.998453 |
| B | -0.539328 | -3.986091 | -0.722612 |
| H | -0.584446 | -4.969872 | -0.047138 |
| B | -1.685662 | -2.656618 | -0.451194 |
| H | -2.529587 | -2.775324 | 0.381015 |
| B | -1.634016 | -3.467213 | -2.033456 |
| H | -2.536994 | -4.170980 | -2.383832 |
| B | 1.054426 | -3.278915 | -1.042507 |
| H | 2.067977 | -3.733348 | -0.616366 |
| B | 0.952546 | -2.322378 | -2.540232 |
| H | 1.938819 | -2.143292 | -3.183055 |
| H | -1.832496 | -0.370396 | 0.663922 |
| Pd | -0.623642 | 0.796399 | 0.168210 |
| O | 1.514282 | 2.245606 | -1.284354 |
| C | 1.081097 | 2.966497 | -0.378824 |
| O | 0.091009 | 2.752077 | 0.414699 |
| C | 1.863736 | 4.267305 | -0.052178 |
| F | 2.358132 | 4.840014 | -1.165115 |
| F | 2.927916 | 3.938373 | 0.742901 |
| F | 1.137774 | 5.186540 | 0.605991 |
| O | -2.504233 | 1.508063 | -0.262973 |
| C | -3.389037 | 0.776956 | 0.267601 |
| O | -3.163105 | -0.267378 | 0.944551 |
| C | -4.863144 | 1.144538 | -0.006394 |
| F | -5.630932 | 0.858271 | 1.057459 |
| F | -5.296053 | 0.413216 | -1.056139 |
| F | -5.000360 | 2.442288 | -0.301156 |

**TS1a-B4**

Lowest frequency = -875.55 $cm^{-1}$

Charge = 0, Multiplicity = 1

65

| | | | |
|---|---|---|---|
| O | -0.363737 | 1.052225 | 0.202486 |
| N | -2.232132 | 1.125118 | 1.410814 |
| C | -1.356123 | 0.426084 | 0.685040 |
| C | -1.357717 | -1.066045 | 0.388821 |
| C | -2.504264 | -1.806956 | -0.598013 |
| C | -3.729764 | -1.004154 | -0.952419 |
| C | -5.004953 | -1.510895 | -0.633170 |
| H | -5.094076 | -2.495908 | -0.168917 |
| C | -6.153276 | -0.757649 | -0.904011 |
| H | -7.137523 | -1.166598 | -0.654822 |
| C | -6.043508 | 0.513926 | -1.485367 |
| H | -6.941910 | 1.104403 | -1.691540 |
| C | -4.777280 | 1.022206 | -1.806455 |
| H | -4.678720 | 2.011012 | -2.265218 |

| | | | |
|---|---|---|---|
| C | -3.625986 | 0.267257 | -1.548634 |
| H | -2.646805 | 0.674347 | -1.810485 |
| C | -1.898208 | 2.562105 | 1.633418 |
| H | -2.404821 | 2.849122 | 2.568833 |
| H | -0.808068 | 2.637085 | 1.774127 |
| C | -2.343372 | 3.442940 | 0.464819 |
| H | -2.098410 | 4.493805 | 0.690036 |
| H | -1.801665 | 3.166143 | -0.452925 |
| H | -3.430406 | 3.365358 | 0.286675 |
| C | -3.513844 | 0.656941 | 1.961950 |
| H | -4.236991 | 1.473398 | 1.795623 |
| H | -3.865602 | -0.194920 | 1.368746 |
| C | -3.415084 | 0.303480 | 3.446683 |
| H | -2.706573 | -0.525816 | 3.606477 |
| H | -3.078584 | 1.166207 | 4.045863 |
| H | -4.405967 | -0.007427 | 3.818338 |
| B | -2.344109 | -2.286011 | 1.068803 |
| B | -1.357709 | -3.746103 | 1.053384 |
| H | -1.530910 | -4.574772 | 1.899494 |
| B | -0.603771 | -2.179389 | 1.446435 |
| H | -0.301099 | -1.776137 | 2.530061 |
| B | 0.245569 | -3.335444 | 0.378439 |
| H | 1.242316 | -3.879384 | 0.749601 |
| B | 0.017726 | -2.799144 | -1.308689 |
| H | 0.836929 | -2.930937 | -2.170463 |
| B | -1.726150 | -2.889354 | -1.680888 |
| H | -2.225001 | -3.001798 | -2.760010 |
| B | -2.566714 | -3.474699 | -0.227073 |
| H | -3.621040 | -4.027858 | -0.309882 |
| B | -0.971496 | -4.132773 | -0.650757 |
| H | -0.867311 | -5.262831 | -1.031820 |
| B | -0.972833 | -1.338687 | -1.280780 |
| H | -0.967165 | -0.406740 | -2.017977 |
| B | 0.257386 | -1.592135 | -0.013764 |
| H | 1.665626 | -1.234709 | 0.781180 |
| Pd | 1.395337 | 0.161840 | -0.252952 |
| O | 1.609185 | 2.750757 | 1.269116 |
| C | 1.834455 | 2.932303 | 0.072740 |
| O | 2.006991 | 2.055777 | -0.861927 |
| C | 1.828383 | 4.388533 | -0.469186 |
| F | 2.204859 | 5.270639 | 0.474722 |
| F | 2.614512 | 4.566768 | -1.546222 |
| F | 0.550729 | 4.710847 | -0.837614 |
| O | 3.228998 | -0.644766 | -0.679106 |
| C | 3.567747 | -1.466029 | 0.225681 |
| O | 2.855244 | -1.808509 | 1.208070 |
| C | 4.936358 | -2.161680 | 0.060635 |
| F | 5.532353 | -2.326495 | 1.252545 |
| F | 4.733236 | -3.379746 | -0.487820 |
| F | 5.754758 | -1.464656 | -0.737163 |
| H | -3.215135 | -2.001086 | 1.823206 |

**TS2-B6**

Lowest frequency = -802.10 $cm^{-1}$

Charge = 1, Multiplicity = 1

79

| | | | |
|---|---|---|---|
| O | 0.376445 | 1.290307 | 0.672795 |
| N | -1.545293 | 2.199312 | 0.022400 |
| C | -0.719767 | 1.153782 | 0.019310 |
| C | -0.894017 | -0.149555 | -0.746951 |
| C | -1.086852 | -1.633879 | 0.022956 |
| C | -1.311090 | -1.753493 | 1.510619 |
| C | -1.465446 | -0.630663 | 2.363131 |
| H | -1.661458 | 0.360218 | 1.950405 |
| C | -1.554982 | -0.804048 | 3.771889 |
| H | -1.813322 | 0.053060 | 4.404880 |
| C | -1.491272 | -2.105249 | 4.328921 |
| H | -1.560291 | -2.238371 | 5.412338 |
| C | -1.388957 | -3.207099 | 3.477531 |
| H | -1.366568 | -4.219424 | 3.890614 |
| C | -1.303976 | -3.033668 | 2.085593 |
| H | -1.208140 | -3.910878 | 1.444038 |
| C | -1.114522 | 3.388945 | 0.814406 |
| H | -1.698766 | 4.236572 | 0.429284 |
| H | -0.050396 | 3.573413 | 0.602870 |
| C | -1.351429 | 3.203651 | 2.314352 |
| H | -1.100712 | 4.139471 | 2.840069 |
| H | -0.705050 | 2.408065 | 2.722007 |
| H | -2.407277 | 2.963102 | 2.526616 |
| C | -2.822930 | 2.342664 | -0.706459 |
| H | -3.565305 | 2.694057 | 0.030871 |
| H | -3.149323 | 1.351258 | -1.029876 |
| C | -2.721672 | 3.306174 | -1.889708 |
| H | -1.966439 | 2.964916 | -2.616098 |
| H | -2.468982 | 4.333013 | -1.577453 |
| H | -3.700214 | 3.340084 | -2.396367 |
| B | -2.371535 | -1.094610 | -1.058749 |
| B | -1.980442 | -1.907268 | -2.599833 |
| H | -2.891690 | -2.167757 | -3.327690 |
| B | -1.448433 | -0.237440 | -2.350693 |
| H | -1.928652 | 0.745723 | -2.821380 |
| B | -0.371076 | -1.391568 | -3.178893 |
| H | -0.122970 | -1.253107 | -4.339752 |
| B | 0.851355 | -1.957650 | -1.994345 |
| H | 1.981781 | -2.237748 | -2.263401 |
| B | -0.024658 | -2.811332 | -0.709584 |
| H | 0.420929 | -3.651768 | 0.006202 |
| B | -1.757603 | -2.773956 | -1.066241 |
| H | -2.493879 | -3.583508 | -0.589754 |
| B | -0.569456 | -2.973251 | -2.385499 |
| H | -0.474647 | -4.022200 | -2.950153 |
| B | 0.534193 | -1.154422 | -0.457188 |
| H | 1.153916 | -1.563604 | 1.019377 |
| B | 0.304698 | -0.264367 | -1.986470 |
| H | 0.954680 | 0.722082 | -2.167532 |
| Pd | 1.859107 | -0.071537 | 0.741340 |
| O | 3.364471 | -1.430631 | 0.983898 |
| C | 2.920973 | -2.451229 | 1.600210 |
| O | 1.713419 | -2.647811 | 1.901678 |
| C | 3.942976 | -3.547185 | 1.994768 |
| F | 3.646747 | -4.669989 | 1.317425 |
| F | 3.831978 | -3.789342 | 3.312624 |

| | | | |
|---|---|---|---|
| F | 5.193853 | -3.181900 | 1.719323 |
| C | -3.833703 | -0.735715 | -0.619906 |
| C | -4.726529 | -0.330056 | -1.644072 |
| C | -4.359021 | -0.827741 | 0.686466 |
| C | -6.055269 | 0.000585 | -1.368036 |
| H | -4.370371 | -0.268238 | -2.677796 |
| C | -5.691563 | -0.495488 | 0.961928 |
| H | -3.736982 | -1.182547 | 1.510875 |
| C | -6.566308 | -0.069101 | -0.055246 |
| H | -6.713161 | 0.310689 | -2.187504 |
| H | -6.063953 | -0.580101 | 1.989041 |
| C | -8.010055 | 0.259525 | 0.235048 |
| H | -8.347601 | 1.134088 | -0.346405 |
| H | -8.661008 | -0.589213 | -0.046688 |
| H | -8.172244 | 0.463549 | 1.305712 |
| Ag | 0.673949 | -0.211681 | 3.377066 |
| O | 3.134822 | 1.368861 | 1.584473 |
| C | 3.205237 | 1.434534 | 2.844778 |
| O | 2.524851 | 0.816617 | 3.709911 |
| C | 4.227510 | 2.461834 | 3.405113 |
| F | 4.742311 | 2.038794 | 4.566203 |
| F | 5.222505 | 2.688218 | 2.541226 |
| F | 3.568873 | 3.624793 | 3.622227 |

**TS2-B4**

Lowest frequency = -828.67 $cm^{-1}$

Charge = 1, Multiplicity = 1

79

| | | | |
|---|---|---|---|
| O | -0.289538 | 1.258080 | 0.057084 |
| N | -2.234915 | 2.264852 | -0.318887 |
| C | -1.549926 | 1.288672 | 0.276612 |
| C | -2.038275 | 0.233626 | 1.260345 |
| C | -3.567177 | -0.645464 | 1.385890 |
| C | -4.757275 | -0.412918 | 0.496189 |
| C | -4.840721 | -0.957305 | -0.798923 |
| H | -4.024357 | -1.563768 | -1.191615 |
| C | -5.981719 | -0.745038 | -1.583493 |
| H | -6.031771 | -1.176901 | -2.587821 |
| C | -7.058953 | -0.002173 | -1.081765 |
| H | -7.950967 | 0.157551 | -1.695325 |
| C | -6.996425 | 0.517426 | 0.220324 |
| H | -7.841233 | 1.078370 | 0.631463 |
| C | -5.857793 | 0.312992 | 1.005322 |
| H | -5.822193 | 0.718083 | 2.019686 |
| C | -1.457349 | 3.190698 | -1.195430 |
| H | -0.531772 | 3.463408 | -0.666148 |
| H | -2.075736 | 4.093440 | -1.302116 |
| C | -1.145544 | 2.584272 | -2.564389 |
| H | -0.655149 | 3.344976 | -3.193657 |
| H | -2.065906 | 2.256530 | -3.077537 |
| H | -0.454569 | 1.730071 | -2.471119 |
| C | -3.666995 | 2.579246 | -0.163400 |
| H | -4.162455 | 1.713172 | 0.280958 |
| H | -4.078999 | 2.690519 | -1.181373 |
| C | -3.913513 | 3.837215 | 0.671010 |
| H | -3.480465 | 4.739235 | 0.208109 |

| | | | |
|---|---|---|---|
| H | -3.493516 | 3.730010 | 1.684455 |
| H | -5.001193 | 3.994720 | 0.759373 |
| B | -2.111327 | -1.437056 | 0.792892 |
| B | -1.482090 | -2.321821 | 2.237872 |
| H | -0.906373 | -3.353968 | 2.070323 |
| B | -0.738009 | -0.791958 | 1.767719 |
| H | 0.314993 | -1.570695 | 0.771037 |
| B | -1.020737 | -1.130224 | 3.484990 |
| H | -0.089758 | -1.293831 | 4.216584 |
| B | -2.510232 | -0.252627 | 3.963202 |
| H | -2.684944 | 0.222081 | 5.045662 |
| B | -3.860963 | -0.946785 | 3.042347 |
| H | -5.004467 | -0.950858 | 3.377936 |
| B | -3.225884 | -2.208970 | 1.961044 |
| H | -3.924214 | -3.077919 | 1.533707 |
| B | -2.560795 | -2.008436 | 3.614706 |
| H | -2.781509 | -2.832547 | 4.451429 |
| B | -3.134483 | 0.591394 | 2.527855 |
| H | -3.712998 | 1.628826 | 2.484824 |
| B | -1.368713 | 0.489576 | 2.827751 |
| H | -0.787158 | 1.523083 | 2.974823 |
| Pd | 1.014448 | -0.042837 | 0.887988 |
| O | 2.630190 | 1.124493 | 0.205794 |
| C | 3.177125 | 0.795991 | -0.884715 |
| O | 2.812408 | -0.073285 | -1.724149 |
| C | 4.438223 | 1.613073 | -1.278093 |
| F | 5.325657 | 0.842067 | -1.920433 |
| F | 5.027841 | 2.159367 | -0.209077 |
| F | 4.048086 | 2.607111 | -2.111135 |
| Ag | 0.861673 | -0.954006 | -1.864675 |
| O | 1.058329 | -2.840020 | 0.490019 |
| C | 2.092659 | -2.548825 | 1.146410 |
| O | 2.379761 | -1.389530 | 1.585197 |
| C | 3.082817 | -3.696424 | 1.463870 |
| F | 4.198653 | -3.246439 | 2.037101 |
| F | 2.477731 | -4.566813 | 2.291356 |
| F | 3.398567 | -4.329610 | 0.320148 |
| C | -1.804391 | -1.970046 | -0.661915 |
| C | -1.637447 | -3.357347 | -0.841374 |
| C | -1.518320 | -1.140892 | -1.780064 |
| C | -1.174380 | -3.903776 | -2.047726 |
| H | -1.845504 | -4.032364 | -0.006802 |
| C | -1.044154 | -1.688653 | -3.005119 |
| H | -1.765543 | -0.075502 | -1.755810 |
| C | -0.848552 | -3.092528 | -3.147537 |
| H | -1.049695 | -4.988607 | -2.127231 |
| H | -0.953894 | -1.041971 | -3.887107 |
| C | -0.367818 | -3.681073 | -4.449242 |
| H | 0.114056 | -2.922531 | -5.086273 |
| H | 0.347601 | -4.501154 | -4.273151 |
| H | -1.219548 | -4.105045 | -5.012906 |

**TS2a-B6**

Lowest frequency = -652.59 $cm^{-1}$

Charge = 0, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | 0.200359 | 1.184047 | 0.519675 |
| N | -1.497228 | 2.252731 | -0.453524 |
| C | -0.792767 | 1.135918 | -0.277250 |
| C | -1.033581 | -0.199274 | -0.977791 |
| C | -1.112021 | -1.543006 | 0.014392 |
| C | -1.192885 | -1.335932 | 1.508998 |
| C | -1.885459 | -0.245601 | 2.068224 |
| H | -2.422039 | 0.456246 | 1.426737 |
| C | -1.920749 | -0.056011 | 3.453061 |
| H | -2.463148 | 0.801257 | 3.863946 |
| C | -1.268758 | -0.958080 | 4.304920 |
| H | -1.293052 | -0.808726 | 5.389030 |
| C | -0.585675 | -2.051802 | 3.757339 |
| H | -0.070306 | -2.764088 | 4.408934 |
| C | -0.544771 | -2.240499 | 2.370335 |
| H | 0.005105 | -3.087186 | 1.957201 |
| C | -0.990278 | 3.482001 | 0.216753 |
| H | -1.449257 | 4.326621 | -0.319323 |
| H | 0.094787 | 3.521951 | 0.048649 |
| C | -1.337210 | 3.525904 | 1.704804 |
| H | -0.961516 | 4.470749 | 2.131875 |
| H | -0.858467 | 2.691663 | 2.240985 |
| H | -2.428952 | 3.482136 | 1.867309 |
| C | -2.707327 | 2.412295 | -1.271888 |
| H | -3.430203 | 2.982622 | -0.662821 |
| H | -3.146187 | 1.424856 | -1.434989 |
| C | -2.423100 | 3.121292 | -2.597507 |
| H | -1.686283 | 2.557479 | -3.191614 |
| H | -2.032131 | 4.140473 | -2.441795 |
| H | -3.359196 | 3.197663 | -3.175959 |
| B | -2.525889 | -1.165188 | -0.990162 |
| B | -2.317428 | -2.194136 | -2.422901 |
| H | -3.312199 | -2.539146 | -2.992729 |
| B | -1.772108 | -0.511106 | -2.481246 |
| H | -2.316687 | 0.378805 | -3.055573 |
| B | -0.790657 | -1.780450 | -3.249241 |
| H | -0.682385 | -1.820859 | -4.440949 |
| B | 0.561400 | -2.175481 | -2.146875 |
| H | 1.652053 | -2.510837 | -2.508839 |
| B | -0.152801 | -2.821770 | -0.652102 |
| H | 0.372703 | -3.588558 | 0.088304 |
| B | -1.909582 | -2.825495 | -0.809250 |
| H | -2.570931 | -3.557783 | -0.136082 |
| B | -0.882843 | -3.225335 | -2.213740 |
| H | -0.841139 | -4.347842 | -2.628372 |
| B | 0.442159 | -1.157858 | -0.717770 |
| H | 1.574145 | -1.483650 | 0.660687 |
| B | 0.005401 | -0.488554 | -2.320948 |
| H | 0.619801 | 0.455109 | -2.718586 |
| Pd | 1.843751 | 0.074989 | 0.105706 |
| O | 1.850291 | 2.666668 | -1.256924 |
| C | 2.658093 | 2.724607 | -0.321719 |
| O | 3.036729 | 1.778389 | 0.460299 |
| C | 3.232381 | 4.117448 | 0.052067 |
| F | 4.358108 | 4.061292 | 0.783209 |
| F | 2.293917 | 4.782314 | 0.794116 |

| | | | |
|---|---|---|---|
| F | 3.478160 | 4.862403 | -1.041658 |
| O | 3.504272 | -1.041163 | -0.325781 |
| C | 3.440063 | -2.169066 | 0.256483 |
| O | 2.497117 | -2.569476 | 0.985141 |
| C | 4.590033 | -3.154649 | -0.047586 |
| F | 4.812443 | -3.970067 | 0.995743 |
| F | 5.728604 | -2.515194 | -0.343713 |
| F | 4.229867 | -3.909616 | -1.109608 |
| C | -3.960503 | -0.795228 | -0.452533 |
| C | -4.875633 | -0.142123 | -1.308988 |
| C | -4.467780 | -1.263600 | 0.780334 |
| C | -6.200397 | 0.098094 | -0.926840 |
| H | -4.554994 | 0.161015 | -2.312020 |
| C | -5.791565 | -1.025652 | 1.163865 |
| H | -3.824645 | -1.839010 | 1.451234 |
| C | -6.681396 | -0.324854 | 0.326451 |
| H | -6.878150 | 0.606950 | -1.621917 |
| H | -6.145362 | -1.404897 | 2.129528 |
| C | -8.100316 | -0.041172 | 0.759549 |
| H | -8.757482 | 0.141750 | -0.106726 |
| H | -8.517005 | -0.879151 | 1.343966 |
| H | -8.140047 | 0.858212 | 1.403384 |

**TS2a-B4**

Lowest frequency = -844.18 $cm^{-1}$

Charge = 0, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | 0.018390 | 1.058923 | 0.676732 |
| N | 1.605411 | 2.257361 | -0.345554 |
| C | 0.883431 | 1.140403 | -0.255086 |
| C | 0.947328 | -0.089804 | -1.154059 |
| C | 2.297940 | -0.958144 | -1.533360 |
| C | 3.653958 | -0.434809 | -1.120414 |
| C | 4.730291 | -0.502021 | -2.026254 |
| H | 4.578158 | -0.943453 | -3.012734 |
| C | 5.989859 | -0.002435 | -1.673262 |
| H | 6.813215 | -0.065181 | -2.391768 |
| C | 6.194484 | 0.575563 | -0.412783 |
| H | 7.179444 | 0.966748 | -0.138411 |
| C | 5.128410 | 0.645194 | 0.494210 |
| H | 5.272612 | 1.086502 | 1.485520 |
| C | 3.869212 | 0.142203 | 0.147443 |
| H | 3.060035 | 0.196870 | 0.875890 |
| C | 1.332349 | 3.304858 | 0.675910 |
| H | 1.717523 | 4.246525 | 0.256380 |
| H | 0.243361 | 3.400126 | 0.776914 |
| C | 2.002376 | 2.983849 | 2.012307 |
| H | 1.782370 | 3.789664 | 2.732475 |
| H | 1.615191 | 2.038418 | 2.425667 |
| H | 3.098248 | 2.906334 | 1.903273 |
| C | 2.553030 | 2.637148 | -1.407552 |
| H | 3.390651 | 3.154440 | -0.910365 |
| H | 2.970909 | 1.732660 | -1.860868 |
| C | 1.882062 | 3.527919 | -2.455606 |
| H | 1.047215 | 2.996526 | -2.939854 |
| H | 1.475613 | 4.448359 | -2.005211 |

| | | | |
|---|---|---|---|
| H | 2.621217 | 3.811191 | -3.223878 |
| B | 1.447408 | -0.101211 | -2.801082 |
| B | 0.424357 | -1.289190 | -3.599346 |
| H | 0.177524 | -1.142846 | -4.761370 |
| B | -0.275145 | -0.217127 | -2.364744 |
| H | -0.950689 | 0.752883 | -2.534957 |
| B | -0.727893 | -1.941987 | -2.398271 |
| H | -1.845293 | -2.264748 | -2.684483 |
| B | 0.206920 | -2.789472 | -1.135495 |
| H | -0.196139 | -3.727545 | -0.516384 |
| B | 1.929127 | -2.638101 | -1.545773 |
| H | 2.808163 | -3.380026 | -1.227582 |
| B | 2.061223 | -1.733684 | -3.058073 |
| H | 3.002924 | -1.883430 | -3.773803 |
| B | 0.722560 | -2.875819 | -2.837854 |
| H | 0.696786 | -3.899232 | -3.458922 |
| B | 1.217930 | -1.622832 | -0.260651 |
| B | -0.407305 | -1.145061 | -0.841821 |
| H | -1.499973 | -1.650801 | 0.391350 |
| Pd | -1.714563 | 0.083986 | 0.200298 |
| O | -1.557909 | 2.874308 | -0.841585 |
| C | -2.343193 | 2.834727 | 0.112653 |
| O | -2.756161 | 1.813662 | 0.776302 |
| C | -2.849122 | 4.185313 | 0.688948 |
| F | -4.009404 | 4.088243 | 1.359563 |
| F | -1.908235 | 4.658490 | 1.563691 |
| F | -2.998097 | 5.112267 | -0.275819 |
| O | -3.467815 | -0.872847 | -0.267481 |
| C | -3.408292 | -2.094462 | 0.063696 |
| O | -2.409028 | -2.667541 | 0.579132 |
| C | -4.637688 | -2.964220 | -0.276736 |
| F | -4.798247 | -3.943197 | 0.627606 |
| F | -5.759832 | -2.234787 | -0.325004 |
| F | -4.438205 | -3.529476 | -1.487785 |
| H | 1.958723 | 0.860401 | -3.270341 |
| C | 1.677905 | -1.754724 | 1.237979 |
| C | 2.884375 | -2.425300 | 1.549617 |
| C | 0.895422 | -1.309834 | 2.325526 |
| C | 3.299712 | -2.610978 | 2.870791 |
| H | 3.519699 | -2.799681 | 0.741494 |
| C | 1.310972 | -1.496691 | 3.649454 |
| H | -0.056192 | -0.804615 | 2.140920 |
| C | 2.522268 | -2.146478 | 3.950060 |
| H | 4.245223 | -3.128825 | 3.069515 |
| H | 0.675508 | -1.132837 | 4.464951 |
| C | 2.954557 | -2.376097 | 5.379059 |
| H | 2.534415 | -1.612819 | 6.055178 |
| H | 2.604559 | -3.363165 | 5.736788 |
| H | 4.053625 | -2.363904 | 5.475001 |

**TS3-B6**

Lowest frequency = -42.63 $cm^{-1}$

Charge = 1, Multiplicity = 1

86

| | | | |
|---|---|---|---|
| O | 0.330778 | -1.169366 | 1.857555 |
| N | 2.475130 | -1.765312 | 1.955053 |

| | | | |
|---|---|---|---|
| C | 1.407603 | -1.440080 | 1.227467 |
| C | 1.315278 | -1.398580 | -0.290441 |
| C | 0.679073 | -0.016994 | -0.939709 |
| C | 0.522236 | 1.220191 | -0.088956 |
| C | 1.376675 | 1.505667 | 0.989559 |
| H | 2.198202 | 0.830158 | 1.231673 |
| C | 1.225403 | 2.676556 | 1.747543 |
| H | 1.907372 | 2.867071 | 2.580861 |
| C | 0.215502 | 3.594361 | 1.441587 |
| H | 0.094867 | 4.506498 | 2.032631 |
| C | -0.639734 | 3.345985 | 0.347238 |
| H | -1.380923 | 4.092783 | 0.044007 |
| C | -0.489503 | 2.164017 | -0.422079 |
| H | -1.079626 | 2.025982 | -1.330894 |
| C | 2.293978 | -1.803151 | 3.434632 |
| H | 3.078689 | -2.471706 | 3.819660 |
| H | 1.311828 | -2.251512 | 3.645426 |
| C | 2.392495 | -0.412649 | 4.064883 |
| H | 2.312447 | -0.506521 | 5.159842 |
| H | 1.567011 | 0.230162 | 3.721649 |
| H | 3.357177 | 0.068664 | 3.827582 |
| C | 3.824429 | -2.085575 | 1.457400 |
| H | 4.533594 | -1.536414 | 2.099962 |
| H | 3.925941 | -1.669036 | 0.451888 |
| C | 4.113142 | -3.587096 | 1.474907 |
| H | 3.404812 | -4.131843 | 0.829621 |
| H | 4.053261 | -4.006137 | 2.493268 |
| H | 5.133843 | -3.762437 | 1.096540 |
| B | 2.343444 | -0.456870 | -1.427762 |
| B | 2.105676 | -1.315532 | -2.957613 |
| H | 3.007938 | -1.274872 | -3.740880 |
| B | 2.233605 | -2.245619 | -1.452128 |
| H | 3.171616 | -2.886007 | -1.095090 |
| B | 1.073884 | -2.745818 | -2.708393 |
| H | 1.235033 | -3.765963 | -3.311511 |
| B | -0.545775 | -2.181334 | -2.221347 |
| H | -1.548615 | -2.757910 | -2.519325 |
| B | -0.497302 | -0.409539 | -2.134275 |
| H | -1.422051 | 0.323259 | -2.297730 |
| B | 1.126772 | 0.126753 | -2.591227 |
| H | 1.286826 | 1.238833 | -2.995901 |
| B | 0.388118 | -1.261624 | -3.422259 |
| H | 0.034612 | -1.171553 | -4.560927 |
| B | -0.446609 | -1.387227 | -0.657108 |
| B | 0.596385 | -2.793767 | -0.992271 |
| H | 0.482347 | -3.748661 | -0.281321 |
| Pd | -1.545799 | -1.344637 | 1.059818 |
| O | -1.922013 | 1.073318 | 3.445040 |
| C | -2.010777 | -0.119411 | 3.840957 |
| O | -2.193586 | -1.171063 | 3.168645 |
| C | -1.815493 | -0.357377 | 5.362143 |
| F | -2.697727 | -1.255258 | 5.832311 |
| F | -1.925900 | 0.769725 | 6.074065 |
| F | -0.563599 | -0.859093 | 5.559075 |
| C | 3.631312 | 0.383665 | -1.114151 |
| C | 4.894212 | -0.254009 | -1.128471 |

| | | | |
|---|---|---|---|
| C | 3.633447 | 1.794911 | -1.030885 |
| C | 6.084395 | 0.467181 | -0.990208 |
| H | 4.954037 | -1.336169 | -1.290056 |
| C | 4.822598 | 2.517632 | -0.892316 |
| H | 2.693992 | 2.349536 | -1.101245 |
| C | 6.072716 | 1.869028 | -0.851100 |
| H | 7.041867 | -0.064953 | -1.013648 |
| H | 4.781678 | 3.611081 | -0.834997 |
| C | 7.352749 | 2.648147 | -0.672939 |
| H | 7.597104 | 2.750989 | 0.401500 |
| H | 8.203480 | 2.140853 | -1.156861 |
| H | 7.266209 | 3.665187 | -1.089491 |
| Ag | -2.014913 | 1.405234 | 1.277604 |
| I | -3.744152 | -0.513251 | -0.274977 |
| C | -3.317078 | -2.622288 | 0.732026 |
| C | -2.935291 | -3.668245 | -0.121400 |
| C | -4.056450 | -2.847000 | 1.910187 |
| C | -3.199240 | -4.984616 | 0.286926 |
| H | -2.439258 | -3.471614 | -1.071854 |
| C | -4.312057 | -4.167474 | 2.277150 |
| H | -4.387076 | -2.019197 | 2.538436 |
| C | -3.885412 | -5.258733 | 1.483316 |
| H | -2.872929 | -5.807219 | -0.358267 |
| H | -4.863845 | -4.353394 | 3.205036 |
| C | -4.177627 | -6.673751 | 1.913436 |
| H | -5.254940 | -6.809559 | 2.114017 |
| H | -3.870542 | -7.402429 | 1.147287 |
| H | -3.642095 | -6.911547 | 2.850786 |

**TS3-B4**

Lowest frequency = -36.850 $cm^{-1}$

Charge = 1, Multiplicity = 1

86

| | | | |
|---|---|---|---|
| O | 0.591412 | 0.950527 | 1.273328 |
| N | 2.574791 | 1.375412 | 2.196122 |
| C | 1.831490 | 1.184303 | 1.104232 |
| C | 2.251006 | 1.258652 | -0.355509 |
| C | 3.608489 | 0.423917 | -1.205150 |
| C | 4.703325 | -0.358009 | -0.536060 |
| C | 5.881567 | 0.296786 | -0.114628 |
| H | 5.975453 | 1.379394 | -0.234220 |
| C | 6.949098 | -0.430397 | 0.421246 |
| H | 7.854725 | 0.095179 | 0.739271 |
| C | 6.867934 | -1.826889 | 0.526302 |
| H | 7.704272 | -2.396562 | 0.943163 |
| C | 5.724869 | -2.490623 | 0.060445 |
| H | 5.667726 | -3.582731 | 0.098805 |
| C | 4.655154 | -1.765418 | -0.477434 |
| H | 3.792834 | -2.300787 | -0.874977 |
| C | 1.868039 | 1.307295 | 3.508236 |
| H | 2.486794 | 1.881103 | 4.214798 |
| H | 0.897760 | 1.813777 | 3.397404 |
| C | 1.667037 | -0.129615 | 3.992121 |
| H | 1.198923 | -0.110827 | 4.989551 |
| H | 0.994878 | -0.679603 | 3.315831 |
| H | 2.629077 | -0.665408 | 4.070575 |

| | | | |
|---|---|---|---|
| C | 4.014733 | 1.673562 | 2.249435 |
| H | 4.438622 | 1.040514 | 3.047719 |
| H | 4.470215 | 1.338039 | 1.313796 |
| C | 4.301754 | 3.153000 | 2.509630 |
| H | 3.884492 | 3.782941 | 1.706825 |
| H | 3.880065 | 3.490089 | 3.471211 |
| H | 5.392622 | 3.310638 | 2.545548 |
| B | 3.557788 | 2.143317 | -1.021749 |
| B | 2.963678 | 2.782753 | -2.572278 |
| H | 3.355094 | 3.839015 | -2.972730 |
| B | 1.863680 | 2.701264 | -1.176351 |
| H | 1.531254 | 3.624260 | -0.492669 |
| B | 1.289869 | 2.203074 | -2.794654 |
| H | 0.480192 | 2.841107 | -3.399079 |
| B | 1.323854 | 0.418919 | -2.837282 |
| H | 0.555825 | -0.246270 | -3.467281 |
| B | 3.012264 | -0.096563 | -2.695925 |
| H | 3.448266 | -1.129126 | -3.106468 |
| B | 4.026829 | 1.364347 | -2.551501 |
| H | 5.183149 | 1.351775 | -2.844813 |
| B | 2.611763 | 1.374759 | -3.625092 |
| H | 2.749943 | 1.400293 | -4.812458 |
| B | 1.935848 | -0.172537 | -1.260773 |
| B | 0.825839 | 1.268788 | -1.363103 |
| Pd | -0.847610 | 1.154358 | -0.177972 |
| H | 4.324466 | 2.686613 | -0.296385 |
| C | 1.476569 | -1.518837 | -0.575376 |
| C | 0.663211 | -2.422729 | -1.323271 |
| C | 1.805528 | -1.899781 | 0.742179 |
| C | 0.182409 | -3.623838 | -0.740911 |
| H | 0.480931 | -2.230154 | -2.385764 |
| C | 1.345071 | -3.094680 | 1.310447 |
| H | 2.459807 | -1.262443 | 1.343252 |
| C | 0.508662 | -3.971514 | 0.594752 |
| H | -0.398771 | -4.321806 | -1.354318 |
| H | 1.630794 | -3.345477 | 2.337287 |
| C | -0.046522 | -5.220579 | 1.229310 |
| H | 0.652713 | -5.637849 | 1.971873 |
| H | -0.989731 | -4.986400 | 1.757886 |
| H | -0.268350 | -5.993876 | 0.476128 |
| C | -2.405555 | 2.451472 | -1.082855 |
| C | -3.538191 | 2.595969 | -0.256897 |
| C | -1.728743 | 3.557788 | -1.618943 |
| C | -3.920758 | 3.885676 | 0.108062 |
| H | -4.080048 | 1.726504 | 0.117160 |
| C | -2.134583 | 4.840779 | -1.219218 |
| H | -0.907471 | 3.430721 | -2.324494 |
| C | -3.227303 | 5.029136 | -0.355249 |
| H | -4.785911 | 4.006040 | 0.769163 |
| H | -1.589925 | 5.706969 | -1.609858 |
| C | -3.668806 | 6.408921 | 0.062967 |
| H | -3.558184 | 6.537443 | 1.155179 |
| H | -3.079203 | 7.192565 | -0.437749 |
| H | -4.735352 | 6.569343 | -0.174466 |
| I | -2.353904 | 0.448352 | -2.312610 |
| Ag | -1.324396 | -1.593495 | -0.325559 |

| | | | |
|---|---|---|---|
| O | -2.239478 | 0.857431 | 1.525845 |
| C | -2.334225 | -0.241496 | 2.135982 |
| O | -2.108821 | -1.408629 | 1.717287 |
| C | -2.730480 | -0.113738 | 3.631044 |
| F | -1.638611 | 0.309618 | 4.328982 |
| F | -3.706411 | 0.793687 | 3.804183 |
| F | -3.128790 | -1.279022 | 4.156257 |

**TS3a-B6**

Lowest frequency = -91.68 $cm^{-1}$

Charge = 1, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | -0.245810 | 1.088329 | -1.164459 |
| N | 1.534819 | 2.418273 | -0.917642 |
| C | 0.787838 | 1.404822 | -0.481670 |
| C | 1.004280 | 0.626720 | 0.808117 |
| C | 1.075877 | -1.042909 | 0.671639 |
| C | 1.152355 | -1.618761 | -0.723970 |
| C | 0.405150 | -2.768269 | -1.047222 |
| H | -0.201426 | -3.254831 | -0.281886 |
| C | 0.436087 | -3.291822 | -2.345602 |
| H | -0.148127 | -4.187567 | -2.576776 |
| C | 1.205810 | -2.672952 | -3.340086 |
| H | 1.228105 | -3.082833 | -4.354511 |
| C | 1.951818 | -1.528503 | -3.025136 |
| H | 2.565629 | -1.041922 | -3.789317 |
| C | 1.926184 | -1.005593 | -1.727789 |
| H | 2.533949 | -0.128099 | -1.496938 |
| C | 1.095286 | 3.097871 | -2.165934 |
| H | -0.001523 | 3.178948 | -2.136436 |
| H | 1.520991 | 4.112026 | -2.128171 |
| C | 1.554902 | 2.351529 | -3.419744 |
| H | 1.252149 | 2.920776 | -4.314206 |
| H | 2.653007 | 2.242803 | -3.440365 |
| H | 1.094495 | 1.352206 | -3.470062 |
| C | 2.782279 | 2.920822 | -0.314162 |
| H | 3.174224 | 2.149522 | 0.353949 |
| H | 3.510352 | 3.021245 | -1.137491 |
| C | 2.591748 | 4.251087 | 0.415181 |
| H | 2.252754 | 5.051136 | -0.264050 |
| H | 1.859793 | 4.152116 | 1.233148 |
| H | 3.556452 | 4.563506 | 0.848044 |
| B | -0.463095 | -0.317287 | 1.057762 |
| B | -0.675008 | -0.429810 | 2.787899 |
| H | -1.779676 | -0.511571 | 3.239547 |
| B | -0.077820 | 1.091532 | 2.063923 |
| H | -0.683961 | 2.106714 | 1.886264 |
| B | 0.660860 | 0.474951 | 3.558385 |
| H | 0.515919 | 1.071304 | 4.584908 |
| B | 2.194208 | -0.327366 | 3.127882 |
| H | 3.157072 | -0.329598 | 3.836464 |
| B | 1.814208 | -1.713700 | 2.073492 |
| H | 2.468723 | -2.697666 | 1.909323 |
| B | 0.060677 | -1.779030 | 1.874746 |
| H | -0.467501 | -2.813353 | 1.618287 |
| B | 0.739731 | -1.303148 | 3.441587 |

| | | | |
|---|---|---|---|
| H | 0.650522 | -2.036737 | 4.381382 |
| B | 2.483395 | -0.215160 | 1.380713 |
| B | 1.699111 | 1.140835 | 2.268678 |
| H | 2.243028 | 2.199495 | 2.305115 |
| Pd | -1.749351 | -0.133638 | -0.481743 |
| C | 3.935911 | -0.202541 | 0.785454 |
| C | 4.850259 | 0.789127 | 1.211580 |
| C | 4.456709 | -1.256840 | 0.000754 |
| C | 6.192325 | 0.768034 | 0.818175 |
| H | 4.514344 | 1.584018 | 1.887316 |
| C | 5.798505 | -1.279408 | -0.391558 |
| H | 3.810736 | -2.085759 | -0.301485 |
| C | 6.692849 | -0.262734 | -0.001077 |
| H | 6.868587 | 1.556118 | 1.167693 |
| H | 6.163377 | -2.111518 | -1.004010 |
| C | 8.147801 | -0.309273 | -0.399597 |
| H | 8.719460 | -0.941047 | 0.306177 |
| H | 8.276367 | -0.743674 | -1.405059 |
| H | 8.602786 | 0.694613 | -0.387741 |
| C | -3.716952 | 0.460403 | 0.138632 |
| C | -4.368167 | 0.841489 | -1.045251 |
| C | -3.786757 | 1.214679 | 1.318024 |
| C | -5.045712 | 2.073101 | -1.052950 |
| H | -4.368665 | 0.203492 | -1.934611 |
| C | -4.481915 | 2.428522 | 1.274021 |
| H | -3.301171 | 0.876604 | 2.236077 |
| C | -5.118952 | 2.880822 | 0.096872 |
| H | -5.547769 | 2.388315 | -1.974093 |
| H | -4.528745 | 3.036563 | 2.184417 |
| I | -3.418708 | -1.953253 | 0.364601 |
| C | -5.889933 | 4.178643 | 0.092664 |
| H | -5.311067 | 4.987154 | 0.571274 |
| H | -6.148368 | 4.491747 | -0.931124 |
| H | -6.831671 | 4.071204 | 0.661824 |

**TS3a-B4**

Lowest frequency = -79.33 $cm^{-1}$

Charge = 1, Multiplicity = 1

78

| | | | |
|---|---|---|---|
| O | -0.297385 | -0.474757 | 2.041406 |
| N | -2.516184 | -0.574431 | 2.372191 |
| C | -1.458395 | -0.741276 | 1.576549 |
| C | -1.437361 | -1.280716 | 0.157191 |
| C | -2.452987 | -0.935007 | -1.121770 |
| C | -3.657444 | -0.047184 | -0.920079 |
| C | -4.919404 | -0.490515 | -1.366215 |
| H | -5.011449 | -1.454486 | -1.869760 |
| C | -6.059931 | 0.295075 | -1.162115 |
| H | -7.030158 | -0.064408 | -1.518313 |
| C | -5.961306 | 1.530207 | -0.506137 |
| H | -6.854419 | 2.142429 | -0.347048 |
| C | -4.709584 | 1.975345 | -0.059409 |
| H | -4.615883 | 2.939923 | 0.449560 |
| C | -3.564544 | 1.196372 | -0.265026 |
| H | -2.602207 | 1.565499 | 0.088177 |
| C | -2.270578 | 0.049049 | 3.702735 |

| | | | |
|---|---|---|---|
| H | -3.055163 | -0.332982 | 4.372863 |
| H | -1.297595 | -0.303277 | 4.073031 |
| C | -2.316714 | 1.575851 | 3.619050 |
| H | -2.182452 | 2.002749 | 4.626696 |
| H | -1.513763 | 1.960862 | 2.970188 |
| H | -3.285695 | 1.924931 | 3.223442 |
| C | -3.914061 | -0.994285 | 2.132905 |
| H | -4.550276 | -0.156400 | 2.463012 |
| H | -4.076184 | -1.102510 | 1.057344 |
| C | -4.262780 | -2.286214 | 2.874282 |
| H | -3.629659 | -3.121711 | 2.532795 |
| H | -4.145998 | -2.184594 | 3.966037 |
| H | -5.315500 | -2.542044 | 2.669408 |
| B | -2.483412 | -2.527146 | -0.401103 |
| B | -1.491408 | -3.560631 | -1.427043 |
| H | -1.763427 | -4.721712 | -1.507569 |
| B | -0.792173 | -2.885924 | 0.059575 |
| H | -0.609445 | -3.433538 | 1.105938 |
| B | 0.180167 | -2.931402 | -1.434396 |
| H | 1.129966 | -3.650134 | -1.512115 |
| B | 0.146158 | -1.284912 | -2.145766 |
| H | 1.058538 | -0.806752 | -2.752636 |
| B | -1.541597 | -0.913265 | -2.572772 |
| H | -1.921020 | -0.163460 | -3.417955 |
| B | -2.535379 | -2.314368 | -2.149582 |
| H | -3.552901 | -2.525647 | -2.730209 |
| B | -0.904149 | -2.566780 | -2.796583 |
| H | -0.748605 | -3.012275 | -3.894976 |
| B | -0.813141 | -0.194004 | -1.103630 |
| B | 0.194500 | -1.491602 | -0.403070 |
| Pd | 1.477439 | -0.721370 | 0.975017 |
| H | -3.421049 | -2.829299 | 0.259839 |
| C | -0.533472 | 1.352779 | -0.982125 |
| C | -0.548408 | 2.112822 | -2.174206 |
| C | -0.193631 | 2.043130 | 0.204593 |
| C | -0.266136 | 3.483242 | -2.175865 |
| H | -0.785173 | 1.625322 | -3.123768 |
| C | 0.086183 | 3.413348 | 0.203331 |
| H | -0.136361 | 1.512034 | 1.156336 |
| C | 0.047994 | 4.166649 | -0.985515 |
| H | -0.292448 | 4.032743 | -3.123598 |
| H | 0.350015 | 3.905542 | 1.145853 |
| C | 0.315379 | 5.651879 | -0.985432 |
| H | 0.859373 | 5.965224 | -0.079884 |
| H | 0.899765 | 5.955839 | -1.870372 |
| H | -0.635437 | 6.216256 | -1.016491 |
| C | 2.983013 | 0.496568 | 0.143836 |
| C | 2.776223 | 1.132150 | -1.084997 |
| C | 3.540498 | 1.153898 | 1.253627 |
| C | 3.076781 | 2.496441 | -1.172573 |
| H | 2.367352 | 0.592754 | -1.940982 |
| C | 3.805758 | 2.527438 | 1.135956 |
| H | 3.778571 | 0.622110 | 2.180942 |
| C | 3.586557 | 3.216634 | -0.073012 |
| H | 2.896322 | 3.010685 | -2.122008 |
| H | 4.222162 | 3.057017 | 2.000008 |

| | | | |
|---|---|---|---|
| C | 3.929857 | 4.681465 | -0.195661 |
| H | 3.494983 | 5.120972 | -1.106780 |
| H | 3.567092 | 5.251679 | 0.676653 |
| H | 5.025531 | 4.821211 | -0.243611 |
| I | 3.544461 | -1.936798 | -0.021084 |

**TS3b-B6**

Lowest frequency = -120.72 $cm^{-1}$

Charge = 0, Multiplicity = 1

85

| | | | |
|---|---|---|---|
| O | -0.123317 | 0.706495 | 1.050401 |
| N | 1.690728 | 0.849008 | 2.326287 |
| C | 0.998068 | 0.216821 | 1.366366 |
| C | 1.400394 | -1.076801 | 0.660983 |
| C | 1.541666 | -1.029744 | -0.989771 |
| C | 1.523248 | 0.320415 | -1.664430 |
| C | 0.858007 | 0.477830 | -2.894805 |
| H | 0.338396 | -0.371266 | -3.341372 |
| C | 0.855565 | 1.717358 | -3.542984 |
| H | 0.324897 | 1.823434 | -4.494198 |
| C | 1.509023 | 2.816463 | -2.973144 |
| H | 1.492303 | 3.788745 | -3.474883 |
| C | 2.156156 | 2.671627 | -1.741405 |
| H | 2.649571 | 3.527787 | -1.271862 |
| C | 2.159237 | 1.435578 | -1.089849 |
| H | 2.684346 | 1.340402 | -0.137634 |
| C | 1.073227 | 2.088707 | 2.870490 |
| H | 0.003122 | 1.890161 | 3.035634 |
| H | 1.551714 | 2.264184 | 3.847054 |
| C | 1.249618 | 3.289262 | 1.937733 |
| H | 0.798230 | 4.178860 | 2.408263 |
| H | 2.319362 | 3.497314 | 1.757493 |
| H | 0.738367 | 3.121613 | 0.975882 |
| C | 2.987521 | 0.456026 | 2.885593 |
| H | 3.463098 | -0.242782 | 2.193301 |
| H | 3.621619 | 1.360054 | 2.901635 |
| C | 2.871781 | -0.154165 | 4.283986 |
| H | 2.430427 | 0.553793 | 5.006032 |
| H | 2.249086 | -1.063641 | 4.262735 |
| H | 3.876701 | -0.428245 | 4.647497 |
| B | -0.034811 | -1.547330 | -0.327967 |
| B | 0.055330 | -3.307223 | -0.340231 |
| H | -0.954733 | -3.936689 | -0.463081 |
| B | 0.463940 | -2.425987 | 1.152127 |
| H | -0.199469 | -2.288324 | 2.137654 |
| B | 1.417748 | -3.849891 | 0.674173 |
| H | 1.371079 | -4.855642 | 1.324226 |
| B | 2.927185 | -3.279211 | -0.080133 |
| H | 3.974637 | -3.853162 | 0.006791 |
| B | 2.488493 | -2.359385 | -1.542475 |
| H | 3.171528 | -2.169371 | -2.503922 |
| B | 0.728504 | -2.377934 | -1.693172 |
| H | 0.233445 | -2.264717 | -2.770969 |
| B | 1.578044 | -3.822618 | -1.101696 |
| H | 1.648181 | -4.809004 | -1.778055 |
| B | 2.976904 | -1.508261 | -0.064760 |

| | | | |
|---|---|---|---|
| B | 2.245330 | -2.404598 | 1.304489 |
| H | 2.734536 | -2.306165 | 2.388540 |
| Pd | -1.409646 | -0.073771 | -0.349770 |
| O | -2.635452 | 1.714514 | -0.235951 |
| C | -1.897176 | 2.748797 | -0.401783 |
| O | -0.754277 | 2.809849 | -0.865478 |
| C | -2.520766 | 4.053896 | 0.162588 |
| F | -2.119272 | 4.208988 | 1.460272 |
| F | -2.111566 | 5.146143 | -0.513727 |
| F | -3.870657 | 4.049474 | 0.160552 |
| C | 4.367805 | -0.762832 | -0.032922 |
| C | 5.278136 | -1.045079 | 1.010698 |
| C | 4.855712 | 0.012455 | -1.108461 |
| C | 6.576357 | -0.521992 | 1.018865 |
| H | 4.973674 | -1.709268 | 1.827562 |
| C | 6.153179 | 0.534524 | -1.103456 |
| H | 4.217099 | 0.205380 | -1.974128 |
| C | 7.035699 | 0.292914 | -0.032488 |
| H | 7.250796 | -0.765230 | 1.848110 |
| H | 6.491580 | 1.133773 | -1.956711 |
| C | 8.424397 | 0.887296 | -0.017841 |
| H | 9.087755 | 0.345636 | 0.676699 |
| H | 8.880040 | 0.867296 | -1.022822 |
| H | 8.394423 | 1.945365 | 0.305393 |
| C | -3.407185 | -1.282806 | 0.249919 |
| C | -4.326122 | -0.332891 | 0.717620 |
| C | -3.120508 | -2.453634 | 0.959068 |
| C | -4.906730 | -0.545431 | 1.973742 |
| H | -4.539009 | 0.573894 | 0.149487 |
| C | -3.716673 | -2.632614 | 2.215932 |
| H | -2.440426 | -3.204727 | 0.556161 |
| C | -4.612837 | -1.687219 | 2.747194 |
| H | -5.607116 | 0.206206 | 2.356103 |
| H | -3.475258 | -3.537216 | 2.785808 |
| I | -2.989447 | -1.299052 | -2.050285 |
| C | -5.245743 | -1.881998 | 4.105439 |
| H | -5.009670 | -2.875346 | 4.520701 |
| H | -4.885630 | -1.120006 | 4.821506 |
| H | -6.344627 | -1.782497 | 4.052151 |

**TS3b-B4**

Lowest frequency = -109.140 $cm^{-1}$

Charge = 0, Multiplicity = 1

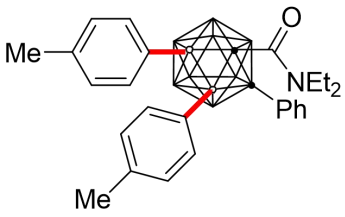
85

| | | | |
|---|---|---|---|
| O | 0.136001 | -0.947359 | -0.940979 |
| N | 1.748870 | -2.484961 | -1.097230 |
| C | 1.140308 | -1.506039 | -0.412775 |
| C | 1.442955 | -1.028186 | 1.002197 |
| C | 2.863516 | -0.428429 | 1.577725 |
| C | 4.077356 | -0.431694 | 0.680252 |
| C | 5.346299 | -0.706515 | 1.224297 |
| H | 5.442126 | -0.907183 | 2.292987 |
| C | 6.481810 | -0.728297 | 0.404660 |
| H | 7.459666 | -0.943705 | 0.847049 |
| C | 6.367928 | -0.479757 | -0.970053 |
| H | 7.256318 | -0.499043 | -1.609589 |

| | | | |
|---|---|---|---|
| C | 5.108125 | -0.202497 | -1.518270 |
| H | 5.001735 | 0.001789 | -2.588401 |
| C | 3.972190 | -0.172672 | -0.701646 |
| H | 3.006510 | 0.064866 | -1.150088 |
| C | 1.120913 | -2.844579 | -2.398146 |
| H | 1.482355 | -3.855666 | -2.642044 |
| H | 0.034650 | -2.896211 | -2.233489 |
| C | 1.474117 | -1.855573 | -3.509698 |
| H | 0.981673 | -2.171143 | -4.444676 |
| H | 1.113236 | -0.845721 | -3.257399 |
| H | 2.564133 | -1.815635 | -3.685008 |
| C | 2.957201 | -3.243174 | -0.736989 |
| H | 3.596347 | -3.262301 | -1.637214 |
| H | 3.515250 | -2.689658 | 0.025375 |
| C | 2.633854 | -4.661934 | -0.263177 |
| H | 1.999755 | -4.638583 | 0.637844 |
| H | 2.104808 | -5.240227 | -1.038832 |
| H | 3.571661 | -5.189870 | -0.020609 |
| B | 2.280144 | -1.961180 | 2.180224 |
| B | 1.479057 | -1.621679 | 3.704972 |
| H | 1.478045 | -2.465256 | 4.555060 |
| B | 0.506819 | -1.789480 | 2.222718 |
| H | -0.142534 | -2.730942 | 1.875831 |
| B | 0.114155 | -0.510986 | 3.393986 |
| H | -0.891772 | -0.561569 | 4.039887 |
| B | 0.778066 | 1.021314 | 2.767655 |
| H | 0.299094 | 2.096715 | 2.974881 |
| B | 2.543988 | 0.847229 | 2.678064 |
| H | 3.352625 | 1.723012 | 2.739482 |
| B | 2.976775 | -0.763978 | 3.264804 |
| H | 4.052803 | -0.973098 | 3.735476 |
| B | 1.649037 | 0.122978 | 4.036248 |
| H | 1.776998 | 0.557259 | 5.145646 |
| B | 1.544238 | 0.741427 | 1.192103 |
| B | 0.055071 | -0.153865 | 1.644776 |
| Pd | -1.440130 | -0.313358 | 0.281417 |
| O | -1.876067 | -2.907847 | -0.805496 |
| C | -2.575586 | -2.153077 | -1.498292 |
| O | -2.824404 | -0.912491 | -1.308150 |
| C | -3.147232 | -2.725292 | -2.822604 |
| F | -4.190366 | -2.023160 | -3.306856 |
| F | -2.162598 | -2.694069 | -3.774036 |
| F | -3.535207 | -4.009411 | -2.695217 |
| H | 2.855662 | -2.945803 | 1.856521 |
| C | 1.738162 | 1.782437 | 0.022539 |
| C | 2.855641 | 2.652614 | 0.037052 |
| C | 0.830134 | 1.937300 | -1.046041 |
| C | 3.064838 | 3.600289 | -0.967762 |
| H | 3.586307 | 2.578816 | 0.847615 |
| C | 1.046630 | 2.877243 | -2.061479 |
| H | -0.070947 | 1.321851 | -1.091285 |
| C | 2.166263 | 3.726258 | -2.046679 |
| H | 3.945358 | 4.251647 | -0.917079 |
| H | 0.316784 | 2.955340 | -2.874686 |
| C | 2.391455 | 4.754870 | -3.130513 |
| H | 3.407851 | 4.673348 | -3.555907 |

| | | | |
|---|---|---|---|
| H | 1.663624 | 4.640630 | -3.950541 |
| H | 2.292070 | 5.780660 | -2.728720 |
| C | -2.491210 | 1.883153 | 0.441678 |
| C | -1.711484 | 2.904139 | 1.005776 |
| C | -3.044756 | 1.998241 | -0.840891 |
| C | -1.434488 | 4.037692 | 0.236627 |
| H | -1.311125 | 2.808859 | 2.015896 |
| C | -2.741479 | 3.147210 | -1.588733 |
| H | -3.649608 | 1.194643 | -1.267121 |
| C | -1.939533 | 4.181169 | -1.071505 |
| H | -0.799955 | 4.821199 | 0.665858 |
| H | -3.146321 | 3.229947 | -2.603961 |
| C | -1.614614 | 5.409944 | -1.887260 |
| H | -0.521289 | 5.533809 | -1.989730 |
| H | -2.050252 | 5.349260 | -2.897958 |
| H | -2.002420 | 6.324498 | -1.402424 |
| I | -3.381784 | 0.369825 | 1.919947 |

# X-Ray crystallographic analysis




**3aa**

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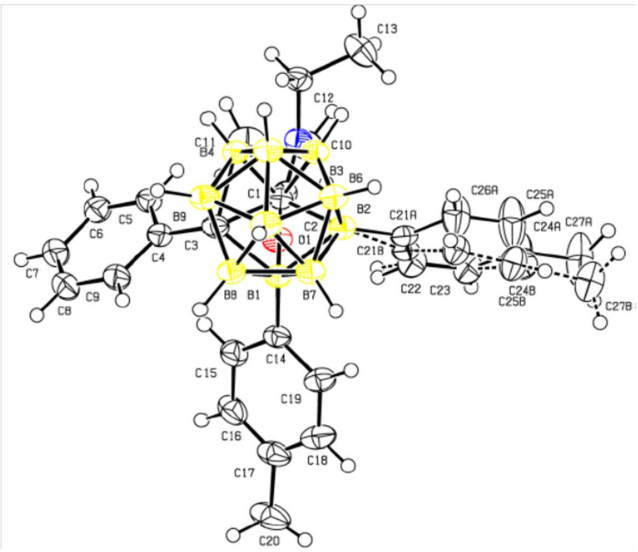



**CCDC 1893305**

**Crystal data and structure refinement for 3aa.**

| | |
|---|---|
| Identification code | 0538_CG_0m |
| CCDC number | 1893305 |
| Empirical formula | $C_{27}H_{37}B_{10}NO$ |
| Formula weight | 499.68 |
| Temperature/K | 100.03 |
| Crystal system | monoclinic |
| Space group | C2/c |
| a/Å | 12.5994(11) |
| b/Å | 23.669(2) |
| c/Å | 21.4198(18) |
| α/° | 90 |
| β/° | 102.169(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 6244.2(9) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.190 |
| μ/mm$^{-1}$ | 1.633 |
| F(000) | 2344.0 |
| Crystal size/mm$^3$ | 0.425 × 0.4 × 0.368 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 7.47 to 149.188 |
| Index ranges | $-15 \le h \le 14$, $-29 \le k \le 29$, $-26 \le l \le 26$ |
| Reflections collected | 38084 |
| Independent reflections | 6321 [$R_{int}$ = 0.0376, $R_{sigma}$ = 0.0261] |
| Data/restraints/parameters | 6321/90/429 |

| | |
|---|---|
| Goodness-of-fit on $F^2$ | 1.025 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0515, $wR_2$ = 0.1443 |
| Final R indexes [all data] | $R_1$ = 0.0526, $wR_2$ = 0.1455 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.36/-0.24 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for 0538_CG_0m. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 7895.7(7) | 3538.7(4) | 4870.3(4) | 36.1(2) |
| N1 | 9698.3(8) | 3611.1(4) | 5235.0(5) | 33.2(2) |
| C1 | 8665.1(9) | 3762.6(5) | 5229.2(5) | 29.8(2) |
| C2 | 8381.0(9) | 4206.9(5) | 5694.3(5) | 28.4(2) |
| C3 | 7618.3(9) | 4767.2(5) | 5377.8(6) | 30.4(2) |
| C4 | 7390.5(9) | 4882.5(5) | 4668.3(6) | 31.6(3) |
| C5 | 8090.4(10) | 4708.2(5) | 4278.5(6) | 33.0(3) |
| C6 | 7855.5(11) | 4822.6(6) | 3629.1(6) | 37.5(3) |
| C7 | 6917.4(12) | 5116.9(7) | 3356.1(7) | 43.7(3) |
| C8 | 6235.3(11) | 5303.7(7) | 3743.9(7) | 46.5(3) |
| C9 | 6466.9(10) | 5192.1(6) | 4393.1(7) | 39.1(3) |
| C10 | 9811.5(12) | 3144.0(6) | 4796.4(7) | 43.7(3) |
| C11 | 9756.9(13) | 3346.6(7) | 4119.9(7) | 51.4(4) |
| C12 | 10726.7(10) | 3884.7(6) | 5534.5(6) | 34.9(3) |
| C13 | 11424.7(13) | 3531.8(7) | 6054.9(8) | 51.6(4) |
| C14 | 5975.6(9) | 3863.5(5) | 5299.1(6) | 33.1(3) |
| C15 | 5650.1(11) | 3858.7(6) | 4634.0(7) | 41.2(3) |
| C16 | 4690.8(13) | 3599.4(6) | 4328.6(8) | 48.9(4) |
| C17 | 4016.7(11) | 3327.7(6) | 4670.0(8) | 48.3(4) |
| C18 | 4345.4(11) | 3316.3(6) | 5328.7(8) | 47.0(4) |
| C19 | 5302.7(11) | 3577.3(6) | 5638.6(7) | 39.6(3) |
| C20 | 2965.1(13) | 3062.6(7) | 4323.6(12) | 69.5(6) |
| C21A | 8103.3(18) | 3332.7(9) | 6577.7(11) | 30.9(3) |
| C21B | 7856(13) | 3279(8) | 6541(10) | 30.9(3) |
| C22 | 7790.4(12) | 2874.7(6) | 6164.4(6) | 40.6(3) |
| C23 | 7920.2(12) | 2320.0(6) | 6371.8(7) | 41.0(3) |
| C24A | 8333(3) | 2191.1(11) | 6990.8(12) | 54.7(7) |
| C24B | 8054(18) | 2201(10) | 7082(11) | 38(2) |
| C25A | 8668(4) | 2638.9(9) | 7406.6(9) | 78.8(13) |
| C25B | 7921(17) | 2637(6) | 7442(7) | 45(3) |
| C26A | 8560(3) | 3194.4(8) | 7201.4(8) | 60.2(8) |
| C26B | 7926(16) | 3180(6) | 7201(6) | 39(3) |
| C27A | 8432(4) | 1586.4(10) | 7214.4(13) | 85.0(12) |
| C27B | 8040(19) | 1584(7) | 7377(10) | 53(4) |
| B1 | 6948.0(10) | 4216.0(6) | 5698.8(6) | 30.8(3) |

| | | | | |
|---|---|---|---|---|
| B2 | 7977.9(11) | 3967.3(6) | 6373.5(6) | 30.9(3) |
| B3 | 9190.7(11) | 4384.0(6) | 6416.6(6) | 31.2(3) |
| B4 | 8960.2(11) | 4871.1(6) | 5771.2(7) | 31.0(3) |
| B5 | 8915.8(12) | 5103.3(6) | 6548.6(7) | 35.3(3) |
| B6 | 8302.8(12) | 4553.1(6) | 6923.4(7) | 34.9(3) |
| B7 | 6955.9(11) | 4457.2(6) | 6488.0(7) | 34.2(3) |
| B8 | 6721.4(11) | 4945.4(6) | 5850.2(7) | 34.1(3) |
| B9 | 7922.2(11) | 5341.9(6) | 5882.2(7) | 34.8(3) |
| B10 | 7528.0(12) | 5148.9(6) | 6599.3(7) | 37.2(3) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for 0538_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 33.7(4) | 40.1(5) | 35.2(4) | -8.8(4) | 9.1(4) | -4.8(3) |
| N1 | 30.6(5) | 33.1(5) | 36.9(5) | -3.4(4) | 9.0(4) | 3.6(4) |
| C1 | 30.5(6) | 30.9(6) | 28.7(5) | -1.2(4) | 7.9(4) | -0.1(4) |
| C2 | 23.9(5) | 31.1(6) | 30.4(6) | -1.8(4) | 6.1(4) | -0.1(4) |
| C3 | 25.8(5) | 30.6(6) | 35.6(6) | -1.8(4) | 8.3(4) | 2.2(4) |
| C4 | 27.2(6) | 32.6(6) | 35.2(6) | 1.4(4) | 6.7(5) | 0.5(4) |
| C5 | 29.0(6) | 33.6(6) | 37.0(6) | 0.5(5) | 8.0(5) | 1.2(4) |
| C6 | 35.8(6) | 40.9(7) | 37.0(7) | 1.1(5) | 10.2(5) | -0.5(5) |
| C7 | 40.3(7) | 52.9(8) | 36.6(7) | 9.1(6) | 5.0(5) | 1.3(6) |
| C8 | 34.1(7) | 55.6(8) | 48.9(8) | 14.4(6) | 6.5(6) | 8.6(6) |
| C9 | 29.7(6) | 44.6(7) | 44.4(7) | 6.9(5) | 11.0(5) | 6.5(5) |
| C10 | 42.1(7) | 39.3(7) | 51.2(8) | -11.4(6) | 13.0(6) | 7.3(6) |
| C11 | 46.5(8) | 63.9(10) | 47.5(8) | -19.4(7) | 18.5(6) | -0.6(7) |
| C12 | 27.5(6) | 40.0(7) | 37.7(6) | -0.6(5) | 8.4(5) | 3.6(5) |
| C13 | 49.2(8) | 49.7(8) | 50.1(8) | -3.4(6) | -2.7(7) | 16.9(7) |
| C14 | 24.5(5) | 33.3(6) | 41.2(7) | -3.1(5) | 6.3(5) | 1.8(4) |
| C15 | 37.6(7) | 38.7(7) | 43.2(7) | 1.4(5) | -0.4(5) | -3.4(5) |
| C16 | 45.6(8) | 38.1(7) | 52.9(8) | -0.5(6) | -12.5(6) | -0.5(6) |
| C17 | 30.0(6) | 29.2(6) | 78.9(11) | -7.6(6) | -3.9(6) | 2.7(5) |
| C18 | 30.6(6) | 37.6(7) | 75.5(10) | -10.6(6) | 17.5(6) | -3.8(5) |
| C19 | 31.2(6) | 39.2(7) | 51.2(8) | -7.3(5) | 14.8(5) | -2.3(5) |
| C20 | 38.4(8) | 35.1(8) | 120.0(16) | -10.9(9) | -17.4(9) | -1.0(6) |
| C21A | 22.9(9) | 37.9(5) | 32.1(5) | -2.8(4) | 6.0(6) | -5.6(5) |
| C21B | 22.9(9) | 37.9(5) | 32.1(5) | -2.8(4) | 6.0(6) | -5.6(5) |
| C22 | 47.8(7) | 39.4(5) | 34.7(5) | -4.7(3) | 8.7(4) | -6.0(4) |
| C23 | 47.6(7) | 38.8(4) | 37.6(5) | -4.7(4) | 11.2(5) | -5.7(4) |
| C24A | 85(2) | 39.3(8) | 38.4(10) | 0.4(7) | 9.7(10) | 1.0(11) |
| C24B | 39(6) | 38.8(10) | 38.1(6) | -3.1(5) | 10.9(10) | -3.7(14) |
| C25A | 148(4) | 46.4(9) | 31.5(8) | 2.9(7) | -5.1(12) | -3.2(12) |
| C25B | 63(9) | 38.1(10) | 37.2(8) | -0.7(6) | 17(2) | -1.1(15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C26A | 102(2) | 41.8(8) | 31.1(7) | -3.1(6) | 0.1(9) | -7.0(10) |
| C26B | 47(8) | 38.2(10) | 33.2(5) | -1.4(6) | 10.4(14) | -2.3(14) |
| C27A | 163(4) | 41.5(10) | 45.0(13) | 6.0(9) | 7.9(16) | 1.1(14) |
| C27B | 84(11) | 38.2(11) | 41(2) | -3.5(10) | 22(3) | -3.7(18) |
| B1 | 25.2(6) | 34.5(7) | 33.9(6) | -2.1(5) | 9.2(5) | 0.2(5) |
| B2 | 28.3(6) | 36.7(7) | 28.3(6) | -4.3(5) | 7.5(5) | -2.5(5) |
| B3 | 28.6(6) | 34.2(7) | 30.1(6) | -4.8(5) | 4.9(5) | -2.5(5) |
| B4 | 27.0(6) | 30.1(6) | 36.1(7) | -2.9(5) | 6.9(5) | -0.5(5) |
| B5 | 32.4(7) | 35.1(7) | 38.7(7) | -9.0(5) | 8.6(5) | -2.6(5) |
| B6 | 33.9(7) | 39.5(7) | 32.2(7) | -8.3(5) | 8.9(5) | -3.3(5) |
| B7 | 30.7(6) | 38.7(7) | 34.9(7) | -6.0(5) | 10.7(5) | -0.8(5) |
| B8 | 28.6(6) | 35.8(7) | 40.0(7) | -4.2(5) | 12.1(5) | 1.8(5) |
| B9 | 30.6(7) | 32.6(7) | 42.5(7) | -5.9(6) | 10.6(6) | 0.8(5) |
| B10 | 35.1(7) | 37.8(7) | 40.7(7) | -9.1(6) | 12.7(6) | -0.4(6) |

**Bond Lengths for 0538_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C1 | 1.2238(15) | C21B | C22 | 1.243(18) |
| N1 | C1 | 1.3478(15) | C21B | C26B | 1.42(2) |
| N1 | C10 | 1.4770(16) | C21B | B2 | 1.68(2) |
| N1 | C12 | 1.4694(16) | C22 | C23 | 1.385(2) |
| C1 | C2 | 1.5417(15) | C23 | C24A | 1.353(3) |
| C2 | C3 | 1.6932(16) | C23 | C24B | 1.52(2) |
| C2 | B1 | 1.8076(17) | C24A | C25A | 1.391(3) |
| C2 | B2 | 1.7342(17) | C24A | C27A | 1.506(3) |
| C2 | B3 | 1.7160(17) | C24B | C25B | 1.32(3) |
| C2 | B4 | 1.7265(17) | C24B | C27B | 1.59(3) |
| C3 | C4 | 1.5108(17) | C25A | C26A | 1.384(3) |
| C3 | B1 | 1.7699(18) | C25B | C26B | 1.385(19) |
| C3 | B4 | 1.7403(17) | B1 | B2 | 1.8243(19) |
| C3 | B8 | 1.7207(17) | B1 | B7 | 1.7823(19) |
| C3 | B9 | 1.7291(18) | B1 | B8 | 1.7904(19) |
| C4 | C5 | 1.3984(17) | B2 | B3 | 1.8047(19) |
| C4 | C9 | 1.3962(17) | B2 | B6 | 1.8094(19) |
| C5 | C6 | 1.3863(18) | B2 | B7 | 1.7877(19) |
| C6 | C7 | 1.3903(19) | B3 | B4 | 1.776(2) |
| C7 | C8 | 1.387(2) | B3 | B5 | 1.772(2) |
| C8 | C9 | 1.385(2) | B3 | B6 | 1.7614(19) |
| C10 | C11 | 1.514(2) | B4 | B5 | 1.766(2) |
| C12 | C13 | 1.5166(19) | B4 | B9 | 1.7719(19) |
| C14 | C15 | 1.3969(18) | B5 | B6 | 1.788(2) |
| C14 | C19 | 1.4023(18) | B5 | B9 | 1.780(2) |
| C14 | B1 | 1.5774(17) | B5 | B10 | 1.778(2) |

| | | | | | |
|---|---|---|---|---|---|
| C15 | C16 | 1.3900(19) | B6 | B7 | 1.770(2) |
| C16 | C17 | 1.390(2) | B6 | B10 | 1.771(2) |
| C17 | C18 | 1.384(2) | B7 | B8 | 1.766(2) |
| C17 | C20 | 1.5117(19) | B7 | B10 | 1.785(2) |
| C18 | C19 | 1.3926(19) | B8 | B9 | 1.769(2) |
| C21A | C22 | 1.403(2) | B8 | B10 | 1.775(2) |
| C21A | C26A | 1.378(3) | B9 | B10 | 1.771(2) |
| C21A | B2 | 1.563(3) | | | |

**Bond Angles for 0538_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 114.57(10) | C21A | B2 | B1 | 123.02(12) |
| C1 | N1 | C12 | 130.38(10) | C21A | B2 | B3 | 118.44(12) |
| C12 | N1 | C10 | 114.40(10) | C21A | B2 | B6 | 123.95(12) |
| O1 | C1 | N1 | 121.75(11) | C21A | B2 | B7 | 128.18(12) |
| O1 | C1 | C2 | 116.12(10) | C21B | B2 | C2 | 123.5(7) |
| N1 | C1 | C2 | 122.07(10) | C21B | B2 | B1 | 113.6(6) |
| C1 | C2 | C3 | 117.70(9) | C21B | B2 | B3 | 129.3(6) |
| C1 | C2 | B1 | 112.33(9) | C21B | B2 | B6 | 128.4(7) |
| C1 | C2 | B2 | 117.91(9) | C21B | B2 | B7 | 119.9(6) |
| C1 | C2 | B3 | 125.05(9) | B3 | B2 | B1 | 108.50(9) |
| C1 | C2 | B4 | 122.11(9) | B3 | B2 | B6 | 58.33(7) |
| C3 | C2 | B1 | 60.63(7) | B6 | B2 | B1 | 107.09(10) |
| C3 | C2 | B2 | 110.50(8) | B7 | B2 | B1 | 59.12(7) |
| C3 | C2 | B3 | 110.43(9) | B7 | B2 | B3 | 105.37(10) |
| C3 | C2 | B4 | 61.17(7) | B7 | B2 | B6 | 58.96(8) |
| B2 | C2 | B1 | 61.97(7) | C2 | B3 | B2 | 58.96(7) |
| B3 | C2 | B1 | 113.39(9) | C2 | B3 | B4 | 59.22(7) |
| B3 | C2 | B2 | 63.08(7) | C2 | B3 | B5 | 106.23(10) |
| B3 | C2 | B4 | 62.13(8) | C2 | B3 | B6 | 106.08(9) |
| B4 | C2 | B1 | 113.03(9) | B4 | B3 | B2 | 108.49(9) |
| B4 | C2 | B2 | 114.24(9) | B5 | B3 | B2 | 109.96(10) |
| C2 | C3 | B1 | 62.88(7) | B5 | B3 | B4 | 59.68(8) |
| C2 | C3 | B4 | 60.36(7) | B6 | B3 | B2 | 60.97(8) |
| C2 | C3 | B8 | 110.13(9) | B6 | B3 | B4 | 108.14(10) |
| C2 | C3 | B9 | 109.49(9) | B6 | B3 | B5 | 60.81(8) |
| C4 | C3 | C2 | 121.05(9) | C2 | B4 | C3 | 58.47(7) |
| C4 | C3 | B1 | 121.26(10) | C2 | B4 | B3 | 58.64(7) |
| C4 | C3 | B4 | 114.88(9) | C2 | B4 | B5 | 106.06(9) |
| C4 | C3 | B8 | 122.56(10) | C2 | B4 | B9 | 106.04(9) |
| C4 | C3 | B9 | 117.16(10) | C3 | B4 | B3 | 105.54(9) |
| B4 | C3 | B1 | 114.24(9) | C3 | B4 | B5 | 106.25(9) |
| B8 | C3 | B1 | 61.70(8) | C3 | B4 | B9 | 58.98(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B8 | C3 | B4 | 111.84(9) | B5 | B4 | B3 | 60.04(8) |
| B8 | C3 | B9 | 61.72(8) | B5 | B4 | B9 | 60.44(8) |
| B9 | C3 | B1 | 113.46(9) | B9 | B4 | B3 | 107.94(10) |
| B9 | C3 | B4 | 61.42(7) | B3 | B5 | B6 | 59.29(8) |
| C5 | C4 | C3 | 122.50(10) | B3 | B5 | B9 | 107.74(10) |
| C9 | C4 | C3 | 118.96(11) | B3 | B5 | B10 | 107.21(10) |
| C9 | C4 | C5 | 118.50(11) | B4 | B5 | B3 | 60.28(8) |
| C6 | C5 | C4 | 120.89(11) | B4 | B5 | B6 | 107.41(9) |
| C5 | C6 | C7 | 120.17(12) | B4 | B5 | B9 | 59.95(8) |
| C8 | C7 | C6 | 119.13(13) | B4 | B5 | B10 | 107.68(10) |
| C9 | C8 | C7 | 120.96(13) | B9 | B5 | B6 | 107.08(10) |
| C8 | C9 | C4 | 120.30(12) | B10 | B5 | B6 | 59.57(8) |
| N1 | C10 | C11 | 112.38(12) | B10 | B5 | B9 | 59.70(8) |
| N1 | C12 | C13 | 113.55(12) | B3 | B6 | B2 | 60.70(7) |
| C15 | C14 | C19 | 116.44(12) | B3 | B6 | B5 | 59.89(8) |
| C15 | C14 | B1 | 125.83(11) | B3 | B6 | B7 | 108.01(9) |
| C19 | C14 | B1 | 117.34(11) | B3 | B6 | B10 | 107.97(10) |
| C16 | C15 | C14 | 121.52(14) | B5 | B6 | B2 | 109.01(9) |
| C17 | C16 | C15 | 121.60(15) | B7 | B6 | B2 | 59.91(8) |
| C16 | C17 | C20 | 120.22(17) | B7 | B6 | B5 | 108.28(10) |
| C18 | C17 | C16 | 117.42(13) | B7 | B6 | B10 | 60.51(8) |
| C18 | C17 | C20 | 122.36(17) | B10 | B6 | B2 | 108.94(10) |
| C17 | C18 | C19 | 121.34(14) | B10 | B6 | B5 | 59.92(8) |
| C18 | C19 | C14 | 121.64(14) | B1 | B7 | B2 | 61.46(7) |
| C22 | C21A | B2 | 124.59(18) | B1 | B7 | B10 | 109.99(10) |
| C26A | C21A | C22 | 115.63(18) | B6 | B7 | B1 | 110.72(9) |
| C26A | C21A | B2 | 119.77(16) | B6 | B7 | B2 | 61.13(8) |
| C22 | C21B | C26B | 120.1(17) | B6 | B7 | B10 | 59.78(8) |
| C22 | C21B | B2 | 127.2(16) | B8 | B7 | B1 | 60.61(8) |
| C26B | C21B | B2 | 112.6(12) | B8 | B7 | B2 | 109.03(9) |
| C21B | C22 | C23 | 122.4(10) | B8 | B7 | B6 | 108.01(10) |
| C23 | C22 | C21A | 122.14(15) | B8 | B7 | B10 | 60.00(9) |
| C22 | C23 | C24B | 118.5(9) | B10 | B7 | B2 | 109.34(10) |
| C24A | C23 | C22 | 121.54(16) | C3 | B8 | B1 | 60.50(7) |
| C23 | C24A | C25A | 117.2(2) | C3 | B8 | B7 | 105.73(9) |
| C23 | C24A | C27A | 121.0(2) | C3 | B8 | B9 | 59.37(7) |
| C25A | C24A | C27A | 121.8(2) | C3 | B8 | B10 | 106.04(10) |
| C23 | C24B | C27B | 124.0(16) | B7 | B8 | B1 | 60.15(8) |
| C25B | C24B | C23 | 116.0(17) | B7 | B8 | B9 | 108.35(10) |
| C25B | C24B | C27B | 118.1(16) | B7 | B8 | B10 | 60.52(8) |
| C26A | C25A | C24A | 121.62(19) | B9 | B8 | B1 | 110.53(9) |
| C24B | C25B | C26B | 119.7(14) | B9 | B8 | B10 | 59.95(8) |
| C21A | C26A | C25A | 121.78(17) | B10 | B8 | B1 | 110.04(10) |
| C25B | C26B | C21B | 121.5(13) | C3 | B9 | B4 | 59.60(7) |
| C2 | B1 | B2 | 57.04(7) | C3 | B9 | B5 | 106.09(10) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C3 | B1 | C2 | 56.48(6) | C3 | B9 | B8 | 58.91(7) |
| C3 | B1 | B2 | 103.16(9) | C3 | B9 | B10 | 105.87(10) |
| C3 | B1 | B7 | 102.99(9) | B4 | B9 | B5 | 59.61(8) |
| C3 | B1 | B8 | 57.80(7) | B8 | B9 | B4 | 108.09(10) |
| C14 | B1 | C2 | 130.78(10) | B8 | B9 | B5 | 108.28(10) |
| C14 | B1 | C3 | 123.96(10) | B8 | B9 | B10 | 60.19(8) |
| C14 | B1 | B2 | 126.91(10) | B10 | B9 | B4 | 107.71(10) |
| C14 | B1 | B7 | 122.19(10) | B10 | B9 | B5 | 60.08(9) |
| C14 | B1 | B8 | 118.23(10) | B5 | B10 | B7 | 108.11(10) |
| B7 | B1 | C2 | 101.71(9) | B6 | B10 | B5 | 60.51(8) |
| B7 | B1 | B2 | 59.42(8) | B6 | B10 | B7 | 59.71(8) |
| B7 | B1 | B8 | 59.24(8) | B6 | B10 | B8 | 107.53(10) |
| B8 | B1 | C2 | 102.13(9) | B8 | B10 | B5 | 108.14(10) |
| B8 | B1 | B2 | 106.36(9) | B8 | B10 | B7 | 59.48(8) |
| C2 | B2 | B1 | 60.99(7) | B9 | B10 | B5 | 60.22(8) |
| C2 | B2 | B3 | 57.97(7) | B9 | B10 | B6 | 108.24(10) |
| C2 | B2 | B6 | 103.26(9) | B9 | B10 | B7 | 107.45(10) |
| C2 | B2 | B7 | 104.46(9) | B9 | B10 | B8 | 59.86(8) |
| C21A | B2 | C2 | 121.25(12) | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for 0538_CG_0m.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | 8735.58 | 4508.79 | 4461.07 | 40 |
| H6 | 8336.83 | 4699.46 | 3370.03 | 45 |
| H7 | 6745.74 | 5189.25 | 2909.89 | 52 |
| H8 | 5600.08 | 5511.08 | 3561.43 | 56 |
| H9 | 5995.29 | 5326.87 | 4652.43 | 47 |
| H10A | 9226.22 | 2864.97 | 4796.4 | 52 |
| H10B | 10514.89 | 2951.7 | 4953.45 | 52 |
| H11A | 9851.61 | 3024.56 | 3849.28 | 77 |
| H11B | 10334.28 | 3623.4 | 4117.22 | 77 |
| H11C | 9049.38 | 3522.82 | 3955.42 | 77 |
| H12A | 10565.44 | 4250.09 | 5719.42 | 42 |
| H12B | 11143.31 | 3965.66 | 5201.17 | 42 |
| H13A | 11682.48 | 3195.6 | 5864.75 | 77 |
| H13B | 10994.33 | 3416.08 | 6364.47 | 77 |
| H13C | 12048.48 | 3755.76 | 6271.76 | 77 |
| H15 | 6094.59 | 4036.69 | 4384.7 | 49 |
| H16 | 4491.08 | 3608.09 | 3875.59 | 59 |
| H18 | 3909.15 | 3126.6 | 5574.36 | 56 |
| H19 | 5504.89 | 3561.11 | 6091.33 | 48 |
| H20A | 2622.83 | 2864.13 | 4631.14 | 104 |

| | | | | |
|---|---|---|---|---|
| H20B | 3115.33 | 2793.67 | 4005.23 | 104 |
| H20C | 2475.5 | 3358.12 | 4109.82 | 104 |
| H22 | 7479.29 | 2947.39 | 5728.05 | 49 |
| H22A | 7646.04 | 2948.74 | 5718.61 | 49 |
| H23 | 7714.65 | 2022.91 | 6072.49 | 49 |
| H23A | 7925.76 | 2020.59 | 6077.11 | 49 |
| H25A | 8978.1 | 2561.37 | 7841.99 | 95 |
| H25B | 7822.03 | 2579.42 | 7865.17 | 54 |
| H26A | 8807.56 | 3488.26 | 7498.55 | 72 |
| H26B | 7978.79 | 3492.64 | 7483.88 | 47 |
| H27A | 7738.25 | 1460.67 | 7304.05 | 128 |
| H27B | 8999.83 | 1557.62 | 7603.71 | 128 |
| H27C | 8622.54 | 1347.45 | 6880.76 | 128 |
| H27D | 8587.6 | 1560.12 | 7775.51 | 80 |
| H27E | 8202.26 | 1304.21 | 7072.64 | 80 |
| H27F | 7320.34 | 1507.08 | 7464.08 | 80 |
| H3 | 9980(12) | 4166(6) | 6544(7) | 36(4) |
| H4 | 9524(12) | 4979(6) | 5466(7) | 34(4) |
| H5A | 9548(14) | 5385(7) | 6803(8) | 47(4) |
| H6A | 8542(12) | 4471(6) | 7449(7) | 37(4) |
| H7A | 6297(13) | 4316(6) | 6729(7) | 40(4) |
| H8A | 5937(14) | 5124(7) | 5608(8) | 42(4) |
| H9A | 7870(12) | 5744(6) | 5639(7) | 34(4) |
| H10 | 7234(14) | 5472(7) | 6886(8) | 48(4) |

**Atomic Occupancy for 0538_CG_0m.**

| Atom | *Occupancy* | Atom | *Occupancy* | Atom | *Occupancy* |
|---|---|---|---|---|---|
| C21A | 0.887(7) | C21B | 0.113(7) | H22 | 0.887(7) |
| H22A | 0.113(7) | H23 | 0.887(7) | H23A | 0.113(7) |
| C24A | 0.887(7) | C24B | 0.113(7) | C25A | 0.887(7) |
| H25A | 0.887(7) | C25B | 0.113(7) | H25B | 0.113(7) |
| C26A | 0.887(7) | H26A | 0.887(7) | C26B | 0.113(7) |
| H26B | 0.113(7) | C27A | 0.887(7) | H27A | 0.887(7) |
| H27B | 0.887(7) | H27C | 0.887(7) | C27B | 0.113(7) |
| H27D | 0.113(7) | H27E | 0.113(7) | H27F | 0.113(7) |

**Solvent masks information for 0538_CG_0m.**

| Number | X | Y | Z | Volume | Electron count | Content |
|---|---|---|---|---|---|---|
| 1 | 0.000 | 0.186 | 0.250 | 195.3 | 49.9 | 0.5 Cl3HC |
| 2 | 0.000 | -0.186 | 0.750 | 195.3 | 49.9 | 0.5 Cl3HC |
| 3 | 0.500 | 0.314 | 0.750 | 195.3 | 49.9 | 0.5 Cl3HC |

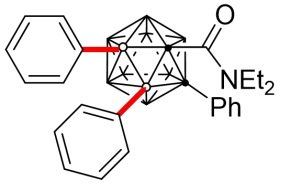
| | | | | | | |
|---|---|---|---|---|---|---|
| 4 | 0.500 | 0.686 | 0.250 | 195.3 | 49.9 | 0.5 Cl3HC |

**Experimental**

Single crystals of $C_{27}H_{37}B_{10}NO$ [0538_CG_0m] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

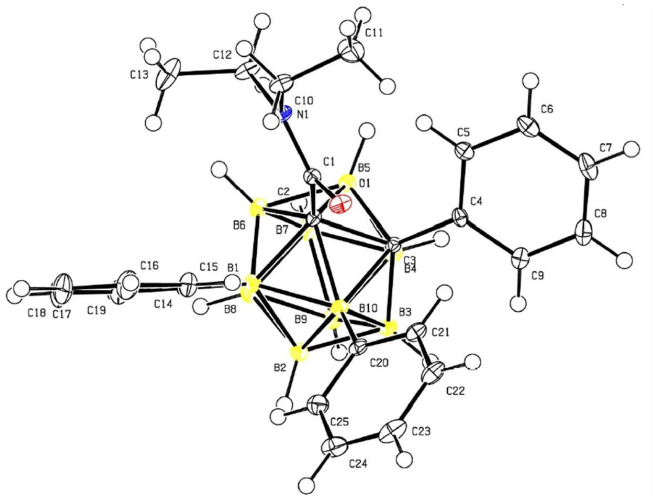
**Crystal structure determination of 3aa**

**Crystal Data** for $C_{27}H_{38}B_{10}NO$ (*M* = 499.68 g/mol): monoclinic, space group C2/c (no. 15), *a* = 12.5994(11) Å, *b* = 23.669(2) Å, *c* = 21.4198(18) Å, *β* = 102.169(3)°, *V* = 6244.2(9) Å$^3$, *Z* = 8, *T* = 100.03 K, μ(CuKα) = 1.633 mm$^{-1}$, *Dcalc* = 1.190 g/cm$^3$, 38084 reflections measured (7.47° ≤ 2Θ ≤ 149.188°), 6321 unique ($R_{int}$ = 0.0376, $R_{sigma}$ = 0.0261) which were used in all calculations. The final $R_1$ was 0.0515 (I > 2σ(I)) and $wR_2$ was 0.1455 (all data).




**3ab**

≡




**CCDC 1983600**

**Crystal data and structure refinement for 3ab.**

| | |
|---|---|
| Identification code | mo_0922_CG_0m |
| CCDC number | 1983600 |
| Empirical formula | $C_{25}H_{33}B_{10}NO$ |
| Formula weight | 471.62 |
| Temperature/K | 100.0 |

| | |
|---|---|
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 13.6114(6) |
| b/Å | 13.9152(8) |
| c/Å | 14.1817(8) |
| α/° | 90 |
| β/° | 93.358(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 2681.5(2) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.168 |
| μ/mm$^{-1}$ | 0.064 |
| F(000) | 992.0 |
| Crystal size/mm$^3$ | 0.405 × 0.28 × 0.122 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.032 to 57.426 |
| Index ranges | -18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -19 ≤ l ≤ 19 |
| Reflections collected | 60954 |
| Independent reflections | 6925 [$R_{int}$ = 0.0319, $R_{sigma}$ = 0.0183] |
| Data/restraints/parameters | 6925/0/368 |
| Goodness-of-fit on $F^2$ | 1.084 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0425, $wR_2$ = 0.1089 |
| Final R indexes [all data] | $R_1$ = 0.0471, $wR_2$ = 0.1132 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.64/-0.21 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0922_CG_0m. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 8016.6(5) | 6425.9(6) | 6714.1(5) | 14.14(15) |
| N1 | 9458.3(6) | 6888.7(6) | 6174.7(6) | 13.08(17) |
| C1 | 8524.9(7) | 6572.4(7) | 6044.0(7) | 10.46(18) |
| C2 | 8029.1(7) | 6388.6(7) | 5048.2(7) | 9.57(17) |
| C3 | 7517.6(7) | 5288.4(7) | 4869.4(7) | 9.65(17) |
| C4 | 7706.9(7) | 4469.4(7) | 5562.1(7) | 10.61(18) |
| C5 | 8580.6(7) | 4390.0(7) | 6119.5(7) | 13.07(19) |
| C6 | 8756.6(8) | 3589.2(8) | 6698.1(7) | 16.8(2) |
| C7 | 8067.1(9) | 2854.7(8) | 6718.4(8) | 18.7(2) |
| C8 | 7198.2(8) | 2929.3(8) | 6160.3(8) | 18.3(2) |
| C9 | 7014.3(8) | 3728.1(7) | 5584.6(7) | 15.2(2) |
| C10 | 9787.5(8) | 7080.1(8) | 7170.0(7) | 16.0(2) |
| C11 | 10073.6(9) | 6163.0(9) | 7705.3(8) | 23.2(2) |
| C12 | 10206.1(7) | 7070.8(8) | 5492.5(7) | 16.9(2) |
| C13 | 10324.2(10) | 8138.0(9) | 5283.7(9) | 27.7(3) |

| | | | | |
|---|---|---|---|---|
| C14 | 7317.6(7) | 8329.2(7) | 4927.1(7) | 12.72(19) |
| C15 | 7264.2(8) | 8543.3(8) | 5888.8(8) | 17.1(2) |
| C16 | 7346.8(9) | 9484.7(8) | 6220.0(8) | 22.4(2) |
| C17 | 7482.0(10) | 10235.2(8) | 5594.9(9) | 24.9(2) |
| C18 | 7526.7(9) | 10044.0(8) | 4637.3(9) | 23.9(2) |
| C19 | 7448.2(8) | 9103.3(8) | 4308.1(8) | 17.7(2) |
| C20 | 6044.8(7) | 6325.4(7) | 5957.2(7) | 11.94(19) |
| C21 | 6072.7(7) | 5680.6(7) | 6719.9(7) | 13.88(19) |
| C22 | 5392.3(8) | 5733.0(8) | 7414.2(8) | 18.3(2) |
| C23 | 4664.1(8) | 6433.5(9) | 7363.4(8) | 21.4(2) |
| C24 | 4626.3(8) | 7085.5(8) | 6623.8(9) | 21.5(2) |
| C25 | 5308.9(8) | 7031.9(8) | 5927.4(8) | 16.5(2) |
| B1 | 7285.4(8) | 7272.2(8) | 4517.7(7) | 11.0(2) |
| B2 | 6286.1(8) | 6622.8(8) | 3940.2(8) | 12.1(2) |
| B3 | 6435.8(8) | 5383.6(8) | 4187.7(8) | 11.1(2) |
| B4 | 7528.0(8) | 4986.6(8) | 3686.6(8) | 11.8(2) |
| B5 | 8534.0(8) | 5616.5(8) | 4252.1(8) | 11.1(2) |
| B6 | 8372.8(8) | 6855.1(8) | 3994.5(8) | 12.0(2) |
| B7 | 8064.9(8) | 5980.5(8) | 3120.4(8) | 12.8(2) |
| B8 | 7284.5(8) | 6993.5(8) | 3275.6(8) | 12.9(2) |
| B9 | 6764.1(8) | 5841.0(8) | 3074.6(8) | 12.8(2) |
| B10 | 6717.2(8) | 6256.3(8) | 5089.4(7) | 10.10(19) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_0922_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 12.1(3) | 19.9(4) | 10.5(3) | -0.4(3) | 0.8(3) | -1.7(3) |
| N1 | 10.7(4) | 17.4(4) | 11.0(4) | -3.2(3) | -0.2(3) | -3.5(3) |
| C1 | 10.7(4) | 10.8(4) | 9.7(4) | -1.2(3) | -0.8(3) | 0.4(3) |
| C2 | 9.6(4) | 9.6(4) | 9.4(4) | -0.2(3) | 0.1(3) | -2.0(3) |
| C3 | 9.4(4) | 9.6(4) | 9.8(4) | -0.5(3) | -0.3(3) | -1.2(3) |
| C4 | 13.0(4) | 9.2(4) | 9.8(4) | 0.1(3) | 2.3(3) | 1.4(3) |
| C5 | 13.6(4) | 13.7(4) | 12.0(4) | -0.3(3) | 1.1(3) | 1.9(3) |
| C6 | 19.8(5) | 17.9(5) | 12.7(5) | 1.5(4) | 1.0(4) | 6.1(4) |
| C7 | 28.8(6) | 13.4(5) | 14.5(5) | 3.5(4) | 6.2(4) | 6.0(4) |
| C8 | 24.1(5) | 12.0(5) | 19.5(5) | 1.6(4) | 6.2(4) | -1.6(4) |
| C9 | 16.8(5) | 12.8(5) | 16.0(5) | 0.3(4) | 1.8(4) | -1.9(4) |
| C10 | 13.7(4) | 22.3(5) | 11.6(4) | -4.8(4) | -2.4(3) | -3.9(4) |
| C11 | 24.5(5) | 26.0(6) | 18.0(5) | -1.6(4) | -7.6(4) | 1.1(4) |
| C12 | 10.5(4) | 24.9(5) | 15.6(5) | -4.1(4) | 2.4(3) | -5.3(4) |
| C13 | 33.9(6) | 27.8(6) | 21.8(6) | -3.7(5) | 4.7(5) | -18.5(5) |
| C14 | 12.4(4) | 10.5(4) | 15.2(5) | -0.6(4) | 0.3(3) | -1.4(3) |
| C15 | 22.1(5) | 13.5(5) | 15.7(5) | -0.5(4) | 1.4(4) | -3.1(4) |
| C16 | 30.6(6) | 17.4(5) | 19.6(5) | -5.2(4) | 3.5(4) | -4.7(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 34.2(6) | 12.0(5) | 28.6(6) | -5.2(4) | 3.5(5) | -4.6(4) |
| C18 | 33.4(6) | 12.2(5) | 26.1(6) | 2.9(4) | 3.2(5) | -4.3(4) |
| C19 | 23.0(5) | 13.9(5) | 16.2(5) | 1.1(4) | 1.3(4) | -2.5(4) |
| C20 | 9.6(4) | 13.1(4) | 13.0(4) | -4.0(3) | -0.1(3) | -2.9(3) |
| C21 | 12.6(4) | 16.1(5) | 13.0(4) | -2.9(4) | 0.7(3) | -3.5(3) |
| C22 | 18.8(5) | 22.8(5) | 13.7(5) | -5.1(4) | 3.6(4) | -8.7(4) |
| C23 | 16.9(5) | 27.4(6) | 20.8(5) | -13.9(4) | 7.8(4) | -7.1(4) |
| C24 | 14.4(5) | 21.2(5) | 28.9(6) | -13.1(4) | 2.6(4) | 0.5(4) |
| C25 | 14.4(4) | 14.9(5) | 20.1(5) | -5.0(4) | -0.8(4) | 0.2(4) |
| B1 | 12.7(5) | 9.6(5) | 10.6(5) | 1.0(4) | -0.5(4) | -0.6(4) |
| B2 | 13.2(5) | 11.8(5) | 11.1(5) | 1.0(4) | -2.2(4) | -0.8(4) |
| B3 | 10.5(4) | 12.0(5) | 10.4(5) | -0.9(4) | -1.6(4) | -1.1(4) |
| B4 | 13.4(5) | 12.5(5) | 9.3(5) | -1.2(4) | 0.4(4) | -1.0(4) |
| B5 | 11.6(5) | 11.6(5) | 10.1(5) | -0.4(4) | 1.6(4) | -1.2(4) |
| B6 | 13.5(5) | 12.5(5) | 10.0(5) | 1.1(4) | 1.7(4) | -2.1(4) |
| B7 | 15.5(5) | 13.0(5) | 9.8(5) | 0.0(4) | 0.8(4) | -1.7(4) |
| B8 | 15.5(5) | 13.2(5) | 9.8(5) | 1.5(4) | -0.8(4) | -1.9(4) |
| B9 | 14.8(5) | 13.8(5) | 9.7(5) | 0.2(4) | -1.1(4) | -1.3(4) |
| B10 | 9.2(4) | 10.5(5) | 10.4(5) | -0.3(4) | -0.8(3) | -0.3(3) |

**Bond Lengths for mo_0922_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C1 | 1.2249(12) | C18 | C19 | 1.3918(15) |
| N1 | C1 | 1.3471(12) | C20 | C21 | 1.4041(14) |
| N1 | C10 | 1.4799(12) | C20 | C25 | 1.4023(14) |
| N1 | C12 | 1.4669(13) | C20 | B10 | 1.5792(14) |
| C1 | C2 | 1.5503(13) | C21 | C22 | 1.3927(14) |
| C2 | C3 | 1.6947(13) | C22 | C23 | 1.3890(17) |
| C2 | B1 | 1.7358(14) | C23 | C24 | 1.3856(18) |
| C2 | B5 | 1.7298(14) | C24 | C25 | 1.3970(15) |
| C2 | B6 | 1.7191(14) | B1 | B2 | 1.7909(15) |
| C2 | B10 | 1.7995(14) | B1 | B6 | 1.7907(16) |
| C3 | C4 | 1.5169(13) | B1 | B8 | 1.8037(16) |
| C3 | B3 | 1.7187(14) | B1 | B10 | 1.8240(15) |
| C3 | B4 | 1.7300(14) | B2 | B3 | 1.7691(16) |
| C3 | B5 | 1.7409(14) | B2 | B8 | 1.7753(16) |
| C3 | B10 | 1.7715(14) | B2 | B9 | 1.7909(16) |
| C4 | C5 | 1.3933(13) | B2 | B10 | 1.7743(15) |
| C4 | C9 | 1.3990(14) | B3 | B4 | 1.7732(16) |
| C5 | C6 | 1.3961(14) | B3 | B9 | 1.7831(16) |
| C6 | C7 | 1.3890(16) | B3 | B10 | 1.7887(15) |
| C7 | C8 | 1.3880(16) | B4 | B5 | 1.7771(15) |
| C8 | C9 | 1.3932(15) | B4 | B7 | 1.7776(16) |

| | | | | | |
|---|---|---|---|---|---|
| C10 | C11 | 1.5237(16) | B4 | B9 | 1.7726(16) |
| C12 | C13 | 1.5246(17) | B5 | B6 | 1.7727(16) |
| C14 | C15 | 1.4020(14) | B5 | B7 | 1.7663(16) |
| C14 | C19 | 1.4073(14) | B6 | B7 | 1.7699(16) |
| C14 | B1 | 1.5810(14) | B6 | B8 | 1.7590(16) |
| C15 | C16 | 1.3939(15) | B7 | B8 | 1.7864(17) |
| C16 | C17 | 1.3891(17) | B7 | B9 | 1.7785(16) |
| C17 | C18 | 1.3887(18) | B8 | B9 | 1.7695(16) |

**Bond Angles for mo_0922_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 114.86(8) | B10 | B2 | B9 | 109.94(8) |
| C1 | N1 | C12 | 130.62(8) | C3 | B3 | B2 | 105.76(7) |
| C12 | N1 | C10 | 114.51(8) | C3 | B3 | B4 | 59.37(6) |
| O1 | C1 | N1 | 121.25(9) | C3 | B3 | B9 | 105.93(7) |
| O1 | C1 | C2 | 116.34(8) | C3 | B3 | B10 | 60.63(6) |
| N1 | C1 | C2 | 122.40(8) | B2 | B3 | B4 | 108.28(8) |
| C1 | C2 | C3 | 116.00(7) | B2 | B3 | B9 | 60.55(6) |
| C1 | C2 | B1 | 119.32(8) | B2 | B3 | B10 | 59.83(6) |
| C1 | C2 | B5 | 121.91(8) | B4 | B3 | B9 | 59.79(6) |
| C1 | C2 | B6 | 127.12(8) | B4 | B3 | B10 | 110.40(7) |
| C1 | C2 | B10 | 111.54(7) | B9 | B3 | B10 | 109.65(8) |
| C3 | C2 | B1 | 110.55(7) | C3 | B4 | B3 | 58.75(6) |
| C3 | C2 | B5 | 61.10(6) | C3 | B4 | B5 | 59.51(6) |
| C3 | C2 | B6 | 109.96(7) | C3 | B4 | B7 | 106.02(7) |
| C3 | C2 | B10 | 60.84(6) | C3 | B4 | B9 | 105.90(7) |
| B1 | C2 | B10 | 62.09(6) | B3 | B4 | B5 | 107.91(7) |
| B5 | C2 | B1 | 113.64(7) | B3 | B4 | B7 | 108.37(8) |
| B5 | C2 | B10 | 112.99(7) | B5 | B4 | B7 | 59.59(6) |
| B6 | C2 | B1 | 62.44(6) | B9 | B4 | B3 | 60.38(6) |
| B6 | C2 | B5 | 61.86(6) | B9 | B4 | B5 | 107.73(8) |
| B6 | C2 | B10 | 112.82(7) | B9 | B4 | B7 | 60.13(6) |
| C2 | C3 | B3 | 110.22(7) | C2 | B5 | C3 | 58.46(6) |
| C2 | C3 | B4 | 109.74(7) | C2 | B5 | B4 | 106.01(7) |
| C2 | C3 | B5 | 60.45(6) | C2 | B5 | B6 | 58.77(6) |
| C2 | C3 | B10 | 62.51(6) | C2 | B5 | B7 | 106.18(8) |
| C4 | C3 | C2 | 121.95(7) | C3 | B5 | B4 | 58.90(6) |
| C4 | C3 | B3 | 121.98(8) | C3 | B5 | B6 | 105.44(7) |
| C4 | C3 | B4 | 115.77(8) | C3 | B5 | B7 | 106.05(7) |
| C4 | C3 | B5 | 114.39(7) | B6 | B5 | B4 | 107.68(8) |
| C4 | C3 | B10 | 122.69(8) | B7 | B5 | B4 | 60.22(6) |
| B3 | C3 | B4 | 61.88(6) | B7 | B5 | B6 | 60.01(6) |
| B3 | C3 | B5 | 112.14(7) | C2 | B6 | B1 | 59.24(6) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B3 | C3 | B10 | 61.64(6) | C2 | B6 | B5 | 59.37(6) |
| B4 | C3 | B5 | 61.59(6) | C2 | B6 | B7 | 106.49(7) |
| B4 | C3 | B10 | 113.29(7) | C2 | B6 | B8 | 106.40(7) |
| B5 | C3 | B10 | 113.84(7) | B5 | B6 | B1 | 108.97(7) |
| C5 | C4 | C3 | 122.27(9) | B7 | B6 | B1 | 110.21(8) |
| C5 | C4 | C9 | 118.85(9) | B7 | B6 | B5 | 59.81(6) |
| C9 | C4 | C3 | 118.66(9) | B8 | B6 | B1 | 61.07(6) |
| C4 | C5 | C6 | 120.53(10) | B8 | B6 | B5 | 108.41(8) |
| C7 | C6 | C5 | 120.44(10) | B8 | B6 | B7 | 60.82(6) |
| C8 | C7 | C6 | 119.17(10) | B4 | B7 | B8 | 107.17(8) |
| C7 | C8 | C9 | 120.78(10) | B4 | B7 | B9 | 59.80(6) |
| C8 | C9 | C4 | 120.23(10) | B5 | B7 | B4 | 60.19(6) |
| N1 | C10 | C11 | 112.26(9) | B5 | B7 | B6 | 60.17(6) |
| N1 | C12 | C13 | 112.43(9) | B5 | B7 | B8 | 107.47(8) |
| C15 | C14 | C19 | 117.38(9) | B5 | B7 | B9 | 107.94(8) |
| C15 | C14 | B1 | 123.57(9) | B6 | B7 | B4 | 107.78(8) |
| C19 | C14 | B1 | 119.00(9) | B6 | B7 | B8 | 59.29(6) |
| C16 | C15 | C14 | 121.31(10) | B6 | B7 | B9 | 107.16(8) |
| C17 | C16 | C15 | 120.17(11) | B9 | B7 | B8 | 59.52(6) |
| C18 | C17 | C16 | 119.68(11) | B2 | B8 | B1 | 60.05(6) |
| C17 | C18 | C19 | 120.09(11) | B2 | B8 | B7 | 108.38(8) |
| C18 | C19 | C14 | 121.37(10) | B6 | B8 | B1 | 60.33(6) |
| C21 | C20 | B10 | 124.80(9) | B6 | B8 | B2 | 107.78(7) |
| C25 | C20 | C21 | 117.28(9) | B6 | B8 | B7 | 59.89(6) |
| C25 | C20 | B10 | 117.69(9) | B6 | B8 | B9 | 108.04(8) |
| C22 | C21 | C20 | 121.47(10) | B7 | B8 | B1 | 108.88(8) |
| C23 | C22 | C21 | 120.14(11) | B9 | B8 | B1 | 109.24(8) |
| C24 | C23 | C22 | 119.57(10) | B9 | B8 | B2 | 60.69(6) |
| C23 | C24 | C25 | 120.23(10) | B9 | B8 | B7 | 60.02(6) |
| C24 | C25 | C20 | 121.30(11) | B3 | B9 | B2 | 59.34(6) |
| C2 | B1 | B2 | 104.41(7) | B4 | B9 | B2 | 107.34(7) |
| C2 | B1 | B6 | 58.32(6) | B4 | B9 | B3 | 59.83(6) |
| C2 | B1 | B8 | 103.77(7) | B4 | B9 | B7 | 60.08(6) |
| C2 | B1 | B10 | 60.67(6) | B7 | B9 | B2 | 108.03(8) |
| C14 | B1 | C2 | 119.80(8) | B7 | B9 | B3 | 107.89(7) |
| C14 | B1 | B2 | 129.89(8) | B8 | B9 | B2 | 59.81(6) |
| C14 | B1 | B6 | 116.61(8) | B8 | B9 | B3 | 107.44(8) |
| C14 | B1 | B8 | 123.85(8) | B8 | B9 | B4 | 108.13(8) |
| C14 | B1 | B10 | 124.14(8) | B8 | B9 | B7 | 60.46(6) |
| B2 | B1 | B8 | 59.19(6) | C2 | B10 | B1 | 57.24(6) |
| B2 | B1 | B10 | 58.78(6) | C3 | B10 | C2 | 56.66(5) |
| B6 | B1 | B2 | 105.73(7) | C3 | B10 | B1 | 103.28(7) |
| B6 | B1 | B8 | 58.60(6) | C3 | B10 | B2 | 103.32(7) |
| B6 | B1 | B10 | 108.38(7) | C3 | B10 | B3 | 57.73(6) |
| B8 | B1 | B10 | 106.94(7) | C20 | B10 | C2 | 129.84(8) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B1 | B2 | B9 | 108.86(8) | C20 | B10 | C3 | 125.03(8) |
| B3 | B2 | B1 | 109.00(7) | C20 | B10 | B1 | 125.41(8) |
| B3 | B2 | B8 | 107.80(8) | C20 | B10 | B2 | 121.52(8) |
| B3 | B2 | B9 | 60.11(6) | C20 | B10 | B3 | 119.27(8) |
| B3 | B2 | B10 | 60.64(6) | B2 | B10 | C2 | 102.49(7) |
| B8 | B2 | B1 | 60.77(6) | B2 | B10 | B1 | 59.68(6) |
| B8 | B2 | B9 | 59.50(6) | B2 | B10 | B3 | 59.54(6) |
| B10 | B2 | B1 | 61.54(6) | B3 | B10 | C2 | 102.57(7) |
| B10 | B2 | B8 | 110.42(8) | B3 | B10 | B1 | 106.68(7) |

**Torsion Angles for mo_0922_CG_0m.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O1 | C1 | C2 | C3 | -53.90(11) | B3 | C3 | B10 | B2 | -40.03(7) |
| O1 | C1 | C2 | B1 | 82.30(11) | B3 | B2 | B8 | B1 | -102.24(8) |
| O1 | C1 | C2 | B5 | -124.65(10) | B3 | B2 | B8 | B6 | -63.94(9) |
| O1 | C1 | C2 | B6 | 158.38(9) | B3 | B2 | B8 | B7 | -0.59(10) |
| O1 | C1 | C2 | B10 | 13.12(12) | B3 | B2 | B8 | B9 | 37.19(7) |
| N1 | C1 | C2 | C3 | 127.00(9) | B3 | B2 | B9 | B4 | -37.13(7) |
| N1 | C1 | C2 | B1 | -96.80(11) | B3 | B2 | B9 | B7 | -100.52(8) |
| N1 | C1 | C2 | B5 | 56.25(13) | B3 | B2 | B9 | B8 | -138.41(8) |
| N1 | C1 | C2 | B6 | -20.72(15) | B3 | B2 | B10 | C2 | 97.37(7) |
| N1 | C1 | C2 | B10 | -165.98(9) | B3 | B2 | B10 | C3 | 39.11(7) |
| C1 | N1 | C10 | C11 | 79.51(11) | B3 | B2 | B10 | C20 | -107.73(10) |
| C1 | N1 | C12 | C13 | 102.55(13) | B3 | B2 | B10 | B1 | 136.87(8) |
| C1 | C2 | C3 | C4 | -11.86(12) | B3 | B4 | B5 | C2 | -1.43(10) |
| C1 | C2 | C3 | B3 | 141.61(8) | B3 | B4 | B5 | C3 | 34.60(7) |
| C1 | C2 | C3 | B4 | -152.06(8) | B3 | B4 | B5 | B6 | -63.10(9) |
| C1 | C2 | C3 | B5 | -113.74(9) | B3 | B4 | B5 | B7 | -101.21(8) |
| C1 | C2 | C3 | B10 | 101.28(8) | B3 | B4 | B7 | B5 | 100.42(8) |
| C1 | C2 | B1 | C14 | 14.52(12) | B3 | B4 | B7 | B6 | 62.21(9) |
| C1 | C2 | B1 | B2 | -141.01(8) | B3 | B4 | B7 | B8 | -0.26(10) |
| C1 | C2 | B1 | B6 | 119.18(9) | B3 | B4 | B7 | B9 | -37.69(7) |
| C1 | C2 | B1 | B8 | 157.77(8) | B3 | B4 | B9 | B2 | 36.92(7) |
| C1 | C2 | B1 | B10 | -100.31(9) | B3 | B4 | B9 | B7 | 138.13(8) |
| C1 | C2 | B5 | C3 | 104.25(9) | B3 | B4 | B9 | B8 | 100.04(8) |
| C1 | C2 | B5 | B4 | 140.48(8) | B4 | C3 | C4 | C5 | 108.65(10) |
| C1 | C2 | B5 | B6 | -118.24(9) | B4 | C3 | C4 | C9 | -65.98(11) |
| C1 | C2 | B5 | B7 | -156.57(8) | B4 | C3 | B3 | B2 | -102.22(8) |
| C1 | C2 | B6 | B1 | -107.32(10) | B4 | C3 | B3 | B9 | -39.01(7) |
| C1 | C2 | B6 | B5 | 110.31(10) | B4 | C3 | B3 | B10 | -142.93(8) |
| C1 | C2 | B6 | B7 | 148.61(9) | B4 | C3 | B5 | C2 | 138.43(8) |
| C1 | C2 | B6 | B8 | -147.68(9) | B4 | C3 | B5 | B6 | 101.62(8) |
| C1 | C2 | B10 | C3 | -108.63(8) | B4 | C3 | B5 | B7 | 39.01(7) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C1 | C2 | B10 | C20 | 1.61(13) | B4 | C3 | B10 | C2 | -100.99(8) |
| C1 | C2 | B10 | B1 | 112.74(8) | B4 | C3 | B10 | C20 | 140.64(9) |
| C1 | C2 | B10 | B2 | 153.51(8) | B4 | C3 | B10 | B1 | -66.16(9) |
| C1 | C2 | B10 | B3 | -145.35(8) | B4 | C3 | B10 | B2 | -4.66(9) |
| C2 | C3 | C4 | C5 | -29.35(13) | B4 | C3 | B10 | B3 | 35.37(7) |
| C2 | C3 | C4 | C9 | 156.02(9) | B4 | B3 | B9 | B2 | -138.20(8) |
| C2 | C3 | B3 | B2 | -0.02(9) | B4 | B3 | B9 | B7 | -37.44(7) |
| C2 | C3 | B3 | B4 | 102.20(8) | B4 | B3 | B9 | B8 | -101.23(8) |
| C2 | C3 | B3 | B9 | 63.19(9) | B4 | B3 | B10 | C2 | 2.61(9) |
| C2 | C3 | B3 | B10 | -40.72(7) | B4 | B3 | B10 | C3 | -33.60(7) |
| C2 | C3 | B4 | B3 | -102.97(8) | B4 | B3 | B10 | C20 | -148.71(8) |
| C2 | C3 | B4 | B5 | 37.82(7) | B4 | B3 | B10 | B1 | 61.81(9) |
| C2 | C3 | B4 | B7 | -0.89(9) | B4 | B3 | B10 | B2 | 99.84(8) |
| C2 | C3 | B4 | B9 | -63.70(9) | B4 | B5 | B6 | C2 | 98.35(8) |
| C2 | C3 | B5 | B4 | -138.43(8) | B4 | B5 | B6 | B1 | 64.66(9) |
| C2 | C3 | B5 | B6 | -36.81(7) | B4 | B5 | B6 | B7 | -38.21(7) |
| C2 | C3 | B5 | B7 | -99.42(8) | B4 | B5 | B6 | B8 | -0.21(10) |
| C2 | C3 | B10 | C20 | -118.37(10) | B4 | B5 | B7 | B6 | 137.24(8) |
| C2 | C3 | B10 | B1 | 34.83(6) | B4 | B5 | B7 | B8 | 100.15(8) |
| C2 | C3 | B10 | B2 | 96.33(7) | B4 | B5 | B7 | B9 | 37.35(7) |
| C2 | C3 | B10 | B3 | 136.35(7) | B4 | B7 | B8 | B1 | 64.26(9) |
| C2 | B1 | B2 | B3 | 2.60(10) | B4 | B7 | B8 | B2 | 0.52(10) |
| C2 | B1 | B2 | B8 | -97.64(8) | B4 | B7 | B8 | B6 | 100.85(8) |
| C2 | B1 | B2 | B9 | -61.33(9) | B4 | B7 | B8 | B9 | -37.55(7) |
| C2 | B1 | B2 | B10 | 41.66(7) | B4 | B7 | B9 | B2 | 100.04(8) |
| C2 | B1 | B6 | B5 | 33.74(7) | B4 | B7 | B9 | B3 | 37.32(7) |
| C2 | B1 | B6 | B7 | 97.63(8) | B4 | B7 | B9 | B8 | 137.64(8) |
| C2 | B1 | B6 | B8 | 134.78(8) | B5 | C2 | C3 | C4 | 101.88(9) |
| C2 | B1 | B8 | B2 | 98.75(8) | B5 | C2 | C3 | B3 | -104.65(8) |
| C2 | B1 | B8 | B6 | -38.46(7) | B5 | C2 | C3 | B4 | -38.32(7) |
| C2 | B1 | B8 | B7 | -2.06(9) | B5 | C2 | C3 | B10 | -144.98(7) |
| C2 | B1 | B8 | B9 | 61.84(9) | B5 | C2 | B1 | C14 | -140.65(9) |
| C2 | B1 | B10 | C3 | -34.57(6) | B5 | C2 | B1 | B2 | 63.82(9) |
| C2 | B1 | B10 | C20 | 118.50(10) | B5 | C2 | B1 | B6 | -35.99(7) |
| C2 | B1 | B10 | B2 | -132.40(8) | B5 | C2 | B1 | B8 | 2.60(10) |
| C2 | B1 | B10 | B3 | -94.44(7) | B5 | C2 | B1 | B10 | 104.51(8) |
| C2 | B5 | B6 | B1 | -33.69(7) | B5 | C2 | B6 | B1 | 142.38(8) |
| C2 | B5 | B6 | B7 | -136.56(8) | B5 | C2 | B6 | B7 | 38.31(7) |
| C2 | B5 | B6 | B8 | -98.56(8) | B5 | C2 | B6 | B8 | 102.02(8) |
| C2 | B5 | B7 | B4 | -99.49(8) | B5 | C2 | B10 | C3 | 33.07(7) |
| C2 | B5 | B7 | B6 | 37.75(7) | B5 | C2 | B10 | C20 | 143.31(10) |
| C2 | B5 | B7 | B8 | 0.66(10) | B5 | C2 | B10 | B1 | -105.55(8) |
| C2 | B5 | B7 | B9 | -62.14(9) | B5 | C2 | B10 | B2 | -64.79(9) |
| C2 | B6 | B7 | B4 | 0.12(10) | B5 | C2 | B10 | B3 | -3.65(9) |
| C2 | B6 | B7 | B5 | -38.10(7) | B5 | C3 | C4 | C5 | 39.82(12) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C2 | B6 | B7 | B8 | 99.91(8) | B5 | C3 | C4 | C9 | -134.81(9) |
| C2 | B6 | B7 | B9 | 63.12(9) | B5 | C3 | B3 | B2 | -65.33(9) |
| C2 | B6 | B8 | B1 | 39.48(7) | B5 | C3 | B3 | B4 | 36.89(7) |
| C2 | B6 | B8 | B2 | 1.30(10) | B5 | C3 | B3 | B9 | -2.12(10) |
| C2 | B6 | B8 | B7 | -100.05(8) | B5 | C3 | B3 | B10 | -106.04(8) |
| C2 | B6 | B8 | B9 | -62.84(9) | B5 | C3 | B4 | B3 | -140.79(8) |
| C3 | C2 | B1 | C14 | 152.89(8) | B5 | C3 | B4 | B7 | -38.71(7) |
| C3 | C2 | B1 | B2 | -2.64(9) | B5 | C3 | B4 | B9 | -101.52(8) |
| C3 | C2 | B1 | B6 | -102.45(8) | B5 | C3 | B10 | C2 | -33.08(7) |
| C3 | C2 | B1 | B8 | -63.86(9) | B5 | C3 | B10 | C20 | -151.45(8) |
| C3 | C2 | B1 | B10 | 38.05(7) | B5 | C3 | B10 | B1 | 1.75(9) |
| C3 | C2 | B5 | B4 | 36.23(7) | B5 | C3 | B10 | B2 | 63.25(9) |
| C3 | C2 | B5 | B6 | 137.51(7) | B5 | C3 | B10 | B3 | 103.28(8) |
| C3 | C2 | B5 | B7 | 99.18(8) | B5 | B4 | B7 | B6 | -38.21(7) |
| C3 | C2 | B6 | B1 | 103.39(8) | B5 | B4 | B7 | B8 | -100.67(8) |
| C3 | C2 | B6 | B5 | -38.98(7) | B5 | B4 | B7 | B9 | -138.10(8) |
| C3 | C2 | B6 | B7 | -0.68(10) | B5 | B4 | B9 | B2 | -64.01(9) |
| C3 | C2 | B6 | B8 | 63.04(9) | B5 | B4 | B9 | B3 | -100.93(8) |
| C3 | C2 | B10 | C20 | 110.24(11) | B5 | B4 | B9 | B7 | 37.20(7) |
| C3 | C2 | B10 | B1 | -138.62(7) | B5 | B4 | B9 | B8 | -0.89(10) |
| C3 | C2 | B10 | B2 | -97.86(7) | B5 | B6 | B7 | B4 | 38.22(7) |
| C3 | C2 | B10 | B3 | -36.72(6) | B5 | B6 | B7 | B8 | 138.01(8) |
| C3 | C4 | C5 | C6 | -175.31(9) | B5 | B6 | B7 | B9 | 101.22(8) |
| C3 | C4 | C9 | C8 | 175.18(9) | B5 | B6 | B8 | B1 | 101.97(8) |
| C3 | B3 | B4 | B5 | -34.92(7) | B5 | B6 | B8 | B2 | 63.79(10) |
| C3 | B3 | B4 | B7 | -97.97(8) | B5 | B6 | B8 | B7 | -37.55(7) |
| C3 | B3 | B4 | B9 | -135.54(8) | B5 | B6 | B8 | B9 | -0.34(10) |
| C3 | B3 | B9 | B2 | -99.39(8) | B5 | B7 | B8 | B1 | 0.89(10) |
| C3 | B3 | B9 | B4 | 38.81(7) | B5 | B7 | B8 | B2 | -62.84(9) |
| C3 | B3 | B9 | B7 | 1.38(10) | B5 | B7 | B8 | B6 | 37.48(7) |
| C3 | B3 | B9 | B8 | -62.42(9) | B5 | B7 | B8 | B9 | -100.92(8) |
| C3 | B3 | B10 | C2 | 36.21(6) | B5 | B7 | B9 | B2 | 62.52(10) |
| C3 | B3 | B10 | C20 | -115.11(9) | B5 | B7 | B9 | B3 | -0.20(10) |
| C3 | B3 | B10 | B1 | 95.42(7) | B5 | B7 | B9 | B4 | -37.52(7) |
| C3 | B3 | B10 | B2 | 133.44(8) | B5 | B7 | B9 | B8 | 100.12(8) |
| C3 | B4 | B5 | C2 | -36.03(7) | B6 | C2 | C3 | C4 | 141.20(8) |
| C3 | B4 | B5 | B6 | -97.70(8) | B6 | C2 | C3 | B3 | -65.33(9) |
| C3 | B4 | B5 | B7 | -135.81(8) | B6 | C2 | C3 | B4 | 1.00(9) |
| C3 | B4 | B7 | B5 | 38.67(7) | B6 | C2 | C3 | B5 | 39.32(7) |
| C3 | B4 | B7 | B6 | 0.46(10) | B6 | C2 | C3 | B10 | -105.66(8) |
| C3 | B4 | B7 | B8 | -62.00(9) | B6 | C2 | B1 | C14 | -104.67(9) |
| C3 | B4 | B7 | B9 | -99.43(8) | B6 | C2 | B1 | B2 | 99.80(8) |
| C3 | B4 | B9 | B2 | -1.59(10) | B6 | C2 | B1 | B8 | 38.59(7) |
| C3 | B4 | B9 | B3 | -38.50(7) | B6 | C2 | B1 | B10 | 140.50(7) |
| C3 | B4 | B9 | B7 | 99.63(8) | B6 | C2 | B5 | C3 | -137.51(7) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | B4 | B9 | B8 | 61.54(9) | B6 | C2 | B5 | B4 | -101.28(8) |
| C3 | B5 | B6 | C2 | 36.67(6) | B6 | C2 | B5 | B7 | -38.33(7) |
| C3 | B5 | B6 | B1 | 2.98(9) | B6 | C2 | B10 | C3 | 100.91(8) |
| C3 | B5 | B6 | B7 | -99.89(8) | B6 | C2 | B10 | C20 | -148.85(10) |
| C3 | B5 | B6 | B8 | -61.89(9) | B6 | C2 | B10 | B1 | -37.72(7) |
| C3 | B5 | B7 | B4 | -38.39(7) | B6 | C2 | B10 | B2 | 3.04(10) |
| C3 | B5 | B7 | B6 | 98.85(8) | B6 | C2 | B10 | B3 | 64.19(9) |
| C3 | B5 | B7 | B8 | 61.76(9) | B6 | B1 | B2 | B3 | 63.20(9) |
| C3 | B5 | B7 | B9 | -1.05(10) | B6 | B1 | B2 | B8 | -37.04(7) |
| C4 | C3 | B3 | B2 | 153.45(8) | B6 | B1 | B2 | B9 | -0.73(10) |
| C4 | C3 | B3 | B4 | -104.33(9) | B6 | B1 | B2 | B10 | 102.26(8) |
| C4 | C3 | B3 | B9 | -143.34(8) | B6 | B1 | B8 | B2 | 137.21(8) |
| C4 | C3 | B3 | B10 | 112.74(9) | B6 | B1 | B8 | B7 | 36.40(7) |
| C4 | C3 | B4 | B3 | 114.13(9) | B6 | B1 | B8 | B9 | 100.29(8) |
| C4 | C3 | B4 | B5 | -105.08(9) | B6 | B1 | B10 | C2 | 34.78(7) |
| C4 | C3 | B4 | B7 | -143.79(8) | B6 | B1 | B10 | C3 | 0.21(9) |
| C4 | C3 | B4 | B9 | 153.41(8) | B6 | B1 | B10 | C20 | 153.28(9) |
| C4 | C3 | B5 | C2 | -114.26(8) | B6 | B1 | B10 | B2 | -97.62(8) |
| C4 | C3 | B5 | B4 | 107.31(9) | B6 | B1 | B10 | B3 | -59.66(9) |
| C4 | C3 | B5 | B6 | -151.07(8) | B6 | B5 | B7 | B4 | -137.24(8) |
| C4 | C3 | B5 | B7 | 146.32(8) | B6 | B5 | B7 | B8 | -37.09(7) |
| C4 | C3 | B10 | C2 | 112.01(9) | B6 | B5 | B7 | B9 | -99.89(8) |
| C4 | C3 | B10 | C20 | -6.36(13) | B6 | B7 | B8 | B1 | -36.59(7) |
| C4 | C3 | B10 | B1 | 146.84(8) | B6 | B7 | B8 | B2 | -100.33(8) |
| C4 | C3 | B10 | B2 | -151.66(8) | B6 | B7 | B8 | B9 | -138.40(8) |
| C4 | C3 | B10 | B3 | -111.63(9) | B6 | B7 | B9 | B2 | -0.92(10) |
| C4 | C5 | C6 | C7 | 0.71(15) | B6 | B7 | B9 | B3 | -63.63(9) |
| C5 | C4 | C9 | C8 | 0.36(15) | B6 | B7 | B9 | B4 | -100.96(8) |
| C5 | C6 | C7 | C8 | -0.37(16) | B6 | B7 | B9 | B8 | 36.68(7) |
| C6 | C7 | C8 | C9 | 0.04(16) | B6 | B8 | B9 | B2 | 100.68(8) |
| C7 | C8 | C9 | C4 | -0.04(16) | B6 | B8 | B9 | B3 | 63.92(9) |
| C9 | C4 | C5 | C6 | -0.70(14) | B6 | B8 | B9 | B4 | 0.76(10) |
| C10 | N1 | C1 | O1 | -2.63(14) | B6 | B8 | B9 | B7 | -37.16(7) |
| C10 | N1 | C1 | C2 | 176.42(9) | B7 | B4 | B5 | C2 | 99.78(8) |
| C10 | N1 | C12 | C13 | -77.80(12) | B7 | B4 | B5 | C3 | 135.81(8) |
| C12 | N1 | C1 | O1 | 177.02(10) | B7 | B4 | B5 | B6 | 38.11(7) |
| C12 | N1 | C1 | C2 | -3.92(16) | B7 | B4 | B9 | B2 | -101.21(8) |
| C12 | N1 | C10 | C11 | -100.20(11) | B7 | B4 | B9 | B3 | -138.13(8) |
| C14 | C15 | C16 | C17 | 0.19(18) | B7 | B4 | B9 | B8 | -38.09(7) |
| C14 | B1 | B2 | B3 | -149.46(10) | B7 | B5 | B6 | C2 | 136.56(8) |
| C14 | B1 | B2 | B8 | 110.30(11) | B7 | B5 | B6 | B1 | 102.87(8) |
| C14 | B1 | B2 | B9 | 146.60(10) | B7 | B5 | B6 | B8 | 38.00(7) |
| C14 | B1 | B2 | B10 | -110.40(11) | B7 | B6 | B8 | B1 | 139.53(8) |
| C14 | B1 | B6 | C2 | 110.12(9) | B7 | B6 | B8 | B2 | 101.35(8) |
| C14 | B1 | B6 | B5 | 143.86(8) | B7 | B6 | B8 | B9 | 37.21(7) |

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|---|---|---|---|---|---|---|---|---|---|
| C14 | B1 | B6 | B7 | -152.25(8) | B7 | B8 | B9 | B2 | 137.84(8) |
| C14 | B1 | B6 | B8 | -115.10(9) | B7 | B8 | B9 | B3 | 101.08(8) |
| C14 | B1 | B8 | B2 | -119.94(10) | B7 | B8 | B9 | B4 | 37.92(7) |
| C14 | B1 | B8 | B6 | 102.85(10) | B8 | B1 | B2 | B3 | 100.24(8) |
| C14 | B1 | B8 | B7 | 139.25(9) | B8 | B1 | B2 | B9 | 36.31(7) |
| C14 | B1 | B8 | B9 | -156.86(9) | B8 | B1 | B2 | B10 | 139.30(8) |
| C14 | B1 | B10 | C2 | -107.92(10) | B8 | B1 | B6 | C2 | -134.78(8) |
| C14 | B1 | B10 | C3 | -142.49(9) | B8 | B1 | B6 | B5 | -101.04(8) |
| C14 | B1 | B10 | C20 | 10.58(14) | B8 | B1 | B6 | B7 | -37.15(7) |
| C14 | B1 | B10 | B2 | 119.68(10) | B8 | B1 | B10 | C2 | 96.56(8) |
| C14 | B1 | B10 | B3 | 157.64(8) | B8 | B1 | B10 | C3 | 62.00(8) |
| C15 | C14 | C19 | C18 | 0.33(16) | B8 | B1 | B10 | C20 | -144.94(9) |
| C15 | C14 | B1 | C2 | -48.00(13) | B8 | B1 | B10 | B2 | -35.84(7) |
| C15 | C14 | B1 | B2 | 100.47(13) | B8 | B1 | B10 | B3 | 2.13(9) |
| C15 | C14 | B1 | B6 | -115.05(11) | B8 | B2 | B3 | C3 | 62.77(9) |
| C15 | C14 | B1 | B8 | 176.40(9) | B8 | B2 | B3 | B4 | 0.43(10) |
| C15 | C14 | B1 | B10 | 24.92(14) | B8 | B2 | B3 | B9 | -36.92(7) |
| C15 | C16 | C17 | C18 | 0.51(19) | B8 | B2 | B3 | B10 | 103.87(8) |
| C16 | C17 | C18 | C19 | -0.8(2) | B8 | B2 | B9 | B3 | 138.41(8) |
| C17 | C18 | C19 | C14 | 0.35(18) | B8 | B2 | B9 | B4 | 101.28(8) |
| C19 | C14 | C15 | C16 | -0.60(16) | B8 | B2 | B9 | B7 | 37.89(7) |
| C19 | C14 | B1 | C2 | 129.20(10) | B8 | B2 | B10 | C2 | -2.11(10) |
| C19 | C14 | B1 | B2 | -82.32(13) | B8 | B2 | B10 | C3 | -60.37(9) |
| C19 | C14 | B1 | B6 | 62.15(12) | B8 | B2 | B10 | C20 | 152.78(9) |
| C19 | C14 | B1 | B8 | -6.40(14) | B8 | B2 | B10 | B1 | 37.39(7) |
| C19 | C14 | B1 | B10 | -157.88(9) | B8 | B2 | B10 | B3 | -99.49(8) |
| C20 | C21 | C22 | C23 | 0.02(15) | B8 | B6 | B7 | B4 | -99.79(8) |
| C21 | C20 | C25 | C24 | -0.59(15) | B8 | B6 | B7 | B5 | -138.01(8) |
| C21 | C20 | B10 | C2 | -65.91(14) | B8 | B6 | B7 | B9 | -36.78(7) |
| C21 | C20 | B10 | C3 | 7.27(14) | B8 | B7 | B9 | B2 | -37.60(7) |
| C21 | C20 | B10 | B1 | -140.15(10) | B8 | B7 | B9 | B3 | -100.31(8) |
| C21 | C20 | B10 | B2 | 146.74(9) | B8 | B7 | B9 | B4 | -137.64(8) |
| C21 | C20 | B10 | B3 | 76.50(12) | B9 | B2 | B3 | C3 | 99.69(8) |
| C21 | C22 | C23 | C24 | -0.72(16) | B9 | B2 | B3 | B4 | 37.35(7) |
| C22 | C23 | C24 | C25 | 0.75(16) | B9 | B2 | B3 | B10 | 140.79(8) |
| C23 | C24 | C25 | C20 | -0.09(16) | B9 | B2 | B8 | B1 | -139.43(8) |
| C25 | C20 | C21 | C22 | 0.62(14) | B9 | B2 | B8 | B6 | -101.12(8) |
| C25 | C20 | B10 | C2 | 119.81(11) | B9 | B2 | B8 | B7 | -37.78(7) |
| C25 | C20 | B10 | C3 | -167.01(9) | B9 | B2 | B10 | C2 | 61.71(9) |
| C25 | C20 | B10 | B1 | 45.56(13) | B9 | B2 | B10 | C3 | 3.45(9) |
| C25 | C20 | B10 | B2 | -27.54(13) | B9 | B2 | B10 | C20 | -143.40(9) |
| C25 | C20 | B10 | B3 | -97.78(11) | B9 | B2 | B10 | B1 | 101.21(8) |
| B1 | C2 | C3 | C4 | -151.73(8) | B9 | B2 | B10 | B3 | -35.66(7) |
| B1 | C2 | C3 | B3 | 1.74(10) | B9 | B3 | B4 | C3 | 135.54(8) |
| B1 | C2 | C3 | B4 | 68.07(9) | B9 | B3 | B4 | B5 | 100.63(8) |

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|---|---|---|---|---|---|---|---|---|---|
| B1 | C2 | C3 | B5 | 106.39(8) | B9 | B3 | B4 | B7 | 37.58(7) |
| B1 | C2 | C3 | B10 | -38.59(7) | B9 | B3 | B10 | C2 | -61.47(9) |
| B1 | C2 | B5 | C3 | -101.30(8) | B9 | B3 | B10 | C3 | -97.68(8) |
| B1 | C2 | B5 | B4 | -65.07(9) | B9 | B3 | B10 | C20 | 147.21(8) |
| B1 | C2 | B5 | B6 | 36.21(7) | B9 | B3 | B10 | B1 | -2.26(10) |
| B1 | C2 | B5 | B7 | -2.12(10) | B9 | B3 | B10 | B2 | 35.77(7) |
| B1 | C2 | B6 | B5 | -142.38(7) | B9 | B4 | B5 | C2 | 62.34(9) |
| B1 | C2 | B6 | B7 | -104.07(8) | B9 | B4 | B5 | C3 | 98.37(8) |
| B1 | C2 | B6 | B8 | -40.36(7) | B9 | B4 | B5 | B6 | 0.67(10) |
| B1 | C2 | B10 | C3 | 138.62(7) | B9 | B4 | B5 | B7 | -37.44(7) |
| B1 | C2 | B10 | C20 | -111.13(11) | B9 | B4 | B7 | B5 | 138.10(8) |
| B1 | C2 | B10 | B2 | 40.76(7) | B9 | B4 | B7 | B6 | 99.89(8) |
| B1 | C2 | B10 | B3 | 101.90(8) | B9 | B4 | B7 | B8 | 37.43(7) |
| B1 | C14 | C15 | C16 | 176.64(10) | B9 | B7 | B8 | B1 | 101.82(8) |
| B1 | C14 | C19 | C18 | -177.04(10) | B9 | B7 | B8 | B2 | 38.08(7) |
| B1 | B2 | B3 | C3 | -1.64(10) | B9 | B7 | B8 | B6 | 138.40(8) |
| B1 | B2 | B3 | B4 | -63.98(9) | B10 | C2 | C3 | C4 | -113.14(9) |
| B1 | B2 | B3 | B9 | -101.33(8) | B10 | C2 | C3 | B3 | 40.33(7) |
| B1 | B2 | B3 | B10 | 39.46(7) | B10 | C2 | C3 | B4 | 106.66(8) |
| B1 | B2 | B8 | B6 | 38.31(7) | B10 | C2 | C3 | B5 | 144.98(7) |
| B1 | B2 | B8 | B7 | 101.65(8) | B10 | C2 | B1 | C14 | 114.83(10) |
| B1 | B2 | B8 | B9 | 139.43(8) | B10 | C2 | B1 | B2 | -40.70(7) |
| B1 | B2 | B9 | B3 | 101.56(8) | B10 | C2 | B1 | B6 | -140.50(7) |
| B1 | B2 | B9 | B4 | 64.43(9) | B10 | C2 | B1 | B8 | -101.91(7) |
| B1 | B2 | B9 | B7 | 1.04(10) | B10 | C2 | B5 | C3 | -32.98(7) |
| B1 | B2 | B9 | B8 | -36.85(7) | B10 | C2 | B5 | B4 | 3.25(10) |
| B1 | B2 | B10 | C2 | -39.50(6) | B10 | C2 | B5 | B6 | 104.53(8) |
| B1 | B2 | B10 | C3 | -97.76(7) | B10 | C2 | B5 | B7 | 66.21(9) |
| B1 | B2 | B10 | C20 | 115.39(10) | B10 | C2 | B6 | B1 | 37.58(7) |
| B1 | B2 | B10 | B3 | -136.87(8) | B10 | C2 | B6 | B5 | -104.80(8) |
| B1 | B6 | B7 | B4 | -62.53(10) | B10 | C2 | B6 | B7 | -66.49(9) |
| B1 | B6 | B7 | B5 | -100.75(8) | B10 | C2 | B6 | B8 | -2.78(10) |
| B1 | B6 | B7 | B8 | 37.26(7) | B10 | C3 | C4 | C5 | -105.09(11) |
| B1 | B6 | B7 | B9 | 0.47(10) | B10 | C3 | C4 | C9 | 80.28(11) |
| B1 | B6 | B8 | B2 | -38.18(7) | B10 | C3 | B3 | B2 | 40.71(7) |
| B1 | B6 | B8 | B7 | -139.53(8) | B10 | C3 | B3 | B4 | 142.93(8) |
| B1 | B6 | B8 | B9 | -102.32(8) | B10 | C3 | B3 | B9 | 103.92(8) |
| B1 | B8 | B9 | B2 | 36.64(7) | B10 | C3 | B4 | B3 | -35.28(7) |
| B1 | B8 | B9 | B3 | -0.12(10) | B10 | C3 | B4 | B5 | 105.52(8) |
| B1 | B8 | B9 | B4 | -63.28(10) | B10 | C3 | B4 | B7 | 66.80(9) |
| B1 | B8 | B9 | B7 | -101.20(8) | B10 | C3 | B4 | B9 | 4.00(10) |
| B2 | B1 | B6 | C2 | -97.47(8) | B10 | C3 | B5 | C2 | 33.82(7) |
| B2 | B1 | B6 | B5 | -63.73(9) | B10 | C3 | B5 | B4 | -104.62(8) |
| B2 | B1 | B6 | B7 | 0.16(10) | B10 | C3 | B5 | B6 | -3.00(10) |
| B2 | B1 | B6 | B8 | 37.31(7) | B10 | C3 | B5 | B7 | -65.60(9) |

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|---|---|---|---|---|---|---|---|---|---|
| B2 | B1 | B8 | B6 | -137.21(8) | B10 | C20 | C21 | C22 | -173.69(9) |
| B2 | B1 | B8 | B7 | -100.81(8) | B10 | C20 | C25 | C24 | 174.13(9) |
| B2 | B1 | B8 | B9 | -36.91(7) | B10 | B1 | B2 | B3 | -39.06(7) |
| B2 | B1 | B10 | C2 | 132.40(8) | B10 | B1 | B2 | B8 | -139.30(8) |
| B2 | B1 | B10 | C3 | 97.83(7) | B10 | B1 | B2 | B9 | -102.99(8) |
| B2 | B1 | B10 | C20 | -109.10(10) | B10 | B1 | B6 | C2 | -35.76(7) |
| B2 | B1 | B10 | B3 | 37.96(7) | B10 | B1 | B6 | B5 | -2.01(10) |
| B2 | B3 | B4 | C3 | 97.86(8) | B10 | B1 | B6 | B7 | 61.88(9) |
| B2 | B3 | B4 | B5 | 62.95(9) | B10 | B1 | B6 | B8 | 99.03(8) |
| B2 | B3 | B4 | B7 | -0.10(10) | B10 | B1 | B8 | B2 | 35.66(7) |
| B2 | B3 | B4 | B9 | -37.68(7) | B10 | B1 | B8 | B6 | -101.55(8) |
| B2 | B3 | B9 | B4 | 138.20(8) | B10 | B1 | B8 | B7 | -65.15(9) |
| B2 | B3 | B9 | B7 | 100.76(8) | B10 | B1 | B8 | B9 | -1.26(10) |
| B2 | B3 | B9 | B8 | 36.97(7) | B10 | B2 | B3 | C3 | -41.11(7) |
| B2 | B3 | B10 | C2 | -97.23(7) | B10 | B2 | B3 | B4 | -103.44(8) |
| B2 | B3 | B10 | C3 | -133.44(8) | B10 | B2 | B3 | B9 | -140.79(8) |
| B2 | B3 | B10 | C20 | 111.45(9) | B10 | B2 | B8 | B1 | -37.71(7) |
| B2 | B3 | B10 | B1 | -38.03(7) | B10 | B2 | B8 | B6 | 0.60(11) |
| B2 | B8 | B9 | B3 | -36.76(7) | B10 | B2 | B8 | B7 | 63.94(10) |
| B2 | B8 | B9 | B4 | -99.92(8) | B10 | B2 | B8 | B9 | 101.72(8) |
| B2 | B8 | B9 | B7 | -137.84(8) | B10 | B2 | B9 | B3 | 35.88(7) |
| B3 | C3 | C4 | C5 | -179.74(9) | B10 | B2 | B9 | B4 | -1.25(10) |
| B3 | C3 | C4 | C9 | 5.63(13) | B10 | B2 | B9 | B7 | -64.64(10) |
| B3 | C3 | B4 | B5 | 140.79(8) | B10 | B2 | B9 | B8 | -102.53(8) |
| B3 | C3 | B4 | B7 | 102.08(8) | B10 | B3 | B4 | C3 | 34.09(7) |
| B3 | C3 | B4 | B9 | 39.28(7) | B10 | B3 | B4 | B5 | -0.83(10) |
| B3 | C3 | B5 | C2 | 101.43(8) | B10 | B3 | B4 | B7 | -63.88(9) |
| B3 | C3 | B5 | B4 | -37.01(7) | B10 | B3 | B4 | B9 | -101.45(8) |
| B3 | C3 | B5 | B6 | 64.62(9) | B10 | B3 | B9 | B2 | -35.47(7) |
| B3 | C3 | B5 | B7 | 2.01(10) | B10 | B3 | B9 | B4 | 102.73(8) |
| B3 | C3 | B10 | C2 | -136.35(7) | B10 | B3 | B9 | B7 | 65.30(9) |
| B3 | C3 | B10 | C20 | 105.27(10) | B10 | B3 | B9 | B8 | 1.50(10) |
| B3 | C3 | B10 | B1 | -101.53(7) | | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0922_CG_0m.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | 9060.51 | 4884.74 | 6105.74 | 16 |
| H6 | 9351.84 | 3546.46 | 7080.44 | 20 |
| H7 | 8188.81 | 2308.18 | 7109.4 | 22 |
| H8 | 6723.22 | 2429.78 | 6171.04 | 22 |
| H9 | 6416.56 | 3769.61 | 5205.92 | 18 |
| H10A | 9251.47 | 7404.75 | 7489.17 | 19 |
| H10B | 10359.92 | 7519.99 | 7186.77 | 19 |

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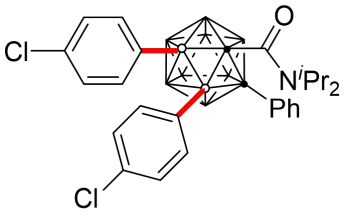
|---|---|---|---|---|
| H11A | 10578.22 | 5820.22 | 7372.25 | 35 |
| H11B | 9492.81 | 5751.92 | 7744.09 | 35 |
| H11C | 10333.9 | 6327.13 | 8344.01 | 35 |
| H12A | 10020.35 | 6728.48 | 4896.55 | 20 |
| H12B | 10845.19 | 6809.55 | 5744.46 | 20 |
| H13A | 10810.19 | 8222.14 | 4807.15 | 42 |
| H13B | 10547.75 | 8474.56 | 5864.23 | 42 |
| H13C | 9690.46 | 8403.39 | 5045.44 | 42 |
| H15 | 7169.87 | 8036.67 | 6323.35 | 21 |
| H16 | 7310.53 | 9613.28 | 6874.96 | 27 |
| H17 | 7543.55 | 10876.13 | 5821.43 | 30 |
| H18 | 7610.97 | 10556.02 | 4206.34 | 29 |
| H19 | 7483.62 | 8981.09 | 3651.91 | 21 |
| H21 | 6566.77 | 5197.79 | 6763.17 | 17 |
| H22 | 5426.27 | 5288.76 | 7923.72 | 22 |
| H23 | 4195 | 6465.32 | 7832.79 | 26 |
| H24 | 4134.48 | 7570.62 | 6590.03 | 26 |
| H25 | 5273.92 | 7482.96 | 5423.75 | 20 |
| H2 | 5567(11) | 6942(11) | 3856(10) | 21(4) |
| H3 | 5850(10) | 4907(10) | 4318(10) | 15(3) |
| H4 | 7636(11) | 4241(11) | 3543(10) | 21(4) |
| H5A | 9216(10) | 5266(10) | 4470(10) | 16(3) |
| H6A | 9001(10) | 7316(10) | 4010(10) | 17(3) |
| H7A | 8509(11) | 5872(11) | 2506(10) | 21(4) |
| H8A | 7230(10) | 7575(11) | 2751(10) | 19(3) |
| H9A | 6343(10) | 5651(10) | 2413(10) | 19(3) |

**Experimental**

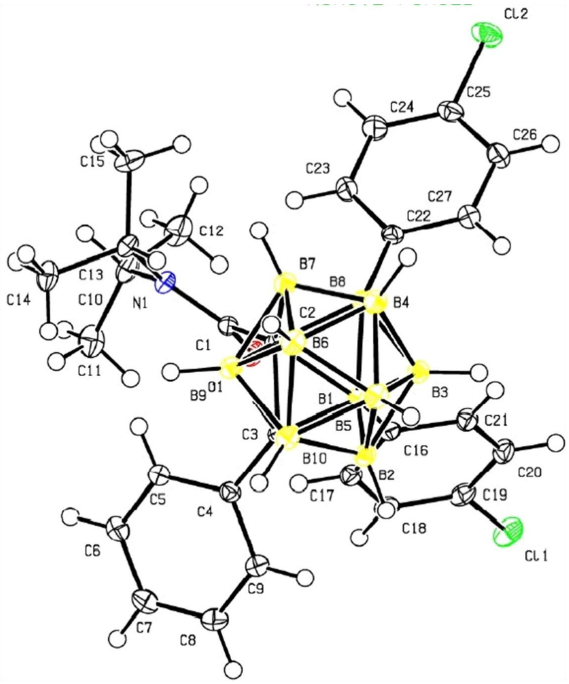
Single crystals of $C_{25}H_{33}B_{10}NO$ [mo_0922_CG_0m] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a Bruker D8 Venture AgMo Dual Source diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

**Crystal structure determination of 3ab**

**Crystal Data** for $C_{25}H_{33}B_{10}NO$ ($M$ =471.62 g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a$ = 13.6114(6) Å, $b$ = 13.9152(8) Å, $c$ = 14.1817(8) Å, $\beta$ = 93.358(2)°, $V$ = 2681.5(2) Å$^3$, $Z$ = 4, $T$ = 100.0 K, μ(MoKα) = 0.064 mm$^{-1}$, *Dcalc* = 1.168 g/cm$^3$, 60954 reflections measured (4.032° ≤ 2Θ ≤ 57.426°), 6925 unique ($R_{int}$ = 0.0319, $R_{sigma}$ = 0.0183) which were used in all calculations. The final $R_1$ was 0.0425 (I > 2σ(I)) and $wR_2$ was 0.1132 (all data).




**3dd**




**CCDC 1983612**

**Crystal data and structure refinement for 3dd.**

| | |
|---|---|
| Identification code | mo_0830_CG_0m |
| CCDC number | 1983612 |
| Empirical formula | $C_{27}H_{35}B_{10}Cl_2NO$ |
| Formula weight | 568.56 |
| Temperature/K | 100.0 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.8615(14) |
| b/Å | 10.9215(14) |
| c/Å | 13.8510(18) |
| α/° | 105.147(4) |
| β/° | 105.960(4) |
| γ/° | 99.055(4) |
| Volume/Å$^3$ | 1477.6(3) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.278 |
| μ/mm$^{-1}$ | 0.245 |
| F(000) | 592.0 |
| Crystal size/mm$^3$ | 0.18 × 0.15 × 0.04 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.244 to 59.328 |
| Index ranges | -15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19 |
| Reflections collected | 77051 |
| Independent reflections | 8309 [$R_{int}$ = 0.0303, $R_{sigma}$ = 0.0150] |
| Data/restraints/parameters | 8309/0/398 |
| Goodness-of-fit on F$^2$ | 1.049 |

| | |
|---|---|
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0310, $wR_2$ = 0.0792 |
| Final R indexes [all data] | $R_1$ = 0.0349, $wR_2$ = 0.0823 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.39/-0.30 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0830_CG_0m. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| Cl1 | 1720.0(2) | 991.8(2) | 1399.7(2) | 25.04(6) |
| Cl2 | 9244.9(3) | 2662.9(3) | -321.5(2) | 26.52(6) |
| O1 | 5234.1(7) | 6365.7(6) | 1759.1(5) | 17.10(13) |
| N1 | 6567.2(8) | 8214.5(7) | 1822.7(6) | 14.08(14) |
| C1 | 6225.8(9) | 7258.9(8) | 2229.3(7) | 12.76(15) |
| C2 | 7073.1(8) | 7211.4(8) | 3319.9(7) | 12.14(15) |
| C3 | 6358.9(9) | 7393.5(8) | 4290.8(7) | 12.93(15) |
| C4 | 5043.5(9) | 7741.5(9) | 4110.3(7) | 14.38(16) |
| C5 | 4679.0(10) | 8541.0(9) | 3501.4(8) | 17.75(17) |
| C6 | 3433.8(11) | 8791.8(11) | 3304.4(9) | 23.1(2) |
| C7 | 2556.9(11) | 8287.4(11) | 3746.3(10) | 26.5(2) |
| C8 | 2931.8(11) | 7531.4(11) | 4385.5(10) | 27.6(2) |
| C9 | 4160.9(10) | 7247.5(10) | 4561.4(8) | 21.18(19) |
| C10 | 5673.3(10) | 8108.3(9) | 748.6(7) | 18.63(18) |
| C11 | 4335.2(11) | 8345.2(11) | 776.9(9) | 25.1(2) |
| C12 | 5551.4(13) | 6849.6(11) | -107.6(8) | 27.9(2) |
| C13 | 7708.7(9) | 9374.3(9) | 2310.6(7) | 15.77(16) |
| C14 | 7267.6(10) | 10654.7(9) | 2481.8(8) | 22.22(19) |
| C15 | 8663.3(11) | 9321.8(11) | 1679.6(9) | 25.3(2) |
| C16 | 5155.2(9) | 4614.6(8) | 2982.8(7) | 13.32(15) |
| C17 | 3854.1(9) | 4708.0(9) | 2556.3(7) | 15.81(16) |
| C18 | 2794.7(9) | 3608.9(9) | 2082.6(7) | 17.69(17) |
| C19 | 3028.3(9) | 2382.6(9) | 2018.3(7) | 17.81(17) |
| C20 | 4291.2(10) | 2241.1(9) | 2423.4(8) | 18.26(17) |
| C21 | 5339.6(9) | 3353.4(9) | 2900.6(7) | 16.01(16) |
| C22 | 8201.7(9) | 5148.9(9) | 2378.8(7) | 15.19(16) |
| C23 | 8058.6(11) | 5448.4(10) | 1439.5(8) | 21.85(19) |
| C24 | 8368.8(11) | 4694.8(10) | 605.3(8) | 23.5(2) |
| C25 | 8843.9(9) | 3617.9(9) | 712.6(8) | 18.98(18) |
| C26 | 9002.2(10) | 3280.5(10) | 1627.4(8) | 20.72(19) |
| C27 | 8681.6(10) | 4049.7(9) | 2451.3(8) | 19.02(18) |
| B1 | 6410.2(10) | 5795.9(9) | 3633.8(8) | 12.93(17) |
| B2 | 6810.4(10) | 6415.5(10) | 5044.2(8) | 15.07(18) |
| B3 | 7850.2(10) | 5582.2(10) | 4503.9(8) | 15.30(18) |
| B4 | 9265.6(10) | 6756.0(11) | 4647.0(8) | 17.15(19) |

| | | | | |
|---|---|---|---|---|
| B5 | 8547.1(10) | 6984.7(11) | 5662.4(8) | 17.60(19) |
| B6 | 9090.8(10) | 8340.8(11) | 5269.9(8) | 17.66(19) |
| B7 | 8751.9(10) | 7754.3(10) | 3881.8(8) | 15.11(18) |
| B8 | 7972.6(10) | 6039.8(10) | 3379.5(8) | 14.12(17) |
| B9 | 7692.3(10) | 8600.5(10) | 4414.9(8) | 14.69(18) |
| B10 | 7564.1(11) | 8113.7(10) | 5516.4(8) | 16.60(18) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_0830_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Cl1 | 23.18(12) | 18.95(11) | 24.67(12) | 4.06(9) | 4.58(9) | -6.81(9) |
| Cl2 | 29.71(13) | 24.73(12) | 25.23(12) | 0.81(9) | 14.95(10) | 8.72(10) |
| O1 | 17.5(3) | 15.0(3) | 15.2(3) | 5.1(2) | 2.5(2) | -1.0(2) |
| N1 | 15.9(3) | 12.9(3) | 12.8(3) | 5.2(3) | 4.1(3) | 1.3(3) |
| C1 | 14.2(4) | 12.8(4) | 12.0(4) | 3.9(3) | 5.1(3) | 3.8(3) |
| C2 | 11.9(4) | 12.2(4) | 12.6(4) | 4.1(3) | 5.0(3) | 2.2(3) |
| C3 | 14.0(4) | 13.2(4) | 12.4(4) | 4.3(3) | 5.8(3) | 2.9(3) |
| C4 | 15.0(4) | 13.5(4) | 15.0(4) | 3.3(3) | 6.6(3) | 4.0(3) |
| C5 | 19.7(4) | 17.6(4) | 20.7(4) | 8.2(3) | 10.6(3) | 7.3(3) |
| C6 | 24.0(5) | 25.0(5) | 28.4(5) | 13.4(4) | 12.6(4) | 13.2(4) |
| C7 | 20.1(5) | 29.6(5) | 37.8(6) | 14.8(5) | 14.5(4) | 12.7(4) |
| C8 | 23.3(5) | 30.9(5) | 41.9(6) | 19.7(5) | 21.0(5) | 11.3(4) |
| C9 | 21.3(5) | 23.0(5) | 27.6(5) | 13.7(4) | 14.0(4) | 8.6(4) |
| C10 | 22.8(4) | 17.0(4) | 13.6(4) | 7.0(3) | 2.5(3) | 0.9(3) |
| C11 | 22.1(5) | 25.2(5) | 23.4(5) | 9.7(4) | -0.7(4) | 4.9(4) |
| C12 | 44.1(6) | 23.8(5) | 13.5(4) | 4.9(4) | 8.5(4) | 5.5(5) |
| C13 | 15.9(4) | 13.4(4) | 17.3(4) | 5.9(3) | 5.3(3) | 0.1(3) |
| C14 | 24.3(5) | 13.4(4) | 25.8(5) | 7.0(4) | 4.6(4) | 1.6(3) |
| C15 | 23.6(5) | 28.4(5) | 27.0(5) | 11.2(4) | 14.0(4) | 1.5(4) |
| C16 | 14.5(4) | 13.4(4) | 12.4(4) | 4.1(3) | 5.9(3) | 1.9(3) |
| C17 | 15.6(4) | 15.1(4) | 16.8(4) | 5.5(3) | 5.9(3) | 2.7(3) |
| C18 | 14.9(4) | 19.4(4) | 17.4(4) | 5.7(3) | 5.1(3) | 1.1(3) |
| C19 | 18.4(4) | 16.0(4) | 15.8(4) | 3.3(3) | 6.2(3) | -2.7(3) |
| C20 | 22.1(4) | 12.7(4) | 19.3(4) | 4.8(3) | 7.4(4) | 2.1(3) |
| C21 | 17.0(4) | 14.6(4) | 16.9(4) | 5.6(3) | 6.1(3) | 3.3(3) |
| C22 | 12.9(4) | 14.7(4) | 18.6(4) | 5.0(3) | 6.7(3) | 3.1(3) |
| C23 | 30.2(5) | 19.7(4) | 23.2(5) | 9.8(4) | 14.2(4) | 12.6(4) |
| C24 | 31.8(5) | 23.4(5) | 21.4(5) | 9.0(4) | 14.1(4) | 11.3(4) |
| C25 | 17.4(4) | 17.5(4) | 20.3(4) | 1.1(3) | 9.0(3) | 3.1(3) |
| C26 | 22.1(5) | 17.6(4) | 24.3(5) | 5.8(4) | 9.5(4) | 8.5(4) |
| C27 | 21.0(4) | 18.3(4) | 21.0(4) | 7.8(3) | 9.0(4) | 7.6(3) |
| B1 | 13.6(4) | 12.4(4) | 13.8(4) | 4.9(3) | 5.3(3) | 3.4(3) |
| B2 | 17.1(4) | 15.5(4) | 13.3(4) | 5.9(3) | 4.8(3) | 4.1(3) |
| B3 | 14.4(4) | 16.3(4) | 15.9(4) | 6.9(4) | 4.5(3) | 3.8(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B4 | 13.5(4) | 18.4(5) | 18.7(5) | 7.2(4) | 3.4(4) | 3.1(4) |
| B5 | 16.6(4) | 18.5(5) | 15.1(4) | 5.9(4) | 1.8(4) | 2.3(4) |
| B6 | 15.6(4) | 17.9(5) | 15.7(4) | 4.9(4) | 1.8(4) | 0.7(4) |
| B7 | 12.4(4) | 14.9(4) | 16.8(4) | 5.3(4) | 4.0(3) | 1.3(3) |
| B8 | 13.4(4) | 13.9(4) | 16.4(4) | 5.9(3) | 5.7(3) | 3.9(3) |
| B9 | 15.0(4) | 13.4(4) | 13.6(4) | 2.9(3) | 4.4(3) | 0.8(3) |
| B10 | 18.6(5) | 16.2(4) | 12.9(4) | 4.0(3) | 3.8(4) | 2.1(4) |

**Bond Lengths for mo_0830_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Cl1 | C19 | 1.7411(10) | C18 | C19 | 1.3869(14) |
| Cl2 | C25 | 1.7420(10) | C19 | C20 | 1.3816(14) |
| O1 | C1 | 1.2196(11) | C20 | C21 | 1.3930(13) |
| N1 | C1 | 1.3580(11) | C22 | C23 | 1.3969(13) |
| N1 | C10 | 1.4997(12) | C22 | C27 | 1.3980(13) |
| N1 | C13 | 1.4819(11) | C22 | B8 | 1.5783(13) |
| C1 | C2 | 1.5565(12) | C23 | C24 | 1.3893(14) |
| C2 | C3 | 1.7124(12) | C24 | C25 | 1.3827(14) |
| C2 | B1 | 1.8085(13) | C25 | C26 | 1.3838(14) |
| C2 | B7 | 1.7089(13) | C26 | C27 | 1.3924(13) |
| C2 | B8 | 1.7329(13) | B1 | B2 | 1.7924(14) |
| C2 | B9 | 1.7232(13) | B1 | B3 | 1.7828(14) |
| C3 | C4 | 1.5075(12) | B1 | B8 | 1.8194(14) |
| C3 | B1 | 1.7619(13) | B2 | B3 | 1.7595(15) |
| C3 | B2 | 1.7136(13) | B2 | B5 | 1.7727(15) |
| C3 | B9 | 1.7345(13) | B2 | B10 | 1.7697(15) |
| C3 | B10 | 1.7234(14) | B3 | B4 | 1.7678(15) |
| C4 | C5 | 1.3930(13) | B3 | B5 | 1.7823(15) |
| C4 | C9 | 1.3941(13) | B3 | B8 | 1.7867(14) |
| C5 | C6 | 1.3897(13) | B4 | B5 | 1.7693(16) |
| C6 | C7 | 1.3845(15) | B4 | B6 | 1.7859(16) |
| C7 | C8 | 1.3859(16) | B4 | B7 | 1.7589(15) |
| C8 | C9 | 1.3888(14) | B4 | B8 | 1.8019(15) |
| C10 | C11 | 1.5249(15) | B5 | B6 | 1.7775(15) |
| C10 | C12 | 1.5226(14) | B5 | B10 | 1.7684(15) |
| C13 | C14 | 1.5301(13) | B6 | B7 | 1.7707(15) |
| C13 | C15 | 1.5275(13) | B6 | B9 | 1.7642(15) |
| C16 | C17 | 1.4051(12) | B6 | B10 | 1.7759(16) |
| C16 | C21 | 1.4027(12) | B7 | B8 | 1.7898(15) |
| C16 | B1 | 1.5806(13) | B7 | B9 | 1.7802(15) |
| C17 | C18 | 1.3906(13) | B9 | B10 | 1.7740(15) |

**Bond Angles for mo_0830_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 116.63(7) | B3 | B2 | B5 | 60.61(6) |
| C1 | N1 | C13 | 128.35(7) | B3 | B2 | B10 | 108.38(7) |
| C13 | N1 | C10 | 115.01(7) | B5 | B2 | B1 | 109.98(7) |
| O1 | C1 | N1 | 122.22(8) | B10 | B2 | B1 | 110.18(7) |
| O1 | C1 | C2 | 115.04(7) | B10 | B2 | B5 | 59.90(6) |
| N1 | C1 | C2 | 122.73(8) | B1 | B3 | B8 | 61.29(6) |
| C1 | C2 | C3 | 116.61(7) | B2 | B3 | B1 | 60.79(6) |
| C1 | C2 | B1 | 112.95(7) | B2 | B3 | B4 | 108.10(7) |
| C1 | C2 | B7 | 126.28(7) | B2 | B3 | B5 | 60.06(6) |
| C1 | C2 | B8 | 120.35(7) | B2 | B3 | B8 | 109.11(7) |
| C1 | C2 | B9 | 120.86(7) | B4 | B3 | B1 | 110.41(7) |
| C3 | C2 | B1 | 59.98(5) | B4 | B3 | B5 | 59.78(6) |
| C3 | C2 | B8 | 109.41(6) | B4 | B3 | B8 | 60.92(6) |
| C3 | C2 | B9 | 60.64(5) | B5 | B3 | B1 | 109.98(7) |
| B7 | C2 | C3 | 109.81(7) | B5 | B3 | B8 | 109.16(7) |
| B7 | C2 | B1 | 112.79(6) | B3 | B4 | B5 | 60.52(6) |
| B7 | C2 | B8 | 62.66(6) | B3 | B4 | B6 | 108.17(7) |
| B7 | C2 | B9 | 62.49(6) | B3 | B4 | B8 | 60.06(6) |
| B8 | C2 | B1 | 61.78(5) | B5 | B4 | B6 | 60.00(6) |
| B9 | C2 | B1 | 112.14(6) | B5 | B4 | B8 | 109.06(7) |
| B9 | C2 | B8 | 113.80(7) | B6 | B4 | B8 | 108.68(7) |
| C2 | C3 | B1 | 62.72(5) | B7 | B4 | B3 | 107.90(7) |
| C2 | C3 | B2 | 110.49(7) | B7 | B4 | B5 | 108.16(7) |
| C2 | C3 | B9 | 59.99(5) | B7 | B4 | B6 | 59.93(6) |
| C2 | C3 | B10 | 109.65(7) | B7 | B4 | B8 | 60.33(6) |
| C4 | C3 | C2 | 120.06(7) | B2 | B5 | B3 | 59.33(6) |
| C4 | C3 | B1 | 119.01(7) | B2 | B5 | B6 | 107.96(7) |
| C4 | C3 | B2 | 121.95(7) | B4 | B5 | B2 | 107.45(7) |
| C4 | C3 | B9 | 116.46(7) | B4 | B5 | B3 | 59.70(6) |
| C4 | C3 | B10 | 118.95(7) | B4 | B5 | B6 | 60.46(6) |
| B2 | C3 | B1 | 62.07(6) | B6 | B5 | B3 | 107.90(7) |
| B2 | C3 | B9 | 112.28(7) | B10 | B5 | B2 | 59.97(6) |
| B2 | C3 | B10 | 61.98(6) | B10 | B5 | B3 | 107.42(7) |
| B9 | C3 | B1 | 113.90(7) | B10 | B5 | B4 | 108.25(7) |
| B10 | C3 | B1 | 113.88(7) | B10 | B5 | B6 | 60.11(6) |
| B10 | C3 | B9 | 61.73(6) | B5 | B6 | B4 | 59.54(6) |
| C5 | C4 | C3 | 121.93(8) | B7 | B6 | B4 | 59.28(6) |
| C5 | C4 | C9 | 118.83(9) | B7 | B6 | B5 | 107.28(7) |
| C9 | C4 | C3 | 119.24(8) | B7 | B6 | B10 | 108.12(7) |
| C6 | C5 | C4 | 120.65(9) | B9 | B6 | B4 | 107.55(7) |
| C7 | C6 | C5 | 120.18(9) | B9 | B6 | B5 | 107.80(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C6 | C7 | C8 | 119.44(10) | B9 | B6 | B7 | 60.48(6) |
| C7 | C8 | C9 | 120.64(10) | B9 | B6 | B10 | 60.15(6) |
| C8 | C9 | C4 | 120.19(9) | B10 | B6 | B4 | 107.18(7) |
| N1 | C10 | C11 | 111.92(8) | B10 | B6 | B5 | 59.69(6) |
| N1 | C10 | C12 | 113.18(8) | C2 | B7 | B4 | 106.69(7) |
| C12 | C10 | C11 | 112.73(9) | C2 | B7 | B6 | 106.48(7) |
| N1 | C13 | C14 | 111.82(8) | C2 | B7 | B8 | 59.33(5) |
| N1 | C13 | C15 | 111.55(8) | C2 | B7 | B9 | 59.15(5) |
| C15 | C13 | C14 | 112.03(8) | B4 | B7 | B6 | 60.79(6) |
| C17 | C16 | B1 | 126.32(8) | B4 | B7 | B8 | 61.02(6) |
| C21 | C16 | C17 | 116.75(8) | B4 | B7 | B9 | 108.03(7) |
| C21 | C16 | B1 | 116.70(8) | B6 | B7 | B8 | 109.92(7) |
| C18 | C17 | C16 | 121.92(9) | B6 | B7 | B9 | 59.58(6) |
| C19 | C18 | C17 | 119.15(9) | B9 | B7 | B8 | 108.39(7) |
| C18 | C19 | Cl1 | 119.83(8) | C2 | B8 | B1 | 61.15(5) |
| C20 | C19 | Cl1 | 119.14(7) | C2 | B8 | B3 | 105.06(7) |
| C20 | C19 | C18 | 121.03(9) | C2 | B8 | B4 | 103.81(7) |
| C19 | C20 | C21 | 119.04(9) | C2 | B8 | B7 | 58.01(5) |
| C20 | C21 | C16 | 122.11(9) | C22 | B8 | C2 | 123.20(7) |
| C23 | C22 | C27 | 116.99(9) | C22 | B8 | B1 | 123.35(7) |
| C23 | C22 | B8 | 123.83(8) | C22 | B8 | B3 | 125.77(8) |
| C27 | C22 | B8 | 118.95(8) | C22 | B8 | B4 | 122.21(8) |
| C24 | C23 | C22 | 122.21(9) | C22 | B8 | B7 | 119.46(7) |
| C25 | C24 | C23 | 118.83(9) | B3 | B8 | B1 | 59.25(5) |
| C24 | C25 | Cl2 | 119.60(8) | B3 | B8 | B4 | 59.02(6) |
| C24 | C25 | C26 | 121.13(9) | B3 | B8 | B7 | 105.74(7) |
| C26 | C25 | Cl2 | 119.28(8) | B4 | B8 | B1 | 107.25(7) |
| C25 | C26 | C27 | 118.95(9) | B7 | B8 | B1 | 108.55(7) |
| C26 | C27 | C22 | 121.88(9) | B7 | B8 | B4 | 58.64(6) |
| C2 | B1 | B8 | 57.07(5) | C2 | B9 | C3 | 59.37(5) |
| C3 | B1 | C2 | 57.30(5) | C2 | B9 | B6 | 106.15(7) |
| C3 | B1 | B2 | 57.64(5) | C2 | B9 | B7 | 58.36(5) |
| C3 | B1 | B3 | 102.80(7) | C2 | B9 | B10 | 106.83(7) |
| C3 | B1 | B8 | 103.47(6) | C3 | B9 | B6 | 105.94(7) |
| C16 | B1 | C2 | 130.94(7) | C3 | B9 | B7 | 105.58(7) |
| C16 | B1 | C3 | 124.76(7) | C3 | B9 | B10 | 58.83(6) |
| C16 | B1 | B2 | 118.13(7) | B6 | B9 | B7 | 59.94(6) |
| C16 | B1 | B3 | 121.19(7) | B6 | B9 | B10 | 60.25(6) |
| C16 | B1 | B8 | 126.36(7) | B10 | B9 | B7 | 107.79(7) |
| B2 | B1 | C2 | 102.83(6) | C3 | B10 | B2 | 58.74(5) |
| B2 | B1 | B8 | 106.24(7) | C3 | B10 | B5 | 105.75(7) |
| B3 | B1 | C2 | 102.13(6) | C3 | B10 | B6 | 105.91(7) |
| B3 | B1 | B2 | 58.96(6) | C3 | B10 | B9 | 59.44(5) |
| B3 | B1 | B8 | 59.46(6) | B2 | B10 | B6 | 108.17(7) |
| C3 | B2 | B1 | 60.29(5) | B2 | B10 | B9 | 107.81(7) |

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|---|---|---|---|---|---|---|---|
| C3 | B2 | B3 | 105.80(7) | B5 | B10 | B2 | 60.14(6) |
| C3 | B2 | B5 | 105.98(7) | B5 | B10 | B6 | 60.20(6) |
| C3 | B2 | B10 | 59.28(6) | B5 | B10 | B9 | 107.77(7) |
| B3 | B2 | B1 | 60.25(6) | B9 | B10 | B6 | 59.60(6) |

**Torsion Angles for mo_0830_CG_0m.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| Cl1 | C19 | C20 | C21 | 178.83(7) | B2 | B5 | B10 | B6 | -138.00(7) |
| Cl2 | C25 | C26 | C27 | 179.90(8) | B2 | B5 | B10 | B9 | -100.74(8) |
| O1 | C1 | C2 | C3 | -65.10(10) | B3 | B1 | B2 | C3 | 133.43(7) |
| O1 | C1 | C2 | B1 | 1.60(10) | B3 | B1 | B2 | B5 | 35.97(7) |
| O1 | C1 | C2 | B7 | 147.98(8) | B3 | B1 | B2 | B10 | 100.18(8) |
| O1 | C1 | C2 | B8 | 71.30(10) | B3 | B1 | B8 | C2 | -132.29(7) |
| O1 | C1 | C2 | B9 | -135.25(8) | B3 | B1 | B8 | C22 | 115.01(9) |
| N1 | C1 | C2 | C3 | 115.51(9) | B3 | B1 | B8 | B4 | -35.73(7) |
| N1 | C1 | C2 | B1 | -177.79(7) | B3 | B1 | B8 | B7 | -97.66(8) |
| N1 | C1 | C2 | B7 | -31.41(13) | B3 | B2 | B5 | B4 | 36.75(7) |
| N1 | C1 | C2 | B8 | -108.10(9) | B3 | B2 | B5 | B6 | 100.56(8) |
| N1 | C1 | C2 | B9 | 45.35(12) | B3 | B2 | B5 | B10 | 138.14(7) |
| C1 | N1 | C10 | C11 | 69.00(10) | B3 | B2 | B10 | C3 | 97.84(7) |
| C1 | N1 | C10 | C12 | -59.70(11) | B3 | B2 | B10 | B5 | -37.78(7) |
| C1 | N1 | C13 | C14 | -117.94(10) | B3 | B2 | B10 | B6 | -0.11(9) |
| C1 | N1 | C13 | C15 | 115.72(10) | B3 | B2 | B10 | B9 | 62.89(9) |
| C1 | C2 | C3 | C4 | -7.02(11) | B3 | B4 | B5 | B2 | -36.59(7) |
| C1 | C2 | C3 | B1 | 102.37(8) | B3 | B4 | B5 | B6 | -137.75(7) |
| C1 | C2 | C3 | B2 | 143.32(7) | B3 | B4 | B5 | B10 | -99.93(8) |
| C1 | C2 | C3 | B9 | -112.11(8) | B3 | B4 | B6 | B5 | 38.03(7) |
| C1 | C2 | C3 | B10 | -150.20(7) | B3 | B4 | B6 | B7 | -100.59(8) |
| C1 | C2 | B1 | C3 | -108.49(7) | B3 | B4 | B6 | B9 | -62.69(9) |
| C1 | C2 | B1 | C16 | 1.39(12) | B3 | B4 | B6 | B10 | 0.66(9) |
| C1 | C2 | B1 | B2 | -145.50(7) | B3 | B4 | B7 | C2 | 1.17(9) |
| C1 | C2 | B1 | B3 | 153.97(7) | B3 | B4 | B7 | B6 | 101.05(8) |
| C1 | C2 | B1 | B8 | 113.30(8) | B3 | B4 | B7 | B8 | -38.04(7) |
| C1 | C2 | B7 | B4 | -149.05(8) | B3 | B4 | B7 | B9 | 63.43(9) |
| C1 | C2 | B7 | B6 | 147.22(8) | B3 | B4 | B8 | C2 | 99.47(7) |
| C1 | C2 | B7 | B8 | -109.03(9) | B3 | B4 | B8 | C22 | -115.32(9) |
| C1 | C2 | B7 | B9 | 109.57(9) | B3 | B4 | B8 | B1 | 35.83(7) |
| C1 | C2 | B8 | C22 | 11.47(12) | B3 | B4 | B8 | B7 | 137.41(7) |
| C1 | C2 | B8 | B1 | -101.45(8) | B3 | B5 | B6 | B4 | -37.59(7) |
| C1 | C2 | B8 | B3 | -142.63(7) | B3 | B5 | B6 | B7 | -1.06(10) |
| C1 | C2 | B8 | B4 | 156.24(7) | B3 | B5 | B6 | B9 | 62.69(9) |
| C1 | C2 | B8 | B7 | 117.99(8) | B3 | B5 | B6 | B10 | 100.21(8) |
| C1 | C2 | B9 | C3 | 105.22(8) | B3 | B5 | B10 | C3 | -1.42(9) |

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|---|---|---|---|---|---|---|---|---|---|
| C1 | C2 | B9 | B6 | -155.52(7) | B3 | B5 | B10 | B2 | 36.98(7) |
| C1 | C2 | B9 | B7 | -117.78(8) | B3 | B5 | B10 | B6 | -101.02(8) |
| C1 | C2 | B9 | B10 | 141.36(8) | B3 | B5 | B10 | B9 | -63.76(9) |
| C2 | C3 | C4 | C5 | -33.38(12) | B4 | B3 | B5 | B2 | 138.61(7) |
| C2 | C3 | C4 | C9 | 146.40(9) | B4 | B3 | B5 | B6 | 37.93(7) |
| C2 | C3 | B1 | C16 | -120.15(9) | B4 | B3 | B5 | B10 | 101.35(8) |
| C2 | C3 | B1 | B2 | 135.98(7) | B4 | B3 | B8 | C2 | -97.28(7) |
| C2 | C3 | B1 | B3 | 96.33(7) | B4 | B3 | B8 | C22 | 109.49(10) |
| C2 | C3 | B1 | B8 | 35.11(6) | B4 | B3 | B8 | B1 | -139.42(7) |
| C2 | C3 | B2 | B1 | -41.24(6) | B4 | B3 | B8 | B7 | -36.90(7) |
| C2 | C3 | B2 | B3 | -0.30(9) | B4 | B5 | B6 | B7 | 36.53(7) |
| C2 | C3 | B2 | B5 | 62.98(8) | B4 | B5 | B6 | B9 | 100.29(8) |
| C2 | C3 | B2 | B10 | 101.99(7) | B4 | B5 | B6 | B10 | 137.80(7) |
| C2 | C3 | B9 | B6 | -99.61(7) | B4 | B5 | B10 | C3 | 61.62(9) |
| C2 | C3 | B9 | B7 | -37.07(6) | B4 | B5 | B10 | B2 | 100.02(8) |
| C2 | C3 | B9 | B10 | -138.72(7) | B4 | B5 | B10 | B6 | -37.98(7) |
| C2 | C3 | B10 | B2 | -103.36(7) | B4 | B5 | B10 | B9 | -0.71(10) |
| C2 | C3 | B10 | B5 | -64.29(8) | B4 | B6 | B7 | C2 | 100.24(7) |
| C2 | C3 | B10 | B6 | -1.46(9) | B4 | B6 | B7 | B8 | 37.54(7) |
| C2 | C3 | B10 | B9 | 37.34(6) | B4 | B6 | B7 | B9 | 137.69(7) |
| C2 | B1 | B2 | C3 | 36.85(6) | B4 | B6 | B9 | C2 | -0.35(9) |
| C2 | B1 | B2 | B3 | -96.58(7) | B4 | B6 | B9 | C3 | 61.69(9) |
| C2 | B1 | B2 | B5 | -60.61(8) | B4 | B6 | B9 | B7 | -37.36(7) |
| C2 | B1 | B2 | B10 | 3.61(9) | B4 | B6 | B9 | B10 | 100.12(8) |
| C2 | B1 | B3 | B2 | 97.80(7) | B4 | B6 | B10 | C3 | -62.02(9) |
| C2 | B1 | B3 | B4 | -2.08(9) | B4 | B6 | B10 | B2 | -0.34(9) |
| C2 | B1 | B3 | B5 | 62.06(8) | B4 | B6 | B10 | B5 | 37.30(7) |
| C2 | B1 | B3 | B8 | -39.42(6) | B4 | B6 | B10 | B9 | -100.74(8) |
| C2 | B1 | B8 | C22 | -112.70(9) | B4 | B7 | B8 | C2 | 135.25(7) |
| C2 | B1 | B8 | B3 | 132.29(7) | B4 | B7 | B8 | C22 | -111.88(9) |
| C2 | B1 | B8 | B4 | 96.56(7) | B4 | B7 | B8 | B1 | 99.31(8) |
| C2 | B1 | B8 | B7 | 34.64(6) | B4 | B7 | B8 | B3 | 37.07(7) |
| C2 | B7 | B8 | C22 | 112.87(9) | B4 | B7 | B9 | C2 | -99.06(7) |
| C2 | B7 | B8 | B1 | -35.94(6) | B4 | B7 | B9 | C3 | -61.52(8) |
| C2 | B7 | B8 | B3 | -98.18(7) | B4 | B7 | B9 | B6 | 38.16(7) |
| C2 | B7 | B8 | B4 | -135.25(7) | B4 | B7 | B9 | B10 | 0.12(9) |
| C2 | B7 | B9 | C3 | 37.53(6) | B5 | B2 | B3 | B1 | -140.69(7) |
| C2 | B7 | B9 | B6 | 137.22(7) | B5 | B2 | B3 | B4 | -36.95(7) |
| C2 | B7 | B9 | B10 | 99.18(7) | B5 | B2 | B3 | B8 | -101.61(8) |
| C2 | B9 | B10 | C3 | -36.37(6) | B5 | B2 | B10 | C3 | 135.62(7) |
| C2 | B9 | B10 | B2 | -1.72(9) | B5 | B2 | B10 | B6 | 37.67(7) |
| C2 | B9 | B10 | B5 | 61.78(9) | B5 | B2 | B10 | B9 | 100.67(8) |
| C2 | B9 | B10 | B6 | 99.31(8) | B5 | B3 | B4 | B6 | -37.80(7) |
| C3 | C2 | B1 | C16 | 109.88(10) | B5 | B3 | B4 | B7 | -101.17(8) |
| C3 | C2 | B1 | B2 | -37.01(6) | B5 | B3 | B4 | B8 | -139.33(7) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | C2 | B1 | B3 | -97.55(7) | B5 | B3 | B8 | C2 | -60.69(8) |
| C3 | C2 | B1 | B8 | -138.21(7) | B5 | B3 | B8 | C22 | 146.09(9) |
| C3 | C2 | B7 | B4 | 62.20(8) | B5 | B3 | B8 | B1 | -102.83(8) |
| C3 | C2 | B7 | B6 | -1.54(9) | B5 | B3 | B8 | B4 | 36.59(7) |
| C3 | C2 | B7 | B8 | 102.21(7) | B5 | B3 | B8 | B7 | -0.30(9) |
| C3 | C2 | B7 | B9 | -39.18(6) | B5 | B4 | B6 | B7 | -138.61(7) |
| C3 | C2 | B8 | C22 | 150.64(8) | B5 | B4 | B6 | B9 | -100.71(8) |
| C3 | C2 | B8 | B1 | 37.72(6) | B5 | B4 | B6 | B10 | -37.37(7) |
| C3 | C2 | B8 | B3 | -3.46(8) | B5 | B4 | B7 | C2 | -62.83(9) |
| C3 | C2 | B8 | B4 | -64.59(8) | B5 | B4 | B7 | B6 | 37.05(7) |
| C3 | C2 | B8 | B7 | -102.84(7) | B5 | B4 | B7 | B8 | -102.04(8) |
| C3 | C2 | B9 | B6 | 99.26(7) | B5 | B4 | B7 | B9 | -0.57(9) |
| C3 | C2 | B9 | B7 | 137.00(7) | B5 | B4 | B8 | C2 | 62.59(8) |
| C3 | C2 | B9 | B10 | 36.14(6) | B5 | B4 | B8 | C22 | -152.20(8) |
| C3 | C4 | C5 | C6 | 176.74(9) | B5 | B4 | B8 | B1 | -1.05(9) |
| C3 | C4 | C9 | C8 | -178.54(10) | B5 | B4 | B8 | B3 | -36.88(7) |
| C3 | B1 | B2 | B3 | -133.43(7) | B5 | B4 | B8 | B7 | 100.53(8) |
| C3 | B1 | B2 | B5 | -97.46(8) | B5 | B6 | B7 | C2 | 63.60(9) |
| C3 | B1 | B2 | B10 | -33.24(7) | B5 | B6 | B7 | B4 | -36.64(7) |
| C3 | B1 | B3 | B2 | 38.99(6) | B5 | B6 | B7 | B8 | 0.90(10) |
| C3 | B1 | B3 | B4 | -60.90(8) | B5 | B6 | B7 | B9 | 101.05(8) |
| C3 | B1 | B3 | B5 | 3.24(9) | B5 | B6 | B9 | C2 | -63.16(9) |
| C3 | B1 | B3 | B8 | -98.24(7) | B5 | B6 | B9 | C3 | -1.13(9) |
| C3 | B1 | B8 | C2 | -35.21(6) | B5 | B6 | B9 | B7 | -100.18(8) |
| C3 | B1 | B8 | C22 | -147.91(8) | B5 | B6 | B9 | B10 | 37.31(7) |
| C3 | B1 | B8 | B3 | 97.08(7) | B5 | B6 | B10 | C3 | -99.32(8) |
| C3 | B1 | B8 | B4 | 61.35(8) | B5 | B6 | B10 | B2 | -37.64(7) |
| C3 | B1 | B8 | B7 | -0.58(8) | B5 | B6 | B10 | B9 | -138.05(7) |
| C3 | B2 | B3 | B1 | -40.96(6) | B6 | B4 | B5 | B2 | 101.15(8) |
| C3 | B2 | B3 | B4 | 62.78(9) | B6 | B4 | B5 | B3 | 137.75(7) |
| C3 | B2 | B3 | B5 | 99.73(8) | B6 | B4 | B5 | B10 | 37.82(7) |
| C3 | B2 | B3 | B8 | -1.88(9) | B6 | B4 | B7 | C2 | -99.89(8) |
| C3 | B2 | B5 | B3 | -99.43(7) | B6 | B4 | B7 | B8 | -139.09(7) |
| C3 | B2 | B5 | B4 | -62.67(9) | B6 | B4 | B7 | B9 | -37.62(7) |
| C3 | B2 | B5 | B6 | 1.14(9) | B6 | B4 | B8 | C2 | -1.20(9) |
| C3 | B2 | B5 | B10 | 38.72(7) | B6 | B4 | B8 | C22 | 144.01(8) |
| C3 | B2 | B10 | B5 | -135.62(7) | B6 | B4 | B8 | B1 | -64.84(9) |
| C3 | B2 | B10 | B6 | -97.95(7) | B6 | B4 | B8 | B3 | -100.67(8) |
| C3 | B2 | B10 | B9 | -34.95(7) | B6 | B4 | B8 | B7 | 36.74(7) |
| C3 | B9 | B10 | B2 | 34.66(7) | B6 | B5 | B10 | C3 | 99.60(7) |
| C3 | B9 | B10 | B5 | 98.15(8) | B6 | B5 | B10 | B2 | 138.00(7) |
| C3 | B9 | B10 | B6 | 135.68(7) | B6 | B5 | B10 | B9 | 37.26(7) |
| C4 | C3 | B1 | C2 | 111.01(8) | B6 | B7 | B8 | C2 | 97.81(8) |
| C4 | C3 | B1 | C16 | -9.14(12) | B6 | B7 | B8 | C22 | -149.32(8) |
| C4 | C3 | B1 | B2 | -113.01(8) | B6 | B7 | B8 | B1 | 61.87(9) |

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|---|---|---|---|---|---|---|---|---|---|
| C4 | C3 | B1 | B3 | -152.66(7) | B6 | B7 | B8 | B3 | -0.37(9) |
| C4 | C3 | B1 | B8 | 146.11(7) | B6 | B7 | B8 | B4 | -37.44(7) |
| C4 | C3 | B2 | B1 | 108.44(9) | B6 | B7 | B9 | C2 | -137.22(7) |
| C4 | C3 | B2 | B3 | 149.38(8) | B6 | B7 | B9 | C3 | -99.68(7) |
| C4 | C3 | B2 | B5 | -147.33(8) | B6 | B7 | B9 | B10 | -38.04(7) |
| C4 | C3 | B2 | B10 | -108.32(9) | B6 | B9 | B10 | C3 | -135.68(7) |
| C4 | C3 | B9 | C2 | -111.02(8) | B6 | B9 | B10 | B2 | -101.02(8) |
| C4 | C3 | B9 | B6 | 149.37(7) | B6 | B9 | B10 | B5 | -37.53(7) |
| C4 | C3 | B9 | B7 | -148.09(7) | B7 | C2 | C3 | C4 | 145.10(8) |
| C4 | C3 | B9 | B10 | 110.26(8) | B7 | C2 | C3 | B1 | -105.51(7) |
| C4 | C3 | B10 | B2 | 113.00(9) | B7 | C2 | C3 | B2 | -64.56(8) |
| C4 | C3 | B10 | B5 | 152.06(8) | B7 | C2 | C3 | B9 | 40.01(7) |
| C4 | C3 | B10 | B6 | -145.10(8) | B7 | C2 | C3 | B10 | 1.92(9) |
| C4 | C3 | B10 | B9 | -106.31(8) | B7 | C2 | B1 | C3 | 100.47(7) |
| C4 | C5 | C6 | C7 | 2.45(16) | B7 | C2 | B1 | C16 | -149.65(9) |
| C5 | C4 | C9 | C8 | 1.25(15) | B7 | C2 | B1 | B2 | 63.46(8) |
| C5 | C6 | C7 | C8 | -0.02(17) | B7 | C2 | B1 | B3 | 2.92(9) |
| C6 | C7 | C8 | C9 | -1.78(18) | B7 | C2 | B1 | B8 | -37.74(7) |
| C7 | C8 | C9 | C4 | 1.15(18) | B7 | C2 | B8 | C22 | -106.52(9) |
| C9 | C4 | C5 | C6 | -3.04(15) | B7 | C2 | B8 | B1 | 140.56(7) |
| C10 | N1 | C1 | O1 | -1.08(13) | B7 | C2 | B8 | B3 | 99.39(7) |
| C10 | N1 | C1 | C2 | 178.27(8) | B7 | C2 | B8 | B4 | 38.25(6) |
| C10 | N1 | C13 | C14 | 61.08(10) | B7 | C2 | B9 | C3 | -137.00(7) |
| C10 | N1 | C13 | C15 | -65.26(10) | B7 | C2 | B9 | B6 | -37.74(7) |
| C13 | N1 | C1 | O1 | 177.92(8) | B7 | C2 | B9 | B10 | -100.86(8) |
| C13 | N1 | C1 | C2 | -2.73(14) | B7 | B4 | B5 | B2 | 64.13(9) |
| C13 | N1 | C10 | C11 | -110.14(9) | B7 | B4 | B5 | B3 | 100.72(8) |
| C13 | N1 | C10 | C12 | 121.16(9) | B7 | B4 | B5 | B6 | -37.03(7) |
| C16 | C17 | C18 | C19 | -0.69(14) | B7 | B4 | B5 | B10 | 0.79(10) |
| C16 | B1 | B2 | C3 | -115.25(8) | B7 | B4 | B6 | B5 | 138.61(7) |
| C16 | B1 | B2 | B3 | 111.32(9) | B7 | B4 | B6 | B9 | 37.90(7) |
| C16 | B1 | B2 | B5 | 147.29(8) | B7 | B4 | B6 | B10 | 101.24(8) |
| C16 | B1 | B2 | B10 | -148.49(8) | B7 | B4 | B8 | C2 | -37.94(6) |
| C16 | B1 | B3 | B2 | -106.20(9) | B7 | B4 | B8 | C22 | 107.27(9) |
| C16 | B1 | B3 | B4 | 153.92(8) | B7 | B4 | B8 | B1 | -101.59(7) |
| C16 | B1 | B3 | B5 | -141.94(8) | B7 | B4 | B8 | B3 | -137.41(7) |
| C16 | B1 | B3 | B8 | 116.58(9) | B7 | B6 | B9 | C2 | 37.02(6) |
| C16 | B1 | B8 | C2 | 119.51(9) | B7 | B6 | B9 | C3 | 99.05(7) |
| C16 | B1 | B8 | C22 | 6.81(13) | B7 | B6 | B9 | B10 | 137.49(7) |
| C16 | B1 | B8 | B3 | -108.20(9) | B7 | B6 | B10 | C3 | 0.50(9) |
| C16 | B1 | B8 | B4 | -143.93(8) | B7 | B6 | B10 | B2 | 62.18(9) |
| C16 | B1 | B8 | B7 | 154.14(8) | B7 | B6 | B10 | B5 | 99.83(8) |
| C17 | C16 | C21 | C20 | -0.15(13) | B7 | B6 | B10 | B9 | -38.22(7) |
| C17 | C16 | B1 | C2 | -53.79(13) | B7 | B9 | B10 | C3 | -97.79(7) |
| C17 | C16 | B1 | C3 | 20.63(13) | B7 | B9 | B10 | B2 | -63.13(9) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C17 | C16 | B1 | B2 | 89.06(11) | B7 | B9 | B10 | B5 | 0.36(9) |
| C17 | C16 | B1 | B3 | 157.97(8) | B7 | B9 | B10 | B6 | 37.89(7) |
| C17 | C16 | B1 | B8 | -129.00(10) | B8 | C2 | C3 | C4 | -147.90(8) |
| C17 | C18 | C19 | Cl1 | -178.46(7) | B8 | C2 | C3 | B1 | -38.50(6) |
| C17 | C18 | C19 | C20 | 0.48(14) | B8 | C2 | C3 | B2 | 2.45(9) |
| C18 | C19 | C20 | C21 | -0.11(14) | B8 | C2 | C3 | B9 | 107.02(7) |
| C19 | C20 | C21 | C16 | -0.05(14) | B8 | C2 | C3 | B10 | 68.92(8) |
| C21 | C16 | C17 | C18 | 0.52(13) | B8 | C2 | B1 | C3 | 138.21(7) |
| C21 | C16 | B1 | C2 | 132.00(9) | B8 | C2 | B1 | C16 | -111.91(10) |
| C21 | C16 | B1 | C3 | -153.58(8) | B8 | C2 | B1 | B2 | 101.20(7) |
| C21 | C16 | B1 | B2 | -85.16(10) | B8 | C2 | B1 | B3 | 40.67(6) |
| C21 | C16 | B1 | B3 | -16.24(12) | B8 | C2 | B7 | B4 | -40.01(7) |
| C21 | C16 | B1 | B8 | 56.78(12) | B8 | C2 | B7 | B6 | -103.74(7) |
| C22 | C23 | C24 | C25 | -0.47(17) | B8 | C2 | B7 | B9 | -141.39(7) |
| C23 | C22 | C27 | C26 | -0.15(14) | B8 | C2 | B9 | C3 | -99.71(7) |
| C23 | C22 | B8 | C2 | 19.47(14) | B8 | C2 | B9 | B6 | -0.45(9) |
| C23 | C22 | B8 | B1 | 94.42(11) | B8 | C2 | B9 | B7 | 37.29(7) |
| C23 | C22 | B8 | B3 | 168.14(9) | B8 | C2 | B9 | B10 | -63.58(9) |
| C23 | C22 | B8 | B4 | -119.07(10) | B8 | C22 | C23 | C24 | 174.82(10) |
| C23 | C22 | B8 | B7 | -49.59(13) | B8 | C22 | C27 | C26 | -174.95(9) |
| C23 | C24 | C25 | Cl2 | -179.76(8) | B8 | B1 | B2 | C3 | 95.89(7) |
| C23 | C24 | C25 | C26 | 0.50(16) | B8 | B1 | B2 | B3 | -37.54(6) |
| C24 | C25 | C26 | C27 | -0.36(15) | B8 | B1 | B2 | B5 | -1.57(9) |
| C25 | C26 | C27 | C22 | 0.19(15) | B8 | B1 | B2 | B10 | 62.65(9) |
| C27 | C22 | C23 | C24 | 0.30(15) | B8 | B1 | B3 | B2 | 137.22(7) |
| C27 | C22 | B8 | C2 | -166.11(8) | B8 | B1 | B3 | B4 | 37.34(7) |
| C27 | C22 | B8 | B1 | -91.16(11) | B8 | B1 | B3 | B5 | 101.48(8) |
| C27 | C22 | B8 | B3 | -17.43(13) | B8 | B3 | B4 | B5 | 139.33(7) |
| C27 | C22 | B8 | B4 | 55.36(12) | B8 | B3 | B4 | B6 | 101.54(8) |
| C27 | C22 | B8 | B7 | 124.84(9) | B8 | B3 | B4 | B7 | 38.17(7) |
| B1 | C2 | C3 | C4 | -109.39(8) | B8 | B3 | B5 | B2 | 101.53(8) |
| B1 | C2 | C3 | B2 | 40.95(6) | B8 | B3 | B5 | B4 | -37.08(7) |
| B1 | C2 | C3 | B9 | 145.52(7) | B8 | B3 | B5 | B6 | 0.86(10) |
| B1 | C2 | C3 | B10 | 107.43(7) | B8 | B3 | B5 | B10 | 64.27(9) |
| B1 | C2 | B7 | B4 | -2.62(9) | B8 | B4 | B5 | B2 | 0.09(10) |
| B1 | C2 | B7 | B6 | -66.36(8) | B8 | B4 | B5 | B3 | 36.69(7) |
| B1 | C2 | B7 | B8 | 37.39(7) | B8 | B4 | B5 | B6 | -101.06(8) |
| B1 | C2 | B7 | B9 | -104.01(7) | B8 | B4 | B5 | B10 | -63.24(9) |
| B1 | C2 | B8 | C22 | 112.93(9) | B8 | B4 | B6 | B5 | 101.70(8) |
| B1 | C2 | B8 | B3 | -41.17(6) | B8 | B4 | B6 | B7 | -36.92(7) |
| B1 | C2 | B8 | B4 | -102.31(7) | B8 | B4 | B6 | B9 | 0.98(10) |
| B1 | C2 | B8 | B7 | -140.56(7) | B8 | B4 | B6 | B10 | 64.33(9) |
| B1 | C2 | B9 | C3 | -31.95(6) | B8 | B4 | B7 | C2 | 39.21(6) |
| B1 | C2 | B9 | B6 | 67.31(8) | B8 | B4 | B7 | B6 | 139.09(7) |
| B1 | C2 | B9 | B7 | 105.05(7) | B8 | B4 | B7 | B9 | 101.47(7) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| B1 | C2 | B9 | B10 | 4.19(9) | B8 | B7 | B9 | C2 | -34.44(6) |
| B1 | C3 | C4 | C5 | -106.85(10) | B8 | B7 | B9 | C3 | 3.09(9) |
| B1 | C3 | C4 | C9 | 72.93(11) | B8 | B7 | B9 | B6 | 102.78(8) |
| B1 | C3 | B2 | B3 | 40.94(6) | B8 | B7 | B9 | B10 | 64.74(9) |
| B1 | C3 | B2 | B5 | 104.23(7) | B9 | C2 | C3 | C4 | 105.09(8) |
| B1 | C3 | B2 | B10 | 143.23(7) | B9 | C2 | C3 | B1 | -145.52(7) |
| B1 | C3 | B9 | C2 | 33.39(7) | B9 | C2 | C3 | B2 | -104.57(7) |
| B1 | C3 | B9 | B6 | -66.22(9) | B9 | C2 | C3 | B10 | -38.09(7) |
| B1 | C3 | B9 | B7 | -3.68(9) | B9 | C2 | B1 | C3 | 32.19(6) |
| B1 | C3 | B9 | B10 | -105.33(8) | B9 | C2 | B1 | C16 | 142.06(9) |
| B1 | C3 | B10 | B2 | -35.33(7) | B9 | C2 | B1 | B2 | -4.83(9) |
| B1 | C3 | B10 | B5 | 3.73(9) | B9 | C2 | B1 | B3 | -65.36(8) |
| B1 | C3 | B10 | B6 | 66.57(9) | B9 | C2 | B1 | B8 | -106.03(7) |
| B1 | C3 | B10 | B9 | 105.36(7) | B9 | C2 | B7 | B4 | 101.38(8) |
| B1 | C16 | C17 | C18 | -173.69(8) | B9 | C2 | B7 | B6 | 37.65(7) |
| B1 | C16 | C21 | C20 | 174.63(8) | B9 | C2 | B7 | B8 | 141.39(7) |
| B1 | B2 | B3 | B4 | 103.74(8) | B9 | C2 | B8 | C22 | -143.73(8) |
| B1 | B2 | B3 | B5 | 140.69(7) | B9 | C2 | B8 | B1 | 103.34(7) |
| B1 | B2 | B3 | B8 | 39.08(7) | B9 | C2 | B8 | B3 | 62.17(8) |
| B1 | B2 | B5 | B3 | -35.82(7) | B9 | C2 | B8 | B4 | 1.03(9) |
| B1 | B2 | B5 | B4 | 0.94(10) | B9 | C2 | B8 | B7 | -37.22(7) |
| B1 | B2 | B5 | B6 | 64.75(9) | B9 | C3 | C4 | C5 | 35.67(12) |
| B1 | B2 | B5 | B10 | 102.32(8) | B9 | C3 | C4 | C9 | -144.55(9) |
| B1 | B2 | B10 | C3 | 33.63(7) | B9 | C3 | B1 | C2 | -32.42(6) |
| B1 | B2 | B10 | B5 | -101.99(8) | B9 | C3 | B1 | C16 | -152.57(8) |
| B1 | B2 | B10 | B6 | -64.32(9) | B9 | C3 | B1 | B2 | 103.56(8) |
| B1 | B2 | B10 | B9 | -1.32(10) | B9 | C3 | B1 | B3 | 63.91(8) |
| B1 | B3 | B4 | B5 | 101.84(8) | B9 | C3 | B1 | B8 | 2.68(9) |
| B1 | B3 | B4 | B6 | 64.04(9) | B9 | C3 | B2 | B1 | -106.16(7) |
| B1 | B3 | B4 | B7 | 0.67(10) | B9 | C3 | B2 | B3 | -65.22(9) |
| B1 | B3 | B4 | B8 | -37.49(7) | B9 | C3 | B2 | B5 | -1.93(9) |
| B1 | B3 | B5 | B2 | 36.04(7) | B9 | C3 | B2 | B10 | 37.07(7) |
| B1 | B3 | B5 | B4 | -102.57(8) | B9 | C3 | B10 | B2 | -140.70(7) |
| B1 | B3 | B5 | B6 | -64.64(9) | B9 | C3 | B10 | B5 | -101.63(8) |
| B1 | B3 | B5 | B10 | -1.22(10) | B9 | C3 | B10 | B6 | -38.80(7) |
| B1 | B3 | B8 | C2 | 42.14(6) | B9 | B6 | B7 | C2 | -37.45(6) |
| B1 | B3 | B8 | C22 | -111.08(10) | B9 | B6 | B7 | B4 | -137.69(7) |
| B1 | B3 | B8 | B4 | 139.42(7) | B9 | B6 | B7 | B8 | -100.16(8) |
| B1 | B3 | B8 | B7 | 102.53(7) | B9 | B6 | B10 | C3 | 38.72(7) |
| B2 | C3 | C4 | C5 | 179.73(8) | B9 | B6 | B10 | B2 | 100.41(8) |
| B2 | C3 | C4 | C9 | -0.49(13) | B9 | B6 | B10 | B5 | 138.05(7) |
| B2 | C3 | B1 | C2 | -135.98(7) | B9 | B7 | B8 | C2 | 34.37(6) |
| B2 | C3 | B1 | C16 | 103.87(9) | B9 | B7 | B8 | C22 | 147.24(8) |
| B2 | C3 | B1 | B3 | -39.65(6) | B9 | B7 | B8 | B1 | -1.57(9) |
| B2 | C3 | B1 | B8 | -100.88(7) | B9 | B7 | B8 | B3 | -63.81(8) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| B2 | C3 | B9 | C2 | 101.55(7) | B9 | B7 | B8 | B4 | -100.88(8) |
| B2 | C3 | B9 | B6 | 1.94(9) | B10 | C3 | C4 | C5 | 106.45(10) |
| B2 | C3 | B9 | B7 | 64.48(8) | B10 | C3 | C4 | C9 | -73.77(11) |
| B2 | C3 | B9 | B10 | -37.18(7) | B10 | C3 | B1 | C2 | -100.69(7) |
| B2 | C3 | B10 | B5 | 39.06(7) | B10 | C3 | B1 | C16 | 139.17(8) |
| B2 | C3 | B10 | B6 | 101.90(8) | B10 | C3 | B1 | B2 | 35.30(7) |
| B2 | C3 | B10 | B9 | 140.70(7) | B10 | C3 | B1 | B3 | -4.36(9) |
| B2 | B1 | B3 | B4 | -99.89(8) | B10 | C3 | B1 | B8 | -65.58(8) |
| B2 | B1 | B3 | B5 | -35.74(7) | B10 | C3 | B2 | B1 | -143.23(7) |
| B2 | B1 | B3 | B8 | -137.22(7) | B10 | C3 | B2 | B3 | -102.29(8) |
| B2 | B1 | B8 | C2 | -94.98(7) | B10 | C3 | B2 | B5 | -39.01(7) |
| B2 | B1 | B8 | C22 | 152.32(8) | B10 | C3 | B9 | C2 | 138.72(7) |
| B2 | B1 | B8 | B3 | 37.31(6) | B10 | C3 | B9 | B6 | 39.11(7) |
| B2 | B1 | B8 | B4 | 1.58(9) | B10 | C3 | B9 | B7 | 101.65(8) |
| B2 | B1 | B8 | B7 | -60.35(8) | B10 | B2 | B3 | B1 | -103.22(7) |
| B2 | B3 | B4 | B5 | 37.07(7) | B10 | B2 | B3 | B4 | 0.52(9) |
| B2 | B3 | B4 | B6 | -0.73(9) | B10 | B2 | B3 | B5 | 37.47(7) |
| B2 | B3 | B4 | B7 | -64.10(9) | B10 | B2 | B3 | B8 | -64.14(9) |
| B2 | B3 | B4 | B8 | -102.27(7) | B10 | B2 | B5 | B3 | -138.14(7) |
| B2 | B3 | B5 | B4 | -138.61(7) | B10 | B2 | B5 | B4 | -101.39(8) |
| B2 | B3 | B5 | B6 | -100.68(8) | B10 | B2 | B5 | B6 | -37.58(7) |
| B2 | B3 | B5 | B10 | -37.26(7) | B10 | B5 | B6 | B4 | -137.80(7) |
| B2 | B3 | B8 | C2 | 3.28(9) | B10 | B5 | B6 | B7 | -101.27(8) |
| B2 | B3 | B8 | C22 | -149.94(8) | B10 | B5 | B6 | B9 | -37.51(7) |
| B2 | B3 | B8 | B1 | -38.86(7) | B10 | B6 | B7 | C2 | 0.62(9) |
| B2 | B3 | B8 | B4 | 100.57(8) | B10 | B6 | B7 | B4 | -99.62(8) |
| B2 | B3 | B8 | B7 | 63.67(9) | B10 | B6 | B7 | B8 | -62.08(9) |
| B2 | B5 | B6 | B4 | -100.29(8) | B10 | B6 | B7 | B9 | 38.07(7) |
| B2 | B5 | B6 | B7 | -63.76(9) | B10 | B6 | B9 | C2 | -100.47(7) |
| B2 | B5 | B6 | B9 | 0.00(10) | B10 | B6 | B9 | C3 | -38.44(6) |
| B2 | B5 | B6 | B10 | 37.52(7) | B10 | B6 | B9 | B7 | -137.49(7) |
| B2 | B5 | B10 | C3 | -38.40(6) | | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0830_CG_0m.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | 5287.57 | 8918.58 | 3218.02 | 21 |
| H6 | 3183.63 | 9310.61 | 2865.33 | 28 |
| H7 | 1705.43 | 8458.16 | 3612.59 | 32 |
| H8 | 2342.28 | 7204.36 | 4706.33 | 33 |
| H9 | 4400.9 | 6714.95 | 4990.45 | 25 |
| H10 | 6102.19 | 8838.75 | 548.45 | 22 |
| H11A | 3871.61 | 7653.76 | 973.06 | 38 |
| H11B | 3807.17 | 8336.97 | 75.38 | 38 |

| | | | | |
|---|---|---|---|---|
| H11C | 4466.69 | 9197.11 | 1300.3 | 38 |
| H12A | 6435.02 | 6752.77 | -101.61 | 42 |
| H12B | 5051 | 6884.71 | -802.08 | 42 |
| H12C | 5089.68 | 6101.17 | 29.63 | 42 |
| H13 | 8201.11 | 9346.59 | 3026.75 | 19 |
| H14A | 6801.31 | 10729.97 | 1793.67 | 33 |
| H14B | 8043.7 | 11395.57 | 2858.49 | 33 |
| H14C | 6675.17 | 10658.49 | 2903.04 | 33 |
| H15A | 8925.5 | 8491.73 | 1591.29 | 38 |
| H15B | 9448.97 | 10051.52 | 2061.21 | 38 |
| H15C | 8228.05 | 9388.55 | 981.32 | 38 |
| H17 | 3693.41 | 5546.41 | 2592.59 | 19 |
| H18 | 1922.01 | 3697.06 | 1806.54 | 21 |
| H20 | 4442.33 | 1397.46 | 2377.14 | 22 |
| H21 | 6207.27 | 3254.7 | 3179.31 | 19 |
| H23 | 7738.49 | 6192.32 | 1368.62 | 26 |
| H24 | 8256.48 | 4915.57 | -27.68 | 28 |
| H26 | 9324.5 | 2535.9 | 1692.28 | 25 |
| H27 | 8792.27 | 3820.9 | 3080.69 | 23 |
| H2 | 6109(13) | 6011(12) | 5362(10) | 18 |
| H3 | 7914(13) | 4606(12) | 4534(10) | 18 |
| H4 | 10219(13) | 6521(13) | 4738(10) | 21 |
| H5A | 8999(13) | 6894(13) | 6445(10) | 21 |
| H6A | 9923(13) | 9159(13) | 5770(10) | 21 |
| H7A | 9286(13) | 8151(12) | 3458(10) | 18 |
| H9A | 7468(13) | 9498(12) | 4323(10) | 18 |
| H10A | 7293(13) | 8787(13) | 6115(10) | 20 |

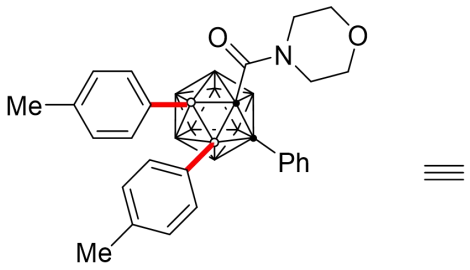
**Experimental**

Single crystals of $C_{27}H_{35}B_{10}Cl_2NO$ [mo_0830_CG_0m] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a Bruker D8 Venture MoCu Dual Source diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

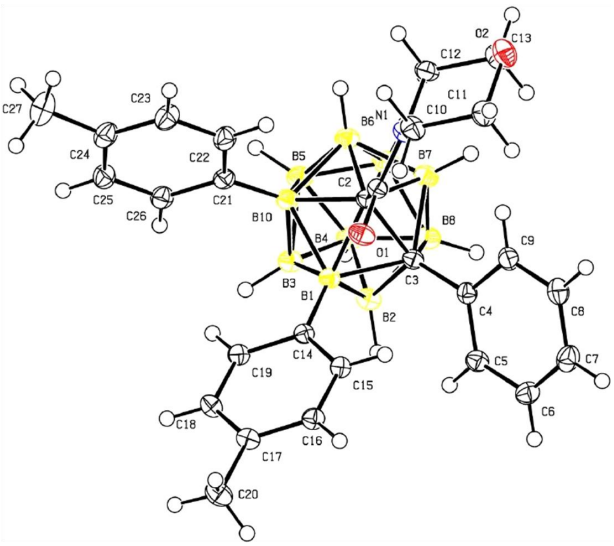
**Crystal structure determination of 3dd**

**Crystal Data** for $C_{27}H_{35}B_{10}Cl_2NO$ ($M$ =568.56 g/mol): triclinic, space group P-1 (no. 2), $a$ = 10.8615(14) Å, $b$ = 10.9215(14) Å, $c$ = 13.8510(18) Å, $\alpha$ = 105.147(4)°, $\beta$ = 105.960(4)°, $\gamma$ = 99.055(4)°, $V$ = 1477.6(3) Å$^3$, $Z$ = 2, $T$ = 100.0 K, μ(MoKα) = 0.245 mm$^{-1}$, *Dcalc* = 1.278 g/cm$^3$, 77051 reflections measured (4.244° ≤ 2Θ ≤ 59.328°), 8309 unique ($R_{int}$ = 0.0303,

$R_{sigma}$ = 0.0150) which were used in all calculations. The final $R_1$ was 0.0310 (I > 2σ(I)) and $wR_2$ was 0.0823 (all data).




**3ea**




**CCDC 1983607**

**Crystal data and structure refinement for 3ea.**

| | |
|---|---|
| Identification code | mo_0804_CG_0m |
| CCDC number | 1983607 |
| Empirical formula | $C_{27}H_{35}B_{10}NO_2$ |
| Formula weight | 513.66 |
| Temperature/K | 100.0 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 11.7623(18) |
| b/Å | 11.821(2) |
| c/Å | 12.371(2) |
| α/° | 108.419(5) |
| β/° | 100.884(5) |
| γ/° | 113.869(6) |
| Volume/Å$^3$ | 1389.5(4) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.228 |
| μ/mm$^{-1}$ | 0.070 |
| F(000) | 540.0 |
| Crystal size/mm$^3$ | 0.215 × 0.134 × 0.074 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.068 to 57.416 |
| Index ranges | -15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16 |
| Reflections collected | 29979 |
| Independent reflections | 7064 [$R_{int}$ = 0.0456, $R_{sigma}$ = 0.0388] |
| Data/restraints/parameters | 7064/0/388 |
| Goodness-of-fit on F$^2$ | 1.073 |

| | |
|---|---|
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0538, $wR_2$ = 0.1248 |
| Final R indexes [all data] | $R_1$ = 0.0744, $wR_2$ = 0.1431 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.95/-0.36 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0804_CG_0m. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 3473.3(12) | 8449.0(12) | 4205.3(10) | 22.9(3) |
| O2 | 4263.2(13) | 8504.8(13) | 8148.6(11) | 28.7(3) |
| N1 | 4162.0(13) | 7923.9(14) | 5706.9(12) | 19.1(3) |
| C1 | 3603.6(15) | 7616.0(16) | 4517.9(14) | 17.5(3) |
| C2 | 3075.7(15) | 6180.9(15) | 3480.2(14) | 17.1(3) |
| C3 | 1387.5(15) | 5238.9(15) | 2701.8(14) | 17.9(3) |
| C4 | 488.1(15) | 5740.7(15) | 3127.6(14) | 17.8(3) |
| C5 | -607.9(16) | 5545.8(16) | 2257.6(15) | 20.8(3) |
| C6 | -1469.4(17) | 5971.4(18) | 2626.1(16) | 24.8(3) |
| C7 | -1249.6(18) | 6600.9(18) | 3857.5(17) | 26.1(4) |
| C8 | -167.7(17) | 6789.9(18) | 4721.8(16) | 25.0(3) |
| C9 | 689.6(16) | 6353.3(16) | 4361.6(15) | 21.2(3) |
| C10 | 4619.7(17) | 9329.2(17) | 6614.7(14) | 23.2(3) |
| C11 | 3963.3(18) | 9254.6(18) | 7544.8(16) | 26.0(4) |
| C12 | 4428.5(17) | 7124.9(18) | 6315.8(15) | 22.8(3) |
| C13 | 3803.9(18) | 7146.1(18) | 7282.2(16) | 26.3(4) |
| C14 | 2352.4(15) | 7178.6(15) | 1594.4(13) | 16.4(3) |
| C15 | 1768.1(15) | 7979.9(15) | 1995.6(14) | 17.5(3) |
| C16 | 1720.5(16) | 8884.4(16) | 1522.5(14) | 19.8(3) |
| C17 | 2266.0(16) | 9051.3(16) | 639.0(14) | 20.3(3) |
| C18 | 2854.3(17) | 8275.1(16) | 238.8(14) | 21.1(3) |
| C19 | 2891.9(16) | 7360.2(16) | 705.1(14) | 18.6(3) |
| C20 | 2231.7(19) | 10056.2(18) | 146.3(16) | 27.5(4) |
| C21 | 5311.5(16) | 7067.6(16) | 2661.6(14) | 19.7(3) |
| C22 | 6240.3(17) | 8160.0(18) | 3786.2(15) | 24.1(3) |
| C23 | 7518.6(17) | 9064.5(18) | 3914.0(16) | 26.6(4) |
| C24 | 7930.3(17) | 8896.1(18) | 2920.1(17) | 26.1(4) |
| C25 | 7005.6(17) | 7822.9(18) | 1784.6(16) | 24.6(3) |
| C26 | 5730.8(17) | 6926.2(17) | 1661.4(15) | 22.2(3) |
| C27 | 9341(2) | 9802(2) | 3059(2) | 37.1(5) |
| B1 | 2390.1(17) | 6041.5(18) | 1975.9(15) | 17.3(3) |
| B2 | 1027.0(19) | 4295.6(18) | 1188.8(16) | 19.8(3) |
| B3 | 2583.5(18) | 4692.3(18) | 1029.6(16) | 20.1(3) |
| B4 | 1644(2) | 3143.0(19) | 1142.0(17) | 23.2(4) |
| B5 | 3400.0(19) | 4141.2(19) | 1924.7(17) | 22.2(4) |
| B6 | 3723.4(19) | 5116.2(19) | 3475.8(17) | 21.2(4) |

| | | | | |
|---|---|---|---|---|
| B7 | 2164.2(19) | 4729.4(18) | 3646.1(17) | 21.5(4) |
| B8 | 874.4(19) | 3509.8(18) | 2201.8(17) | 22.0(4) |
| B9 | 2341(2) | 3410(2) | 2666.9(18) | 24.4(4) |
| B10 | 3894.6(18) | 5939.4(18) | 2473.2(16) | 18.9(3) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_0804_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 29.8(6) | 19.1(5) | 18.5(5) | 7.8(4) | 5.6(5) | 13.0(5) |
| O2 | 34.6(7) | 30.0(6) | 20.1(6) | 10.3(5) | 12.7(5) | 14.3(6) |
| N1 | 21.4(6) | 19.5(6) | 14.5(6) | 7.6(5) | 5.1(5) | 9.0(5) |
| C1 | 17.4(7) | 18.5(7) | 16.4(7) | 7.6(6) | 6.0(5) | 9.0(6) |
| C2 | 18.3(7) | 17.7(7) | 16.8(7) | 8.2(6) | 6.1(6) | 10.1(6) |
| C3 | 19.8(7) | 17.2(7) | 18.2(7) | 8.4(6) | 6.4(6) | 10.1(6) |
| C4 | 19.5(7) | 15.5(7) | 20.4(7) | 9.0(6) | 8.9(6) | 8.9(6) |
| C5 | 22.9(8) | 20.5(7) | 19.7(7) | 8.9(6) | 7.3(6) | 11.7(6) |
| C6 | 24.5(8) | 27.8(8) | 29.0(9) | 14.8(7) | 10.8(7) | 16.6(7) |
| C7 | 26.8(8) | 25.8(8) | 33.0(9) | 13.6(7) | 15.8(7) | 16.6(7) |
| C8 | 27.5(8) | 25.2(8) | 22.8(8) | 9.5(7) | 13.0(7) | 12.7(7) |
| C9 | 21.2(8) | 22.5(7) | 19.7(7) | 10.0(6) | 8.9(6) | 9.5(6) |
| C10 | 24.2(8) | 19.5(7) | 15.5(7) | 3.8(6) | 3.8(6) | 6.3(6) |
| C11 | 28.0(9) | 25.3(8) | 22.7(8) | 8.3(7) | 9.8(7) | 12.9(7) |
| C12 | 25.5(8) | 26.8(8) | 18.7(7) | 11.4(6) | 6.4(6) | 14.9(7) |
| C13 | 29.6(9) | 26.1(8) | 22.7(8) | 12.7(7) | 10.0(7) | 11.7(7) |
| C14 | 17.2(7) | 16.0(7) | 14.2(6) | 4.8(5) | 4.7(5) | 8.3(6) |
| C15 | 18.6(7) | 16.1(7) | 17.3(7) | 6.1(6) | 6.8(6) | 8.8(6) |
| C16 | 22.1(7) | 18.3(7) | 21.2(7) | 8.1(6) | 8.0(6) | 12.2(6) |
| C17 | 22.5(8) | 17.6(7) | 18.3(7) | 7.4(6) | 4.9(6) | 9.3(6) |
| C18 | 25.9(8) | 21.3(7) | 17.9(7) | 9.5(6) | 9.1(6) | 12.0(6) |
| C19 | 20.8(7) | 18.7(7) | 16.2(7) | 5.8(6) | 6.3(6) | 11.3(6) |
| C20 | 36.1(10) | 24.0(8) | 27.5(9) | 14.8(7) | 11.4(7) | 16.7(7) |
| C21 | 21.7(7) | 22.3(7) | 21.2(7) | 10.4(6) | 9.2(6) | 15.1(6) |
| C22 | 22.9(8) | 28.4(8) | 21.5(8) | 8.4(7) | 9.5(6) | 14.5(7) |
| C23 | 22.3(8) | 27.5(8) | 26.2(8) | 7.0(7) | 8.3(7) | 12.8(7) |
| C24 | 23.9(8) | 27.2(8) | 32.7(9) | 12.9(7) | 13.1(7) | 16.4(7) |
| C25 | 27.6(8) | 28.8(8) | 27.0(8) | 13.9(7) | 14.9(7) | 18.9(7) |
| C26 | 24.1(8) | 24.3(8) | 21.7(8) | 9.3(6) | 9.5(6) | 15.3(7) |
| C27 | 28.3(10) | 34.3(10) | 47.1(12) | 14.5(9) | 20.0(9) | 14.1(8) |
| B1 | 19.6(8) | 18.2(8) | 13.7(7) | 5.3(6) | 5.5(6) | 10.7(7) |
| B2 | 24.3(9) | 15.1(7) | 18.3(8) | 5.8(6) | 5.7(7) | 10.3(7) |
| B3 | 23.7(9) | 18.3(8) | 18.3(8) | 5.9(6) | 6.1(7) | 12.7(7) |
| B4 | 26.8(9) | 18.4(8) | 22.6(9) | 6.5(7) | 5.0(7) | 13.2(7) |
| B5 | 26.9(9) | 20.6(8) | 21.4(8) | 7.9(7) | 6.9(7) | 15.4(7) |
| B6 | 23.7(9) | 21.9(8) | 22.7(8) | 11.3(7) | 7.5(7) | 14.6(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B7 | 25.0(9) | 18.9(8) | 21.7(8) | 10.8(7) | 7.3(7) | 11.0(7) |
| B8 | 23.8(9) | 17.2(8) | 22.6(9) | 8.5(7) | 5.2(7) | 9.8(7) |
| B9 | 29.9(10) | 21.1(8) | 25.7(9) | 11.7(7) | 7.9(8) | 15.5(8) |
| B10 | 22.0(8) | 21.4(8) | 16.9(8) | 7.9(7) | 7.4(6) | 14.1(7) |

**Bond Lengths for mo_0804_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C1 | 1.2177(19) | C17 | C20 | 1.507(2) |
| O2 | C11 | 1.428(2) | C18 | C19 | 1.388(2) |
| O2 | C13 | 1.418(2) | C21 | C22 | 1.395(2) |
| N1 | C1 | 1.3532(19) | C21 | C26 | 1.403(2) |
| N1 | C10 | 1.476(2) | C21 | B10 | 1.571(2) |
| N1 | C12 | 1.469(2) | C22 | C23 | 1.390(2) |
| C1 | C2 | 1.543(2) | C23 | C24 | 1.391(2) |
| C2 | C3 | 1.709(2) | C24 | C25 | 1.395(3) |
| C2 | B1 | 1.809(2) | C24 | C27 | 1.506(3) |
| C2 | B6 | 1.714(2) | C25 | C26 | 1.386(2) |
| C2 | B7 | 1.718(2) | B1 | B2 | 1.800(3) |
| C2 | B10 | 1.736(2) | B1 | B3 | 1.783(2) |
| C3 | C4 | 1.506(2) | B1 | B10 | 1.826(2) |
| C3 | B1 | 1.769(2) | B2 | B3 | 1.764(3) |
| C3 | B2 | 1.710(2) | B2 | B4 | 1.776(3) |
| C3 | B7 | 1.746(2) | B2 | B8 | 1.775(3) |
| C3 | B8 | 1.728(2) | B3 | B4 | 1.782(3) |
| C4 | C5 | 1.397(2) | B3 | B5 | 1.770(3) |
| C4 | C9 | 1.392(2) | B3 | B10 | 1.788(3) |
| C5 | C6 | 1.389(2) | B4 | B5 | 1.774(3) |
| C6 | C7 | 1.386(2) | B4 | B8 | 1.770(3) |
| C7 | C8 | 1.385(3) | B4 | B9 | 1.778(3) |
| C8 | C9 | 1.388(2) | B5 | B6 | 1.768(3) |
| C10 | C11 | 1.507(2) | B5 | B9 | 1.790(3) |
| C12 | C13 | 1.516(2) | B5 | B10 | 1.804(3) |
| C14 | C15 | 1.405(2) | B6 | B7 | 1.773(3) |
| C14 | C19 | 1.401(2) | B6 | B9 | 1.780(3) |
| C14 | B1 | 1.573(2) | B6 | B10 | 1.796(3) |
| C15 | C16 | 1.386(2) | B7 | B8 | 1.775(3) |
| C16 | C17 | 1.394(2) | B7 | B9 | 1.763(3) |
| C17 | C18 | 1.386(2) | B8 | B9 | 1.776(3) |

**Bond Angles for mo_0804_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C13 | O2 | C11 | 110.04(13) | B3 | B2 | B8 | 108.09(13) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 116.75(13) | B4 | B2 | B1 | 109.86(13) |
| C1 | N1 | C12 | 132.66(14) | B8 | B2 | B1 | 110.32(12) |
| C12 | N1 | C10 | 110.59(12) | B8 | B2 | B4 | 59.80(11) |
| O1 | C1 | N1 | 121.99(14) | B1 | B3 | B10 | 61.49(10) |
| O1 | C1 | C2 | 116.11(13) | B2 | B3 | B1 | 61.00(10) |
| N1 | C1 | C2 | 121.90(13) | B2 | B3 | B4 | 60.11(10) |
| C1 | C2 | C3 | 115.93(12) | B2 | B3 | B5 | 108.36(13) |
| C1 | C2 | B1 | 113.12(12) | B2 | B3 | B10 | 109.36(12) |
| C1 | C2 | B6 | 125.78(13) | B4 | B3 | B1 | 110.34(13) |
| C1 | C2 | B7 | 119.96(12) | B4 | B3 | B10 | 109.29(13) |
| C1 | C2 | B10 | 120.98(12) | B5 | B3 | B1 | 110.83(12) |
| C3 | C2 | B1 | 60.30(9) | B5 | B3 | B4 | 59.91(11) |
| C3 | C2 | B6 | 110.42(12) | B5 | B3 | B10 | 60.94(10) |
| C3 | C2 | B7 | 61.25(10) | B2 | B4 | B3 | 59.43(10) |
| C3 | C2 | B10 | 109.86(11) | B2 | B4 | B9 | 108.15(13) |
| B6 | C2 | B1 | 113.37(12) | B5 | B4 | B2 | 107.66(13) |
| B6 | C2 | B7 | 62.22(10) | B5 | B4 | B3 | 59.71(10) |
| B6 | C2 | B10 | 62.73(10) | B5 | B4 | B9 | 60.52(11) |
| B7 | C2 | B1 | 112.90(12) | B8 | B4 | B2 | 60.08(10) |
| B7 | C2 | B10 | 113.72(12) | B8 | B4 | B3 | 107.50(13) |
| B10 | C2 | B1 | 61.96(9) | B8 | B4 | B5 | 108.30(13) |
| C2 | C3 | B1 | 62.65(9) | B8 | B4 | B9 | 60.08(11) |
| C2 | C3 | B2 | 110.47(12) | B9 | B4 | B3 | 107.96(13) |
| C2 | C3 | B7 | 59.63(9) | B3 | B5 | B4 | 60.38(11) |
| C2 | C3 | B8 | 109.27(12) | B3 | B5 | B9 | 107.96(13) |
| C4 | C3 | C2 | 120.42(12) | B3 | B5 | B10 | 60.02(10) |
| C4 | C3 | B1 | 119.71(12) | B4 | B5 | B9 | 59.86(11) |
| C4 | C3 | B2 | 122.11(13) | B4 | B5 | B10 | 108.93(12) |
| C4 | C3 | B7 | 116.22(13) | B6 | B5 | B3 | 107.78(12) |
| C4 | C3 | B8 | 118.38(13) | B6 | B5 | B4 | 108.07(13) |
| B2 | C3 | B1 | 62.28(10) | B6 | B5 | B9 | 60.04(11) |
| B2 | C3 | B7 | 112.06(12) | B6 | B5 | B10 | 60.33(10) |
| B2 | C3 | B8 | 62.16(10) | B9 | B5 | B10 | 108.73(13) |
| B7 | C3 | B1 | 113.52(12) | C2 | B6 | B5 | 106.16(12) |
| B8 | C3 | B1 | 114.08(12) | C2 | B6 | B7 | 59.01(10) |
| B8 | C3 | B7 | 61.45(10) | C2 | B6 | B9 | 105.99(13) |
| C5 | C4 | C3 | 119.13(14) | C2 | B6 | B10 | 59.22(9) |
| C9 | C4 | C3 | 121.99(14) | B5 | B6 | B7 | 107.73(13) |
| C9 | C4 | C5 | 118.85(15) | B5 | B6 | B9 | 60.58(11) |
| C6 | C5 | C4 | 120.23(15) | B5 | B6 | B10 | 60.83(10) |
| C7 | C6 | C5 | 120.57(16) | B7 | B6 | B9 | 59.48(11) |
| C8 | C7 | C6 | 119.34(16) | B7 | B6 | B10 | 108.26(12) |
| C7 | C8 | C9 | 120.49(16) | B9 | B6 | B10 | 109.55(13) |
| C8 | C9 | C4 | 120.51(15) | C2 | B7 | C3 | 59.12(9) |
| N1 | C10 | C11 | 109.48(13) | C2 | B7 | B6 | 58.77(10) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O2 | C11 | C10 | 111.14(14) | C2 | B7 | B8 | 106.71(12) |
| N1 | C12 | C13 | 109.61(14) | C2 | B7 | B9 | 106.56(13) |
| O2 | C13 | C12 | 112.09(14) | C3 | B7 | B6 | 106.03(12) |
| C15 | C14 | B1 | 127.12(14) | C3 | B7 | B8 | 58.78(10) |
| C19 | C14 | C15 | 116.20(14) | C3 | B7 | B9 | 106.03(13) |
| C19 | C14 | B1 | 116.56(13) | B6 | B7 | B8 | 108.40(13) |
| C16 | C15 | C14 | 121.46(14) | B9 | B7 | B6 | 60.45(11) |
| C15 | C16 | C17 | 121.40(14) | B9 | B7 | B8 | 60.26(11) |
| C16 | C17 | C20 | 121.03(15) | C3 | B8 | B2 | 58.43(10) |
| C18 | C17 | C16 | 117.88(14) | C3 | B8 | B4 | 105.52(13) |
| C18 | C17 | C20 | 121.09(15) | C3 | B8 | B7 | 59.77(10) |
| C17 | C18 | C19 | 120.73(15) | C3 | B8 | B9 | 106.23(13) |
| C18 | C19 | C14 | 122.33(14) | B2 | B8 | B9 | 108.26(14) |
| C22 | C21 | C26 | 116.67(15) | B4 | B8 | B2 | 60.12(11) |
| C22 | C21 | B10 | 124.44(14) | B4 | B8 | B7 | 107.49(14) |
| C26 | C21 | B10 | 118.70(14) | B4 | B8 | B9 | 60.18(11) |
| C23 | C22 | C21 | 121.84(16) | B7 | B8 | B2 | 107.69(13) |
| C22 | C23 | C24 | 120.90(16) | B7 | B8 | B9 | 59.53(11) |
| C23 | C24 | C25 | 117.93(16) | B4 | B9 | B5 | 59.62(11) |
| C23 | C24 | C27 | 121.66(17) | B4 | B9 | B6 | 107.36(13) |
| C25 | C24 | C27 | 120.37(16) | B6 | B9 | B5 | 59.39(11) |
| C26 | C25 | C24 | 120.91(16) | B7 | B9 | B4 | 107.68(13) |
| C25 | C26 | C21 | 121.72(16) | B7 | B9 | B5 | 107.25(13) |
| C2 | B1 | B10 | 57.04(9) | B7 | B9 | B6 | 60.07(11) |
| C3 | B1 | C2 | 57.05(9) | B7 | B9 | B8 | 60.21(11) |
| C3 | B1 | B2 | 57.25(9) | B8 | B9 | B4 | 59.75(11) |
| C3 | B1 | B3 | 102.41(12) | B8 | B9 | B5 | 107.33(13) |
| C3 | B1 | B10 | 103.29(11) | B8 | B9 | B6 | 108.06(13) |
| C14 | B1 | C2 | 129.42(13) | C2 | B10 | B1 | 60.99(9) |
| C14 | B1 | C3 | 126.19(13) | C2 | B10 | B3 | 104.51(12) |
| C14 | B1 | B2 | 120.90(13) | C2 | B10 | B5 | 103.70(12) |
| C14 | B1 | B3 | 121.95(13) | C2 | B10 | B6 | 58.04(9) |
| C14 | B1 | B10 | 124.16(13) | C21 | B10 | C2 | 123.43(13) |
| B2 | B1 | C2 | 102.21(11) | C21 | B10 | B1 | 122.37(13) |
| B2 | B1 | B10 | 106.11(12) | C21 | B10 | B3 | 125.59(14) |
| B3 | B1 | C2 | 101.73(11) | C21 | B10 | B5 | 122.75(13) |
| B3 | B1 | B2 | 58.96(10) | C21 | B10 | B6 | 120.03(13) |
| B3 | B1 | B10 | 59.38(10) | B3 | B10 | B1 | 59.13(10) |
| C3 | B2 | B1 | 60.46(9) | B3 | B10 | B5 | 59.04(10) |
| C3 | B2 | B3 | 105.68(12) | B3 | B10 | B6 | 105.82(13) |
| C3 | B2 | B4 | 106.04(12) | B5 | B10 | B1 | 107.39(12) |
| C3 | B2 | B8 | 59.41(10) | B6 | B10 | B1 | 108.80(12) |
| B3 | B2 | B1 | 60.04(10) | B6 | B10 | B5 | 58.84(10) |
| B3 | B2 | B4 | 60.46(11) | | | | |

**Torsion Angles for mo_0804_CG_0m.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O1 | C1 | C2 | C3 | -65.63(18) | B2 | B3 | B4 | B8 | -37.48(12) |
| O1 | C1 | C2 | B1 | 1.33(19) | B2 | B3 | B4 | B9 | -100.89(14) |
| O1 | C1 | C2 | B6 | 148.40(15) | B2 | B3 | B5 | B4 | 36.94(12) |
| O1 | C1 | C2 | B7 | -135.94(15) | B2 | B3 | B5 | B6 | -64.15(16) |
| O1 | C1 | C2 | B10 | 71.47(18) | B2 | B3 | B5 | B9 | -0.73(16) |
| N1 | C1 | C2 | C3 | 113.49(15) | B2 | B3 | B5 | B10 | -102.42(13) |
| N1 | C1 | C2 | B1 | -179.55(13) | B2 | B3 | B10 | C2 | 3.28(16) |
| N1 | C1 | C2 | B6 | -32.5(2) | B2 | B3 | B10 | C21 | -148.97(14) |
| N1 | C1 | C2 | B7 | 43.2(2) | B2 | B3 | B10 | B1 | -39.13(12) |
| N1 | C1 | C2 | B10 | -109.41(16) | B2 | B3 | B10 | B5 | 100.76(14) |
| N1 | C10 | C11 | O2 | 58.47(18) | B2 | B3 | B10 | B6 | 63.62(15) |
| N1 | C12 | C13 | O2 | -56.52(18) | B2 | B4 | B5 | B3 | -36.48(12) |
| C1 | N1 | C10 | C11 | 124.18(15) | B2 | B4 | B5 | B6 | 64.12(16) |
| C1 | N1 | C12 | C13 | -125.60(18) | B2 | B4 | B5 | B9 | 101.28(14) |
| C1 | C2 | C3 | C4 | -7.05(19) | B2 | B4 | B5 | B10 | 0.13(17) |
| C1 | C2 | C3 | B1 | 103.02(13) | B2 | B4 | B8 | C3 | -38.15(11) |
| C1 | C2 | C3 | B2 | 144.25(12) | B2 | B4 | B8 | B7 | -100.75(13) |
| C1 | C2 | C3 | B7 | -111.51(14) | B2 | B4 | B8 | B9 | -138.24(13) |
| C1 | C2 | C3 | B8 | -149.17(13) | B2 | B4 | B9 | B5 | -100.45(14) |
| C1 | C2 | B1 | C3 | -107.69(13) | B2 | B4 | B9 | B6 | -63.75(17) |
| C1 | C2 | B1 | C14 | 4.5(2) | B2 | B4 | B9 | B7 | -0.44(18) |
| C1 | C2 | B1 | B2 | -144.57(12) | B2 | B4 | B9 | B8 | 37.41(13) |
| C1 | C2 | B1 | B3 | 155.02(12) | B2 | B8 | B9 | B4 | -37.45(12) |
| C1 | C2 | B1 | B10 | 114.00(14) | B2 | B8 | B9 | B5 | -0.13(17) |
| C1 | C2 | B6 | B5 | -150.27(14) | B2 | B8 | B9 | B6 | 62.52(16) |
| C1 | C2 | B6 | B7 | 108.43(16) | B2 | B8 | B9 | B7 | 100.21(14) |
| C1 | C2 | B6 | B9 | 146.41(14) | B3 | B1 | B2 | C3 | 133.25(12) |
| C1 | C2 | B6 | B10 | -110.02(16) | B3 | B1 | B2 | B4 | 35.60(12) |
| C1 | C2 | B7 | C3 | 105.04(14) | B3 | B1 | B2 | B8 | 99.71(14) |
| C1 | C2 | B7 | B6 | -117.33(15) | B3 | B1 | B10 | C2 | -131.70(13) |
| C1 | C2 | B7 | B8 | 140.93(14) | B3 | B1 | B10 | C21 | 115.07(16) |
| C1 | C2 | B7 | B9 | -155.88(13) | B3 | B1 | B10 | B5 | -35.38(12) |
| C1 | C2 | B10 | C21 | 10.1(2) | B3 | B1 | B10 | B6 | -97.59(14) |
| C1 | C2 | B10 | B1 | -101.49(14) | B3 | B2 | B4 | B5 | 36.60(12) |
| C1 | C2 | B10 | B3 | -142.94(13) | B3 | B2 | B4 | B8 | 137.96(13) |
| C1 | C2 | B10 | B5 | 156.00(13) | B3 | B2 | B4 | B9 | 100.56(14) |
| C1 | C2 | B10 | B6 | 117.24(15) | B3 | B2 | B8 | C3 | 97.89(13) |
| C2 | C3 | C4 | C5 | 141.68(14) | B3 | B2 | B8 | B4 | -37.80(12) |
| C2 | C3 | C4 | C9 | -40.5(2) | B3 | B2 | B8 | B7 | 62.60(16) |
| C2 | C3 | B1 | C14 | -117.61(16) | B3 | B2 | B8 | B9 | -0.32(16) |
| C2 | C3 | B1 | B2 | 135.78(12) | B3 | B4 | B5 | B6 | 100.60(13) |

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|---|---|---|---|---|---|---|---|---|---|
| C2 | C3 | B1 | B3 | 96.05(12) | B3 | B4 | B5 | B9 | 137.76(13) |
| C2 | C3 | B1 | B10 | 34.99(10) | B3 | B4 | B5 | B10 | 36.61(12) |
| C2 | C3 | B2 | B1 | -41.40(11) | B3 | B4 | B8 | C3 | -0.96(16) |
| C2 | C3 | B2 | B3 | -0.44(15) | B3 | B4 | B8 | B2 | 37.19(12) |
| C2 | C3 | B2 | B4 | 62.68(15) | B3 | B4 | B8 | B7 | -63.55(15) |
| C2 | C3 | B2 | B8 | 101.61(13) | B3 | B4 | B8 | B9 | -101.05(14) |
| C2 | C3 | B7 | B6 | -36.84(11) | B3 | B4 | B9 | B5 | -37.61(12) |
| C2 | C3 | B7 | B8 | -138.96(13) | B3 | B4 | B9 | B6 | -0.90(17) |
| C2 | C3 | B7 | B9 | -100.00(14) | B3 | B4 | B9 | B7 | 62.41(17) |
| C2 | C3 | B8 | B2 | -103.55(13) | B3 | B4 | B9 | B8 | 100.26(14) |
| C2 | C3 | B8 | B4 | -64.60(15) | B3 | B5 | B6 | C2 | 1.35(17) |
| C2 | C3 | B8 | B7 | 36.88(12) | B3 | B5 | B6 | B7 | 63.30(16) |
| C2 | C3 | B8 | B9 | -1.78(16) | B3 | B5 | B6 | B9 | 100.89(14) |
| C2 | B1 | B2 | C3 | 36.79(10) | B3 | B5 | B6 | B10 | -38.13(12) |
| C2 | B1 | B2 | B3 | -96.46(12) | B3 | B5 | B9 | B4 | 37.90(12) |
| C2 | B1 | B2 | B4 | -60.86(15) | B3 | B5 | B9 | B6 | -100.58(13) |
| C2 | B1 | B2 | B8 | 3.25(16) | B3 | B5 | B9 | B7 | -62.85(16) |
| C2 | B1 | B3 | B2 | 97.31(12) | B3 | B5 | B9 | B8 | 0.52(17) |
| C2 | B1 | B3 | B4 | 61.73(15) | B3 | B5 | B10 | C2 | 98.88(13) |
| C2 | B1 | B3 | B5 | -2.73(16) | B3 | B5 | B10 | C21 | -114.90(17) |
| C2 | B1 | B3 | B10 | -39.78(11) | B3 | B5 | B10 | B1 | 35.41(12) |
| C2 | B1 | B10 | C21 | -113.23(16) | B3 | B5 | B10 | B6 | 137.25(14) |
| C2 | B1 | B10 | B3 | 131.70(13) | B4 | B2 | B3 | B1 | -141.00(13) |
| C2 | B1 | B10 | B5 | 96.32(13) | B4 | B2 | B3 | B5 | -36.86(12) |
| C2 | B1 | B10 | B6 | 34.11(11) | B4 | B2 | B3 | B10 | -101.65(14) |
| C2 | B6 | B7 | C3 | 36.99(11) | B4 | B2 | B8 | C3 | 135.68(13) |
| C2 | B6 | B7 | B8 | 98.77(13) | B4 | B2 | B8 | B7 | 100.40(14) |
| C2 | B6 | B7 | B9 | 136.63(13) | B4 | B2 | B8 | B9 | 37.48(12) |
| C2 | B6 | B9 | B4 | 63.03(16) | B4 | B3 | B5 | B6 | -101.09(15) |
| C2 | B6 | B9 | B5 | 99.83(13) | B4 | B3 | B5 | B9 | -37.67(12) |
| C2 | B6 | B9 | B7 | -37.76(12) | B4 | B3 | B5 | B10 | -139.37(13) |
| C2 | B6 | B9 | B8 | -0.02(17) | B4 | B3 | B10 | C2 | -60.82(15) |
| C2 | B6 | B10 | C21 | 112.92(16) | B4 | B3 | B10 | C21 | 146.93(15) |
| C2 | B6 | B10 | B1 | -35.31(11) | B4 | B3 | B10 | B1 | -103.24(14) |
| C2 | B6 | B10 | B3 | -97.47(13) | B4 | B3 | B10 | B5 | 36.65(12) |
| C2 | B6 | B10 | B5 | -134.70(13) | B4 | B3 | B10 | B6 | -0.49(16) |
| C2 | B7 | B8 | C3 | -36.04(11) | B4 | B5 | B6 | C2 | -62.46(15) |
| C2 | B7 | B8 | B2 | -1.32(17) | B4 | B5 | B6 | B7 | -0.51(16) |
| C2 | B7 | B8 | B4 | 62.08(15) | B4 | B5 | B6 | B9 | 37.08(12) |
| C2 | B7 | B8 | B9 | 99.86(14) | B4 | B5 | B6 | B10 | -101.94(13) |
| C2 | B7 | B9 | B4 | -62.47(16) | B4 | B5 | B9 | B6 | -138.49(13) |
| C2 | B7 | B9 | B5 | 0.35(17) | B4 | B5 | B9 | B7 | -100.76(14) |
| C2 | B7 | B9 | B6 | 37.78(12) | B4 | B5 | B9 | B8 | -37.38(12) |
| C2 | B7 | B9 | B8 | -100.11(13) | B4 | B5 | B10 | C2 | 62.12(15) |
| C3 | C2 | B1 | C14 | 112.22(17) | B4 | B5 | B10 | C21 | -151.66(15) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | C2 | B1 | B2 | -36.89(10) | B4 | B5 | B10 | B1 | -1.35(17) |
| C3 | C2 | B1 | B3 | -97.29(12) | B4 | B5 | B10 | B3 | -36.76(12) |
| C3 | C2 | B1 | B10 | -138.31(12) | B4 | B5 | B10 | B6 | 100.49(14) |
| C3 | C2 | B6 | B5 | 62.22(15) | B4 | B8 | B9 | B5 | 37.32(12) |
| C3 | C2 | B6 | B7 | -39.08(12) | B4 | B8 | B9 | B6 | 99.97(14) |
| C3 | C2 | B6 | B9 | -1.10(16) | B4 | B8 | B9 | B7 | 137.66(14) |
| C3 | C2 | B6 | B10 | 102.47(13) | B5 | B3 | B4 | B2 | 138.85(13) |
| C3 | C2 | B7 | B6 | 137.63(13) | B5 | B3 | B4 | B8 | 101.37(14) |
| C3 | C2 | B7 | B8 | 35.89(11) | B5 | B3 | B4 | B9 | 37.96(12) |
| C3 | C2 | B7 | B9 | 99.08(13) | B5 | B3 | B10 | C2 | -97.48(13) |
| C3 | C2 | B10 | C21 | 149.47(14) | B5 | B3 | B10 | C21 | 110.27(17) |
| C3 | C2 | B10 | B1 | 37.90(11) | B5 | B3 | B10 | B1 | -139.89(13) |
| C3 | C2 | B10 | B3 | -3.55(15) | B5 | B3 | B10 | B6 | -37.14(12) |
| C3 | C2 | B10 | B5 | -64.61(14) | B5 | B4 | B8 | C3 | 62.12(15) |
| C3 | C2 | B10 | B6 | -103.37(13) | B5 | B4 | B8 | B2 | 100.28(14) |
| C3 | C4 | C5 | C6 | 178.55(14) | B5 | B4 | B8 | B7 | -0.47(16) |
| C3 | C4 | C9 | C8 | -179.25(15) | B5 | B4 | B8 | B9 | -37.96(12) |
| C3 | B1 | B2 | B3 | -133.25(12) | B5 | B4 | B9 | B6 | 36.70(12) |
| C3 | B1 | B2 | B4 | -97.65(13) | B5 | B4 | B9 | B7 | 100.02(14) |
| C3 | B1 | B2 | B8 | -33.53(12) | B5 | B4 | B9 | B8 | 137.86(13) |
| C3 | B1 | B3 | B2 | 38.85(11) | B5 | B6 | B7 | C2 | -98.56(13) |
| C3 | B1 | B3 | B4 | 3.27(16) | B5 | B6 | B7 | C3 | -61.56(15) |
| C3 | B1 | B3 | B5 | -61.19(15) | B5 | B6 | B7 | B8 | 0.22(16) |
| C3 | B1 | B3 | B10 | -98.24(12) | B5 | B6 | B7 | B9 | 38.08(12) |
| C3 | B1 | B10 | C2 | -34.99(10) | B5 | B6 | B9 | B4 | -36.81(12) |
| C3 | B1 | B10 | C21 | -148.22(14) | B5 | B6 | B9 | B7 | -137.59(13) |
| C3 | B1 | B10 | B3 | 96.71(12) | B5 | B6 | B9 | B8 | -99.85(14) |
| C3 | B1 | B10 | B5 | 61.33(14) | B5 | B6 | B10 | C2 | 134.70(13) |
| C3 | B1 | B10 | B6 | -0.89(15) | B5 | B6 | B10 | C21 | -112.38(16) |
| C3 | B2 | B3 | B1 | -41.17(11) | B5 | B6 | B10 | B1 | 99.39(13) |
| C3 | B2 | B3 | B4 | 99.84(13) | B5 | B6 | B10 | B3 | 37.23(12) |
| C3 | B2 | B3 | B5 | 62.98(15) | B6 | C2 | C3 | C4 | 143.96(13) |
| C3 | B2 | B3 | B10 | -1.81(16) | B6 | C2 | C3 | B1 | -105.96(13) |
| C3 | B2 | B4 | B3 | -99.23(13) | B6 | C2 | C3 | B2 | -64.73(15) |
| C3 | B2 | B4 | B5 | -62.62(16) | B6 | C2 | C3 | B7 | 39.51(12) |
| C3 | B2 | B4 | B8 | 38.74(12) | B6 | C2 | C3 | B8 | 1.85(16) |
| C3 | B2 | B4 | B9 | 1.33(17) | B6 | C2 | B1 | C3 | 101.02(13) |
| C3 | B2 | B8 | B4 | -135.68(13) | B6 | C2 | B1 | C14 | -146.76(15) |
| C3 | B2 | B8 | B7 | -35.29(12) | B6 | C2 | B1 | B2 | 64.13(15) |
| C3 | B2 | B8 | B9 | -98.20(14) | B6 | C2 | B1 | B3 | 3.73(16) |
| C3 | B7 | B8 | B2 | 34.72(12) | B6 | C2 | B1 | B10 | -37.29(12) |
| C3 | B7 | B8 | B4 | 98.12(13) | B6 | C2 | B7 | C3 | -137.63(12) |
| C3 | B7 | B8 | B9 | 135.90(13) | B6 | C2 | B7 | B8 | -101.74(14) |
| C3 | B7 | B9 | B4 | -0.62(17) | B6 | C2 | B7 | B9 | -38.55(12) |
| C3 | B7 | B9 | B5 | 62.21(16) | B6 | C2 | B10 | C21 | -107.16(16) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | B7 | B9 | B6 | 99.63(13) | B6 | C2 | B10 | B1 | 141.27(13) |
| C3 | B7 | B9 | B8 | -38.25(12) | B6 | C2 | B10 | B3 | 99.82(13) |
| C3 | B8 | B9 | B4 | -98.88(14) | B6 | C2 | B10 | B5 | 38.76(12) |
| C3 | B8 | B9 | B5 | -61.56(16) | B6 | B5 | B9 | B4 | 138.49(13) |
| C3 | B8 | B9 | B6 | 1.09(17) | B6 | B5 | B9 | B7 | 37.73(12) |
| C3 | B8 | B9 | B7 | 38.77(12) | B6 | B5 | B9 | B8 | 101.11(14) |
| C4 | C3 | B1 | C2 | 111.18(15) | B6 | B5 | B10 | C2 | -38.37(11) |
| C4 | C3 | B1 | C14 | -6.4(2) | B6 | B5 | B10 | C21 | 107.85(16) |
| C4 | C3 | B1 | B2 | -113.05(15) | B6 | B5 | B10 | B1 | -101.84(13) |
| C4 | C3 | B1 | B3 | -152.77(13) | B6 | B5 | B10 | B3 | -137.25(14) |
| C4 | C3 | B1 | B10 | 146.17(13) | B6 | B7 | B8 | C3 | -97.96(13) |
| C4 | C3 | B2 | B1 | 109.34(15) | B6 | B7 | B8 | B2 | -63.24(16) |
| C4 | C3 | B2 | B3 | 150.30(13) | B6 | B7 | B8 | B4 | 0.15(16) |
| C4 | C3 | B2 | B4 | -146.58(14) | B6 | B7 | B8 | B9 | 37.94(12) |
| C4 | C3 | B2 | B8 | -107.65(16) | B6 | B7 | B9 | B4 | -100.25(14) |
| C4 | C3 | B7 | C2 | -111.45(14) | B6 | B7 | B9 | B5 | -37.43(12) |
| C4 | C3 | B7 | B6 | -148.29(13) | B6 | B7 | B9 | B8 | -137.89(13) |
| C4 | C3 | B7 | B8 | 109.59(15) | B7 | C2 | C3 | C4 | 104.46(15) |
| C4 | C3 | B7 | B9 | 148.54(14) | B7 | C2 | C3 | B1 | -145.47(12) |
| C4 | C3 | B8 | B2 | 113.45(15) | B7 | C2 | C3 | B2 | -104.24(13) |
| C4 | C3 | B8 | B4 | 152.40(13) | B7 | C2 | C3 | B8 | -37.66(12) |
| C4 | C3 | B8 | B7 | -106.12(15) | B7 | C2 | B1 | C3 | 32.65(12) |
| C4 | C3 | B8 | B9 | -144.78(14) | B7 | C2 | B1 | C14 | 144.87(15) |
| C4 | C5 | C6 | C7 | 0.4(2) | B7 | C2 | B1 | B2 | -4.23(15) |
| C5 | C4 | C9 | C8 | -1.4(2) | B7 | C2 | B1 | B3 | -64.64(15) |
| C5 | C6 | C7 | C8 | -0.7(3) | B7 | C2 | B1 | B10 | -105.66(14) |
| C6 | C7 | C8 | C9 | -0.1(3) | B7 | C2 | B6 | B5 | 101.30(14) |
| C7 | C8 | C9 | C4 | 1.1(3) | B7 | C2 | B6 | B9 | 37.98(12) |
| C9 | C4 | C5 | C6 | 0.6(2) | B7 | C2 | B6 | B10 | 141.55(13) |
| C10 | N1 | C1 | O1 | -0.5(2) | B7 | C2 | B10 | C21 | -144.10(15) |
| C10 | N1 | C1 | C2 | -179.56(13) | B7 | C2 | B10 | B1 | 104.33(13) |
| C10 | N1 | C12 | C13 | 54.74(17) | B7 | C2 | B10 | B3 | 62.88(15) |
| C11 | O2 | C13 | C12 | 58.79(18) | B7 | C2 | B10 | B5 | 1.82(16) |
| C12 | N1 | C1 | O1 | 179.87(16) | B7 | C2 | B10 | B6 | -36.94(12) |
| C12 | N1 | C1 | C2 | 0.8(3) | B7 | C3 | C4 | C5 | -149.68(14) |
| C12 | N1 | C10 | C11 | -56.10(17) | B7 | C3 | C4 | C9 | 28.2(2) |
| C13 | O2 | C11 | C10 | -59.72(18) | B7 | C3 | B1 | C2 | -32.24(11) |
| C14 | C15 | C16 | C17 | -0.8(2) | B7 | C3 | B1 | C14 | -149.85(14) |
| C14 | B1 | B2 | C3 | -115.68(15) | B7 | C3 | B1 | B2 | 103.54(13) |
| C14 | B1 | B2 | B3 | 111.07(16) | B7 | C3 | B1 | B3 | 63.82(15) |
| C14 | B1 | B2 | B4 | 146.67(14) | B7 | C3 | B1 | B10 | 2.75(15) |
| C14 | B1 | B2 | B8 | -149.21(14) | B7 | C3 | B2 | B1 | -105.87(13) |
| C14 | B1 | B3 | B2 | -109.33(16) | B7 | C3 | B2 | B3 | -64.91(15) |
| C14 | B1 | B3 | B4 | -144.91(14) | B7 | C3 | B2 | B4 | -1.79(17) |
| C14 | B1 | B3 | B5 | 150.62(14) | B7 | C3 | B2 | B8 | 37.14(13) |

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|---|---|---|---|---|---|---|---|---|---|
| C14 | B1 | B3 | B10 | 113.58(16) | B7 | C3 | B8 | B2 | -140.43(14) |
| C14 | B1 | B10 | C2 | 118.34(16) | B7 | C3 | B8 | B4 | -101.48(14) |
| C14 | B1 | B10 | C21 | 5.1(2) | B7 | C3 | B8 | B9 | -38.66(12) |
| C14 | B1 | B10 | B3 | -109.96(16) | B7 | B6 | B9 | B4 | 100.79(14) |
| C14 | B1 | B10 | B5 | -145.34(14) | B7 | B6 | B9 | B5 | 137.59(13) |
| C14 | B1 | B10 | B6 | 152.44(14) | B7 | B6 | B9 | B8 | 37.74(12) |
| C15 | C14 | C19 | C18 | -0.1(2) | B7 | B6 | B10 | C2 | 34.15(12) |
| C15 | C14 | B1 | C2 | -58.4(2) | B7 | B6 | B10 | C21 | 147.07(14) |
| C15 | C14 | B1 | C3 | 15.9(2) | B7 | B6 | B10 | B1 | -1.16(16) |
| C15 | C14 | B1 | B2 | 85.78(19) | B7 | B6 | B10 | B3 | -63.32(15) |
| C15 | C14 | B1 | B3 | 156.21(15) | B7 | B6 | B10 | B5 | -100.55(14) |
| C15 | C14 | B1 | B10 | -131.38(16) | B7 | B8 | B9 | B4 | -137.66(14) |
| C15 | C16 | C17 | C18 | 0.4(2) | B7 | B8 | B9 | B5 | -100.33(14) |
| C15 | C16 | C17 | C20 | -178.89(15) | B7 | B8 | B9 | B6 | -37.68(12) |
| C16 | C17 | C18 | C19 | 0.2(2) | B8 | C3 | C4 | C5 | -79.53(18) |
| C17 | C18 | C19 | C14 | -0.3(2) | B8 | C3 | C4 | C9 | 98.33(18) |
| C19 | C14 | C15 | C16 | 0.7(2) | B8 | C3 | B1 | C2 | -100.12(13) |
| C19 | C14 | B1 | C2 | 125.54(16) | B8 | C3 | B1 | C14 | 142.27(15) |
| C19 | C14 | B1 | C3 | -160.18(14) | B8 | C3 | B1 | B2 | 35.65(12) |
| C19 | C14 | B1 | B2 | -90.26(17) | B8 | C3 | B1 | B3 | -4.07(16) |
| C19 | C14 | B1 | B3 | -19.8(2) | B8 | C3 | B1 | B10 | -65.13(15) |
| C19 | C14 | B1 | B10 | 52.6(2) | B8 | C3 | B2 | B1 | -143.00(13) |
| C20 | C17 | C18 | C19 | 179.45(15) | B8 | C3 | B2 | B3 | -102.05(13) |
| C21 | C22 | C23 | C24 | -1.2(3) | B8 | C3 | B2 | B4 | -38.92(12) |
| C22 | C21 | C26 | C25 | 0.3(2) | B8 | C3 | B7 | C2 | 138.96(13) |
| C22 | C21 | B10 | C2 | 22.1(2) | B8 | C3 | B7 | B6 | 102.12(14) |
| C22 | C21 | B10 | B1 | 96.51(19) | B8 | C3 | B7 | B9 | 38.95(13) |
| C22 | C21 | B10 | B3 | 169.44(15) | B8 | B2 | B3 | B1 | -103.50(13) |
| C22 | C21 | B10 | B5 | -117.52(18) | B8 | B2 | B3 | B4 | 37.50(12) |
| C22 | C21 | B10 | B6 | -47.3(2) | B8 | B2 | B3 | B5 | 0.65(16) |
| C22 | C23 | C24 | C25 | 2.3(3) | B8 | B2 | B3 | B10 | -64.14(15) |
| C22 | C23 | C24 | C27 | -175.49(17) | B8 | B2 | B4 | B3 | -137.96(13) |
| C23 | C24 | C25 | C26 | -2.1(3) | B8 | B2 | B4 | B5 | -101.36(14) |
| C24 | C25 | C26 | C21 | 0.8(3) | B8 | B2 | B4 | B9 | -37.41(13) |
| C26 | C21 | C22 | C23 | -0.1(2) | B8 | B4 | B5 | B3 | -99.99(14) |
| C26 | C21 | B10 | C2 | -163.12(14) | B8 | B4 | B5 | B6 | 0.61(17) |
| C26 | C21 | B10 | B1 | -88.75(18) | B8 | B4 | B5 | B9 | 37.77(12) |
| C26 | C21 | B10 | B3 | -15.8(2) | B8 | B4 | B5 | B10 | -63.38(16) |
| C26 | C21 | B10 | B5 | 57.2(2) | B8 | B4 | B9 | B5 | -137.86(13) |
| C26 | C21 | B10 | B6 | 127.42(16) | B8 | B4 | B9 | B6 | -101.16(14) |
| C27 | C24 | C25 | C26 | 175.70(17) | B8 | B4 | B9 | B7 | -37.85(13) |
| B1 | C2 | C3 | C4 | -110.08(14) | B8 | B7 | B9 | B4 | 37.64(13) |
| B1 | C2 | C3 | B2 | 41.23(11) | B8 | B7 | B9 | B5 | 100.46(14) |
| B1 | C2 | C3 | B7 | 145.47(12) | B8 | B7 | B9 | B6 | 137.89(13) |
| B1 | C2 | C3 | B8 | 107.80(13) | B9 | B4 | B5 | B3 | -137.76(13) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| B1 | C2 | B6 | B5 | -3.27(17) | B9 | B4 | B5 | B6 | -37.16(12) |
| B1 | C2 | B6 | B7 | -104.56(13) | B9 | B4 | B5 | B10 | -101.15(14) |
| B1 | C2 | B6 | B9 | -66.58(15) | B9 | B4 | B8 | C3 | 100.09(13) |
| B1 | C2 | B6 | B10 | 36.98(12) | B9 | B4 | B8 | B2 | 138.24(13) |
| B1 | C2 | B7 | C3 | -32.32(11) | B9 | B4 | B8 | B7 | 37.49(12) |
| B1 | C2 | B7 | B6 | 105.32(13) | B9 | B5 | B6 | C2 | -99.54(14) |
| B1 | C2 | B7 | B8 | 3.58(17) | B9 | B5 | B6 | B7 | -37.59(12) |
| B1 | C2 | B7 | B9 | 66.77(15) | B9 | B5 | B6 | B10 | -139.02(13) |
| B1 | C2 | B10 | C21 | 111.57(16) | B9 | B5 | B10 | C2 | -1.50(16) |
| B1 | C2 | B10 | B3 | -41.45(11) | B9 | B5 | B10 | C21 | 144.71(15) |
| B1 | C2 | B10 | B5 | -102.51(13) | B9 | B5 | B10 | B1 | -64.98(15) |
| B1 | C2 | B10 | B6 | -141.27(13) | B9 | B5 | B10 | B3 | -100.39(14) |
| B1 | C3 | C4 | C5 | 67.85(19) | B9 | B5 | B10 | B6 | 36.86(12) |
| B1 | C3 | C4 | C9 | -114.30(16) | B9 | B6 | B7 | C2 | -136.63(13) |
| B1 | C3 | B2 | B3 | 40.96(11) | B9 | B6 | B7 | C3 | -99.64(13) |
| B1 | C3 | B2 | B4 | 104.08(14) | B9 | B6 | B7 | B8 | -37.86(12) |
| B1 | C3 | B2 | B8 | 143.00(13) | B9 | B6 | B10 | C2 | 97.39(14) |
| B1 | C3 | B7 | C2 | 33.31(12) | B9 | B6 | B10 | C21 | -149.69(14) |
| B1 | C3 | B7 | B6 | -3.53(16) | B9 | B6 | B10 | B1 | 62.08(16) |
| B1 | C3 | B7 | B8 | -105.65(14) | B9 | B6 | B10 | B3 | -0.08(17) |
| B1 | C3 | B7 | B9 | -66.70(15) | B9 | B6 | B10 | B5 | -37.31(13) |
| B1 | C3 | B8 | B2 | -35.70(12) | B9 | B7 | B8 | C3 | -135.90(13) |
| B1 | C3 | B8 | B4 | 3.26(17) | B9 | B7 | B8 | B2 | -101.18(14) |
| B1 | C3 | B8 | B7 | 104.74(14) | B9 | B7 | B8 | B4 | -37.79(12) |
| B1 | C3 | B8 | B9 | 66.08(16) | B10 | C2 | C3 | C4 | -148.70(13) |
| B1 | C14 | C15 | C16 | -175.37(15) | B10 | C2 | C3 | B1 | -38.62(11) |
| B1 | C14 | C19 | C18 | 176.36(14) | B10 | C2 | C3 | B2 | 2.61(15) |
| B1 | B2 | B3 | B4 | 141.00(13) | B10 | C2 | C3 | B7 | 106.84(13) |
| B1 | B2 | B3 | B5 | 104.15(13) | B10 | C2 | C3 | B8 | 69.18(14) |
| B1 | B2 | B3 | B10 | 39.36(11) | B10 | C2 | B1 | C3 | 138.31(12) |
| B1 | B2 | B4 | B3 | -35.43(12) | B10 | C2 | B1 | C14 | -109.47(17) |
| B1 | B2 | B4 | B5 | 1.18(17) | B10 | C2 | B1 | B2 | 101.42(12) |
| B1 | B2 | B4 | B8 | 102.54(14) | B10 | C2 | B1 | B3 | 41.02(11) |
| B1 | B2 | B4 | B9 | 65.13(16) | B10 | C2 | B6 | B5 | -40.25(12) |
| B1 | B2 | B8 | C3 | 33.94(12) | B10 | C2 | B6 | B7 | -141.55(13) |
| B1 | B2 | B8 | B4 | -101.74(14) | B10 | C2 | B6 | B9 | -103.57(14) |
| B1 | B2 | B8 | B7 | -1.35(17) | B10 | C2 | B7 | C3 | -100.49(13) |
| B1 | B2 | B8 | B9 | -64.26(16) | B10 | C2 | B7 | B6 | 37.14(12) |
| B1 | B3 | B4 | B2 | 35.94(12) | B10 | C2 | B7 | B8 | -64.60(16) |
| B1 | B3 | B4 | B5 | -102.91(14) | B10 | C2 | B7 | B9 | -1.41(17) |
| B1 | B3 | B4 | B8 | -1.54(17) | B10 | C21 | C22 | C23 | 174.77(16) |
| B1 | B3 | B4 | B9 | -64.95(16) | B10 | C21 | C26 | C25 | -174.89(15) |
| B1 | B3 | B5 | B4 | 102.09(14) | B10 | B1 | B2 | C3 | 95.66(12) |
| B1 | B3 | B5 | B6 | 0.99(18) | B10 | B1 | B2 | B3 | -37.58(11) |
| B1 | B3 | B5 | B9 | 64.42(16) | B10 | B1 | B2 | B4 | -1.99(16) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| B1 | B3 | B5 | B10 | -37.28(12) | B10 | B1 | B2 | B8 | 62.13(15) |
| B1 | B3 | B10 | C2 | 42.42(11) | B10 | B1 | B3 | B2 | 137.09(13) |
| B1 | B3 | B10 | C21 | -109.83(17) | B10 | B1 | B3 | B4 | 101.51(14) |
| B1 | B3 | B10 | B5 | 139.89(13) | B10 | B1 | B3 | B5 | 37.05(12) |
| B1 | B3 | B10 | B6 | 102.75(13) | B10 | B3 | B4 | B2 | 101.76(13) |
| B2 | C3 | C4 | C5 | -6.2(2) | B10 | B3 | B4 | B5 | -37.09(12) |
| B2 | C3 | C4 | C9 | 171.62(14) | B10 | B3 | B4 | B8 | 64.28(16) |
| B2 | C3 | B1 | C2 | -135.78(12) | B10 | B3 | B4 | B9 | 0.87(17) |
| B2 | C3 | B1 | C14 | 106.62(16) | B10 | B3 | B5 | B4 | 139.37(13) |
| B2 | C3 | B1 | B3 | -39.72(11) | B10 | B3 | B5 | B6 | 38.27(12) |
| B2 | C3 | B1 | B10 | -100.78(12) | B10 | B3 | B5 | B9 | 101.70(14) |
| B2 | C3 | B7 | C2 | 101.53(13) | B10 | B5 | B6 | C2 | 39.48(12) |
| B2 | C3 | B7 | B6 | 64.70(16) | B10 | B5 | B6 | B7 | 101.43(13) |
| B2 | C3 | B7 | B8 | -37.43(13) | B10 | B5 | B6 | B9 | 139.02(13) |
| B2 | C3 | B7 | B9 | 1.53(17) | B10 | B5 | B9 | B4 | 101.50(14) |
| B2 | C3 | B8 | B4 | 38.95(12) | B10 | B5 | B9 | B6 | -36.99(12) |
| B2 | C3 | B8 | B7 | 140.43(14) | B10 | B5 | B9 | B7 | 0.74(17) |
| B2 | C3 | B8 | B9 | 101.78(14) | B10 | B5 | B9 | B8 | 64.12(16) |
| B2 | B1 | B3 | B4 | -35.58(12) | B10 | B6 | B7 | C2 | -34.24(11) |
| B2 | B1 | B3 | B5 | -100.04(14) | B10 | B6 | B7 | C3 | 2.75(16) |
| B2 | B1 | B3 | B10 | -137.09(13) | B10 | B6 | B7 | B8 | 64.54(15) |
| B2 | B1 | B10 | C2 | -94.31(12) | B10 | B6 | B7 | B9 | 102.39(14) |
| B2 | B1 | B10 | C21 | 152.46(14) | B10 | B6 | B9 | B4 | 0.61(17) |
| B2 | B1 | B10 | B3 | 37.39(11) | B10 | B6 | B9 | B5 | 37.42(12) |
| B2 | B1 | B10 | B5 | 2.01(15) | B10 | B6 | B9 | B7 | -100.17(14) |
| B2 | B1 | B10 | B6 | -60.20(15) | B10 | B6 | B9 | B8 | -62.43(17) |
| B2 | B3 | B4 | B5 | -138.85(13) | | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0804_CG_0m.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | -764.46 | 5120.91 | 1411.28 | 25 |
| H6 | -2215.72 | 5829.67 | 2028.76 | 30 |
| H7 | -1835.23 | 6899.87 | 4106.31 | 31 |
| H8 | -10.94 | 7221.46 | 5567.42 | 30 |
| H9 | 1419.39 | 6473.6 | 4962.05 | 25 |
| H10A | 4386.4 | 9838.66 | 6198.06 | 28 |
| H10B | 5602.21 | 9826.4 | 7029.24 | 28 |
| H11A | 4278.33 | 10197.27 | 8157.97 | 31 |
| H11B | 2984.05 | 8801.03 | 7131.38 | 31 |
| H12A | 5404.12 | 7523.65 | 6701.47 | 27 |
| H12B | 4050.44 | 6164.25 | 5705.42 | 27 |
| H13A | 2820.89 | 6668.41 | 6879.85 | 32 |
| H13B | 4019.19 | 6639.07 | 7712.37 | 32 |

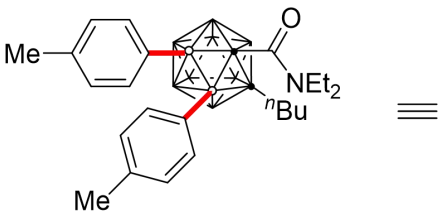
| | | | | |
|---|---|---|---|---|
| H15 | 1397.47 | 7899.74 | 2604.67 | 21 |
| H16 | 1307.45 | 9401.77 | 1806.2 | 24 |
| H18 | 3235.9 | 8370.21 | -361.06 | 25 |
| H19 | 3297.79 | 6838.85 | 410.48 | 22 |
| H20A | 2562.72 | 9955.9 | -528.63 | 41 |
| H20B | 2798.07 | 10995.74 | 798.57 | 41 |
| H20C | 1311.89 | 9870.3 | -151.51 | 41 |
| H22 | 5992.04 | 8289.4 | 4484.34 | 29 |
| H23 | 8119.43 | 9807.85 | 4690.8 | 32 |
| H25 | 7253.14 | 7705.08 | 1086.23 | 30 |
| H26 | 5125.02 | 6196.74 | 879.39 | 27 |
| H27A | 9335.73 | 10302.57 | 2561.26 | 56 |
| H27B | 9741.6 | 9233.81 | 2785.75 | 56 |
| H27C | 9864.68 | 10460.57 | 3920.25 | 56 |
| H2 | 150(20) | 4120(20) | 496(18) | 24 |
| H3 | 2720(20) | 4680(20) | 164(18) | 24 |
| H4 | 1120(20) | 2130(20) | 331(19) | 28 |
| H5A | 4190(20) | 3810(20) | 1639(18) | 27 |
| H6A | 4610(20) | 5490(20) | 4253(18) | 25 |
| H7A | 2000(20) | 4870(20) | 4503(19) | 26 |
| H8A | -110(20) | 2870(20) | 2200(18) | 26 |
| H9A | 2330(20) | 2600(20) | 2921(19) | 29 |

**Experimental**

Single crystals of $C_{27}H_{35}B_{10}NO_2$ [mo_0804_CG_0m] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a Bruker D8 Venture Source diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

**Crystal structure determination of 3ea**

**Crystal Data** for $C_{27}H_{35}B_{10}NO_2$ ($M$ =513.66 g/mol): triclinic, space group P-1 (no. 2), $a$ = 11.7623(18) Å, $b$ = 11.821(2) Å, $c$ = 12.371(2) Å, $\alpha$ = 108.419(5)°, $\beta$ = 100.884(5)°, $\gamma$ = 113.869(6)°, $V$ = 1389.5(4) Å$^3$, $Z$ = 2, $T$ = 100.0 K, μ(MoKα) = 0.070 mm$^{-1}$, *Dcalc* = 1.228 g/cm$^3$, 29979 reflections measured (4.068° ≤ 2Θ ≤ 57.416°), 7064 unique ($R_{int}$ = 0.0456, $R_{sigma}$ = 0.0388) which were used in all calculations. The final $R_1$ was 0.0538 (I > 2σ(I)) and $wR_2$ was 0.1431 (all data).




**3fa**

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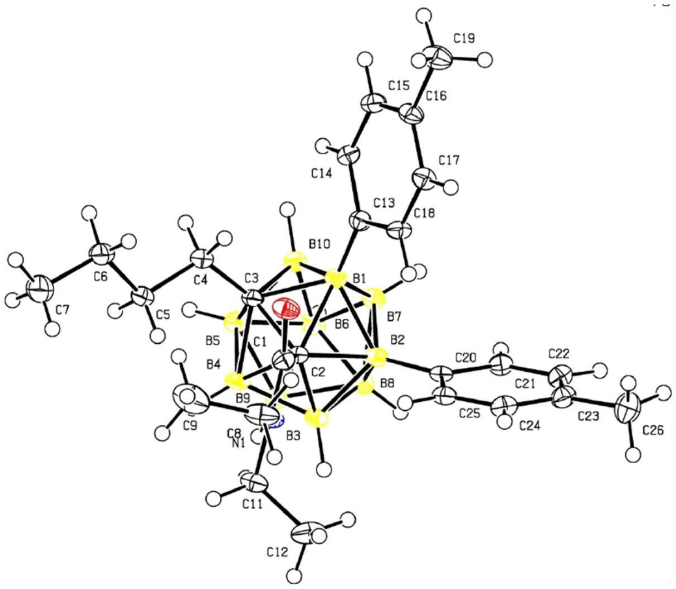


**CCDC 1983615**

**Crystal data and structure refinement for 3fa.**

| | |
|---|---|
| Identification code | mo_0848_CG_0m_4 |
| CCDC number | 1983615 |
| Empirical formula | $C_{25}H_{41}B_{10}NO$ |
| Formula weight | 479.69 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 12.2842(10) |
| b/Å | 12.2978(10) |
| c/Å | 19.8427(15) |
| α/° | 90 |
| β/° | 106.783(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 2869.9(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.110 |
| μ/mm$^{-1}$ | 0.060 |
| F(000) | 1024.0 |
| Crystal size/mm$^3$ | 0.188 × 0.185 × 0.142 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.946 to 52.818 |
| Index ranges | -15 ≤ h ≤ 14, 0 ≤ k ≤ 15, 0 ≤ l ≤ 24 |
| Reflections collected | 11362 |
| Independent reflections | 11362 [$R_{int}$ = ?, $R_{sigma}$ = 0.0660] |
| Data/restraints/parameters | 11362/0/343 |
| Goodness-of-fit on F$^2$ | 1.138 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0861, $wR_2$ = 0.1800 |
| Final R indexes [all data] | $R_1$ = 0.1194, $wR_2$ = 0.1966 |

Largest diff. peak/hole / e Å$^{-3}$ 0.31/-0.34

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0848_CG_0m_4. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 3691(2) | 8136(2) | 6392.6(15) | 23.9(7) |
| N1 | 2207(3) | 8638(3) | 6767.4(19) | 21.9(8) |
| C1 | 2842(4) | 7885(3) | 6559(2) | 20.3(9) |
| C2 | 2560(3) | 6655(3) | 6536(2) | 17.3(8) |
| C3 | 2503(3) | 6074(3) | 5764(2) | 18.9(9) |
| C4 | 2701(3) | 6766(3) | 5167(2) | 22.3(9) |
| C5 | 1797(4) | 7618(3) | 4835(2) | 23.8(10) |
| C6 | 2183(4) | 8349(4) | 4330(2) | 31.2(11) |
| C7 | 1272(5) | 9169(4) | 3959(3) | 42.3(13) |
| C8 | 2642(4) | 9770(3) | 6800(3) | 31.2(11) |
| C9 | 2209(5) | 10343(4) | 6092(3) | 44.5(14) |
| C11 | 1075(4) | 8562(3) | 6874(2) | 25.7(10) |
| C12 | 1114(4) | 8654(4) | 7650(2) | 34.7(12) |
| C13 | 4964(3) | 6115(3) | 6512(2) | 19.5(9) |
| C14 | 5509(4) | 5635(3) | 6055(2) | 20.2(9) |
| C15 | 6640(4) | 5845(3) | 6107(2) | 22.9(9) |
| C16 | 7281(3) | 6547(3) | 6613(2) | 22.9(9) |
| C17 | 6759(4) | 7013(3) | 7081(2) | 22.0(9) |
| C18 | 5633(4) | 6803(3) | 7027(2) | 21.7(9) |
| C19 | 8505(4) | 6814(4) | 6660(3) | 33.4(11) |
| C20 | 3873(3) | 6080(3) | 7985(2) | 18.0(9) |
| C21 | 4396(4) | 5250(3) | 8445(2) | 21.1(9) |
| C22 | 5090(4) | 5467(4) | 9118(2) | 25.7(10) |
| C23 | 5315(4) | 6529(3) | 9363(2) | 25.0(10) |
| C24 | 4789(4) | 7360(3) | 8911(2) | 23.5(9) |
| C25 | 4086(3) | 7148(3) | 8240(2) | 21.4(9) |
| C26 | 6094(4) | 6770(4) | 10085(2) | 34.6(11) |
| B1 | 3712(4) | 5784(4) | 6479(2) | 17.7(9) |
| B2 | 3138(4) | 5756(4) | 7226(2) | 18.1(10) |
| B3 | 1645(4) | 6012(4) | 6915(2) | 19.3(10) |
| B4 | 1246(4) | 6257(4) | 5995(3) | 20.9(10) |
| B5 | 1513(4) | 5057(4) | 5580(3) | 21.0(10) |
| B6 | 2034(4) | 4052(4) | 6242(3) | 22.8(11) |
| B7 | 3366(4) | 4528(4) | 6795(2) | 18.6(10) |
| B8 | 2118(4) | 4665(4) | 7067(3) | 19.5(10) |
| B9 | 958(4) | 4983(4) | 6313(2) | 20.7(10) |
| B10 | 2976(4) | 4769(4) | 5880(2) | 19.6(10) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_0848_CG_0m_4. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 21.3(16) | 19.3(15) | 34.1(18) | 1.2(13) | 12.7(14) | -0.2(12) |
| N1 | 19.4(18) | 16.8(18) | 33(2) | -1.5(15) | 12.8(16) | 0.6(14) |
| C1 | 21(2) | 20(2) | 21(2) | -0.4(17) | 7.1(17) | -1.9(17) |
| C2 | 16(2) | 20(2) | 18(2) | -0.7(17) | 7.2(16) | 1.6(16) |
| C3 | 15(2) | 24(2) | 20(2) | -1.4(17) | 7.8(17) | 1.3(16) |
| C4 | 20(2) | 26(2) | 23(2) | 0.2(18) | 9.7(18) | 3.5(18) |
| C5 | 19(2) | 29(2) | 25(2) | 3.9(19) | 9.3(18) | 4.7(18) |
| C6 | 30(3) | 38(3) | 30(3) | 10(2) | 16(2) | 11(2) |
| C7 | 42(3) | 49(3) | 41(3) | 19(3) | 19(3) | 17(3) |
| C8 | 33(3) | 17(2) | 52(3) | -5(2) | 25(2) | -1.5(19) |
| C9 | 40(3) | 28(3) | 71(4) | 11(3) | 26(3) | 4(2) |
| C11 | 21(2) | 25(2) | 35(3) | 0(2) | 14(2) | 4.3(18) |
| C12 | 37(3) | 33(3) | 42(3) | -12(2) | 24(2) | -6(2) |
| C13 | 20(2) | 18(2) | 22(2) | 3.4(17) | 8.8(17) | 1.6(17) |
| C14 | 23(2) | 20(2) | 19(2) | -1.3(17) | 9.3(17) | 0.0(17) |
| C15 | 25(2) | 23(2) | 26(2) | 1.1(19) | 14.3(19) | 2.2(18) |
| C16 | 17(2) | 23(2) | 30(2) | 1.8(19) | 9.9(19) | -0.6(17) |
| C17 | 20(2) | 21(2) | 26(2) | -3.0(18) | 6.5(18) | -1.1(18) |
| C18 | 21(2) | 23(2) | 24(2) | -4.5(18) | 11.0(18) | 0.6(18) |
| C19 | 25(3) | 34(3) | 44(3) | 1(2) | 16(2) | -2(2) |
| C20 | 16(2) | 18(2) | 22(2) | -1.5(17) | 10.6(17) | 0.4(16) |
| C21 | 23(2) | 19(2) | 23(2) | -2.9(17) | 8.5(18) | -1.4(17) |
| C22 | 28(2) | 29(2) | 23(2) | 0.9(19) | 10.4(19) | 0.5(19) |
| C23 | 23(2) | 32(2) | 22(2) | -3.7(19) | 8.6(18) | -4.8(19) |
| C24 | 24(2) | 23(2) | 26(2) | -5.9(19) | 10.8(19) | -5.4(18) |
| C25 | 20(2) | 22(2) | 26(2) | -0.1(18) | 12.0(18) | 1.6(17) |
| C26 | 38(3) | 35(3) | 27(3) | -4(2) | 4(2) | -5(2) |
| B1 | 18(2) | 18(2) | 19(2) | -2.6(19) | 6.9(19) | 2.3(19) |
| B2 | 16(2) | 18(2) | 23(2) | -0.1(19) | 8.7(19) | -0.6(18) |
| B3 | 14(2) | 22(2) | 24(2) | -1(2) | 7.3(19) | -2.3(18) |
| B4 | 13(2) | 26(3) | 26(3) | -4(2) | 9.5(19) | -2.2(19) |
| B5 | 19(2) | 23(3) | 21(2) | -6(2) | 6(2) | -3(2) |
| B6 | 21(3) | 22(3) | 26(3) | -2(2) | 7(2) | 0(2) |
| B7 | 18(2) | 16(2) | 23(2) | -1.4(19) | 7.7(19) | -0.5(18) |
| B8 | 17(2) | 17(2) | 25(3) | 0(2) | 6(2) | -2.0(19) |
| B9 | 17(2) | 20(2) | 26(3) | 1(2) | 8(2) | -1.2(19) |
| B10 | 19(2) | 21(2) | 20(2) | -3(2) | 7.0(19) | -0.3(19) |

**Bond Lengths for mo_0848_CG_0m_4.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C1 | 1.221(4) | C20 | C25 | 1.405(5) |
| N1 | C1 | 1.349(5) | C20 | B2 | 1.568(6) |
| N1 | C8 | 1.486(5) | C21 | C22 | 1.387(6) |
| N1 | C11 | 1.470(5) | C22 | C23 | 1.393(6) |
| C1 | C2 | 1.550(5) | C23 | C24 | 1.390(6) |
| C2 | C3 | 1.673(5) | C23 | C26 | 1.505(6) |
| C2 | B1 | 1.804(6) | C24 | C25 | 1.386(6) |
| C2 | B2 | 1.742(6) | B1 | B2 | 1.815(6) |
| C2 | B3 | 1.715(6) | B1 | B7 | 1.764(6) |
| C2 | B4 | 1.731(6) | B1 | B10 | 1.781(6) |
| C3 | C4 | 1.535(5) | B2 | B3 | 1.786(7) |
| C3 | B1 | 1.769(6) | B2 | B7 | 1.796(6) |
| C3 | B4 | 1.747(6) | B2 | B8 | 1.801(6) |
| C3 | B5 | 1.708(6) | B3 | B4 | 1.774(7) |
| C3 | B10 | 1.699(6) | B3 | B8 | 1.753(6) |
| C4 | C5 | 1.530(5) | B3 | B9 | 1.778(7) |
| C5 | C6 | 1.521(5) | B4 | B5 | 1.767(6) |
| C6 | C7 | 1.529(6) | B4 | B9 | 1.762(7) |
| C8 | C9 | 1.524(7) | B5 | B6 | 1.783(7) |
| C11 | C12 | 1.532(6) | B5 | B9 | 1.778(6) |
| C13 | C14 | 1.404(5) | B5 | B10 | 1.758(7) |
| C13 | C18 | 1.398(6) | B6 | B7 | 1.785(7) |
| C13 | B1 | 1.574(6) | B6 | B8 | 1.779(6) |
| C14 | C15 | 1.386(6) | B6 | B9 | 1.785(7) |
| C15 | C16 | 1.384(6) | B6 | B10 | 1.764(6) |
| C16 | C17 | 1.394(5) | B7 | B8 | 1.774(6) |
| C16 | C19 | 1.516(6) | B7 | B10 | 1.765(6) |
| C17 | C18 | 1.380(6) | B8 | B9 | 1.788(7) |
| C20 | C21 | 1.397(5) | | | |

**Bond Angles for mo_0848_CG_0m_4.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C8 | 115.1(3) | B3 | B2 | B7 | 105.6(3) |
| C1 | N1 | C11 | 130.9(3) | B3 | B2 | B8 | 58.5(2) |
| C11 | N1 | C8 | 113.4(3) | B7 | B2 | B1 | 58.5(2) |
| O1 | C1 | N1 | 121.6(4) | B7 | B2 | B8 | 59.1(2) |
| O1 | C1 | C2 | 116.1(3) | B8 | B2 | B1 | 106.6(3) |
| N1 | C1 | C2 | 122.3(3) | C2 | B3 | B2 | 59.6(2) |
| C1 | C2 | C3 | 113.2(3) | C2 | B3 | B4 | 59.5(2) |
| C1 | C2 | B1 | 114.1(3) | C2 | B3 | B8 | 106.5(3) |
| C1 | C2 | B2 | 124.0(3) | C2 | B3 | B9 | 106.1(3) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C1 | C2 | B3 | 127.3(3) | B4 | B3 | B2 | 109.6(3) |
| C1 | C2 | B4 | 117.0(3) | B4 | B3 | B9 | 59.5(3) |
| C3 | C2 | B1 | 61.0(2) | B8 | B3 | B2 | 61.2(3) |
| C3 | C2 | B2 | 110.4(3) | B8 | B3 | B4 | 108.5(3) |
| C3 | C2 | B3 | 110.2(3) | B8 | B3 | B9 | 60.8(3) |
| C3 | C2 | B4 | 61.7(2) | B9 | B3 | B2 | 110.3(3) |
| B2 | C2 | B1 | 61.6(2) | C2 | B4 | C3 | 57.5(2) |
| B3 | C2 | B1 | 112.3(3) | C2 | B4 | B3 | 58.6(2) |
| B3 | C2 | B2 | 62.2(2) | C2 | B4 | B5 | 105.1(3) |
| B3 | C2 | B4 | 62.0(3) | C2 | B4 | B9 | 106.1(3) |
| B4 | C2 | B1 | 113.7(3) | C3 | B4 | B3 | 104.2(3) |
| B4 | C2 | B2 | 113.8(3) | C3 | B4 | B5 | 58.2(2) |
| C2 | C3 | B1 | 63.1(2) | C3 | B4 | B9 | 105.2(3) |
| C2 | C3 | B4 | 60.8(2) | B5 | B4 | B3 | 107.8(3) |
| C2 | C3 | B5 | 110.4(3) | B9 | B4 | B3 | 60.4(3) |
| C2 | C3 | B10 | 111.0(3) | B9 | B4 | B5 | 60.5(3) |
| C4 | C3 | C2 | 119.8(3) | C3 | B5 | B4 | 60.3(2) |
| C4 | C3 | B1 | 116.6(3) | C3 | B5 | B6 | 105.5(3) |
| C4 | C3 | B4 | 118.7(3) | C3 | B5 | B9 | 106.2(3) |
| C4 | C3 | B5 | 120.1(3) | C3 | B5 | B10 | 58.7(2) |
| C4 | C3 | B10 | 120.2(3) | B4 | B5 | B6 | 108.1(3) |
| B4 | C3 | B1 | 114.6(3) | B4 | B5 | B9 | 59.6(2) |
| B5 | C3 | B1 | 113.9(3) | B9 | B5 | B6 | 60.2(3) |
| B5 | C3 | B4 | 61.5(3) | B10 | B5 | B4 | 108.6(3) |
| B10 | C3 | B1 | 61.7(3) | B10 | B5 | B6 | 59.8(3) |
| B10 | C3 | B4 | 112.4(3) | B10 | B5 | B9 | 108.0(3) |
| B10 | C3 | B5 | 62.1(3) | B5 | B6 | B7 | 107.2(3) |
| C5 | C4 | C3 | 117.0(3) | B5 | B6 | B9 | 59.8(3) |
| C6 | C5 | C4 | 111.2(3) | B7 | B6 | B9 | 108.0(3) |
| C5 | C6 | C7 | 112.5(4) | B8 | B6 | B5 | 107.3(3) |
| N1 | C8 | C9 | 111.6(4) | B8 | B6 | B7 | 59.7(3) |
| N1 | C11 | C12 | 112.6(4) | B8 | B6 | B9 | 60.2(3) |
| C14 | C13 | B1 | 120.5(4) | B10 | B6 | B5 | 59.4(3) |
| C18 | C13 | C14 | 116.0(4) | B10 | B6 | B7 | 59.6(3) |
| C18 | C13 | B1 | 123.2(3) | B10 | B6 | B8 | 107.0(3) |
| C15 | C14 | C13 | 121.9(4) | B10 | B6 | B9 | 107.4(3) |
| C16 | C15 | C14 | 121.2(4) | B1 | B7 | B2 | 61.3(2) |
| C15 | C16 | C17 | 117.7(4) | B1 | B7 | B6 | 109.9(3) |
| C15 | C16 | C19 | 121.7(4) | B1 | B7 | B8 | 110.1(3) |
| C17 | C16 | C19 | 120.6(4) | B1 | B7 | B10 | 60.6(3) |
| C18 | C17 | C16 | 121.0(4) | B6 | B7 | B2 | 109.1(3) |
| C17 | C18 | C13 | 122.3(4) | B8 | B7 | B2 | 60.6(2) |
| C21 | C20 | C25 | 116.5(4) | B8 | B7 | B6 | 60.0(3) |
| C21 | C20 | B2 | 118.1(3) | B10 | B7 | B2 | 108.4(3) |
| C25 | C20 | B2 | 125.4(4) | B10 | B7 | B6 | 59.6(3) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C22 | C21 | C20 | 121.8(4) | B10 | B7 | B8 | 107.2(3) |
| C21 | C22 | C23 | 121.4(4) | B3 | B8 | B2 | 60.3(3) |
| C22 | C23 | C26 | 121.6(4) | B3 | B8 | B6 | 108.3(3) |
| C24 | C23 | C22 | 117.1(4) | B3 | B8 | B7 | 108.0(3) |
| C24 | C23 | C26 | 121.3(4) | B3 | B8 | B9 | 60.3(3) |
| C25 | C24 | C23 | 121.8(4) | B6 | B8 | B2 | 109.2(3) |
| C24 | C25 | C20 | 121.4(4) | B6 | B8 | B9 | 60.1(3) |
| C2 | B1 | B2 | 57.5(2) | B7 | B8 | B2 | 60.3(2) |
| C3 | B1 | C2 | 55.8(2) | B7 | B8 | B6 | 60.3(3) |
| C3 | B1 | B2 | 102.9(3) | B7 | B8 | B9 | 108.4(3) |
| C3 | B1 | B10 | 57.2(2) | B9 | B8 | B2 | 109.2(3) |
| C13 | B1 | C2 | 128.2(3) | B3 | B9 | B5 | 107.1(3) |
| C13 | B1 | C3 | 124.4(3) | B3 | B9 | B6 | 106.9(3) |
| C13 | B1 | B2 | 125.2(4) | B3 | B9 | B8 | 58.9(3) |
| C13 | B1 | B7 | 123.0(3) | B4 | B9 | B3 | 60.1(3) |
| C13 | B1 | B10 | 120.7(3) | B4 | B9 | B5 | 59.9(3) |
| B7 | B1 | C2 | 102.9(3) | B4 | B9 | B6 | 108.2(3) |
| B7 | B1 | C3 | 103.2(3) | B4 | B9 | B8 | 107.5(3) |
| B7 | B1 | B2 | 60.2(2) | B5 | B9 | B6 | 60.1(3) |
| B7 | B1 | B10 | 59.7(3) | B5 | B9 | B8 | 107.2(3) |
| B10 | B1 | C2 | 101.6(3) | B6 | B9 | B8 | 59.7(3) |
| B10 | B1 | B2 | 106.9(3) | C3 | B10 | B1 | 61.0(2) |
| C2 | B2 | B1 | 60.9(2) | C3 | B10 | B5 | 59.2(3) |
| C2 | B2 | B3 | 58.2(2) | C3 | B10 | B6 | 106.7(3) |
| C2 | B2 | B7 | 104.1(3) | C3 | B10 | B7 | 106.1(3) |
| C2 | B2 | B8 | 103.3(3) | B5 | B10 | B1 | 110.9(3) |
| C20 | B2 | C2 | 125.8(3) | B5 | B10 | B6 | 60.8(3) |
| C20 | B2 | B1 | 121.9(3) | B5 | B10 | B7 | 109.2(3) |
| C20 | B2 | B3 | 122.4(3) | B6 | B10 | B1 | 110.1(3) |
| C20 | B2 | B7 | 123.0(4) | B6 | B10 | B7 | 60.8(3) |
| C20 | B2 | B8 | 122.4(3) | B7 | B10 | B1 | 59.7(3) |
| B3 | B2 | B1 | 108.5(3) | | | | |

**Torsion Angles for mo_0848_CG_0m_4.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O1 | C1 | C2 | C3 | -52.8(5) | B2 | C2 | B4 | C3 | -101.2(3) |
| O1 | C1 | C2 | B1 | 14.5(5) | B2 | C2 | B4 | B3 | 35.7(3) |
| O1 | C1 | C2 | B2 | 85.4(5) | B2 | C2 | B4 | B5 | -66.2(4) |
| O1 | C1 | C2 | B3 | 164.3(4) | B2 | C2 | B4 | B9 | -3.1(4) |
| O1 | C1 | C2 | B4 | -121.7(4) | B2 | C20 | C21 | C22 | 177.9(4) |
| N1 | C1 | C2 | C3 | 128.9(4) | B2 | C20 | C25 | C24 | -177.1(4) |
| N1 | C1 | C2 | B1 | -163.8(4) | B2 | B1 | B7 | B6 | 101.5(3) |
| N1 | C1 | C2 | B2 | -92.9(5) | B2 | B1 | B7 | B8 | 37.2(3) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| N1 | C1 | C2 | B3 | -14.0(6) | B2 | B1 | B7 | B10 | 136.1(3) |
| N1 | C1 | C2 | B4 | 60.0(5) | B2 | B1 | B10 | C3 | 94.8(3) |
| C1 | N1 | C8 | C9 | 87.1(5) | B2 | B1 | B10 | B5 | 61.7(4) |
| C1 | N1 | C11 | C12 | 111.3(5) | B2 | B1 | B10 | B6 | -3.7(4) |
| C1 | C2 | C3 | C4 | -1.0(5) | B2 | B1 | B10 | B7 | -38.9(3) |
| C1 | C2 | C3 | B1 | 105.8(3) | B2 | B3 | B4 | C2 | -33.5(3) |
| C1 | C2 | C3 | B4 | -109.3(4) | B2 | B3 | B4 | C3 | 2.9(4) |
| C1 | C2 | C3 | B5 | -147.0(3) | B2 | B3 | B4 | B5 | 63.6(4) |
| C1 | C2 | C3 | B10 | 146.1(3) | B2 | B3 | B4 | B9 | 102.6(4) |
| C1 | C2 | B1 | C3 | -104.1(3) | B2 | B3 | B8 | B6 | -102.1(3) |
| C1 | C2 | B1 | C13 | 5.4(6) | B2 | B3 | B8 | B7 | -38.3(3) |
| C1 | C2 | B1 | B2 | 117.1(4) | B2 | B3 | B8 | B9 | -139.6(3) |
| C1 | C2 | B1 | B7 | 158.5(3) | B2 | B3 | B9 | B4 | -101.4(3) |
| C1 | C2 | B1 | B10 | -140.2(3) | B2 | B3 | B9 | B5 | -62.8(4) |
| C1 | C2 | B2 | C20 | 8.8(6) | B2 | B3 | B9 | B6 | 0.3(4) |
| C1 | C2 | B2 | B1 | -101.3(4) | B2 | B3 | B9 | B8 | 37.3(3) |
| C1 | C2 | B2 | B3 | 118.1(4) | B2 | B7 | B8 | B3 | 38.3(3) |
| C1 | C2 | B2 | B7 | -142.1(3) | B2 | B7 | B8 | B6 | 139.5(3) |
| C1 | C2 | B2 | B8 | 156.9(3) | B2 | B7 | B8 | B9 | 102.1(3) |
| C1 | C2 | B3 | B2 | -113.2(4) | B2 | B7 | B10 | C3 | -1.4(4) |
| C1 | C2 | B3 | B4 | 103.9(4) | B2 | B7 | B10 | B1 | 39.8(3) |
| C1 | C2 | B3 | B8 | -154.0(4) | B2 | B7 | B10 | B5 | -63.7(4) |
| C1 | C2 | B3 | B9 | 142.3(4) | B2 | B7 | B10 | B6 | -101.9(4) |
| C1 | C2 | B4 | C3 | 103.1(3) | B2 | B8 | B9 | B3 | -36.6(3) |
| C1 | C2 | B4 | B3 | -120.0(4) | B2 | B8 | B9 | B4 | 0.3(4) |
| C1 | C2 | B4 | B5 | 138.1(3) | B2 | B8 | B9 | B5 | 63.4(4) |
| C1 | C2 | B4 | B9 | -158.8(3) | B2 | B8 | B9 | B6 | 101.6(3) |
| C2 | C3 | C4 | C5 | -67.9(5) | B3 | C2 | C3 | C4 | 148.3(3) |
| C2 | C3 | B1 | C13 | -116.2(4) | B3 | C2 | C3 | B1 | -105.0(3) |
| C2 | C3 | B1 | B2 | 34.8(3) | B3 | C2 | C3 | B4 | 40.0(3) |
| C2 | C3 | B1 | B7 | 96.8(3) | B3 | C2 | C3 | B5 | 2.3(4) |
| C2 | C3 | B1 | B10 | 136.7(3) | B3 | C2 | C3 | B10 | -64.6(4) |
| C2 | C3 | B4 | B3 | -37.0(3) | B3 | C2 | B1 | C3 | 101.5(3) |
| C2 | C3 | B4 | B5 | -139.3(3) | B3 | C2 | B1 | C13 | -148.9(4) |
| C2 | C3 | B4 | B9 | -99.6(3) | B3 | C2 | B1 | B2 | -37.3(3) |
| C2 | C3 | B5 | B4 | 37.4(3) | B3 | C2 | B1 | B7 | 4.1(4) |
| C2 | C3 | B5 | B6 | -64.9(4) | B3 | C2 | B1 | B10 | 65.4(4) |
| C2 | C3 | B5 | B9 | -2.1(4) | B3 | C2 | B2 | C20 | -109.3(4) |
| C2 | C3 | B5 | B10 | -103.6(3) | B3 | C2 | B2 | B1 | 140.6(3) |
| C2 | C3 | B10 | B1 | -41.0(3) | B3 | C2 | B2 | B7 | 99.8(3) |
| C2 | C3 | B10 | B5 | 102.7(3) | B3 | C2 | B2 | B8 | 38.8(3) |
| C2 | C3 | B10 | B6 | 63.2(4) | B3 | C2 | B4 | C3 | -136.9(3) |
| C2 | C3 | B10 | B7 | -0.4(4) | B3 | C2 | B4 | B5 | -101.9(3) |
| C2 | B1 | B2 | C20 | -116.2(4) | B3 | C2 | B4 | B9 | -38.8(3) |
| C2 | B1 | B2 | B3 | 34.6(3) | B3 | B2 | B7 | B1 | 102.4(3) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C2 | B1 | B2 | B7 | 132.0(3) | B3 | B2 | B7 | B6 | -0.4(4) |
| C2 | B1 | B2 | B8 | 96.3(3) | B3 | B2 | B7 | B8 | -36.9(3) |
| C2 | B1 | B7 | B2 | -40.1(3) | B3 | B2 | B7 | B10 | 62.9(4) |
| C2 | B1 | B7 | B6 | 61.4(4) | B3 | B2 | B8 | B6 | 100.6(4) |
| C2 | B1 | B7 | B8 | -2.9(4) | B3 | B2 | B8 | B7 | 137.3(3) |
| C2 | B1 | B7 | B10 | 96.1(3) | B3 | B2 | B8 | B9 | 36.6(3) |
| C2 | B1 | B10 | C3 | 35.4(3) | B3 | B4 | B5 | C3 | -96.0(3) |
| C2 | B1 | B10 | B5 | 2.4(4) | B3 | B4 | B5 | B6 | 1.9(4) |
| C2 | B1 | B10 | B6 | -63.1(4) | B3 | B4 | B5 | B9 | 39.0(3) |
| C2 | B1 | B10 | B7 | -98.3(3) | B3 | B4 | B5 | B10 | -61.4(4) |
| C2 | B2 | B3 | B4 | 33.5(3) | B3 | B4 | B9 | B5 | -136.5(3) |
| C2 | B2 | B3 | B8 | 134.3(3) | B3 | B4 | B9 | B6 | -99.4(4) |
| C2 | B2 | B3 | B9 | 97.2(3) | B3 | B4 | B9 | B8 | -36.4(3) |
| C2 | B2 | B7 | B1 | 42.1(3) | B3 | B8 | B9 | B4 | 36.9(3) |
| C2 | B2 | B7 | B6 | -60.7(4) | B3 | B8 | B9 | B5 | 100.0(3) |
| C2 | B2 | B7 | B8 | -97.3(3) | B3 | B8 | B9 | B6 | 138.2(3) |
| C2 | B2 | B7 | B10 | 2.6(4) | B4 | C2 | C3 | C4 | 108.3(4) |
| C2 | B2 | B8 | B3 | -38.7(3) | B4 | C2 | C3 | B1 | -145.0(3) |
| C2 | B2 | B8 | B6 | 61.9(4) | B4 | C2 | C3 | B5 | -37.7(3) |
| C2 | B2 | B8 | B7 | 98.6(3) | B4 | C2 | C3 | B10 | -104.6(3) |
| C2 | B2 | B8 | B9 | -2.1(4) | B4 | C2 | B1 | C3 | 33.5(3) |
| C2 | B3 | B4 | C3 | 36.5(3) | B4 | C2 | B1 | C13 | 143.1(4) |
| C2 | B3 | B4 | B5 | 97.1(3) | B4 | C2 | B1 | B2 | -105.3(3) |
| C2 | B3 | B4 | B9 | 136.1(3) | B4 | C2 | B1 | B7 | -63.8(4) |
| C2 | B3 | B8 | B2 | 40.1(3) | B4 | C2 | B1 | B10 | -2.6(4) |
| C2 | B3 | B8 | B6 | -62.1(4) | B4 | C2 | B2 | C20 | -144.8(4) |
| C2 | B3 | B8 | B7 | 1.8(4) | B4 | C2 | B2 | B1 | 105.1(3) |
| C2 | B3 | B8 | B9 | -99.5(3) | B4 | C2 | B2 | B3 | -35.6(3) |
| C2 | B3 | B9 | B4 | -38.4(3) | B4 | C2 | B2 | B7 | 64.3(4) |
| C2 | B3 | B9 | B5 | 0.2(4) | B4 | C2 | B2 | B8 | 3.2(4) |
| C2 | B3 | B9 | B6 | 63.3(4) | B4 | C2 | B3 | B2 | 142.9(3) |
| C2 | B3 | B9 | B8 | 100.3(3) | B4 | C2 | B3 | B8 | 102.1(3) |
| C2 | B4 | B5 | C3 | -34.7(3) | B4 | C2 | B3 | B9 | 38.4(3) |
| C2 | B4 | B5 | B6 | 63.2(4) | B4 | C3 | C4 | C5 | 3.0(5) |
| C2 | B4 | B5 | B9 | 100.2(3) | B4 | C3 | B1 | C2 | -33.5(3) |
| C2 | B4 | B5 | B10 | -0.1(4) | B4 | C3 | B1 | C13 | -149.7(4) |
| C2 | B4 | B9 | B3 | 38.0(3) | B4 | C3 | B1 | B2 | 1.3(4) |
| C2 | B4 | B9 | B5 | -98.5(3) | B4 | C3 | B1 | B7 | 63.3(4) |
| C2 | B4 | B9 | B6 | -61.5(4) | B4 | C3 | B1 | B10 | 103.2(3) |
| C2 | B4 | B9 | B8 | 1.6(4) | B4 | C3 | B5 | B6 | -102.3(3) |
| C3 | C2 | B1 | C13 | 109.6(4) | B4 | C3 | B5 | B9 | -39.5(3) |
| C3 | C2 | B1 | B2 | -138.8(3) | B4 | C3 | B5 | B10 | -141.0(3) |
| C3 | C2 | B1 | B7 | -97.3(3) | B4 | C3 | B10 | B1 | -106.9(3) |
| C3 | C2 | B1 | B10 | -36.1(3) | B4 | C3 | B10 | B5 | 36.7(3) |
| C3 | C2 | B2 | C20 | 148.0(4) | B4 | C3 | B10 | B6 | -2.7(4) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | C2 | B2 | B1 | 37.9(3) | B4 | C3 | B10 | B7 | -66.4(4) |
| C3 | C2 | B2 | B3 | -102.7(3) | B4 | B3 | B8 | B2 | 102.7(3) |
| C3 | C2 | B2 | B7 | -2.9(4) | B4 | B3 | B8 | B6 | 0.6(4) |
| C3 | C2 | B2 | B8 | -63.9(4) | B4 | B3 | B8 | B7 | 64.4(4) |
| C3 | C2 | B3 | B2 | 103.0(3) | B4 | B3 | B8 | B9 | -36.9(3) |
| C3 | C2 | B3 | B4 | -39.9(3) | B4 | B3 | B9 | B5 | 38.6(3) |
| C3 | C2 | B3 | B8 | 62.2(4) | B4 | B3 | B9 | B6 | 101.7(3) |
| C3 | C2 | B3 | B9 | -1.5(4) | B4 | B3 | B9 | B8 | 138.7(3) |
| C3 | C2 | B4 | B3 | 136.9(3) | B4 | B5 | B6 | B7 | -64.4(4) |
| C3 | C2 | B4 | B5 | 35.0(3) | B4 | B5 | B6 | B8 | -1.6(4) |
| C3 | C2 | B4 | B9 | 98.1(3) | B4 | B5 | B6 | B9 | 36.8(3) |
| C3 | C4 | C5 | C6 | 171.7(4) | B4 | B5 | B6 | B10 | -101.5(3) |
| C3 | B1 | B2 | C2 | -34.0(3) | B4 | B5 | B9 | B3 | -38.7(3) |
| C3 | B1 | B2 | C20 | -150.2(4) | B4 | B5 | B9 | B6 | -138.7(4) |
| C3 | B1 | B2 | B3 | 0.6(4) | B4 | B5 | B9 | B8 | -100.6(4) |
| C3 | B1 | B2 | B7 | 98.0(3) | B4 | B5 | B10 | C3 | -35.3(3) |
| C3 | B1 | B2 | B8 | 62.3(4) | B4 | B5 | B10 | B1 | -1.5(4) |
| C3 | B1 | B7 | B2 | -97.5(3) | B4 | B5 | B10 | B6 | 100.5(4) |
| C3 | B1 | B7 | B6 | 3.9(4) | B4 | B5 | B10 | B7 | 62.4(4) |
| C3 | B1 | B7 | B8 | -60.3(4) | B5 | C3 | C4 | C5 | 74.8(5) |
| C3 | B1 | B7 | B10 | 38.6(3) | B5 | C3 | B1 | C2 | -101.7(3) |
| C3 | B1 | B10 | B5 | -33.1(3) | B5 | C3 | B1 | C13 | 142.1(4) |
| C3 | B1 | B10 | B6 | -98.5(3) | B5 | C3 | B1 | B2 | -66.9(4) |
| C3 | B1 | B10 | B7 | -133.7(3) | B5 | C3 | B1 | B7 | -4.9(4) |
| C3 | B4 | B5 | B6 | 97.9(3) | B5 | C3 | B1 | B10 | 35.0(3) |
| C3 | B4 | B5 | B9 | 135.0(3) | B5 | C3 | B4 | C2 | 139.3(3) |
| C3 | B4 | B5 | B10 | 34.6(3) | B5 | C3 | B4 | B3 | 102.3(3) |
| C3 | B4 | B9 | B3 | 97.9(3) | B5 | C3 | B4 | B9 | 39.7(3) |
| C3 | B4 | B9 | B5 | -38.5(3) | B5 | C3 | B10 | B1 | -143.6(3) |
| C3 | B4 | B9 | B6 | -1.5(4) | B5 | C3 | B10 | B6 | -39.5(3) |
| C3 | B4 | B9 | B8 | 61.5(4) | B5 | C3 | B10 | B7 | -103.1(3) |
| C3 | B5 | B6 | B7 | -1.1(4) | B5 | B4 | B9 | B3 | 136.5(3) |
| C3 | B5 | B6 | B8 | 61.7(4) | B5 | B4 | B9 | B6 | 37.0(3) |
| C3 | B5 | B6 | B9 | 100.1(3) | B5 | B4 | B9 | B8 | 100.1(3) |
| C3 | B5 | B6 | B10 | -38.2(3) | B5 | B6 | B7 | B1 | -1.9(4) |
| C3 | B5 | B9 | B3 | 1.1(4) | B5 | B6 | B7 | B2 | 63.6(4) |
| C3 | B5 | B9 | B4 | 39.8(3) | B5 | B6 | B7 | B8 | 100.4(3) |
| C3 | B5 | B9 | B6 | -98.9(3) | B5 | B6 | B7 | B10 | -37.0(3) |
| C3 | B5 | B9 | B8 | -60.8(4) | B5 | B6 | B8 | B2 | -63.5(4) |
| C3 | B5 | B10 | B1 | 33.8(3) | B5 | B6 | B8 | B3 | 0.6(4) |
| C3 | B5 | B10 | B6 | 135.8(3) | B5 | B6 | B8 | B7 | -100.2(3) |
| C3 | B5 | B10 | B7 | 97.7(3) | B5 | B6 | B8 | B9 | 38.2(3) |
| C4 | C3 | B1 | C2 | 111.6(4) | B5 | B6 | B9 | B3 | -100.3(3) |
| C4 | C3 | B1 | C13 | -4.6(5) | B5 | B6 | B9 | B4 | -36.9(3) |
| C4 | C3 | B1 | B2 | 146.4(3) | B5 | B6 | B9 | B8 | -137.0(3) |

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|---|---|---|---|---|---|---|---|---|---|
| C4 | C3 | B1 | B7 | -151.6(3) | B5 | B6 | B10 | C3 | 38.7(3) |
| C4 | C3 | B1 | B10 | -111.7(4) | B5 | B6 | B10 | B1 | 103.4(4) |
| C4 | C3 | B4 | C2 | -110.0(4) | B5 | B6 | B10 | B7 | 138.1(3) |
| C4 | C3 | B4 | B3 | -147.0(3) | B6 | B5 | B9 | B3 | 100.0(4) |
| C4 | C3 | B4 | B5 | 110.7(4) | B6 | B5 | B9 | B4 | 138.7(4) |
| C4 | C3 | B4 | B9 | 150.4(4) | B6 | B5 | B9 | B8 | 38.1(3) |
| C4 | C3 | B5 | B4 | -108.5(4) | B6 | B5 | B10 | C3 | -135.8(3) |
| C4 | C3 | B5 | B6 | 149.2(3) | B6 | B5 | B10 | B1 | -102.0(4) |
| C4 | C3 | B5 | B9 | -148.0(3) | B6 | B5 | B10 | B7 | -38.1(3) |
| C4 | C3 | B5 | B10 | 110.5(4) | B6 | B7 | B8 | B2 | -139.5(3) |
| C4 | C3 | B10 | B1 | 106.0(4) | B6 | B7 | B8 | B3 | -101.2(4) |
| C4 | C3 | B10 | B5 | -110.4(4) | B6 | B7 | B8 | B9 | -37.4(3) |
| C4 | C3 | B10 | B6 | -149.9(4) | B6 | B7 | B10 | C3 | 100.5(3) |
| C4 | C3 | B10 | B7 | 146.5(4) | B6 | B7 | B10 | B1 | 141.7(3) |
| C4 | C5 | C6 | C7 | 176.8(4) | B6 | B7 | B10 | B5 | 38.1(3) |
| C8 | N1 | C1 | O1 | -1.9(6) | B6 | B8 | B9 | B3 | -138.2(3) |
| C8 | N1 | C1 | C2 | 176.3(4) | B6 | B8 | B9 | B4 | -101.3(3) |
| C8 | N1 | C11 | C12 | -78.4(5) | B6 | B8 | B9 | B5 | -38.2(3) |
| C11 | N1 | C1 | O1 | 168.3(4) | B7 | B1 | B2 | C2 | -132.0(3) |
| C11 | N1 | C1 | C2 | -13.6(7) | B7 | B1 | B2 | C20 | 111.8(4) |
| C11 | N1 | C8 | C9 | -84.8(4) | B7 | B1 | B2 | B3 | -97.4(3) |
| C13 | C14 | C15 | C16 | -0.4(6) | B7 | B1 | B2 | B8 | -35.7(3) |
| C13 | B1 | B2 | C2 | 116.7(4) | B7 | B1 | B10 | C3 | 133.7(3) |
| C13 | B1 | B2 | C20 | 0.5(6) | B7 | B1 | B10 | B5 | 100.6(4) |
| C13 | B1 | B2 | B3 | 151.3(4) | B7 | B1 | B10 | B6 | 35.2(3) |
| C13 | B1 | B2 | B7 | -111.3(4) | B7 | B2 | B3 | C2 | -97.2(3) |
| C13 | B1 | B2 | B8 | -147.0(4) | B7 | B2 | B3 | B4 | -63.7(4) |
| C13 | B1 | B7 | B2 | 114.9(4) | B7 | B2 | B3 | B8 | 37.2(3) |
| C13 | B1 | B7 | B6 | -143.7(4) | B7 | B2 | B3 | B9 | 0.1(4) |
| C13 | B1 | B7 | B8 | 152.0(4) | B7 | B2 | B8 | B3 | -137.3(3) |
| C13 | B1 | B7 | B10 | -109.0(4) | B7 | B2 | B8 | B6 | -36.7(3) |
| C13 | B1 | B10 | C3 | -113.6(4) | B7 | B2 | B8 | B9 | -100.7(3) |
| C13 | B1 | B10 | B5 | -146.6(4) | B7 | B6 | B8 | B2 | 36.7(3) |
| C13 | B1 | B10 | B6 | 147.9(4) | B7 | B6 | B8 | B3 | 100.8(3) |
| C13 | B1 | B10 | B7 | 112.7(4) | B7 | B6 | B8 | B9 | 138.3(3) |
| C14 | C13 | C18 | C17 | 0.8(6) | B7 | B6 | B9 | B3 | -0.5(4) |
| C14 | C13 | B1 | C2 | -138.3(4) | B7 | B6 | B9 | B4 | 62.9(4) |
| C14 | C13 | B1 | C3 | -67.3(5) | B7 | B6 | B9 | B5 | 99.8(4) |
| C14 | C13 | B1 | B2 | 148.0(4) | B7 | B6 | B9 | B8 | -37.1(3) |
| C14 | C13 | B1 | B7 | 73.5(5) | B7 | B6 | B10 | C3 | -99.4(3) |
| C14 | C13 | B1 | B10 | 1.8(6) | B7 | B6 | B10 | B1 | -34.8(3) |
| C14 | C15 | C16 | C17 | 1.7(6) | B7 | B6 | B10 | B5 | -138.1(3) |
| C14 | C15 | C16 | C19 | -177.9(4) | B7 | B8 | B9 | B3 | -100.7(3) |
| C15 | C16 | C17 | C18 | -1.7(6) | B7 | B8 | B9 | B4 | -63.8(4) |
| C16 | C17 | C18 | C13 | 0.5(6) | B7 | B8 | B9 | B5 | -0.8(4) |

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|---|---|---|---|---|---|---|---|---|---|
| C18 | C13 | C14 | C15 | -0.8(6) | B7 | B8 | B9 | B6 | 37.5(3) |
| C18 | C13 | B1 | C2 | 48.1(6) | B8 | B2 | B3 | C2 | -134.3(3) |
| C18 | C13 | B1 | C3 | 119.1(4) | B8 | B2 | B3 | B4 | -100.9(4) |
| C18 | C13 | B1 | B2 | -25.6(6) | B8 | B2 | B3 | B9 | -37.1(3) |
| C18 | C13 | B1 | B7 | -100.1(5) | B8 | B2 | B7 | B1 | 139.3(3) |
| C18 | C13 | B1 | B10 | -171.8(4) | B8 | B2 | B7 | B6 | 36.5(3) |
| C19 | C16 | C17 | C18 | 177.8(4) | B8 | B2 | B7 | B10 | 99.8(4) |
| C20 | C21 | C22 | C23 | -1.3(6) | B8 | B3 | B4 | C2 | -98.7(3) |
| C20 | B2 | B3 | C2 | 114.9(4) | B8 | B3 | B4 | C3 | -62.2(4) |
| C20 | B2 | B3 | B4 | 148.4(4) | B8 | B3 | B4 | B5 | -1.6(4) |
| C20 | B2 | B3 | B8 | -110.8(4) | B8 | B3 | B4 | B9 | 37.5(3) |
| C20 | B2 | B3 | B9 | -147.9(4) | B8 | B3 | B9 | B4 | -138.7(3) |
| C20 | B2 | B7 | B1 | -109.9(4) | B8 | B3 | B9 | B5 | -100.1(3) |
| C20 | B2 | B7 | B6 | 147.3(4) | B8 | B3 | B9 | B6 | -37.0(3) |
| C20 | B2 | B7 | B8 | 110.8(4) | B8 | B6 | B7 | B1 | -102.3(3) |
| C20 | B2 | B7 | B10 | -149.4(4) | B8 | B6 | B7 | B2 | -36.8(3) |
| C20 | B2 | B8 | B3 | 110.8(4) | B8 | B6 | B7 | B10 | -137.3(3) |
| C20 | B2 | B8 | B6 | -148.6(4) | B8 | B6 | B9 | B3 | 36.6(3) |
| C20 | B2 | B8 | B7 | -111.9(4) | B8 | B6 | B9 | B4 | 100.0(4) |
| C20 | B2 | B8 | B9 | 147.4(4) | B8 | B6 | B9 | B5 | 137.0(3) |
| C21 | C20 | C25 | C24 | 0.7(5) | B8 | B6 | B10 | C3 | -61.7(4) |
| C21 | C20 | B2 | C2 | -171.5(3) | B8 | B6 | B10 | B1 | 3.0(4) |
| C21 | C20 | B2 | B1 | -96.5(4) | B8 | B6 | B10 | B5 | -100.4(3) |
| C21 | C20 | B2 | B3 | 116.7(4) | B8 | B6 | B10 | B7 | 37.7(3) |
| C21 | C20 | B2 | B7 | -25.7(5) | B8 | B7 | B10 | C3 | 62.6(4) |
| C21 | C20 | B2 | B8 | 46.0(5) | B8 | B7 | B10 | B1 | 103.8(3) |
| C21 | C22 | C23 | C24 | 1.9(6) | B8 | B7 | B10 | B5 | 0.2(4) |
| C21 | C22 | C23 | C26 | -178.2(4) | B8 | B7 | B10 | B6 | -37.9(3) |
| C22 | C23 | C24 | C25 | -1.2(6) | B9 | B3 | B4 | C2 | -136.1(3) |
| C23 | C24 | C25 | C20 | 0.0(6) | B9 | B3 | B4 | C3 | -99.7(3) |
| C25 | C20 | C21 | C22 | 0.0(6) | B9 | B3 | B4 | B5 | -39.0(3) |
| C25 | C20 | B2 | C2 | 6.2(6) | B9 | B3 | B8 | B2 | 139.6(3) |
| C25 | C20 | B2 | B1 | 81.3(5) | B9 | B3 | B8 | B6 | 37.5(3) |
| C25 | C20 | B2 | B3 | -65.5(5) | B9 | B3 | B8 | B7 | 101.3(3) |
| C25 | C20 | B2 | B7 | 152.0(4) | B9 | B4 | B5 | C3 | -135.0(3) |
| C25 | C20 | B2 | B8 | -136.3(4) | B9 | B4 | B5 | B6 | -37.0(3) |
| C26 | C23 | C24 | C25 | 178.9(4) | B9 | B4 | B5 | B10 | -100.4(4) |
| B1 | C2 | C3 | C4 | -106.8(4) | B9 | B5 | B6 | B7 | -101.2(3) |
| B1 | C2 | C3 | B4 | 145.0(3) | B9 | B5 | B6 | B8 | -38.3(3) |
| B1 | C2 | C3 | B5 | 107.3(3) | B9 | B5 | B6 | B10 | -138.3(3) |
| B1 | C2 | C3 | B10 | 40.3(3) | B9 | B5 | B10 | C3 | -98.4(3) |
| B1 | C2 | B2 | C20 | 110.1(4) | B9 | B5 | B10 | B1 | -64.6(4) |
| B1 | C2 | B2 | B3 | -140.6(3) | B9 | B5 | B10 | B6 | 37.4(3) |
| B1 | C2 | B2 | B7 | -40.8(3) | B9 | B5 | B10 | B7 | -0.7(4) |
| B1 | C2 | B2 | B8 | -101.8(3) | B9 | B6 | B7 | B1 | -64.9(4) |

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|---|---|---|---|---|---|---|---|---|---|
| B1 | C2 | B3 | B2 | 37.1(3) | B9 | B6 | B7 | B2 | 0.5(4) |
| B1 | C2 | B3 | B4 | -105.8(3) | B9 | B6 | B7 | B8 | 37.3(3) |
| B1 | C2 | B3 | B8 | -3.8(4) | B9 | B6 | B7 | B10 | -100.0(4) |
| B1 | C2 | B3 | B9 | -67.4(4) | B9 | B6 | B8 | B2 | -101.6(3) |
| B1 | C2 | B4 | C3 | -33.3(3) | B9 | B6 | B8 | B3 | -37.6(3) |
| B1 | C2 | B4 | B3 | 103.6(3) | B9 | B6 | B8 | B7 | -138.3(3) |
| B1 | C2 | B4 | B5 | 1.8(4) | B9 | B6 | B10 | C3 | 1.6(4) |
| B1 | C2 | B4 | B9 | 64.8(4) | B9 | B6 | B10 | B1 | 66.3(4) |
| B1 | C3 | C4 | C5 | -140.7(4) | B9 | B6 | B10 | B5 | -37.1(3) |
| B1 | C3 | B4 | C2 | 34.3(3) | B9 | B6 | B10 | B7 | 101.1(4) |
| B1 | C3 | B4 | B3 | -2.7(4) | B10 | C3 | C4 | C5 | 148.1(4) |
| B1 | C3 | B4 | B5 | -105.0(4) | B10 | C3 | B1 | C2 | -136.7(3) |
| B1 | C3 | B4 | B9 | -65.3(4) | B10 | C3 | B1 | C13 | 107.1(4) |
| B1 | C3 | B5 | B4 | 106.1(3) | B10 | C3 | B1 | B2 | -101.9(3) |
| B1 | C3 | B5 | B6 | 3.8(4) | B10 | C3 | B1 | B7 | -39.9(3) |
| B1 | C3 | B5 | B9 | 66.6(4) | B10 | C3 | B4 | C2 | 102.3(3) |
| B1 | C3 | B5 | B10 | -34.9(3) | B10 | C3 | B4 | B3 | 65.3(4) |
| B1 | C3 | B10 | B5 | 143.6(3) | B10 | C3 | B4 | B5 | -37.0(3) |
| B1 | C3 | B10 | B6 | 104.1(3) | B10 | C3 | B4 | B9 | 2.7(4) |
| B1 | C3 | B10 | B7 | 40.5(3) | B10 | C3 | B5 | B4 | 141.0(3) |
| B1 | C13 | C14 | C15 | -174.9(4) | B10 | C3 | B5 | B6 | 38.7(3) |
| B1 | C13 | C18 | C17 | 174.6(4) | B10 | C3 | B5 | B9 | 101.5(3) |
| B1 | B2 | B3 | C2 | -35.8(3) | B10 | B1 | B2 | C2 | -93.3(3) |
| B1 | B2 | B3 | B4 | -2.3(4) | B10 | B1 | B2 | C20 | 150.5(4) |
| B1 | B2 | B3 | B8 | 98.6(3) | B10 | B1 | B2 | B3 | -58.7(4) |
| B1 | B2 | B3 | B9 | 61.5(4) | B10 | B1 | B2 | B7 | 38.7(3) |
| B1 | B2 | B7 | B6 | -102.8(4) | B10 | B1 | B2 | B8 | 3.0(4) |
| B1 | B2 | B7 | B8 | -139.3(3) | B10 | B1 | B7 | B2 | -136.1(3) |
| B1 | B2 | B7 | B10 | -39.5(3) | B10 | B1 | B7 | B6 | -34.7(3) |
| B1 | B2 | B8 | B3 | -101.9(3) | B10 | B1 | B7 | B8 | -99.0(4) |
| B1 | B2 | B8 | B6 | -1.3(4) | B10 | B5 | B6 | B7 | 37.1(3) |
| B1 | B2 | B8 | B7 | 35.4(3) | B10 | B5 | B6 | B8 | 99.9(4) |
| B1 | B2 | B8 | B9 | -65.3(4) | B10 | B5 | B6 | B9 | 138.3(3) |
| B1 | B7 | B8 | B2 | -37.5(3) | B10 | B5 | B9 | B3 | 62.8(4) |
| B1 | B7 | B8 | B3 | 0.8(4) | B10 | B5 | B9 | B4 | 101.5(4) |
| B1 | B7 | B8 | B6 | 102.0(4) | B10 | B5 | B9 | B6 | -37.2(3) |
| B1 | B7 | B8 | B9 | 64.6(4) | B10 | B5 | B9 | B8 | 0.9(4) |
| B1 | B7 | B10 | C3 | -41.2(3) | B10 | B6 | B7 | B1 | 35.1(3) |
| B1 | B7 | B10 | B5 | -103.5(3) | B10 | B6 | B7 | B2 | 100.5(3) |
| B1 | B7 | B10 | B6 | -141.7(3) | B10 | B6 | B7 | B8 | 137.3(3) |
| B2 | C2 | C3 | C4 | -144.9(3) | B10 | B6 | B8 | B2 | -1.0(4) |
| B2 | C2 | C3 | B1 | -38.2(3) | B10 | B6 | B8 | B3 | 63.1(4) |
| B2 | C2 | C3 | B4 | 106.8(3) | B10 | B6 | B8 | B7 | -37.7(3) |
| B2 | C2 | C3 | B5 | 69.1(4) | B10 | B6 | B8 | B9 | 100.6(4) |
| B2 | C2 | C3 | B10 | 2.2(4) | B10 | B6 | B9 | B3 | -63.4(4) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| B2 | C2 | B1 | C3 | 138.8(3) | B10 | B6 | B9 | B4 | 0.0(4) |
| B2 | C2 | B1 | C13 | -111.6(5) | B10 | B6 | B9 | B5 | 36.9(3) |
| B2 | C2 | B1 | B7 | 41.5(3) | B10 | B6 | B9 | B8 | -100.0(4) |
| B2 | C2 | B1 | B10 | 102.7(3) | B10 | B7 | B8 | B2 | -101.8(3) |
| B2 | C2 | B3 | B4 | -142.9(3) | B10 | B7 | B8 | B3 | -63.5(4) |
| B2 | C2 | B3 | B8 | -40.8(3) | B10 | B7 | B8 | B6 | 37.7(3) |
| B2 | C2 | B3 | B9 | -104.5(3) | B10 | B7 | B8 | B9 | 0.3(4) |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0848_CG_0m_4.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H4A | 3438.8 | 7144.07 | 5349.5 | 27 |
| H4B | 2771.38 | 6268.1 | 4789.27 | 27 |
| H5A | 1081.63 | 7247.77 | 4578.66 | 29 |
| H5B | 1641.83 | 8067.21 | 5211.34 | 29 |
| H6A | 2382.52 | 7892.1 | 3971.77 | 37 |
| H6B | 2876.23 | 8745.94 | 4593.65 | 37 |
| H7A | 1560.01 | 9621.47 | 3642.01 | 63 |
| H7B | 1079.93 | 9630.89 | 4310.82 | 63 |
| H7C | 590.22 | 8779.32 | 3686.93 | 63 |
| H8A | 3484.06 | 9756.83 | 6943.07 | 37 |
| H8B | 2399.21 | 10181.36 | 7159.81 | 37 |
| H9A | 2518.01 | 11082.77 | 6130.2 | 67 |
| H9B | 1376.45 | 10376.11 | 5954.99 | 67 |
| H9C | 2452.91 | 9939.98 | 5734.73 | 67 |
| H11A | 725.06 | 7858.53 | 6686.21 | 31 |
| H11B | 587.33 | 9149.8 | 6605.26 | 31 |
| H12A | 337.1 | 8662.42 | 7690.3 | 52 |
| H12B | 1503.64 | 9327.27 | 7847.65 | 52 |
| H12C | 1526.01 | 8029.58 | 7910.34 | 52 |
| H14 | 5092.17 | 5153.33 | 5699.78 | 24 |
| H15 | 6980.23 | 5501.34 | 5789.71 | 27 |
| H17 | 7184.43 | 7481.88 | 7441.65 | 26 |
| H18 | 5301.96 | 7138.75 | 7352.28 | 26 |
| H19A | 8575.94 | 7595.66 | 6585.22 | 50 |
| H19B | 8733.63 | 6407.16 | 6298.51 | 50 |
| H19C | 8996.62 | 6612.8 | 7126.5 | 50 |
| H21 | 4273.73 | 4515.82 | 8292.84 | 25 |
| H22 | 5417.56 | 4878.92 | 9418.55 | 31 |
| H24 | 4913.86 | 8092.38 | 9065.74 | 28 |
| H25 | 3740.13 | 7738.11 | 7946.75 | 26 |
| H26A | 5651.59 | 7076.56 | 10378.77 | 52 |
| H26B | 6675.13 | 7293.1 | 10047.52 | 52 |
| H26C | 6461.99 | 6095.92 | 10299.22 | 52 |

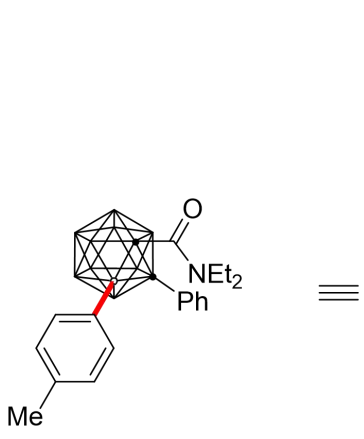
| | | | | |
|---|---|---|---|---|
| H3 | 1205.5 | 6430.25 | 7265.09 | 23 |
| H4 | 552 | 6838.36 | 5731.14 | 25 |
| H5 | 990.87 | 4844.53 | 5033.13 | 25 |
| H6 | 1852.61 | 3164.31 | 6142.01 | 27 |
| H7 | 4058.64 | 3947.21 | 7061.35 | 22 |
| H8 | 1987.47 | 4177.52 | 7514.71 | 23 |
| H9 | 66.29 | 4711.67 | 6258.06 | 25 |
| H10 | 3410.67 | 4356.29 | 5525.16 | 23 |

**Experimental**

Single crystals of $C_{25}H_{41}B_{10}NO$ [mo_0848_CG_0m_4] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a Bruker D8 Venture AgCu Dual Source diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

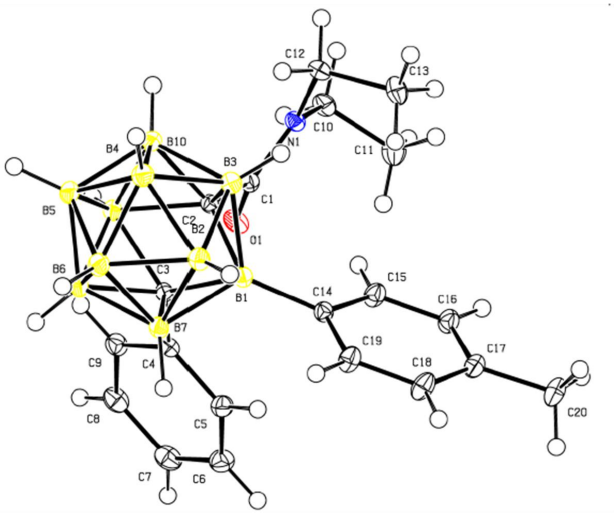
**Crystal structure determination of 3fa**

**Crystal Data** for $C_{25}H_{41}B_{10}NO$ (*M* =479.69 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 12.2842(10) Å, *b* = 12.2978(10) Å, *c* = 19.8427(15) Å, *β* = 106.783(2)°, *V* = 2869.9(4) Å$^3$, *Z* = 4, *T* = 100.0 K, μ(MoKα) = 0.060 mm$^{-1}$, *Dcalc* = 1.110 g/cm$^3$, 11362 reflections measured (3.946° ≤ 2Θ ≤ 52.818°), 11362 unique ($R_{int}$ = ?, $R_{sigma}$ = 0.0660) which were used in all calculations. The final $R_1$ was 0.0861 (I > 2σ(I)) and $wR_2$ was 0.1966 (all data).




**4aa**

≡




**CCDC 1893313**

**Crystal data and structure refinement for 4aa.**

| | |
|---|---|
| Identification code | 0544_CG_0m |
| CCDC number | 1893305 |
| Empirical formula | $C_{20}H_{31}B_{10}NO$ |
| Formula weight | 409.56 |
| Temperature/K | 100.02 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 9.9001(6) |
| b/Å | 10.5092(9) |
| c/Å | 21.5172(15) |
| α/° | 90 |
| β/° | 90.643(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 2238.6(3) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.215 |
| μ/mm$^{-1}$ | 0.066 |
| F(000) | 864.0 |
| Crystal size/mm$^3$ | 0.601 × 0.531 × 0.45 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.314 to 61.04 |
| Index ranges | $-14 \le h \le 11$, $-15 \le k \le 15$, $-30 \le l \le 30$ |
| Reflections collected | 42852 |
| Independent reflections | 6725 [$R_{int}$ = 0.0241, $R_{sigma}$ = 0.0168] |
| Data/restraints/parameters | 6725/0/328 |
| Goodness-of-fit on $F^2$ | 1.048 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0380, $wR_2$ = 0.1027 |
| Final R indexes [all data] | $R_1$ = 0.0401, $wR_2$ = 0.1045 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.41/-0.20 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for 0544_CG_0m. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O1 | 4102.8(6) | 8491.8(6) | 5408.1(3) | 17.17(13) |
| N1 | 5820.9(7) | 8610.4(6) | 6100.3(3) | 12.73(13) |
| C1 | 4505.6(8) | 8448.2(7) | 5948.5(4) | 12.26(14) |
| C2 | 3415.3(7) | 8262.8(7) | 6449.3(4) | 11.79(14) |
| C3 | 1825.9(7) | 7836.8(7) | 6137.2(4) | 12.27(14) |
| C4 | 1530.0(7) | 7547.0(8) | 5460.4(4) | 13.20(14) |
| C5 | 1502.1(8) | 6293.7(8) | 5247.3(4) | 16.61(15) |
| C6 | 1101.7(9) | 6023.3(9) | 4638.1(4) | 19.94(17) |
| C7 | 703.2(9) | 6993.1(9) | 4238.2(4) | 20.42(17) |

| | | | | |
|---|---|---|---|---|
| C8 | 714.4(9) | 8241.0(9) | 4450.9(4) | 19.81(17) |
| C9 | 1123.7(8) | 8520.2(8) | 5055.4(4) | 16.78(15) |
| C10 | 6717.8(8) | 8879.9(8) | 5570.3(4) | 16.00(15) |
| C11 | 7187.7(10) | 7699.3(10) | 5224.3(4) | 23.65(18) |
| C12 | 6477.8(8) | 8538.0(8) | 6715.2(4) | 15.21(15) |
| C13 | 7102.9(9) | 7240.0(9) | 6846.1(4) | 20.46(17) |
| C14 | 3425.4(8) | 5481.2(7) | 6391.2(4) | 12.78(14) |
| C15 | 4528.6(8) | 5398.7(8) | 5992.4(4) | 17.32(16) |
| C16 | 5174.0(9) | 4245.5(8) | 5880.0(4) | 17.96(16) |
| C17 | 4735.7(9) | 3124.2(8) | 6154.9(4) | 15.98(15) |
| C18 | 3592.8(10) | 3185.4(8) | 6528.5(4) | 19.80(17) |
| C19 | 2959.7(9) | 4337.8(8) | 6648.3(4) | 17.73(16) |
| C20 | 5461.9(10) | 1883.5(8) | 6055.8(4) | 21.19(17) |
| B1 | 2753.1(9) | 6758.9(8) | 6605.0(4) | 12.55(15) |
| B2 | 2007.1(9) | 6952.4(9) | 7359.1(4) | 14.64(16) |
| B3 | 3548.5(9) | 7719.9(9) | 7195.7(4) | 13.85(16) |
| B4 | 2297.1(9) | 8546.9(9) | 7621.7(4) | 16.35(17) |
| B5 | 1433.8(9) | 9591.2(9) | 7095.6(4) | 16.49(17) |
| B6 | 602.7(9) | 8639.4(9) | 6530.1(4) | 15.07(16) |
| B7 | 966.5(9) | 7014.1(8) | 6687.0(4) | 13.87(16) |
| B8 | 697.7(9) | 8105.3(9) | 7310.8(4) | 16.05(17) |
| B9 | 2155.2(9) | 9396.0(8) | 6352.7(4) | 14.20(16) |
| B10 | 3204.6(9) | 9346.7(8) | 7032.2(4) | 14.58(16) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for 0544_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 14.1(3) | 23.2(3) | 14.2(3) | 3.9(2) | -0.7(2) | -1.5(2) |
| N1 | 10.9(3) | 13.4(3) | 13.9(3) | 1.6(2) | 0.4(2) | -0.6(2) |
| C1 | 11.6(3) | 10.4(3) | 14.8(3) | 1.5(2) | 1.4(2) | 0.0(2) |
| C2 | 10.3(3) | 11.3(3) | 13.7(3) | 0.6(2) | 0.3(2) | -0.1(2) |
| C3 | 10.4(3) | 11.4(3) | 14.9(3) | 0.9(3) | -0.2(2) | 0.5(2) |
| C4 | 10.5(3) | 15.0(3) | 14.0(3) | 0.9(3) | -0.4(2) | -0.6(3) |
| C5 | 17.0(3) | 15.6(4) | 17.2(4) | -0.4(3) | -1.8(3) | -0.2(3) |
| C6 | 20.0(4) | 21.2(4) | 18.6(4) | -4.0(3) | -1.0(3) | -1.1(3) |
| C7 | 17.4(4) | 28.8(4) | 15.1(4) | -0.7(3) | -0.6(3) | -1.7(3) |
| C8 | 18.2(4) | 24.1(4) | 17.1(4) | 5.2(3) | -2.1(3) | -0.1(3) |
| C9 | 15.8(3) | 16.4(4) | 18.1(4) | 2.7(3) | -1.5(3) | 0.1(3) |
| C10 | 12.2(3) | 18.7(4) | 17.2(3) | 3.2(3) | 2.7(3) | -2.0(3) |
| C11 | 24.6(4) | 27.0(4) | 19.5(4) | 0.1(3) | 6.2(3) | 5.4(3) |
| C12 | 12.0(3) | 18.2(4) | 15.4(3) | -0.2(3) | -1.9(3) | -1.7(3) |
| C13 | 17.6(4) | 25.2(4) | 18.5(4) | 3.7(3) | -1.0(3) | 6.0(3) |
| C14 | 12.7(3) | 11.9(3) | 13.7(3) | 1.3(2) | -0.1(2) | 0.6(3) |
| C15 | 17.5(3) | 12.6(3) | 22.0(4) | 1.0(3) | 5.6(3) | -0.5(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 16.4(3) | 15.3(4) | 22.3(4) | -1.9(3) | 4.7(3) | 0.6(3) |
| C17 | 20.1(4) | 13.5(3) | 14.3(3) | -1.2(3) | -1.0(3) | 2.9(3) |
| C18 | 28.2(4) | 12.0(3) | 19.4(4) | 2.7(3) | 6.7(3) | 1.1(3) |
| C19 | 20.6(4) | 13.7(3) | 19.0(4) | 2.3(3) | 6.5(3) | 0.2(3) |
| C20 | 29.0(4) | 14.9(4) | 19.7(4) | -1.4(3) | 1.6(3) | 7.2(3) |
| B1 | 11.9(3) | 11.6(3) | 14.2(4) | 1.8(3) | 1.2(3) | 0.2(3) |
| B2 | 14.0(4) | 15.5(4) | 14.5(4) | 1.0(3) | 2.8(3) | 0.1(3) |
| B3 | 13.7(3) | 14.9(4) | 13.0(3) | 0.7(3) | 0.9(3) | 0.2(3) |
| B4 | 15.8(4) | 17.1(4) | 16.1(4) | -1.7(3) | 2.6(3) | 0.1(3) |
| B5 | 14.6(4) | 15.1(4) | 19.9(4) | -2.6(3) | 2.3(3) | 1.4(3) |
| B6 | 12.0(3) | 13.9(4) | 19.4(4) | -0.5(3) | 1.5(3) | 1.7(3) |
| B7 | 11.8(3) | 13.6(4) | 16.2(4) | 0.9(3) | 2.3(3) | -0.2(3) |
| B8 | 14.0(4) | 16.3(4) | 18.0(4) | -1.1(3) | 3.5(3) | 0.5(3) |
| B9 | 12.6(3) | 11.8(4) | 18.2(4) | 0.2(3) | 0.2(3) | 1.2(3) |
| B10 | 14.3(4) | 13.1(4) | 16.4(4) | -1.9(3) | 1.0(3) | 0.1(3) |

**Bond Lengths for 0544_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O1 | C1 | 1.2259(10) | C15 | C16 | 1.3924(11) |
| N1 | C1 | 1.3497(10) | C16 | C17 | 1.3902(12) |
| N1 | C10 | 1.4804(10) | C17 | C18 | 1.3968(12) |
| N1 | C12 | 1.4698(10) | C17 | C20 | 1.5052(12) |
| C1 | C2 | 1.5461(10) | C18 | C19 | 1.3891(12) |
| C2 | C3 | 1.7617(11) | B1 | B2 | 1.8018(12) |
| C2 | B1 | 1.7449(12) | B1 | B3 | 1.7981(13) |
| C2 | B3 | 1.7080(12) | B1 | B7 | 1.7996(12) |
| C2 | B9 | 1.7355(12) | B2 | B3 | 1.7649(13) |
| C2 | B10 | 1.7088(12) | B2 | B4 | 1.7905(13) |
| C3 | C4 | 1.5132(11) | B2 | B7 | 1.7673(13) |
| C3 | B1 | 1.7659(12) | B2 | B8 | 1.7766(13) |
| C3 | B6 | 1.7075(12) | B3 | B4 | 1.7764(13) |
| C3 | B7 | 1.7010(12) | B3 | B10 | 1.7775(13) |
| C3 | B9 | 1.7329(12) | B4 | B5 | 1.7873(14) |
| C4 | C5 | 1.3947(11) | B4 | B8 | 1.7738(13) |
| C4 | C9 | 1.3997(11) | B4 | B10 | 1.7743(13) |
| C5 | C6 | 1.3945(11) | B5 | B6 | 1.7709(13) |
| C6 | C7 | 1.3882(13) | B5 | B8 | 1.7865(14) |
| C7 | C8 | 1.3890(13) | B5 | B9 | 1.7701(13) |
| C8 | C9 | 1.3894(12) | B5 | B10 | 1.7787(13) |
| C10 | C11 | 1.5225(13) | B6 | B7 | 1.7772(13) |
| C12 | C13 | 1.5229(12) | B6 | B8 | 1.7726(14) |
| C14 | C15 | 1.3992(11) | B6 | B9 | 1.7758(13) |
| C14 | C19 | 1.4029(11) | B7 | B8 | 1.7876(13) |

| | | | | | |
|---|---|---|---|---|---|
| C14 | B1 | 1.5699(12) | B9 | B10 | 1.7849(13) |

**Bond Angles for 0544_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 115.04(7) | C2 | B3 | B1 | 59.63(5) |
| C1 | N1 | C12 | 128.84(7) | C2 | B3 | B2 | 106.38(6) |
| C12 | N1 | C10 | 116.12(6) | C2 | B3 | B4 | 105.95(6) |
| O1 | C1 | N1 | 121.83(7) | C2 | B3 | B10 | 58.67(5) |
| O1 | C1 | C2 | 116.33(7) | B2 | B3 | B1 | 60.75(5) |
| N1 | C1 | C2 | 121.78(7) | B2 | B3 | B4 | 60.74(5) |
| C1 | C2 | C3 | 113.20(6) | B2 | B3 | B10 | 108.35(6) |
| C1 | C2 | B1 | 120.97(6) | B4 | B3 | B1 | 109.70(6) |
| C1 | C2 | B3 | 130.56(6) | B4 | B3 | B10 | 59.90(5) |
| C1 | C2 | B9 | 109.67(6) | B10 | B3 | B1 | 108.60(6) |
| C1 | C2 | B10 | 121.29(6) | B3 | B4 | B2 | 59.31(5) |
| B1 | C2 | C3 | 60.47(5) | B3 | B4 | B5 | 107.76(6) |
| B3 | C2 | C3 | 109.44(6) | B5 | B4 | B2 | 107.52(6) |
| B3 | C2 | B1 | 62.75(5) | B8 | B4 | B2 | 59.79(5) |
| B3 | C2 | B9 | 112.93(6) | B8 | B4 | B3 | 107.59(6) |
| B3 | C2 | B10 | 62.69(5) | B8 | B4 | B5 | 60.22(5) |
| B9 | C2 | C3 | 59.40(5) | B8 | B4 | B10 | 108.14(6) |
| B9 | C2 | B1 | 111.93(6) | B10 | B4 | B2 | 107.37(6) |
| B10 | C2 | C3 | 109.48(6) | B10 | B4 | B3 | 60.08(5) |
| B10 | C2 | B1 | 114.44(6) | B10 | B4 | B5 | 59.92(5) |
| B10 | C2 | B9 | 62.42(5) | B6 | B5 | B4 | 107.67(7) |
| C2 | C3 | B1 | 59.29(4) | B6 | B5 | B8 | 59.77(5) |
| C4 | C3 | C2 | 125.49(6) | B6 | B5 | B10 | 108.45(6) |
| C4 | C3 | B1 | 120.88(6) | B8 | B5 | B4 | 59.52(5) |
| C4 | C3 | B6 | 116.44(6) | B9 | B5 | B4 | 107.81(6) |
| C4 | C3 | B7 | 118.30(6) | B9 | B5 | B6 | 60.20(5) |
| C4 | C3 | B9 | 118.80(6) | B9 | B5 | B8 | 107.61(6) |
| B6 | C3 | C2 | 108.73(6) | B9 | B5 | B10 | 60.39(5) |
| B6 | C3 | B1 | 113.68(6) | B10 | B5 | B4 | 59.68(5) |
| B6 | C3 | B9 | 62.15(5) | B10 | B5 | B8 | 107.39(6) |
| B7 | C3 | C2 | 108.39(6) | C3 | B6 | B5 | 107.02(6) |
| B7 | C3 | B1 | 62.51(5) | C3 | B6 | B7 | 58.40(5) |
| B7 | C3 | B6 | 62.85(5) | C3 | B6 | B8 | 106.40(6) |
| B7 | C3 | B9 | 112.86(6) | C3 | B6 | B9 | 59.63(5) |
| B9 | C3 | C2 | 59.54(5) | B5 | B6 | B7 | 108.71(6) |
| B9 | C3 | B1 | 111.04(6) | B5 | B6 | B8 | 60.55(5) |
| C5 | C4 | C3 | 120.62(7) | B5 | B6 | B9 | 59.88(5) |
| C5 | C4 | C9 | 118.75(7) | B8 | B6 | B7 | 60.47(5) |
| C9 | C4 | C3 | 120.21(7) | B8 | B6 | B9 | 107.97(6) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C6 | C5 | C4 | 120.38(8) | B9 | B6 | B7 | 107.28(6) |
| C7 | C6 | C5 | 120.59(8) | C3 | B7 | B1 | 60.51(5) |
| C6 | C7 | C8 | 119.19(8) | C3 | B7 | B2 | 107.23(6) |
| C7 | C8 | C9 | 120.60(8) | C3 | B7 | B6 | 58.75(5) |
| C8 | C9 | C4 | 120.48(8) | C3 | B7 | B8 | 106.02(6) |
| N1 | C10 | C11 | 114.20(7) | B2 | B7 | B1 | 60.67(5) |
| N1 | C12 | C13 | 112.81(7) | B2 | B7 | B6 | 107.80(6) |
| C15 | C14 | C19 | 116.81(7) | B2 | B7 | B8 | 59.97(5) |
| C15 | C14 | B1 | 124.69(7) | B6 | B7 | B1 | 108.78(6) |
| C19 | C14 | B1 | 118.35(7) | B6 | B7 | B8 | 59.64(5) |
| C16 | C15 | C14 | 121.56(8) | B8 | B7 | B1 | 108.91(6) |
| C17 | C16 | C15 | 121.19(8) | B2 | B8 | B5 | 108.17(6) |
| C16 | C17 | C18 | 117.68(8) | B2 | B8 | B7 | 59.45(5) |
| C16 | C17 | C20 | 121.48(8) | B4 | B8 | B2 | 60.57(5) |
| C18 | C17 | C20 | 120.84(8) | B4 | B8 | B5 | 60.27(5) |
| C19 | C18 | C17 | 121.14(8) | B4 | B8 | B7 | 108.13(6) |
| C18 | C19 | C14 | 121.50(8) | B5 | B8 | B7 | 107.55(6) |
| C2 | B1 | C3 | 60.23(4) | B6 | B8 | B2 | 107.59(6) |
| C2 | B1 | B2 | 103.26(6) | B6 | B8 | B4 | 108.19(6) |
| C2 | B1 | B3 | 57.62(5) | B6 | B8 | B5 | 59.68(5) |
| C2 | B1 | B7 | 104.81(6) | B6 | B8 | B7 | 59.89(5) |
| C3 | B1 | B2 | 103.02(6) | C2 | B9 | B5 | 105.55(6) |
| C3 | B1 | B3 | 105.27(6) | C2 | B9 | B6 | 106.84(6) |
| C3 | B1 | B7 | 56.98(5) | C2 | B9 | B10 | 58.06(5) |
| C14 | B1 | C2 | 123.85(6) | C3 | B9 | C2 | 61.05(5) |
| C14 | B1 | C3 | 126.95(7) | C3 | B9 | B5 | 105.94(6) |
| C14 | B1 | B2 | 122.67(6) | C3 | B9 | B6 | 58.22(5) |
| C14 | B1 | B3 | 120.25(6) | C3 | B9 | B10 | 107.33(6) |
| C14 | B1 | B7 | 125.21(7) | B5 | B9 | B6 | 59.92(5) |
| B3 | B1 | B2 | 58.72(5) | B5 | B9 | B10 | 60.04(5) |
| B3 | B1 | B7 | 105.67(6) | B6 | B9 | B10 | 107.95(6) |
| B7 | B1 | B2 | 58.78(5) | C2 | B10 | B3 | 58.63(5) |
| B3 | B2 | B1 | 60.54(5) | C2 | B10 | B4 | 106.01(6) |
| B3 | B2 | B4 | 59.95(5) | C2 | B10 | B5 | 106.33(6) |
| B3 | B2 | B7 | 108.52(6) | C2 | B10 | B9 | 59.52(5) |
| B3 | B2 | B8 | 107.98(6) | B3 | B10 | B5 | 108.09(6) |
| B4 | B2 | B1 | 108.90(6) | B3 | B10 | B9 | 107.37(6) |
| B7 | B2 | B1 | 60.55(5) | B4 | B10 | B3 | 60.02(5) |
| B7 | B2 | B4 | 108.29(6) | B4 | B10 | B5 | 60.40(5) |
| B7 | B2 | B8 | 60.58(5) | B4 | B10 | B9 | 107.73(6) |
| B8 | B2 | B1 | 109.30(6) | B5 | B10 | B9 | 59.57(5) |
| B8 | B2 | B4 | 59.64(5) | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for 0544_CG_0m.**

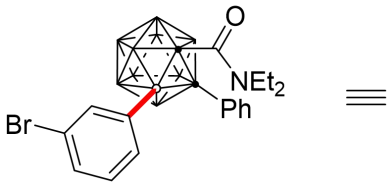
| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | 1757.48 | 5620.4 | 5518.81 | 20 |
| H6 | 1101.62 | 5167.86 | 4495.47 | 24 |
| H7 | 426.16 | 6805.57 | 3824.13 | 25 |
| H8 | 439.69 | 8909.68 | 4180.64 | 24 |
| H9 | 1127.96 | 9377.85 | 5194.95 | 20 |
| H10A | 7521.43 | 9346.87 | 5726.1 | 19 |
| H10B | 6234.07 | 9443.43 | 5273.87 | 19 |
| H11A | 7729.81 | 7954.75 | 4867.05 | 35 |
| H11B | 6399.88 | 7214.18 | 5079.16 | 35 |
| H11C | 7736.03 | 7168.88 | 5504.13 | 35 |
| H12A | 5802.23 | 8726.85 | 7038.19 | 18 |
| H12B | 7191.85 | 9195.8 | 6742.69 | 18 |
| H13A | 7784.33 | 7053.27 | 6532.13 | 31 |
| H13B | 6396.89 | 6586.71 | 6831.2 | 31 |
| H13C | 7529.57 | 7244.8 | 7259.29 | 31 |
| H15 | 4844.83 | 6147.12 | 5793.69 | 21 |
| H16 | 5927.34 | 4224.71 | 5610.54 | 22 |
| H18 | 3242.42 | 2425.81 | 6703.59 | 24 |
| H19 | 2193.99 | 4351.96 | 6910.38 | 21 |
| H20A | 4820.69 | 1244.24 | 5901.09 | 32 |
| H20B | 5858.35 | 1594.18 | 6450.54 | 32 |
| H20C | 6179.4 | 2004.35 | 5751.34 | 32 |
| H2 | 2010(13) | 6141(13) | 7678(6) | 25(3) |
| H3 | 4479(12) | 7391(12) | 7364(6) | 20(3) |
| H4 | 2466(14) | 8783(13) | 8106(6) | 26(3) |
| H5A | 1012(13) | 10514(13) | 7217(6) | 26(3) |
| H6A | -281(12) | 8886(12) | 6259(6) | 20(3) |
| H7A | 292(13) | 6263(12) | 6524(6) | 21(3) |
| H8A | -224(13) | 8031(12) | 7604(6) | 24(3) |
| H9A | 2292(12) | 10088(12) | 6002(6) | 20(3) |
| H10 | 3960(13) | 10055(13) | 7077(6) | 24(3) |

## Experimental

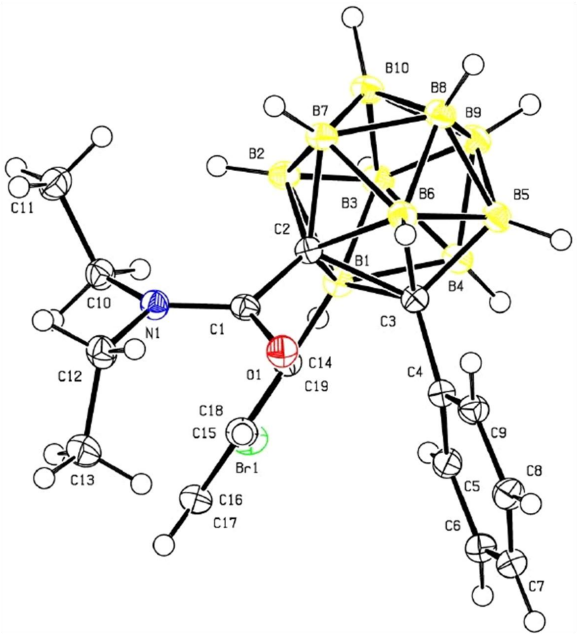
Single crystals of $C_{20}H_{31}B_{10}NO$ [0544_CG_0m] were recrystallised from a mixture of Chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 100.02 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

**Crystal structure determination of 4aa**

**Crystal Data** for $C_{20}H_{31}B_{10}NO$ ($M$ =409.56 g/mol): monoclinic, space group $P2_1/c$ (no. 14), $a$ = 9.9001(6) Å, $b$ = 10.5092(9) Å, $c$ = 21.5172(15) Å, $\beta$ = 90.643(3)°, $V$ = 2238.6(3) Å$^3$, $Z$ = 4, $T$ = 100.02 K, μ(MoKα) = 0.066 mm$^{-1}$, *Dcalc* = 1.215 g/cm$^3$, 42852 reflections measured (4.314° ≤ 2Θ ≤ 61.04°), 6725 unique ($R_{int}$ = 0.0241, $R_{sigma}$ = 0.0168) which were used in all calculations. The final $R_1$was 0.0380 (I > 2σ(I)) and $wR_2$ was 0.1045 (all data).




**4ai**




**CCDC 1983611**

**Crystal data and structure refinement for 4ai.**

| | |
|---|---|
| Identification code | mo_0828_CG_0m |
| CCDC number | 1983611 |
| Empirical formula | $C_{19}H_{28}B_{10}BrNO$ |
| Formula weight | 474.43 |
| Temperature/K | 100.0 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 11.5021(12) |
| b/Å | 11.2242(12) |
| c/Å | 17.6391(19) |
| α/° | 90 |
| β/° | 97.227(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 2259.1(4) |
| Z | 4 |

| | |
|---|---|
| $\rho_{calc}$g/cm$^3$ | 1.395 |
| $\mu$/mm$^{-1}$ | 1.833 |
| F(000) | 968.0 |
| Crystal size/mm$^3$ | 0.3 × 0.25 × 0.25 |
| Radiation | MoK$\alpha$ ($\lambda$ = 0.71073) |
| 2$\Theta$ range for data collection/° | 4.312 to 59.356 |
| Index ranges | $-15 \leq h \leq 15$, $-15 \leq k \leq 15$, $-23 \leq l \leq 24$ |
| Reflections collected | 69892 |
| Independent reflections | 6364 [$R_{int}$ = 0.0329, $R_{sigma}$ = 0.0179] |
| Data/restraints/parameters | 6364/0/318 |
| Goodness-of-fit on $F^2$ | 1.055 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0276, $wR_2$ = 0.0735 |
| Final R indexes [all data] | $R_1$ = 0.0306, $wR_2$ = 0.0749 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.84/-0.59 |

**Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0828_CG_0m. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| Br1 | 5976.2(2) | 2014.7(2) | 3329.9(2) | 22.78(5) |
| O1 | 6018.8(9) | 9339.2(10) | 3282.3(6) | 20.6(2) |
| N1 | 6859.0(11) | 8446.1(12) | 4355.0(7) | 18.7(2) |
| C1 | 5957.7(13) | 8630.1(13) | 3805.1(8) | 17.1(3) |
| C2 | 4753.3(13) | 8017.0(13) | 3822.6(8) | 16.4(3) |
| C3 | 3984.4(13) | 7749.4(13) | 2921.7(8) | 17.1(3) |
| C4 | 4469.8(13) | 7930.0(13) | 2171.0(8) | 17.9(3) |
| C5 | 4810.6(14) | 6951.1(14) | 1763.2(9) | 20.4(3) |
| C6 | 5146.6(14) | 7106.5(15) | 1037.4(9) | 23.1(3) |
| C7 | 5110.3(14) | 8222.3(16) | 702.9(9) | 24.0(3) |
| C8 | 4739.5(14) | 9194.7(15) | 1096.8(9) | 23.5(3) |
| C9 | 4428.7(14) | 9053.3(14) | 1827.4(9) | 20.5(3) |
| C10 | 7045.3(14) | 7465.7(14) | 4911.7(9) | 21.0(3) |
| C11 | 6865.0(16) | 7854.7(16) | 5711.2(9) | 26.5(3) |
| C12 | 7898.2(14) | 9211.6(15) | 4330.5(9) | 22.7(3) |
| C13 | 8777.5(15) | 8667.3(17) | 3853.6(10) | 28.4(3) |
| C14 | 5516.6(13) | 5699.6(13) | 3378.0(8) | 17.5(3) |
| C15 | 6602.4(13) | 6092.6(14) | 3189.4(9) | 19.5(3) |
| C16 | 7491.5(14) | 5304.2(14) | 3086.5(9) | 21.3(3) |
| C17 | 7316.5(14) | 4081.6(14) | 3147.1(9) | 20.6(3) |
| C18 | 6236.4(14) | 3680.0(13) | 3310.4(8) | 19.1(3) |
| C19 | 5345.9(13) | 4466.5(13) | 3435.5(8) | 18.4(3) |
| B1 | 4486.7(15) | 6556.7(15) | 3532.0(10) | 17.8(3) |
| B2 | 4281.1(15) | 7048.8(15) | 4477.1(10) | 19.1(3) |

| | | | | |
|---|---|---|---|---|
| B3 | 3205.8(15) | 6149.4(16) | 3956.2(10) | 20.1(3) |
| B4 | 3049.1(15) | 6590.1(15) | 2987.0(10) | 19.2(3) |
| B5 | 2534.7(15) | 8090.3(16) | 2932.8(10) | 19.7(3) |
| B6 | 3644.1(15) | 8983.0(15) | 3439.9(10) | 18.3(3) |
| B7 | 3805.1(15) | 8550.3(16) | 4418.9(10) | 19.3(3) |
| B8 | 2396.3(15) | 8580.4(16) | 3869.1(10) | 20.1(3) |
| B9 | 2015.4(15) | 7088.3(16) | 3592.6(11) | 21.0(3) |
| B10 | 2789.9(15) | 7380.6(16) | 4507.6(10) | 20.6(3) |

**Anisotropic Displacement Parameters ($Å^2×10^3$) for mo_0828_CG_0m. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Br1 | 29.49(9) | 14.46(7) | 25.50(8) | 0.02(5) | 7.82(6) | 1.09(6) |
| O1 | 21.4(5) | 19.3(5) | 21.1(5) | 4.1(4) | 2.5(4) | -2.5(4) |
| N1 | 18.0(6) | 18.9(6) | 19.2(6) | 1.0(5) | 1.6(5) | -1.8(5) |
| C1 | 17.3(6) | 15.6(6) | 18.9(6) | -2.2(5) | 4.5(5) | -0.7(5) |
| C2 | 17.1(6) | 15.7(6) | 16.6(6) | -0.3(5) | 2.6(5) | -0.8(5) |
| C3 | 17.5(6) | 16.1(6) | 17.7(6) | -0.5(5) | 2.2(5) | -0.2(5) |
| C4 | 16.7(6) | 20.1(7) | 16.9(6) | -0.1(5) | 1.9(5) | 0.4(5) |
| C5 | 21.0(7) | 20.4(7) | 19.5(7) | -0.9(5) | 1.7(5) | 2.2(6) |
| C6 | 22.8(7) | 26.6(8) | 20.1(7) | -3.0(6) | 3.4(6) | 3.1(6) |
| C7 | 21.3(7) | 32.8(8) | 18.2(7) | 0.9(6) | 3.5(6) | 1.1(6) |
| C8 | 24.7(7) | 24.0(8) | 21.9(7) | 4.4(6) | 3.6(6) | 1.3(6) |
| C9 | 21.0(7) | 19.9(7) | 20.7(7) | 0.8(6) | 3.7(5) | 1.3(6) |
| C10 | 20.1(7) | 21.9(7) | 20.6(7) | 3.4(6) | 1.8(5) | 1.1(6) |
| C11 | 27.5(8) | 32.2(9) | 19.8(7) | 1.1(6) | 2.6(6) | -3.0(7) |
| C12 | 18.8(7) | 23.7(7) | 25.2(7) | 0.5(6) | 1.3(6) | -4.6(6) |
| C13 | 21.5(7) | 36.4(9) | 28.3(8) | 2.5(7) | 6.4(6) | -2.2(7) |
| C14 | 18.7(6) | 16.6(6) | 17.3(6) | 0.3(5) | 2.7(5) | 0.8(5) |
| C15 | 21.3(7) | 16.2(6) | 21.4(7) | 0.3(5) | 4.5(5) | -0.9(5) |
| C16 | 20.5(7) | 20.9(7) | 23.3(7) | 0.2(6) | 5.8(6) | -0.5(6) |
| C17 | 22.1(7) | 19.2(7) | 20.7(7) | 0.3(5) | 4.0(5) | 3.4(6) |
| C18 | 25.5(7) | 14.7(6) | 17.4(6) | -0.7(5) | 3.5(5) | 2.1(5) |
| C19 | 19.2(7) | 16.9(6) | 19.5(6) | 0.5(5) | 4.3(5) | 0.3(5) |
| B1 | 18.5(7) | 15.2(7) | 20.2(7) | 0.2(6) | 3.9(6) | -0.6(6) |
| B2 | 20.0(7) | 18.7(7) | 19.3(7) | 1.0(6) | 4.9(6) | -1.0(6) |
| B3 | 19.7(8) | 18.2(7) | 23.3(8) | 0.1(6) | 5.4(6) | -2.4(6) |
| B4 | 18.3(7) | 17.0(7) | 22.6(8) | -2.4(6) | 3.3(6) | -1.5(6) |
| B5 | 17.4(7) | 19.2(7) | 22.3(8) | -2.0(6) | 2.1(6) | 1.4(6) |
| B6 | 18.6(7) | 16.6(7) | 19.8(7) | -1.5(6) | 2.5(6) | 1.6(6) |
| B7 | 19.8(7) | 18.8(7) | 20.0(7) | -2.2(6) | 5.8(6) | -0.8(6) |
| B8 | 18.4(7) | 19.5(8) | 22.9(8) | -2.9(6) | 4.8(6) | 0.2(6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| B9 | 17.7(7) | 20.8(8) | 24.9(8) | -2.7(6) | 4.6(6) | -2.0(6) |
| B10 | 19.2(8) | 21.6(8) | 22.2(8) | -0.8(6) | 6.8(6) | -2.0(6) |

**Bond Lengths for mo_0828_CG_0m.**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Br1 | C18 | 1.8940(15) | C14 | B1 | 1.576(2) |
| O1 | C1 | 1.2267(18) | C15 | C16 | 1.382(2) |
| N1 | C1 | 1.3437(19) | C16 | C17 | 1.393(2) |
| N1 | C10 | 1.472(2) | C17 | C18 | 1.386(2) |
| N1 | C12 | 1.4771(19) | C18 | C19 | 1.391(2) |
| C1 | C2 | 1.551(2) | B1 | B2 | 1.800(2) |
| C2 | C3 | 1.745(2) | B1 | B3 | 1.794(2) |
| C2 | B1 | 1.733(2) | B1 | B4 | 1.806(2) |
| C2 | B2 | 1.722(2) | B2 | B3 | 1.763(2) |
| C2 | B6 | 1.744(2) | B2 | B7 | 1.771(2) |
| C2 | B7 | 1.715(2) | B2 | B10 | 1.763(2) |
| C3 | C4 | 1.514(2) | B3 | B4 | 1.767(3) |
| C3 | B1 | 1.769(2) | B3 | B9 | 1.782(3) |
| C3 | B4 | 1.701(2) | B3 | B10 | 1.789(3) |
| C3 | B5 | 1.713(2) | B4 | B5 | 1.783(2) |
| C3 | B6 | 1.731(2) | B4 | B9 | 1.785(2) |
| C4 | C5 | 1.396(2) | B5 | B6 | 1.773(2) |
| C4 | C9 | 1.397(2) | B5 | B8 | 1.767(2) |
| C5 | C6 | 1.394(2) | B5 | B9 | 1.775(3) |
| C6 | C7 | 1.383(2) | B6 | B7 | 1.781(2) |
| C7 | C8 | 1.389(2) | B6 | B8 | 1.764(2) |
| C8 | C9 | 1.389(2) | B7 | B8 | 1.781(3) |
| C10 | C11 | 1.515(2) | B7 | B10 | 1.777(3) |
| C12 | C13 | 1.522(2) | B8 | B9 | 1.784(3) |
| C14 | C15 | 1.403(2) | B8 | B10 | 1.777(3) |
| C14 | C19 | 1.403(2) | B9 | B10 | 1.773(3) |

**Bond Angles for mo_0828_CG_0m.**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C1 | N1 | C10 | 129.10(13) | B2 | B3 | B1 | 60.80(10) |
| C1 | N1 | C12 | 116.31(13) | B2 | B3 | B4 | 108.87(12) |
| C10 | N1 | C12 | 113.82(12) | B2 | B3 | B9 | 107.81(12) |
| O1 | C1 | N1 | 122.03(14) | B2 | B3 | B10 | 59.49(10) |
| O1 | C1 | C2 | 116.02(13) | B4 | B3 | B1 | 60.93(10) |
| N1 | C1 | C2 | 121.84(13) | B4 | B3 | B9 | 60.40(10) |
| C1 | C2 | C3 | 114.20(11) | B4 | B3 | B10 | 107.94(12) |
| C1 | C2 | B1 | 122.62(12) | B9 | B3 | B1 | 109.47(12) |

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|---|---|---|---|---|---|---|---|
| C1 | C2 | B2 | 130.63(12) | B9 | B3 | B10 | 59.54(10) |
| C1 | C2 | B6 | 109.16(11) | B10 | B3 | B1 | 108.64(12) |
| C1 | C2 | B7 | 119.73(12) | C3 | B4 | B1 | 60.49(9) |
| B1 | C2 | C3 | 61.14(9) | C3 | B4 | B3 | 106.93(12) |
| B1 | C2 | B6 | 112.33(11) | C3 | B4 | B5 | 58.84(9) |
| B2 | C2 | C3 | 109.60(11) | C3 | B4 | B9 | 105.98(12) |
| B2 | C2 | B1 | 62.78(9) | B3 | B4 | B1 | 60.26(10) |
| B2 | C2 | B6 | 112.01(11) | B3 | B4 | B5 | 107.99(12) |
| B6 | C2 | C3 | 59.49(9) | B3 | B4 | B9 | 60.22(10) |
| B7 | C2 | C3 | 109.27(11) | B5 | B4 | B1 | 108.88(12) |
| B7 | C2 | B1 | 114.13(11) | B5 | B4 | B9 | 59.66(10) |
| B7 | C2 | B2 | 62.01(10) | B9 | B4 | B1 | 108.79(12) |
| B7 | C2 | B6 | 61.96(10) | C3 | B5 | B4 | 58.19(9) |
| C2 | C3 | B1 | 59.11(9) | C3 | B5 | B6 | 59.50(9) |
| C4 | C3 | C2 | 124.97(12) | C3 | B5 | B8 | 106.41(12) |
| C4 | C3 | B1 | 120.37(12) | C3 | B5 | B9 | 105.92(12) |
| C4 | C3 | B4 | 117.87(12) | B6 | B5 | B4 | 107.08(12) |
| C4 | C3 | B5 | 116.53(12) | B6 | B5 | B9 | 107.91(12) |
| C4 | C3 | B6 | 119.18(12) | B8 | B5 | B4 | 108.20(12) |
| B4 | C3 | C2 | 108.81(11) | B8 | B5 | B6 | 59.76(10) |
| B4 | C3 | B1 | 62.67(10) | B8 | B5 | B9 | 60.47(10) |
| B4 | C3 | B5 | 62.96(10) | B9 | B5 | B4 | 60.23(10) |
| B4 | C3 | B6 | 112.90(12) | C2 | B6 | B5 | 106.79(11) |
| B5 | C3 | C2 | 109.49(11) | C2 | B6 | B7 | 58.23(9) |
| B5 | C3 | B1 | 113.95(11) | C2 | B6 | B8 | 105.65(12) |
| B5 | C3 | B6 | 61.98(10) | C3 | B6 | C2 | 60.27(9) |
| B6 | C3 | C2 | 60.24(9) | C3 | B6 | B5 | 58.52(9) |
| B6 | C3 | B1 | 111.24(11) | C3 | B6 | B7 | 106.92(12) |
| C5 | C4 | C3 | 120.23(13) | C3 | B6 | B8 | 105.78(12) |
| C5 | C4 | C9 | 118.89(14) | B5 | B6 | B7 | 108.38(12) |
| C9 | C4 | C3 | 120.28(13) | B8 | B6 | B5 | 59.93(10) |
| C6 | C5 | C4 | 120.19(15) | B8 | B6 | B7 | 60.32(10) |
| C7 | C6 | C5 | 120.55(15) | C2 | B7 | B2 | 59.19(9) |
| C6 | C7 | C8 | 119.52(15) | C2 | B7 | B6 | 59.81(9) |
| C9 | C8 | C7 | 120.34(15) | C2 | B7 | B8 | 106.13(12) |
| C8 | C9 | C4 | 120.46(15) | C2 | B7 | B10 | 105.76(12) |
| N1 | C10 | C11 | 112.32(14) | B2 | B7 | B6 | 108.02(12) |
| N1 | C12 | C13 | 112.27(14) | B2 | B7 | B8 | 107.65(12) |
| C15 | C14 | B1 | 124.03(13) | B2 | B7 | B10 | 59.58(10) |
| C19 | C14 | C15 | 117.63(14) | B6 | B7 | B8 | 59.36(10) |
| C19 | C14 | B1 | 118.34(13) | B10 | B7 | B6 | 107.31(12) |
| C16 | C15 | C14 | 121.70(14) | B10 | B7 | B8 | 59.94(10) |
| C15 | C16 | C17 | 120.29(15) | B5 | B8 | B7 | 108.68(12) |
| C18 | C17 | C16 | 118.58(14) | B5 | B8 | B9 | 59.99(10) |
| C17 | C18 | Br1 | 118.21(11) | B5 | B8 | B10 | 108.10(12) |

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|---|---|---|---|---|---|---|---|
| C17 | C18 | C19 | 121.60(14) | B6 | B8 | B5 | 60.31(10) |
| C19 | C18 | Br1 | 120.16(12) | B6 | B8 | B7 | 60.32(10) |
| C18 | C19 | C14 | 120.14(14) | B6 | B8 | B9 | 107.96(12) |
| C2 | B1 | C3 | 59.75(9) | B6 | B8 | B10 | 108.06(12) |
| C2 | B1 | B2 | 58.32(9) | B7 | B8 | B9 | 107.85(12) |
| C2 | B1 | B3 | 103.99(11) | B10 | B8 | B7 | 59.92(10) |
| C2 | B1 | B4 | 104.71(11) | B10 | B8 | B9 | 59.74(10) |
| C3 | B1 | B2 | 105.10(11) | B3 | B9 | B4 | 59.38(10) |
| C3 | B1 | B3 | 102.96(11) | B3 | B9 | B8 | 107.80(12) |
| C3 | B1 | B4 | 56.84(9) | B5 | B9 | B3 | 107.70(12) |
| C14 | B1 | C2 | 121.30(12) | B5 | B9 | B4 | 60.12(10) |
| C14 | B1 | C3 | 123.52(12) | B5 | B9 | B8 | 59.54(10) |
| C14 | B1 | B2 | 122.43(13) | B8 | B9 | B4 | 107.37(12) |
| C14 | B1 | B3 | 126.23(13) | B10 | B9 | B3 | 60.43(10) |
| C14 | B1 | B4 | 125.36(13) | B10 | B9 | B4 | 107.84(12) |
| B2 | B1 | B4 | 105.58(12) | B10 | B9 | B5 | 107.91(12) |
| B3 | B1 | B2 | 58.75(10) | B10 | B9 | B8 | 59.96(10) |
| B3 | B1 | B4 | 58.81(10) | B2 | B10 | B3 | 59.50(10) |
| C2 | B2 | B1 | 58.90(9) | B2 | B10 | B7 | 60.04(10) |
| C2 | B2 | B3 | 105.76(12) | B2 | B10 | B8 | 108.18(12) |
| C2 | B2 | B7 | 58.80(9) | B2 | B10 | B9 | 108.21(12) |
| C2 | B2 | B10 | 106.10(12) | B7 | B10 | B3 | 107.41(12) |
| B3 | B2 | B1 | 60.45(10) | B7 | B10 | B8 | 60.15(10) |
| B3 | B2 | B7 | 108.86(12) | B8 | B10 | B3 | 107.76(12) |
| B7 | B2 | B1 | 108.30(12) | B9 | B10 | B3 | 60.03(10) |
| B10 | B2 | B1 | 109.56(12) | B9 | B10 | B7 | 108.48(12) |
| B10 | B2 | B3 | 61.00(10) | B9 | B10 | B8 | 60.31(10) |
| B10 | B2 | B7 | 60.38(10) | | | | |

**Torsion Angles for mo_0828_CG_0m.**

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| Br1 | C18 | C19 | C14 | -176.36(11) | B2 | C2 | B6 | C3 | -100.48(12) |
| O1 | C1 | C2 | C3 | 33.64(17) | B2 | C2 | B6 | B5 | -63.64(14) |
| O1 | C1 | C2 | B1 | 103.72(16) | B2 | C2 | B6 | B7 | 37.94(12) |
| O1 | C1 | C2 | B2 | -175.86(14) | B2 | C2 | B6 | B8 | -0.96(15) |
| O1 | C1 | C2 | B6 | -30.70(17) | B2 | C2 | B7 | B6 | -139.80(12) |
| O1 | C1 | C2 | B7 | -98.69(16) | B2 | C2 | B7 | B8 | -101.24(13) |
| N1 | C1 | C2 | C3 | -150.06(13) | B2 | C2 | B7 | B10 | -38.64(11) |
| N1 | C1 | C2 | B1 | -79.98(18) | B2 | B1 | B3 | B4 | 137.27(12) |
| N1 | C1 | C2 | B2 | 0.4(2) | B2 | B1 | B3 | B9 | 100.02(13) |
| N1 | C1 | C2 | B6 | 145.61(13) | B2 | B1 | B3 | B10 | 36.65(12) |
| N1 | C1 | C2 | B7 | 77.61(18) | B2 | B1 | B4 | C3 | 98.10(12) |
| C1 | N1 | C10 | C11 | -106.55(18) | B2 | B1 | B4 | B3 | -37.03(11) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C1 | N1 | C12 | C13 | -90.05(17) | B2 | B1 | B4 | B5 | 63.38(14) |
| C1 | C2 | C3 | C4 | 7.80(19) | B2 | B1 | B4 | B9 | -0.03(15) |
| C1 | C2 | C3 | B1 | 115.28(13) | B2 | B3 | B4 | C3 | -1.17(16) |
| C1 | C2 | C3 | B4 | 155.02(12) | B2 | B3 | B4 | B1 | 38.75(11) |
| C1 | C2 | C3 | B5 | -137.86(12) | B2 | B3 | B4 | B5 | -63.15(15) |
| C1 | C2 | C3 | B6 | -98.78(13) | B2 | B3 | B4 | B9 | -100.23(13) |
| C1 | C2 | B1 | C3 | -101.71(14) | B2 | B3 | B9 | B4 | 102.02(13) |
| C1 | C2 | B1 | C14 | 11.5(2) | B2 | B3 | B9 | B5 | 64.81(15) |
| C1 | C2 | B1 | B2 | 122.70(15) | B2 | B3 | B9 | B8 | 1.97(16) |
| C1 | C2 | B1 | B3 | 161.26(13) | B2 | B3 | B9 | B10 | -36.15(11) |
| C1 | C2 | B1 | B4 | -137.84(13) | B2 | B3 | B10 | B7 | 37.63(12) |
| C1 | C2 | B2 | B1 | -110.94(16) | B2 | B3 | B10 | B8 | 101.05(13) |
| C1 | C2 | B2 | B3 | -150.70(14) | B2 | B3 | B10 | B9 | 139.32(13) |
| C1 | C2 | B2 | B7 | 106.49(16) | B2 | B7 | B8 | B5 | -63.50(15) |
| C1 | C2 | B2 | B10 | 145.59(14) | B2 | B7 | B8 | B6 | -100.89(13) |
| C1 | C2 | B6 | C3 | 107.40(12) | B2 | B7 | B8 | B9 | 0.02(16) |
| C1 | C2 | B6 | B5 | 144.24(12) | B2 | B7 | B8 | B10 | 37.05(11) |
| C1 | C2 | B6 | B7 | -114.19(13) | B2 | B7 | B10 | B3 | -37.39(12) |
| C1 | C2 | B6 | B8 | -153.08(12) | B2 | B7 | B10 | B8 | -138.25(12) |
| C1 | C2 | B7 | B2 | -123.08(14) | B2 | B7 | B10 | B9 | -100.82(13) |
| C1 | C2 | B7 | B6 | 97.13(14) | B3 | B1 | B2 | C2 | -134.97(12) |
| C1 | C2 | B7 | B8 | 135.68(13) | B3 | B1 | B2 | B7 | -101.76(13) |
| C1 | C2 | B7 | B10 | -161.72(13) | B3 | B1 | B2 | B10 | -37.54(12) |
| C2 | C3 | C4 | C5 | 104.15(17) | B3 | B1 | B4 | C3 | 135.13(12) |
| C2 | C3 | C4 | C9 | -84.84(18) | B3 | B1 | B4 | B5 | 100.40(13) |
| C2 | C3 | B1 | C14 | -109.58(15) | B3 | B1 | B4 | B9 | 37.00(12) |
| C2 | C3 | B1 | B2 | 38.09(10) | B3 | B2 | B7 | C2 | -97.40(13) |
| C2 | C3 | B1 | B3 | 98.80(12) | B3 | B2 | B7 | B6 | -61.47(15) |
| C2 | C3 | B1 | B4 | 137.06(12) | B3 | B2 | B7 | B8 | 1.21(16) |
| C2 | C3 | B4 | B1 | -38.14(10) | B3 | B2 | B7 | B10 | 38.42(12) |
| C2 | C3 | B4 | B3 | 1.68(15) | B3 | B2 | B10 | B7 | -137.75(13) |
| C2 | C3 | B4 | B5 | 102.82(12) | B3 | B2 | B10 | B8 | -100.32(13) |
| C2 | C3 | B4 | B9 | 64.75(14) | B3 | B2 | B10 | B9 | -36.47(12) |
| C2 | C3 | B5 | B4 | -101.73(12) | B3 | B4 | B5 | C3 | 99.29(13) |
| C2 | C3 | B5 | B6 | 38.30(11) | B3 | B4 | B5 | B6 | 63.91(15) |
| C2 | C3 | B5 | B8 | -0.17(15) | B3 | B4 | B5 | B8 | 0.89(16) |
| C2 | C3 | B5 | B9 | -63.41(14) | B3 | B4 | B5 | B9 | -37.32(11) |
| C2 | C3 | B6 | B5 | -137.70(12) | B3 | B4 | B9 | B5 | 138.36(12) |
| C2 | C3 | B6 | B7 | -36.14(10) | B3 | B4 | B9 | B8 | 100.78(13) |
| C2 | C3 | B6 | B8 | -99.28(12) | B3 | B4 | B9 | B10 | 37.55(12) |
| C2 | B1 | B2 | B3 | 134.97(12) | B3 | B9 | B10 | B2 | 36.25(12) |
| C2 | B1 | B2 | B7 | 33.21(11) | B3 | B9 | B10 | B7 | 99.87(13) |
| C2 | B1 | B2 | B10 | 97.43(13) | B3 | B9 | B10 | B8 | 137.23(12) |
| C2 | B1 | B3 | B2 | -38.35(11) | B4 | C3 | C4 | C5 | -40.4(2) |
| C2 | B1 | B3 | B4 | 98.92(12) | B4 | C3 | C4 | C9 | 130.59(15) |

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|---|---|---|---|---|---|---|---|---|---|
| C2 | B1 | B3 | B9 | 61.67(14) | B4 | C3 | B1 | C2 | -137.06(12) |
| C2 | B1 | B3 | B10 | -1.70(15) | B4 | C3 | B1 | C14 | 113.36(16) |
| C2 | B1 | B4 | C3 | 37.48(10) | B4 | C3 | B1 | B2 | -98.98(12) |
| C2 | B1 | B4 | B3 | -97.66(12) | B4 | C3 | B1 | B3 | -38.26(11) |
| C2 | B1 | B4 | B5 | 2.75(15) | B4 | C3 | B5 | B6 | 140.04(12) |
| C2 | B1 | B4 | B9 | -60.66(14) | B4 | C3 | B5 | B8 | 101.56(13) |
| C2 | B2 | B3 | B1 | 39.01(11) | B4 | C3 | B5 | B9 | 38.32(11) |
| C2 | B2 | B3 | B4 | 0.20(16) | B4 | C3 | B6 | C2 | 99.30(12) |
| C2 | B2 | B3 | B9 | -63.79(14) | B4 | C3 | B6 | B5 | -38.39(12) |
| C2 | B2 | B3 | B10 | -99.96(13) | B4 | C3 | B6 | B7 | 63.16(15) |
| C2 | B2 | B7 | B6 | 35.93(11) | B4 | C3 | B6 | B8 | 0.02(16) |
| C2 | B2 | B7 | B8 | 98.61(12) | B4 | B1 | B2 | C2 | -97.91(12) |
| C2 | B2 | B7 | B10 | 135.82(12) | B4 | B1 | B2 | B3 | 37.05(11) |
| C2 | B2 | B10 | B3 | 99.40(13) | B4 | B1 | B2 | B7 | -64.71(14) |
| C2 | B2 | B10 | B7 | -38.35(11) | B4 | B1 | B2 | B10 | -0.49(15) |
| C2 | B2 | B10 | B8 | -0.92(16) | B4 | B1 | B3 | B2 | -137.27(12) |
| C2 | B2 | B10 | B9 | 62.92(15) | B4 | B1 | B3 | B9 | -37.25(12) |
| C2 | B6 | B7 | B2 | -35.66(11) | B4 | B1 | B3 | B10 | -100.62(13) |
| C2 | B6 | B7 | B8 | -135.90(12) | B4 | B3 | B9 | B5 | -37.21(11) |
| C2 | B6 | B7 | B10 | -98.51(13) | B4 | B3 | B9 | B8 | -100.05(13) |
| C2 | B6 | B8 | B5 | -100.63(12) | B4 | B3 | B9 | B10 | -138.17(12) |
| C2 | B6 | B8 | B7 | 37.91(11) | B4 | B3 | B10 | B2 | -101.76(13) |
| C2 | B6 | B8 | B9 | -62.82(14) | B4 | B3 | B10 | B7 | -64.14(15) |
| C2 | B6 | B8 | B10 | 0.34(15) | B4 | B3 | B10 | B8 | -0.71(16) |
| C2 | B7 | B8 | B5 | -1.38(16) | B4 | B3 | B10 | B9 | 37.55(11) |
| C2 | B7 | B8 | B6 | -38.77(11) | B4 | B5 | B6 | C2 | -2.80(15) |
| C2 | B7 | B8 | B9 | 62.15(15) | B4 | B5 | B6 | C3 | 34.82(11) |
| C2 | B7 | B8 | B10 | 99.17(13) | B4 | B5 | B6 | B7 | -64.16(15) |
| C2 | B7 | B10 | B2 | 38.46(11) | B4 | B5 | B6 | B8 | -101.48(13) |
| C2 | B7 | B10 | B3 | 1.07(16) | B4 | B5 | B8 | B6 | 99.57(13) |
| C2 | B7 | B10 | B8 | -99.79(13) | B4 | B5 | B8 | B7 | 62.17(15) |
| C2 | B7 | B10 | B9 | -62.36(15) | B4 | B5 | B8 | B9 | -38.10(11) |
| C3 | C2 | B1 | C14 | 113.18(15) | B4 | B5 | B8 | B10 | -1.33(16) |
| C3 | C2 | B1 | B2 | -135.59(11) | B4 | B5 | B9 | B3 | 36.88(11) |
| C3 | C2 | B1 | B3 | -97.02(12) | B4 | B5 | B9 | B8 | 137.52(13) |
| C3 | C2 | B1 | B4 | -36.13(10) | B4 | B5 | B9 | B10 | 100.70(13) |
| C3 | C2 | B2 | B1 | 40.59(11) | B4 | B9 | B10 | B2 | -0.83(16) |
| C3 | C2 | B2 | B3 | 0.83(15) | B4 | B9 | B10 | B3 | -37.08(11) |
| C3 | C2 | B2 | B7 | -101.98(12) | B4 | B9 | B10 | B7 | 62.79(15) |
| C3 | C2 | B2 | B10 | -62.88(14) | B4 | B9 | B10 | B8 | 100.15(13) |
| C3 | C2 | B6 | B5 | 36.84(10) | B5 | C3 | C4 | C5 | -112.32(16) |
| C3 | C2 | B6 | B7 | 138.41(12) | B5 | C3 | C4 | C9 | 58.69(19) |
| C3 | C2 | B6 | B8 | 99.52(12) | B5 | C3 | B1 | C2 | -99.19(12) |
| C3 | C2 | B7 | B2 | 102.51(12) | B5 | C3 | B1 | C14 | 151.23(14) |
| C3 | C2 | B7 | B6 | -37.28(11) | B5 | C3 | B1 | B2 | -61.10(14) |

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|---|---|---|---|---|---|---|---|---|---|
| C3 | C2 | B7 | B8 | 1.27(15) | B5 | C3 | B1 | B3 | -0.39(15) |
| C3 | C2 | B7 | B10 | 63.87(14) | B5 | C3 | B1 | B4 | 37.87(12) |
| C3 | C4 | C5 | C6 | 173.58(14) | B5 | C3 | B4 | B1 | -140.96(12) |
| C3 | C4 | C9 | C8 | -172.10(14) | B5 | C3 | B4 | B3 | -101.15(13) |
| C3 | B1 | B2 | C2 | -38.77(10) | B5 | C3 | B4 | B9 | -38.08(11) |
| C3 | B1 | B2 | B3 | 96.20(12) | B5 | C3 | B6 | C2 | 137.70(12) |
| C3 | B1 | B2 | B7 | -5.56(15) | B5 | C3 | B6 | B7 | 101.55(13) |
| C3 | B1 | B2 | B10 | 58.66(14) | B5 | C3 | B6 | B8 | 38.41(11) |
| C3 | B1 | B3 | B2 | -99.97(12) | B5 | B4 | B9 | B3 | -138.36(12) |
| C3 | B1 | B3 | B4 | 37.30(10) | B5 | B4 | B9 | B8 | -37.58(12) |
| C3 | B1 | B3 | B9 | 0.05(15) | B5 | B4 | B9 | B10 | -100.82(13) |
| C3 | B1 | B3 | B10 | -63.32(14) | B5 | B6 | B7 | C2 | 98.75(12) |
| C3 | B1 | B4 | B3 | -135.13(12) | B5 | B6 | B7 | B2 | 63.09(15) |
| C3 | B1 | B4 | B5 | -34.73(11) | B5 | B6 | B7 | B8 | -37.15(11) |
| C3 | B1 | B4 | B9 | -98.14(13) | B5 | B6 | B7 | B10 | 0.24(16) |
| C3 | B4 | B5 | B6 | -35.38(11) | B5 | B6 | B8 | B7 | 138.53(12) |
| C3 | B4 | B5 | B8 | -98.40(13) | B5 | B6 | B8 | B9 | 37.81(12) |
| C3 | B4 | B5 | B9 | -136.61(12) | B5 | B6 | B8 | B10 | 100.97(13) |
| C3 | B4 | B9 | B3 | -100.67(13) | B5 | B8 | B9 | B3 | 100.46(13) |
| C3 | B4 | B9 | B5 | 37.70(11) | B5 | B8 | B9 | B4 | 37.85(12) |
| C3 | B4 | B9 | B8 | 0.11(16) | B5 | B8 | B9 | B10 | 138.80(13) |
| C3 | B4 | B9 | B10 | -63.12(15) | B5 | B8 | B10 | B2 | 64.15(15) |
| C3 | B5 | B6 | C2 | -37.63(11) | B5 | B8 | B10 | B3 | 1.26(16) |
| C3 | B5 | B6 | B7 | -98.98(12) | B5 | B8 | B10 | B7 | 101.54(13) |
| C3 | B5 | B6 | B8 | -136.30(12) | B5 | B8 | B10 | B9 | -36.88(11) |
| C3 | B5 | B8 | B6 | 38.35(11) | B5 | B9 | B10 | B2 | -64.35(15) |
| C3 | B5 | B8 | B7 | 0.96(16) | B5 | B9 | B10 | B3 | -100.60(13) |
| C3 | B5 | B8 | B9 | -99.31(13) | B5 | B9 | B10 | B7 | -0.73(16) |
| C3 | B5 | B8 | B10 | -62.54(15) | B5 | B9 | B10 | B8 | 36.64(11) |
| C3 | B5 | B9 | B3 | -0.50(16) | B6 | C2 | C3 | C4 | 106.59(15) |
| C3 | B5 | B9 | B4 | -37.38(11) | B6 | C2 | C3 | B1 | -145.93(12) |
| C3 | B5 | B9 | B8 | 100.14(13) | B6 | C2 | C3 | B4 | -106.19(13) |
| C3 | B5 | B9 | B10 | 63.32(15) | B6 | C2 | C3 | B5 | -39.07(11) |
| C3 | B6 | B7 | C2 | 37.05(10) | B6 | C2 | B1 | C3 | 31.45(11) |
| C3 | B6 | B7 | B2 | 1.39(15) | B6 | C2 | B1 | C14 | 144.62(13) |
| C3 | B6 | B7 | B8 | -98.85(13) | B6 | C2 | B1 | B2 | -104.14(13) |
| C3 | B6 | B7 | B10 | -61.46(14) | B6 | C2 | B1 | B3 | -65.58(14) |
| C3 | B6 | B8 | B5 | -37.76(11) | B6 | C2 | B1 | B4 | -4.68(15) |
| C3 | B6 | B8 | B7 | 100.78(12) | B6 | C2 | B2 | B1 | 104.65(12) |
| C3 | B6 | B8 | B9 | 0.06(16) | B6 | C2 | B2 | B3 | 64.90(14) |
| C3 | B6 | B8 | B10 | 63.21(14) | B6 | C2 | B2 | B7 | -37.91(11) |
| C4 | C3 | B1 | C2 | 115.06(14) | B6 | C2 | B2 | B10 | 1.18(15) |
| C4 | C3 | B1 | C14 | 5.5(2) | B6 | C2 | B7 | B2 | 139.80(12) |
| C4 | C3 | B1 | B2 | 153.15(13) | B6 | C2 | B7 | B8 | 38.56(11) |
| C4 | C3 | B1 | B3 | -146.14(13) | B6 | C2 | B7 | B10 | 101.15(13) |

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|---|---|---|---|---|---|---|---|---|---|
| C4 | C3 | B1 | B4 | -107.88(15) | B6 | C3 | C4 | C5 | 176.50(13) |
| C4 | C3 | B4 | B1 | 111.74(14) | B6 | C3 | C4 | C9 | -12.5(2) |
| C4 | C3 | B4 | B3 | 151.56(13) | B6 | C3 | B1 | C2 | -31.45(11) |
| C4 | C3 | B4 | B5 | -107.30(14) | B6 | C3 | B1 | C14 | -141.03(14) |
| C4 | C3 | B4 | B9 | -145.37(13) | B6 | C3 | B1 | B2 | 6.64(15) |
| C4 | C3 | B5 | B4 | 109.38(14) | B6 | C3 | B1 | B3 | 67.35(14) |
| C4 | C3 | B5 | B6 | -110.59(14) | B6 | C3 | B1 | B4 | 105.61(13) |
| C4 | C3 | B5 | B8 | -149.06(13) | B6 | C3 | B4 | B1 | -102.97(13) |
| C4 | C3 | B5 | B9 | 147.70(13) | B6 | C3 | B4 | B3 | -63.15(15) |
| C4 | C3 | B6 | C2 | -115.91(14) | B6 | C3 | B4 | B5 | 37.99(12) |
| C4 | C3 | B6 | B5 | 106.40(14) | B6 | C3 | B4 | B9 | -0.08(16) |
| C4 | C3 | B6 | B7 | -152.05(13) | B6 | C3 | B5 | B4 | -140.04(12) |
| C4 | C3 | B6 | B8 | 144.81(13) | B6 | C3 | B5 | B8 | -38.48(11) |
| C4 | C5 | C6 | C7 | -2.1(2) | B6 | C3 | B5 | B9 | -101.71(13) |
| C5 | C4 | C9 | C8 | -1.0(2) | B6 | B5 | B8 | B7 | -37.39(11) |
| C5 | C6 | C7 | C8 | 0.2(2) | B6 | B5 | B8 | B9 | -137.67(12) |
| C6 | C7 | C8 | C9 | 1.2(2) | B6 | B5 | B8 | B10 | -100.90(13) |
| C7 | C8 | C9 | C4 | -0.9(2) | B6 | B5 | B9 | B3 | -62.95(15) |
| C9 | C4 | C5 | C6 | 2.4(2) | B6 | B5 | B9 | B4 | -99.83(13) |
| C10 | N1 | C1 | O1 | -164.61(15) | B6 | B5 | B9 | B8 | 37.69(11) |
| C10 | N1 | C1 | C2 | 19.3(2) | B6 | B5 | B9 | B10 | 0.87(16) |
| C10 | N1 | C12 | C13 | 80.79(17) | B6 | B7 | B8 | B5 | 37.39(12) |
| C12 | N1 | C1 | O1 | 4.6(2) | B6 | B7 | B8 | B9 | 100.92(13) |
| C12 | N1 | C1 | C2 | -171.51(13) | B6 | B7 | B8 | B10 | 137.94(12) |
| C12 | N1 | C10 | C11 | 84.05(16) | B6 | B7 | B10 | B2 | 101.12(13) |
| C14 | C15 | C16 | C17 | 1.9(2) | B6 | B7 | B10 | B3 | 63.73(15) |
| C14 | B1 | B2 | C2 | 109.34(15) | B6 | B7 | B10 | B8 | -37.14(11) |
| C14 | B1 | B2 | B3 | -115.69(16) | B6 | B7 | B10 | B9 | 0.30(16) |
| C14 | B1 | B2 | B7 | 142.55(14) | B6 | B8 | B9 | B3 | 62.51(15) |
| C14 | B1 | B2 | B10 | -153.23(14) | B6 | B8 | B9 | B4 | -0.11(16) |
| C14 | B1 | B3 | B2 | 109.45(17) | B6 | B8 | B9 | B5 | -37.95(11) |
| C14 | B1 | B3 | B4 | -113.27(17) | B6 | B8 | B9 | B10 | 100.84(13) |
| C14 | B1 | B3 | B9 | -150.53(14) | B6 | B8 | B10 | B2 | 0.36(16) |
| C14 | B1 | B3 | B10 | 146.10(14) | B6 | B8 | B10 | B3 | -62.53(15) |
| C14 | B1 | B4 | C3 | -110.19(16) | B6 | B8 | B10 | B7 | 37.75(11) |
| C14 | B1 | B4 | B3 | 114.68(16) | B6 | B8 | B10 | B9 | -100.68(13) |
| C14 | B1 | B4 | B5 | -144.92(14) | B7 | C2 | C3 | C4 | 144.95(14) |
| C14 | B1 | B4 | B9 | 151.67(14) | B7 | C2 | C3 | B1 | -107.57(12) |
| C15 | C14 | C19 | C18 | 0.3(2) | B7 | C2 | C3 | B4 | -67.83(14) |
| C15 | C14 | B1 | C2 | -23.9(2) | B7 | C2 | C3 | B5 | -0.71(15) |
| C15 | C14 | B1 | C3 | 48.4(2) | B7 | C2 | C3 | B6 | 38.36(11) |
| C15 | C14 | B1 | B2 | -93.90(18) | B7 | C2 | B1 | C3 | 99.56(12) |
| C15 | C14 | B1 | B3 | -166.66(15) | B7 | C2 | B1 | C14 | -147.27(13) |
| C15 | C14 | B1 | B4 | 118.85(17) | B7 | C2 | B1 | B2 | -36.03(12) |
| C15 | C16 | C17 | C18 | 0.1(2) | B7 | C2 | B1 | B3 | 2.53(16) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C16 | C17 | C18 | Br1 | 176.21(12) | B7 | C2 | B1 | B4 | 63.43(14) |
| C16 | C17 | C18 | C19 | -1.9(2) | B7 | C2 | B2 | B1 | 142.56(12) |
| C17 | C18 | C19 | C14 | 1.7(2) | B7 | C2 | B2 | B3 | 102.81(13) |
| C19 | C14 | C15 | C16 | -2.0(2) | B7 | C2 | B2 | B10 | 39.09(11) |
| C19 | C14 | B1 | C2 | 155.79(13) | B7 | C2 | B6 | C3 | -138.41(12) |
| C19 | C14 | B1 | C3 | -131.94(15) | B7 | C2 | B6 | B5 | -101.57(13) |
| C19 | C14 | B1 | B2 | 85.78(18) | B7 | C2 | B6 | B8 | -38.90(11) |
| C19 | C14 | B1 | B3 | 13.0(2) | B7 | B2 | B3 | B1 | 100.82(13) |
| C19 | C14 | B1 | B4 | -61.5(2) | B7 | B2 | B3 | B4 | 62.01(15) |
| B1 | C2 | C3 | C4 | -107.48(15) | B7 | B2 | B3 | B9 | -1.98(16) |
| B1 | C2 | C3 | B4 | 39.74(11) | B7 | B2 | B3 | B10 | -38.15(12) |
| B1 | C2 | C3 | B5 | 106.86(12) | B7 | B2 | B10 | B3 | 137.75(13) |
| B1 | C2 | C3 | B6 | 145.93(12) | B7 | B2 | B10 | B8 | 37.43(12) |
| B1 | C2 | B2 | B3 | -39.75(11) | B7 | B2 | B10 | B9 | 101.28(13) |
| B1 | C2 | B2 | B7 | -142.56(12) | B7 | B6 | B8 | B5 | -138.53(12) |
| B1 | C2 | B2 | B10 | -103.47(13) | B7 | B6 | B8 | B9 | -100.72(13) |
| B1 | C2 | B6 | C3 | -32.03(11) | B7 | B6 | B8 | B10 | -37.57(12) |
| B1 | C2 | B6 | B5 | 4.81(15) | B7 | B8 | B9 | B3 | -1.23(16) |
| B1 | C2 | B6 | B7 | 106.38(13) | B7 | B8 | B9 | B4 | -63.84(15) |
| B1 | C2 | B6 | B8 | 67.49(14) | B7 | B8 | B9 | B5 | -101.69(13) |
| B1 | C2 | B7 | B2 | 36.32(12) | B7 | B8 | B9 | B10 | 37.11(11) |
| B1 | C2 | B7 | B6 | -103.48(13) | B7 | B8 | B10 | B2 | -37.39(11) |
| B1 | C2 | B7 | B8 | -64.92(15) | B7 | B8 | B10 | B3 | -100.28(13) |
| B1 | C2 | B7 | B10 | -2.32(16) | B7 | B8 | B10 | B9 | -138.42(12) |
| B1 | C3 | C4 | C5 | 32.6(2) | B8 | B5 | B6 | C2 | 98.68(13) |
| B1 | C3 | C4 | C9 | -156.40(14) | B8 | B5 | B6 | C3 | 136.30(12) |
| B1 | C3 | B4 | B3 | 39.81(11) | B8 | B5 | B6 | B7 | 37.32(11) |
| B1 | C3 | B4 | B5 | 140.96(12) | B8 | B5 | B9 | B3 | -100.64(13) |
| B1 | C3 | B4 | B9 | 102.88(13) | B8 | B5 | B9 | B4 | -137.52(13) |
| B1 | C3 | B5 | B4 | -37.75(12) | B8 | B5 | B9 | B10 | -36.82(12) |
| B1 | C3 | B5 | B6 | 102.28(13) | B8 | B6 | B7 | C2 | 135.90(12) |
| B1 | C3 | B5 | B8 | 63.80(15) | B8 | B6 | B7 | B2 | 100.24(13) |
| B1 | C3 | B5 | B9 | 0.57(16) | B8 | B6 | B7 | B10 | 37.39(11) |
| B1 | C3 | B6 | C2 | 31.05(11) | B8 | B7 | B10 | B2 | 138.25(12) |
| B1 | C3 | B6 | B5 | -106.65(13) | B8 | B7 | B10 | B3 | 100.87(13) |
| B1 | C3 | B6 | B7 | -5.09(15) | B8 | B7 | B10 | B9 | 37.43(12) |
| B1 | C3 | B6 | B8 | -68.23(14) | B8 | B9 | B10 | B2 | -100.98(13) |
| B1 | C14 | C15 | C16 | 177.66(14) | B8 | B9 | B10 | B3 | -137.23(12) |
| B1 | C14 | C19 | C18 | -179.44(13) | B8 | B9 | B10 | B7 | -37.36(12) |
| B1 | B2 | B3 | B4 | -38.81(11) | B9 | B3 | B4 | C3 | 99.05(13) |
| B1 | B2 | B3 | B9 | -102.80(13) | B9 | B3 | B4 | B1 | 138.98(12) |
| B1 | B2 | B3 | B10 | -138.97(13) | B9 | B3 | B4 | B5 | 37.07(11) |
| B1 | B2 | B7 | C2 | -33.25(11) | B9 | B3 | B10 | B2 | -139.32(13) |
| B1 | B2 | B7 | B6 | 2.68(16) | B9 | B3 | B10 | B7 | -101.69(13) |
| B1 | B2 | B7 | B8 | 65.36(14) | B9 | B3 | B10 | B8 | -38.27(11) |

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|---|---|---|---|---|---|---|---|---|---|
| B1 | B2 | B7 | B10 | 102.57(13) | B9 | B4 | B5 | C3 | 136.61(12) |
| B1 | B2 | B10 | B3 | 37.30(12) | B9 | B4 | B5 | B6 | 101.23(13) |
| B1 | B2 | B10 | B7 | -100.45(13) | B9 | B4 | B5 | B8 | 38.21(12) |
| B1 | B2 | B10 | B8 | -63.02(15) | B9 | B5 | B6 | C2 | 60.67(14) |
| B1 | B2 | B10 | B9 | 0.83(16) | B9 | B5 | B6 | C3 | 98.29(13) |
| B1 | B3 | B4 | C3 | -39.92(11) | B9 | B5 | B6 | B7 | -0.69(16) |
| B1 | B3 | B4 | B5 | -101.90(13) | B9 | B5 | B6 | B8 | -38.01(12) |
| B1 | B3 | B4 | B9 | -138.98(12) | B9 | B5 | B8 | B6 | 137.67(12) |
| B1 | B3 | B9 | B4 | 37.48(11) | B9 | B5 | B8 | B7 | 100.27(13) |
| B1 | B3 | B9 | B5 | 0.28(16) | B9 | B5 | B8 | B10 | 36.77(12) |
| B1 | B3 | B9 | B8 | -62.56(15) | B9 | B8 | B10 | B2 | 101.03(13) |
| B1 | B3 | B9 | B10 | -100.69(13) | B9 | B8 | B10 | B3 | 38.14(11) |
| B1 | B3 | B10 | B2 | -37.21(12) | B9 | B8 | B10 | B7 | 138.42(12) |
| B1 | B3 | B10 | B7 | 0.41(16) | B10 | B2 | B3 | B1 | 138.97(13) |
| B1 | B3 | B10 | B8 | 63.84(15) | B10 | B2 | B3 | B4 | 100.16(13) |
| B1 | B3 | B10 | B9 | 102.11(13) | B10 | B2 | B3 | B9 | 36.17(12) |
| B1 | B4 | B5 | C3 | 35.40(11) | B10 | B2 | B7 | C2 | -135.82(12) |
| B1 | B4 | B5 | B6 | 0.03(16) | B10 | B2 | B7 | B6 | -99.89(13) |
| B1 | B4 | B5 | B8 | -63.00(15) | B10 | B2 | B7 | B8 | -37.21(12) |
| B1 | B4 | B5 | B9 | -101.21(13) | B10 | B3 | B4 | C3 | 61.88(15) |
| B1 | B4 | B9 | B3 | -37.01(11) | B10 | B3 | B4 | B1 | 101.80(13) |
| B1 | B4 | B9 | B5 | 101.35(13) | B10 | B3 | B4 | B5 | -0.10(15) |
| B1 | B4 | B9 | B8 | 63.77(15) | B10 | B3 | B4 | B9 | -37.18(11) |
| B1 | B4 | B9 | B10 | 0.53(16) | B10 | B3 | B9 | B4 | 138.17(12) |
| B2 | C2 | C3 | C4 | -148.83(13) | B10 | B3 | B9 | B5 | 100.96(13) |
| B2 | C2 | C3 | B1 | -41.35(11) | B10 | B3 | B9 | B8 | 38.12(11) |
| B2 | C2 | C3 | B4 | -1.61(15) | B10 | B7 | B8 | B5 | -100.55(13) |
| B2 | C2 | C3 | B5 | 65.51(14) | B10 | B7 | B8 | B6 | -137.94(12) |
| B2 | C2 | C3 | B6 | 104.58(12) | B10 | B7 | B8 | B9 | -37.03(12) |
| B2 | C2 | B1 | C3 | 135.59(11) | B10 | B8 | B9 | B3 | -38.34(12) |
| B2 | C2 | B1 | C14 | -111.24(15) | B10 | B8 | B9 | B4 | -100.95(13) |
| B2 | C2 | B1 | B3 | 38.56(11) | B10 | B8 | B9 | B5 | -138.80(13) |
| B2 | C2 | B1 | B4 | 99.46(12) | | | | | |

**Hydrogen Atom Coordinates (Å×10$^4$) and Isotropic Displacement Parameters (Å$^2$×10$^3$) for mo_0828_CG_0m.**

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H5 | 4813.59 | 6176.88 | 1981.04 | 24 |
| H6 | 5402.57 | 6440.38 | 770.38 | 28 |
| H7 | 5337.21 | 8323.25 | 207.3 | 29 |
| H8 | 4698.2 | 9960.29 | 865.32 | 28 |
| H9 | 4186.68 | 9725.04 | 2095.35 | 25 |
| H10A | 7852.56 | 7156.22 | 4918.46 | 25 |
| H10B | 6495.09 | 6809.51 | 4748.35 | 25 |

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|---|---|---|---|---|
| H11A | 6044.25 | 8083.32 | 5718.94 | 40 |
| H11B | 7372.63 | 8537.27 | 5863.22 | 40 |
| H11C | 7061.37 | 7195.17 | 6068.46 | 40 |
| H12A | 8284.39 | 9342.63 | 4857.78 | 27 |
| H12B | 7643.83 | 9996.45 | 4113.47 | 27 |
| H13A | 8424.71 | 8611.85 | 3319.32 | 43 |
| H13B | 8995.42 | 7868.96 | 4046.85 | 43 |
| H13C | 9478.32 | 9170.57 | 3887.6 | 43 |
| H15 | 6729.22 | 6922.07 | 3130.99 | 23 |
| H16 | 8225.52 | 5597.18 | 2973.92 | 26 |
| H17 | 7924.76 | 3534.79 | 3077.92 | 25 |
| H19 | 4620.55 | 4168.43 | 3560.04 | 22 |
| H2 | 4865(18) | 6714(18) | 4942(12) | 23 |
| H3 | 3076(18) | 5212(19) | 4142(11) | 24 |
| H4 | 2866(17) | 6042(19) | 2502(11) | 23 |
| H5A | 2095(17) | 8469(19) | 2401(12) | 24 |
| H6A | 3891(17) | 9881(18) | 3258(11) | 22 |
| H7A | 4157(17) | 9175(18) | 4847(12) | 23 |
| H8A | 1758(18) | 9247(19) | 3946(12) | 24 |
| H9A | 1120(18) | 6813(19) | 3505(12) | 25 |
| H10 | 2359(18) | 7235(19) | 5048(12) | 25 |

**Experimental**

Single crystals of $C_{19}H_{28}B_{10}BrNO$ [mo_0828_CG_0m] were recrystallised from a mixture of chloroform and hexane by slow evaporation. A suitable crystal was selected and the crystal was mounted on a MITIGEN holder oil on a Bruker D8 Venture MoCu Dual Source diffractometer. The crystal was kept at 100.03 K during data collection. Using Olex2[2], the structure was solved with the XT[3] structure solution program using Intrinsic Phasing and refined with the XL[4] refinement package using Least Squares minimisation.

**Crystal structure determination of 4ai**

**Crystal Data** for $C_{19}H_{28}B_{10}BrNO$ ($M$ =474.43 g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a$ = 11.5021(12) Å, $b$ = 11.2242(12) Å, $c$ = 17.6391(19) Å, $\beta$ = 97.227(3)°, $V$ = 2259.1(4) Å$^3$, $Z$ = 4, $T$ = 100.0 K, μ(MoKα) = 1.833 mm$^{-1}$, *Dcalc* = 1.395 g/cm$^3$, 69892 reflections measured (4.312° ≤ 2Θ ≤ 59.356°), 6364 unique ($R_{int}$ = 0.0329, $R_{sigma}$ = 0.0179) which were used in all calculations. The final $R_1$ was 0.0276 (I > 2σ(I)) and $wR_2$ was 0.0749 (all data).

## References


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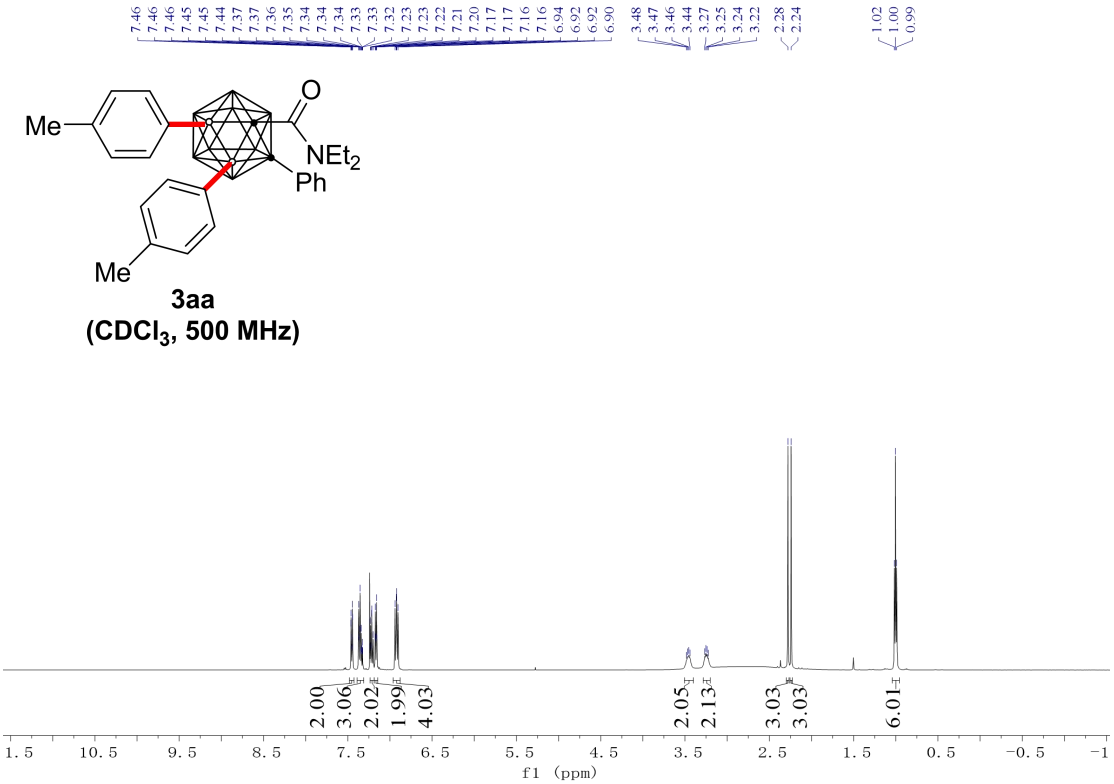
# $^{1}H$, $^{13}C$, and $^{11}B$ NMR spectra

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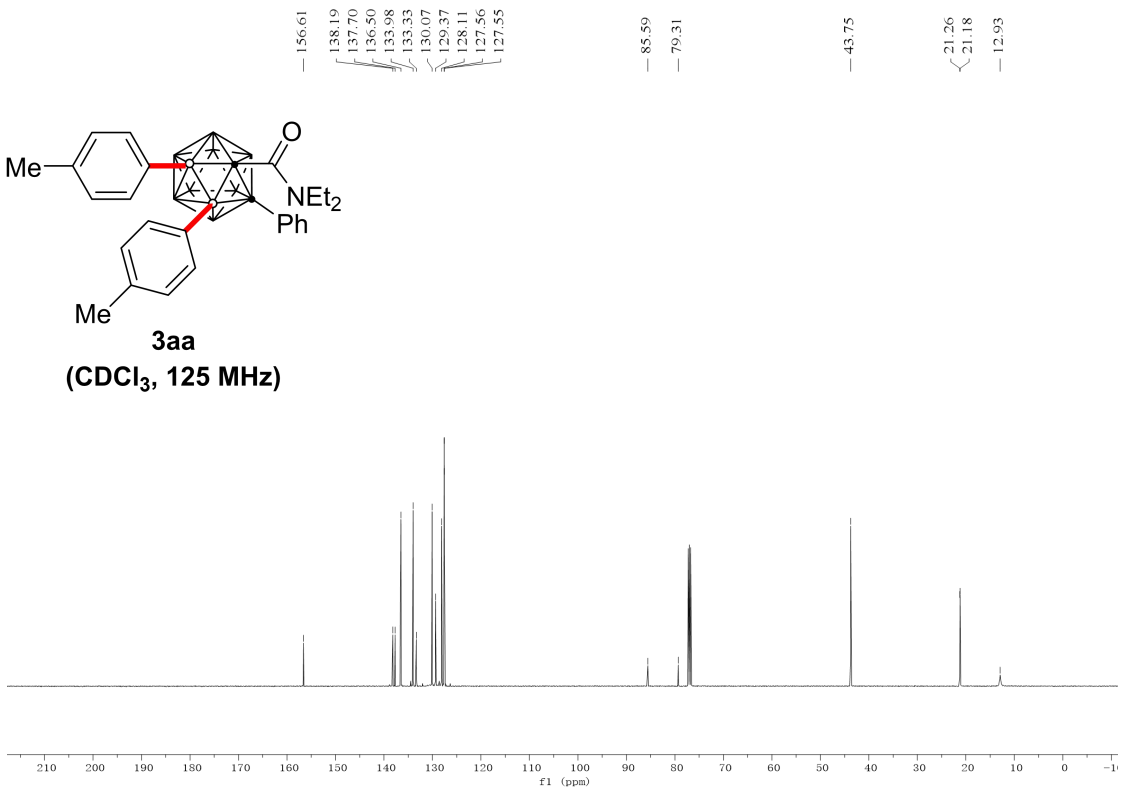


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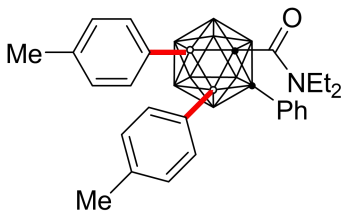


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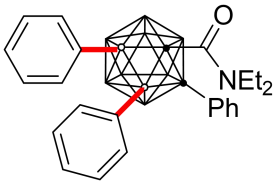


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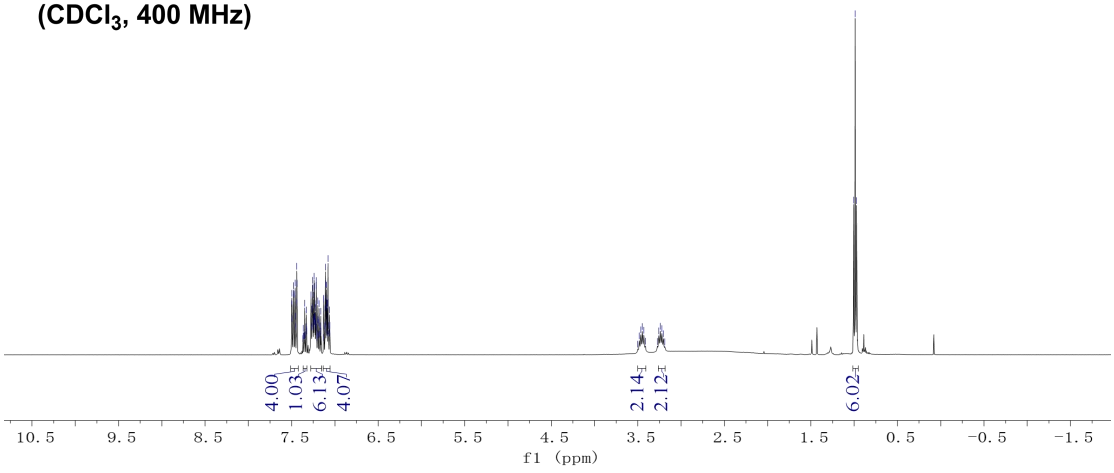

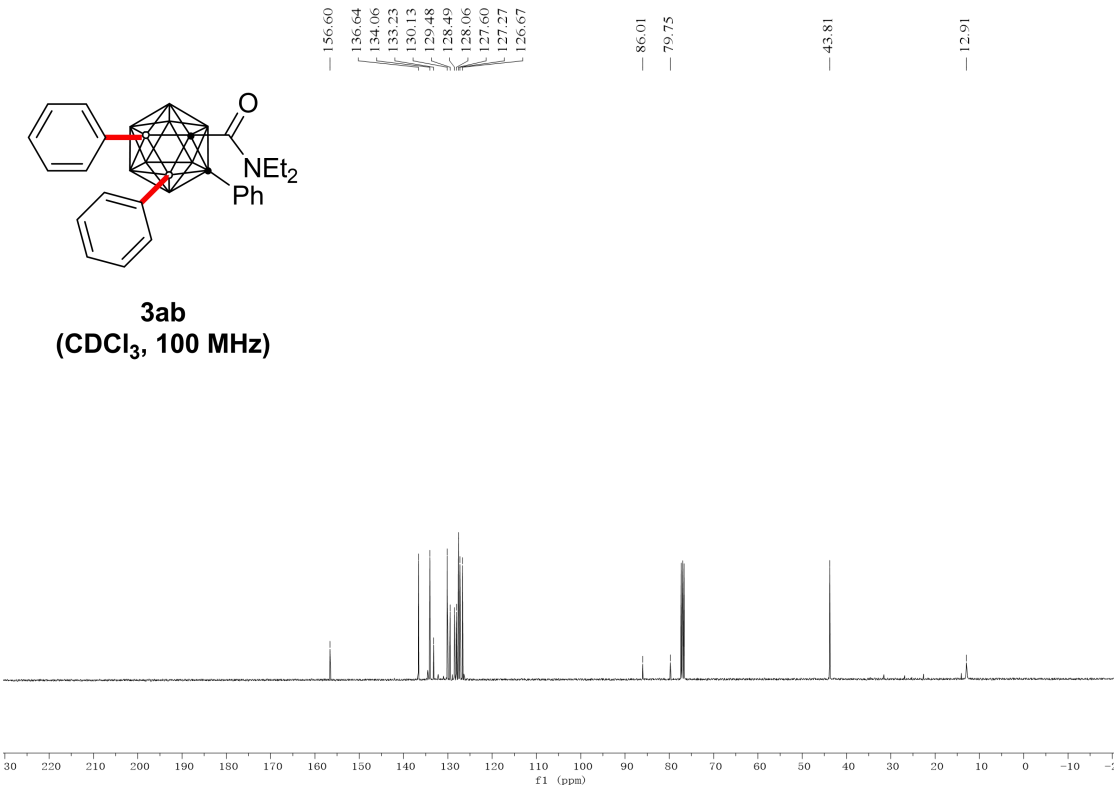


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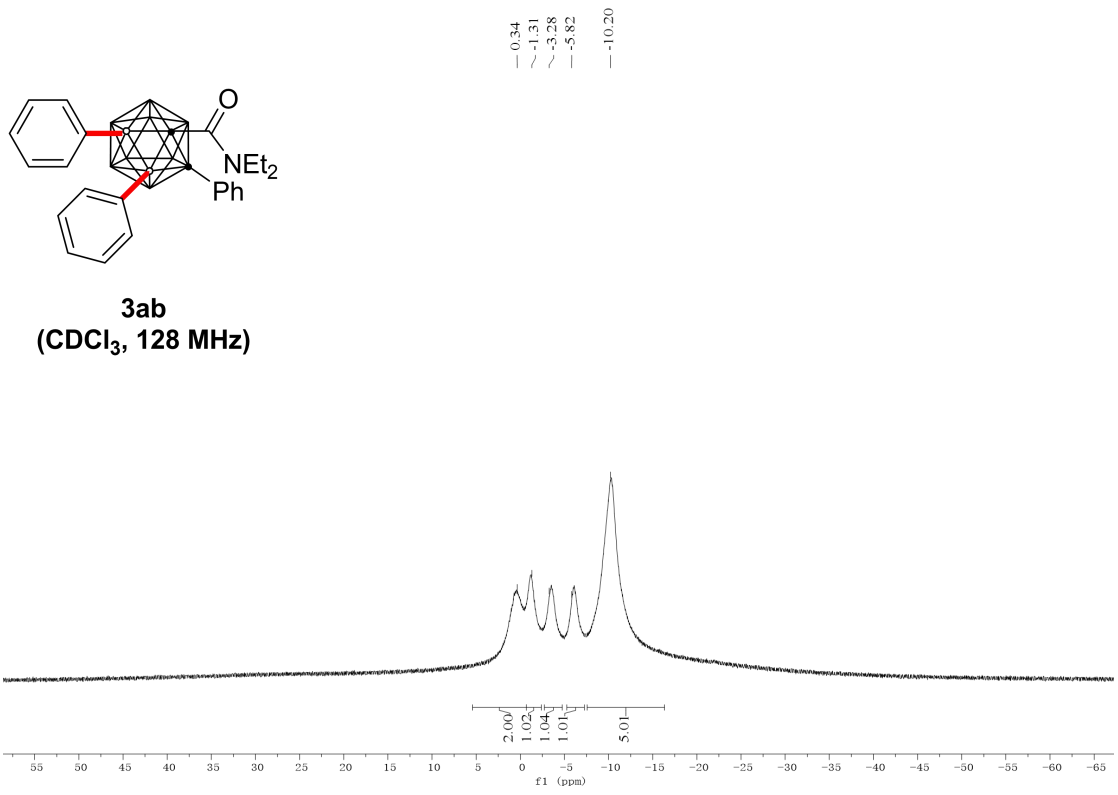
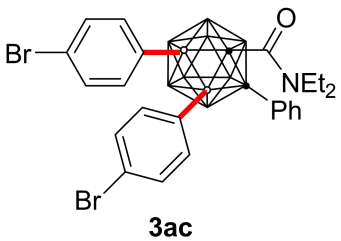



**3ab**
**($CDCl_3$, 128 MHz)**

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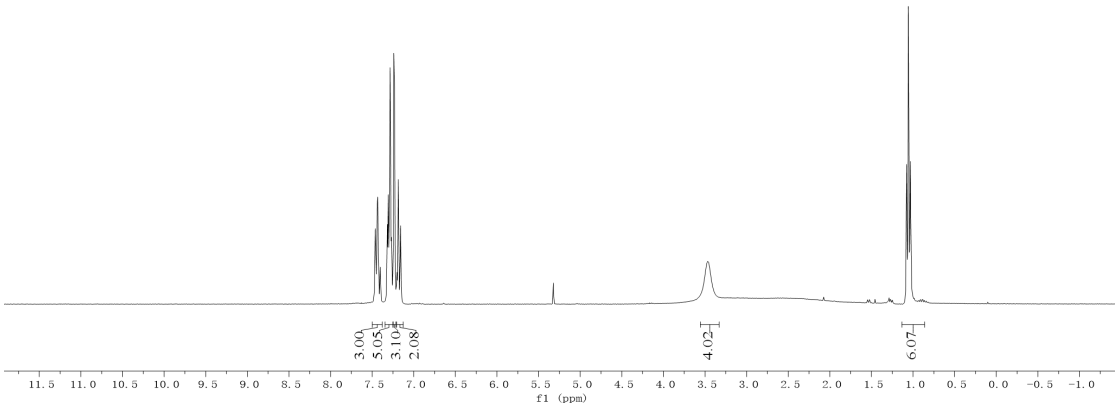
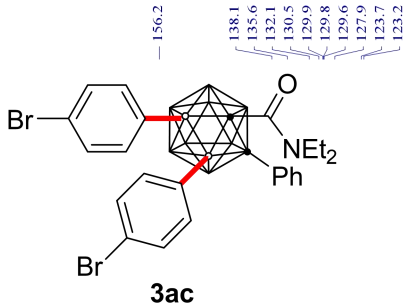
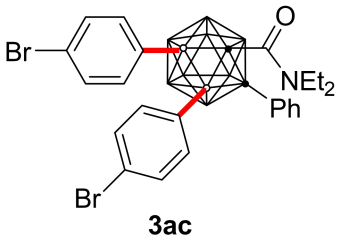



**3ac**
**($CDCl_3$, 75 MHz)**

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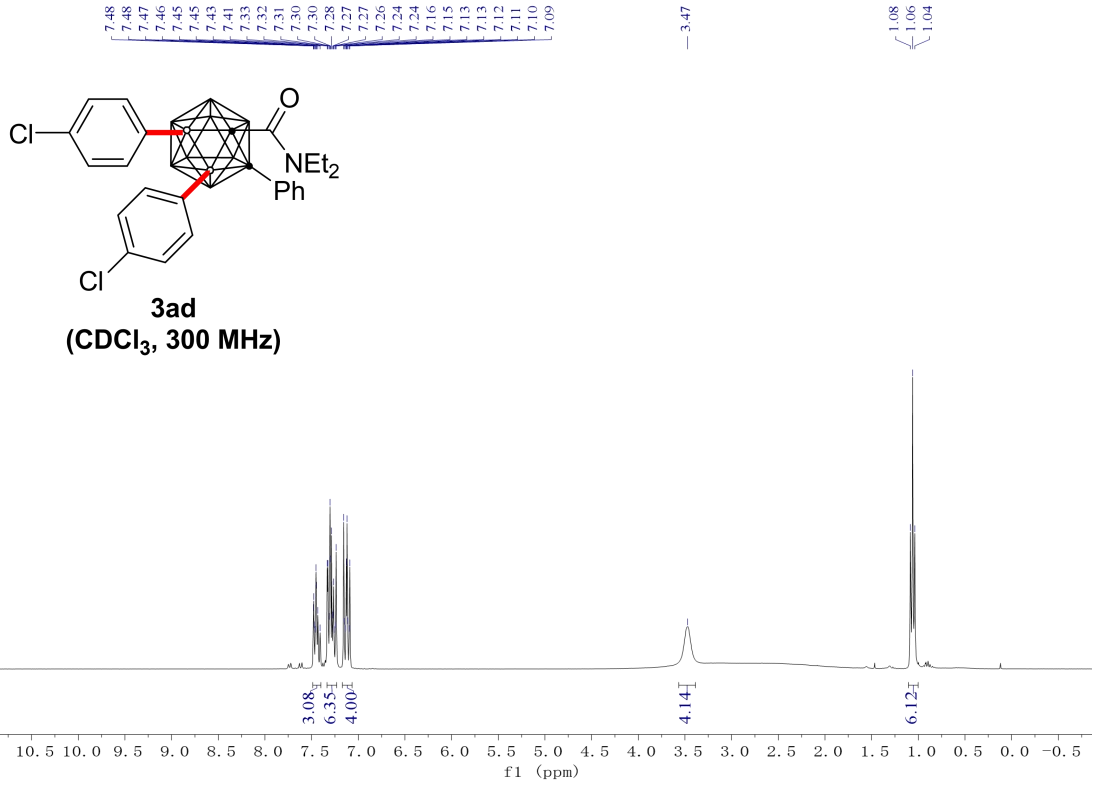


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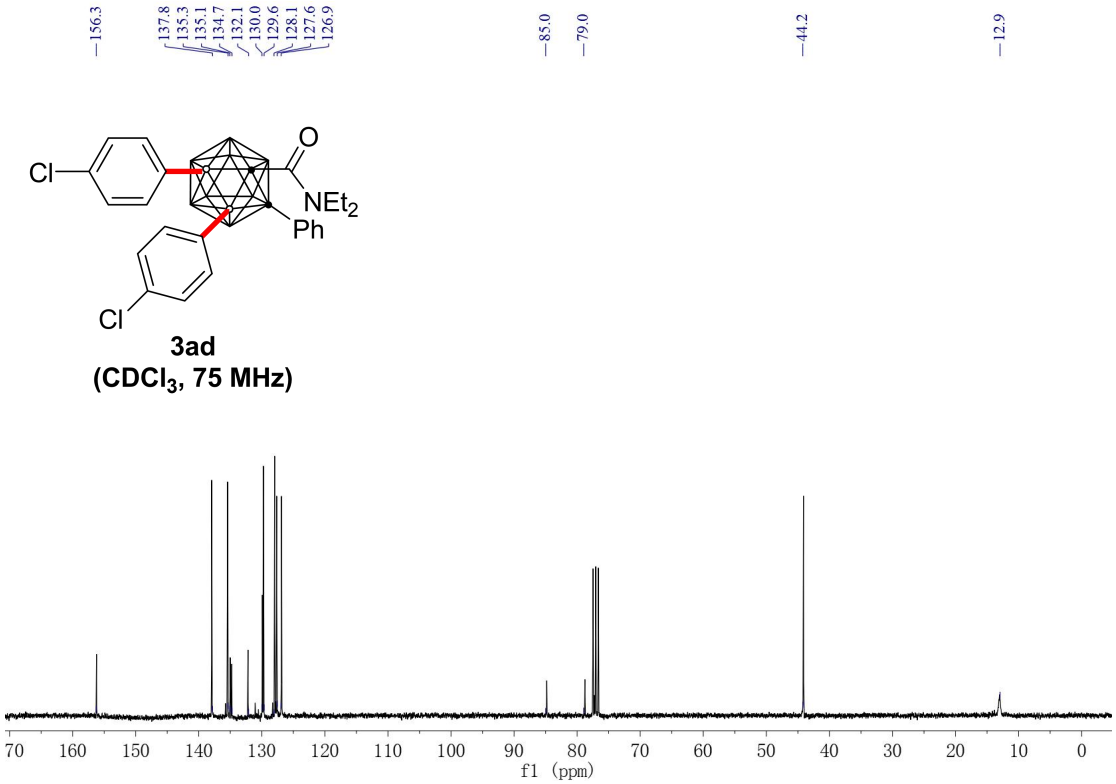


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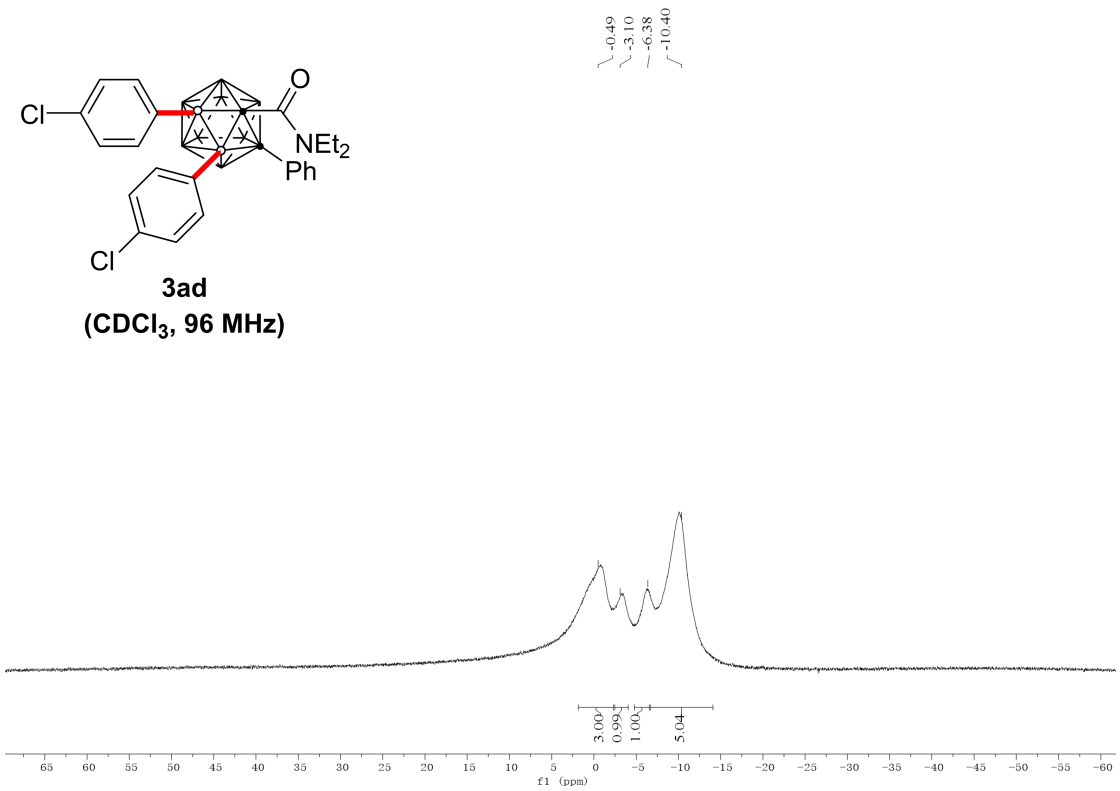


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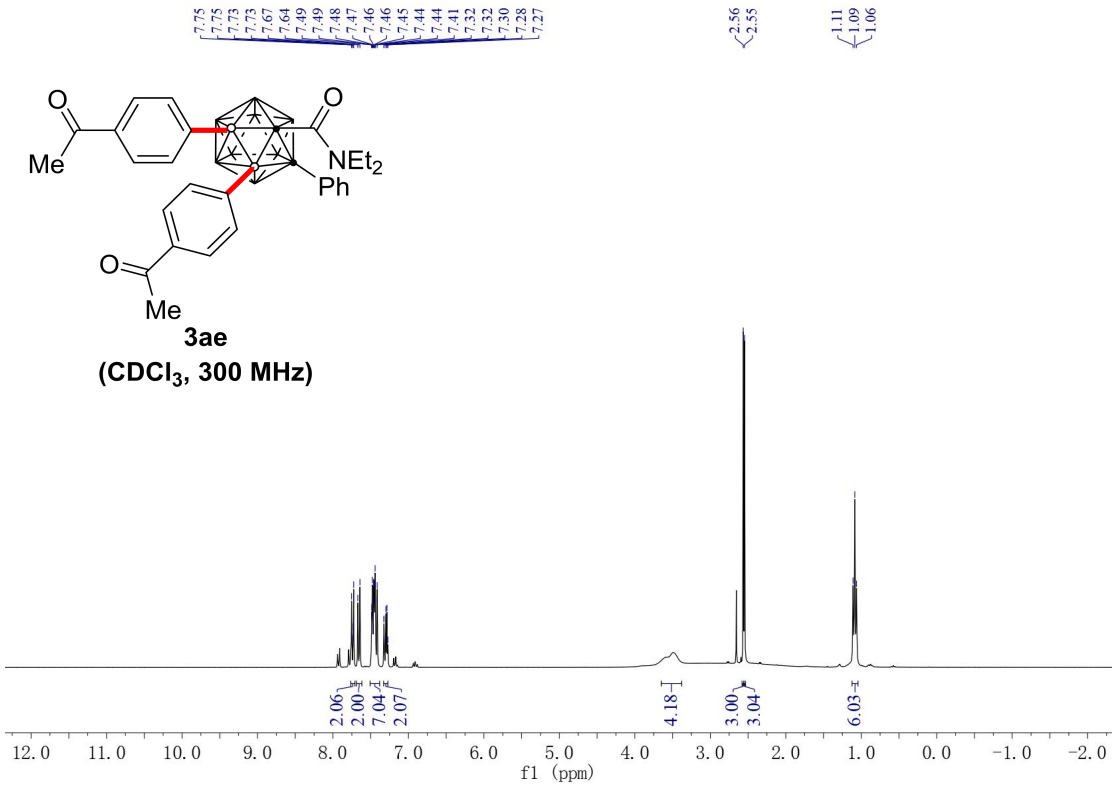
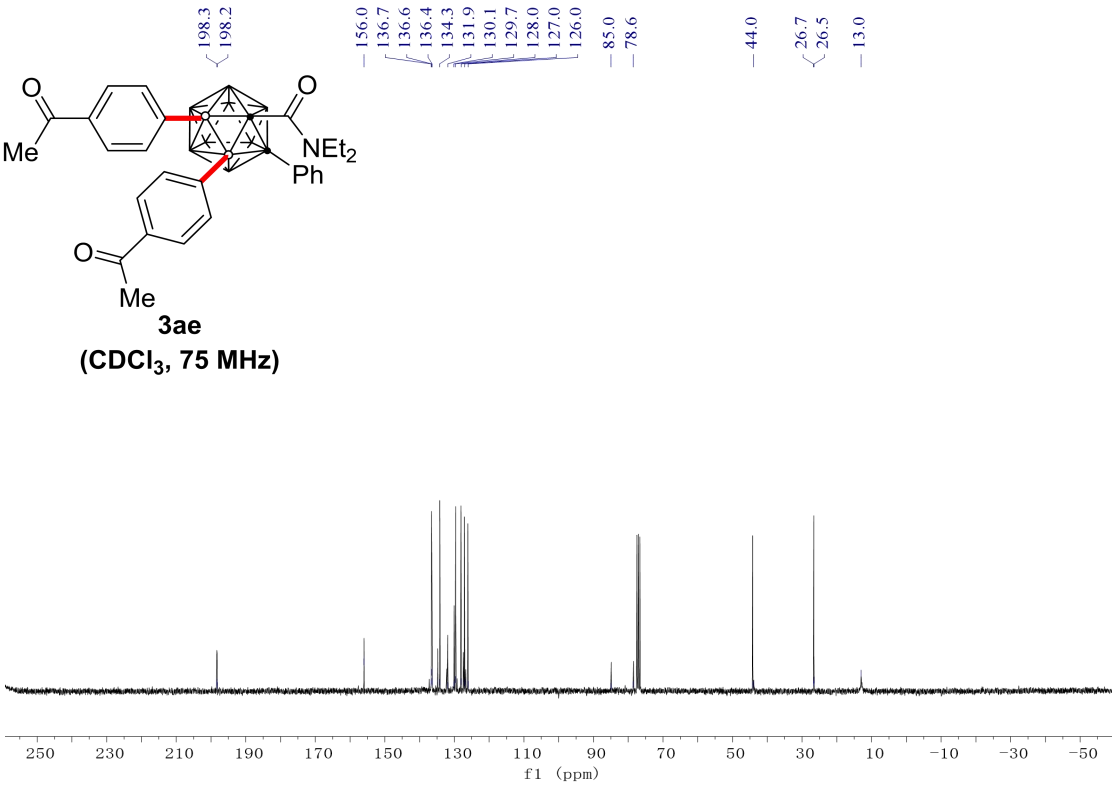



**3ae**

**($CDCl_3$, 300 MHz)**

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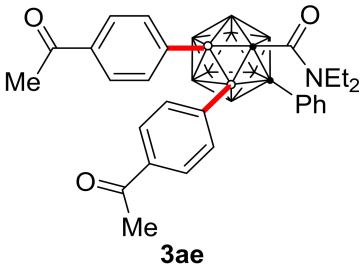


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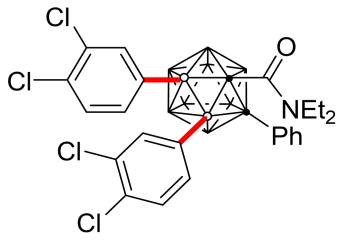


**3af**

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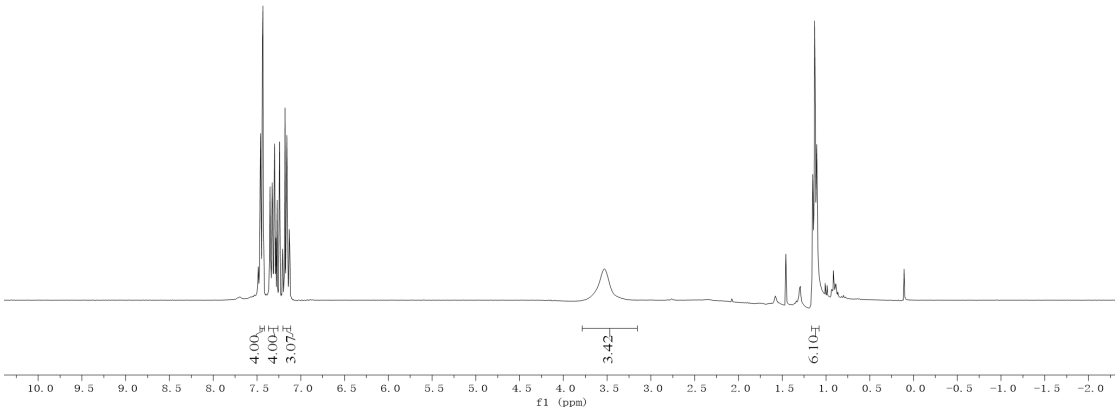

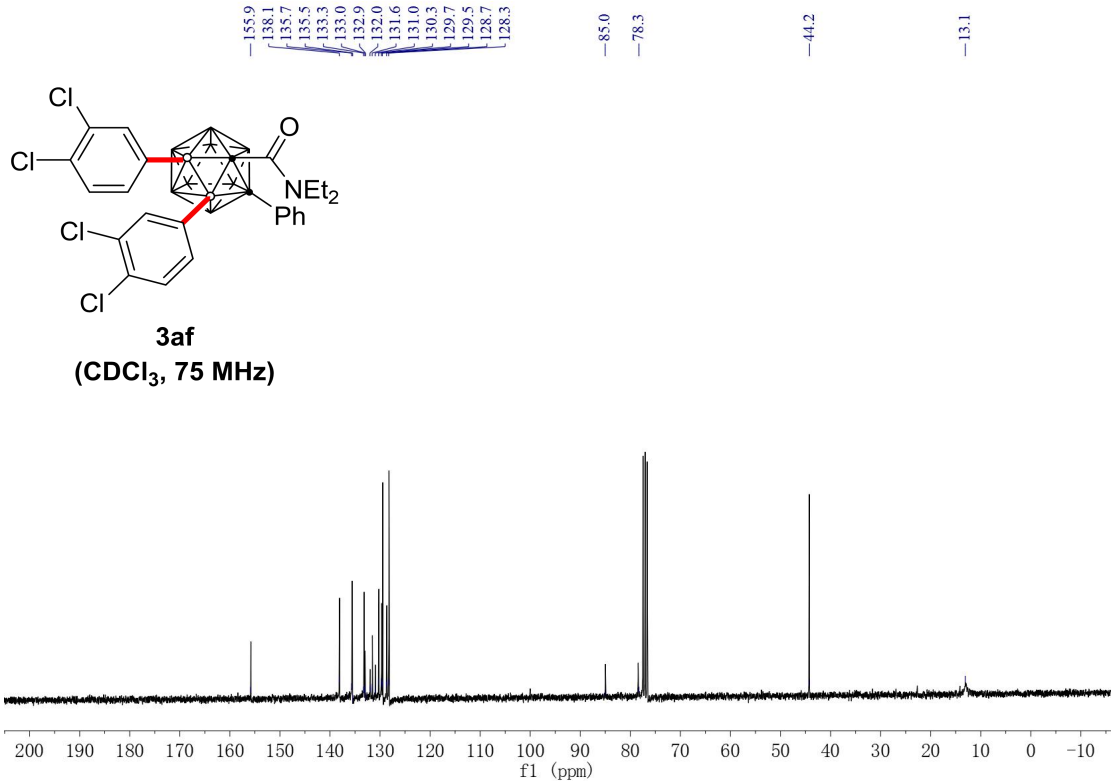


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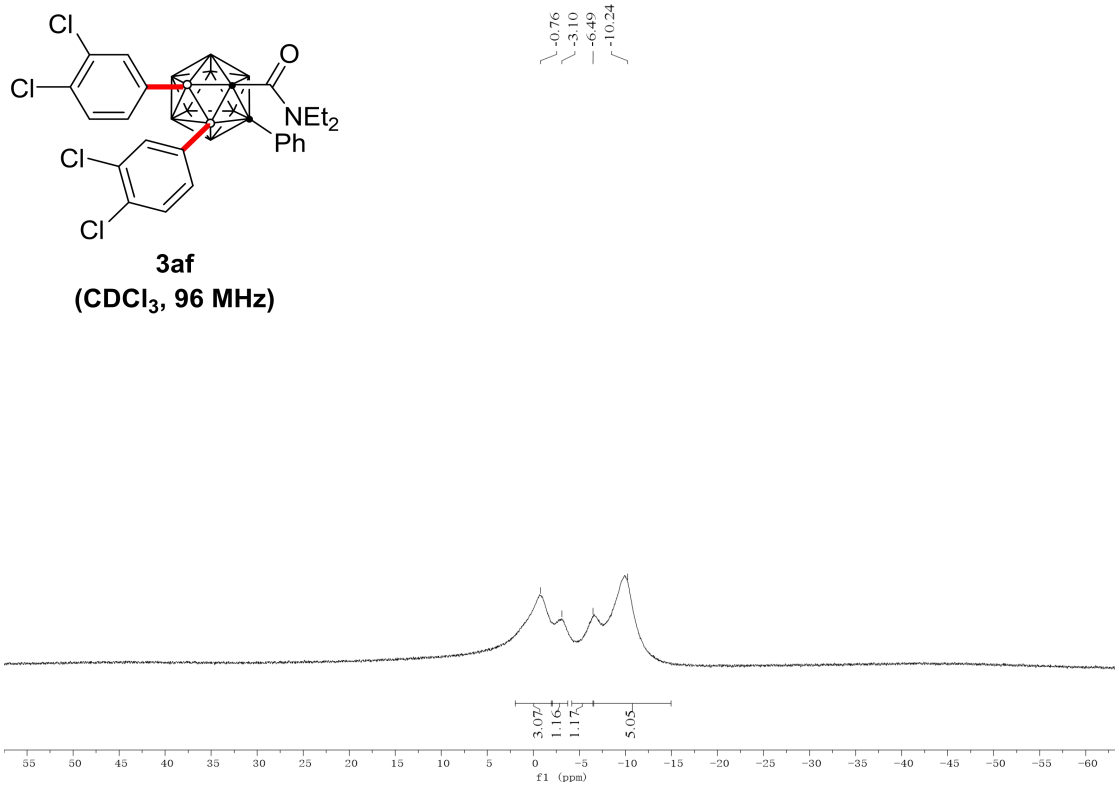


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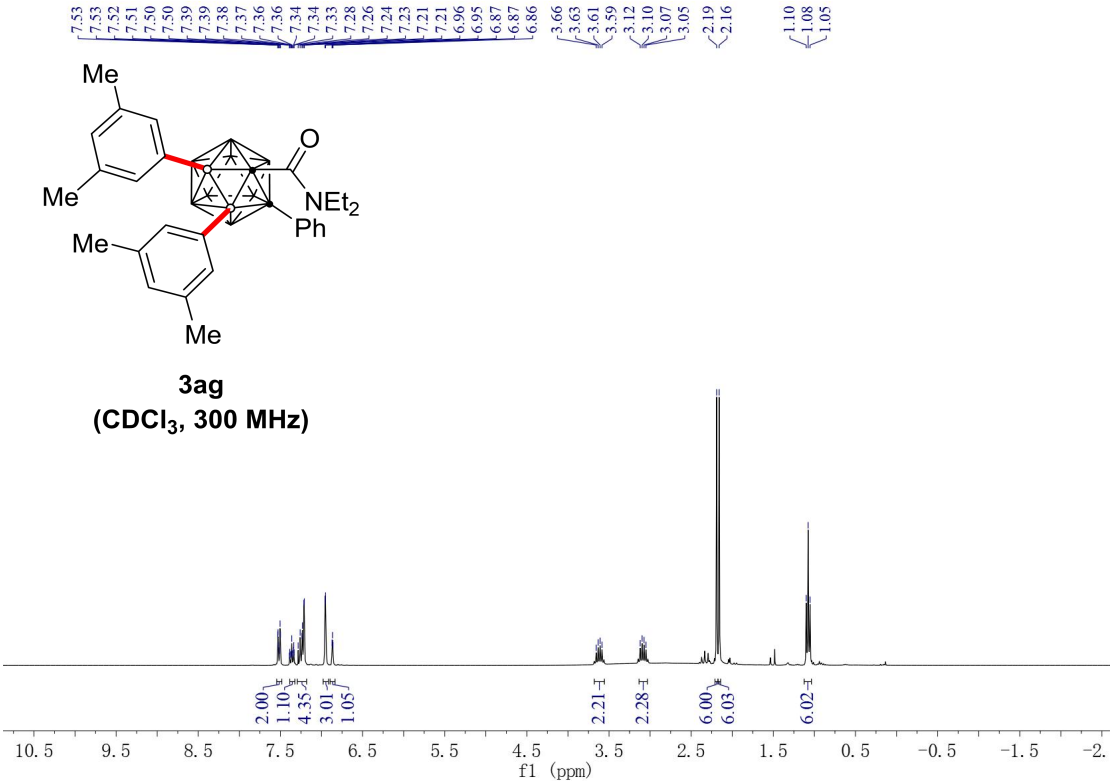


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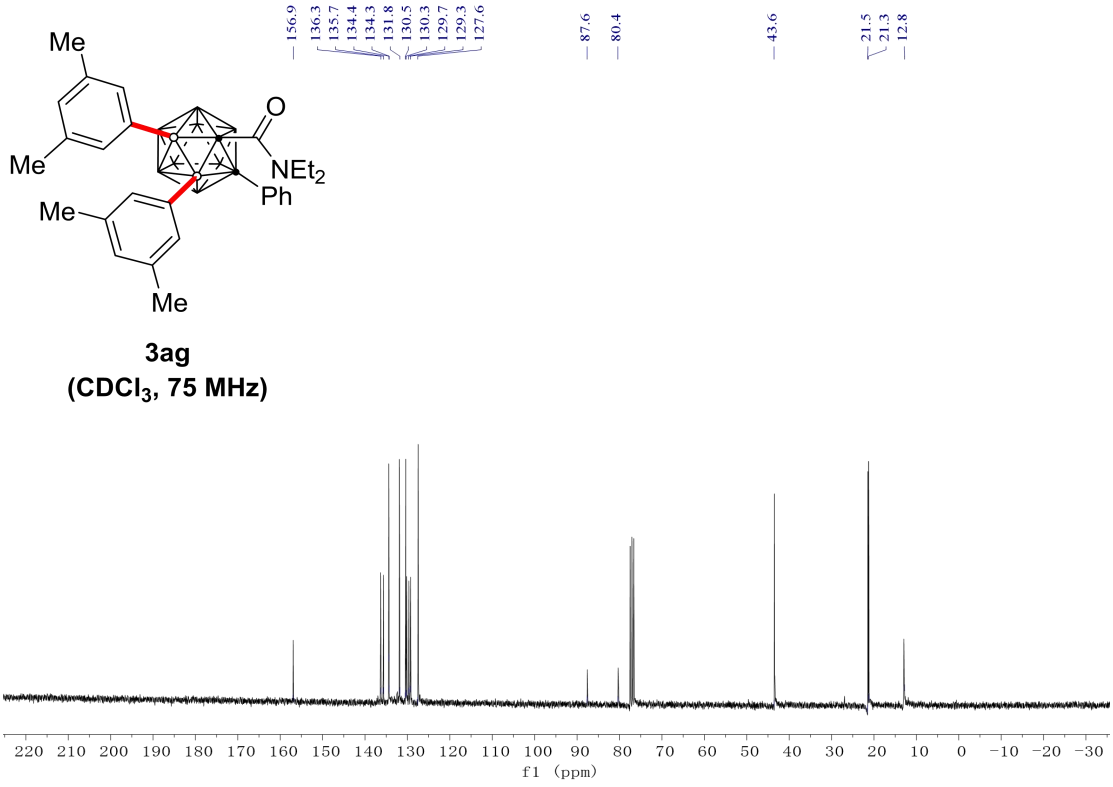


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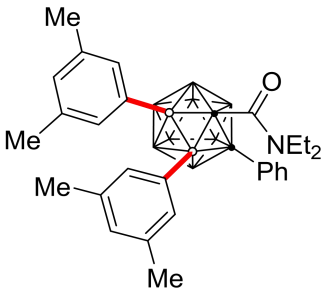


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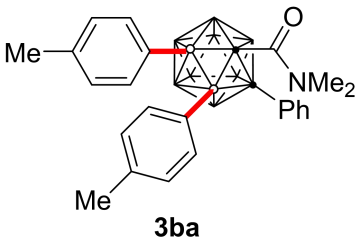


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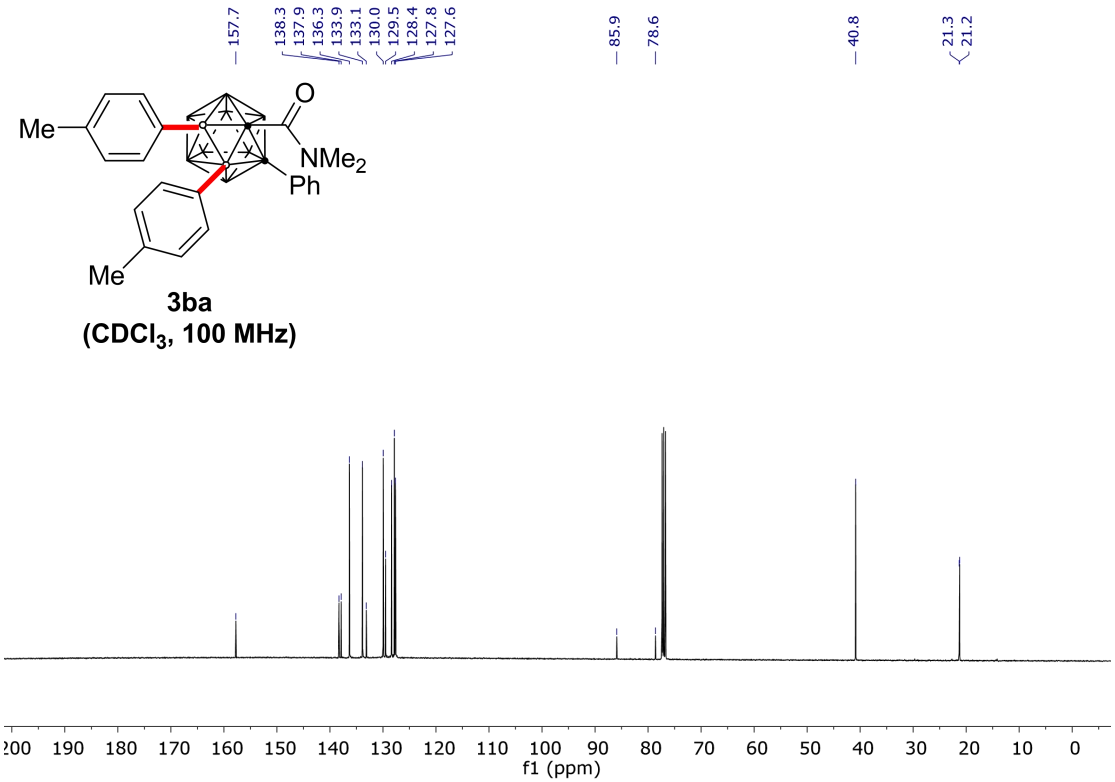


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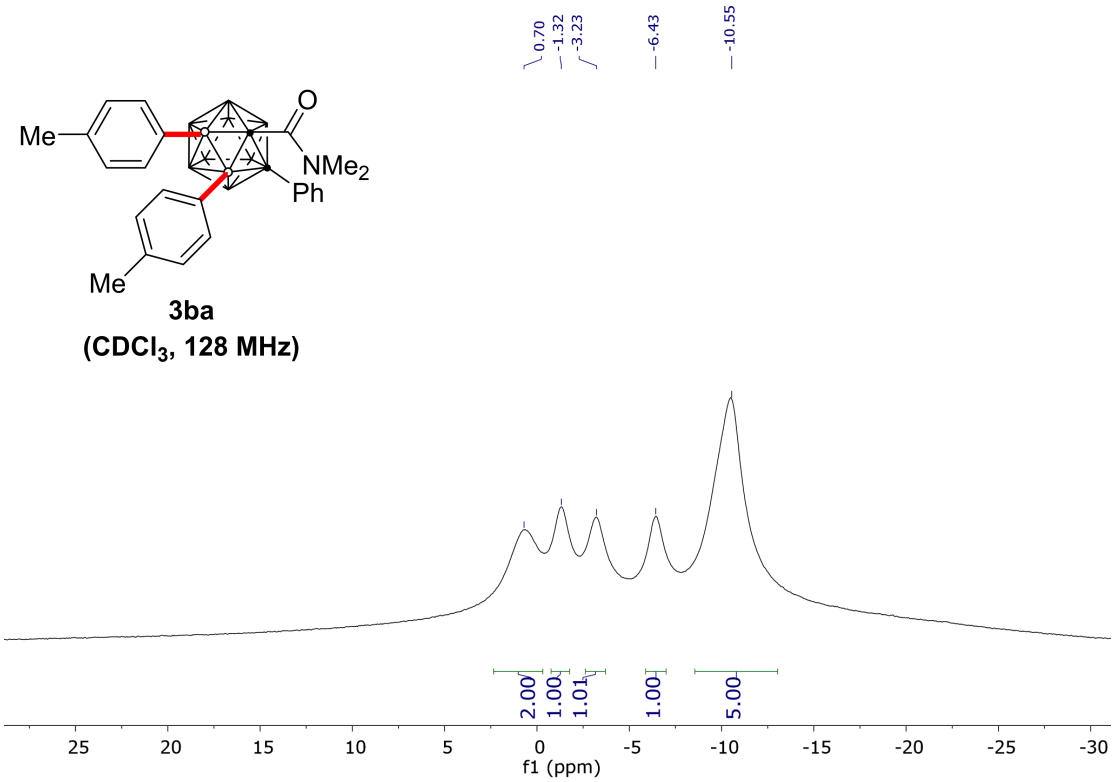


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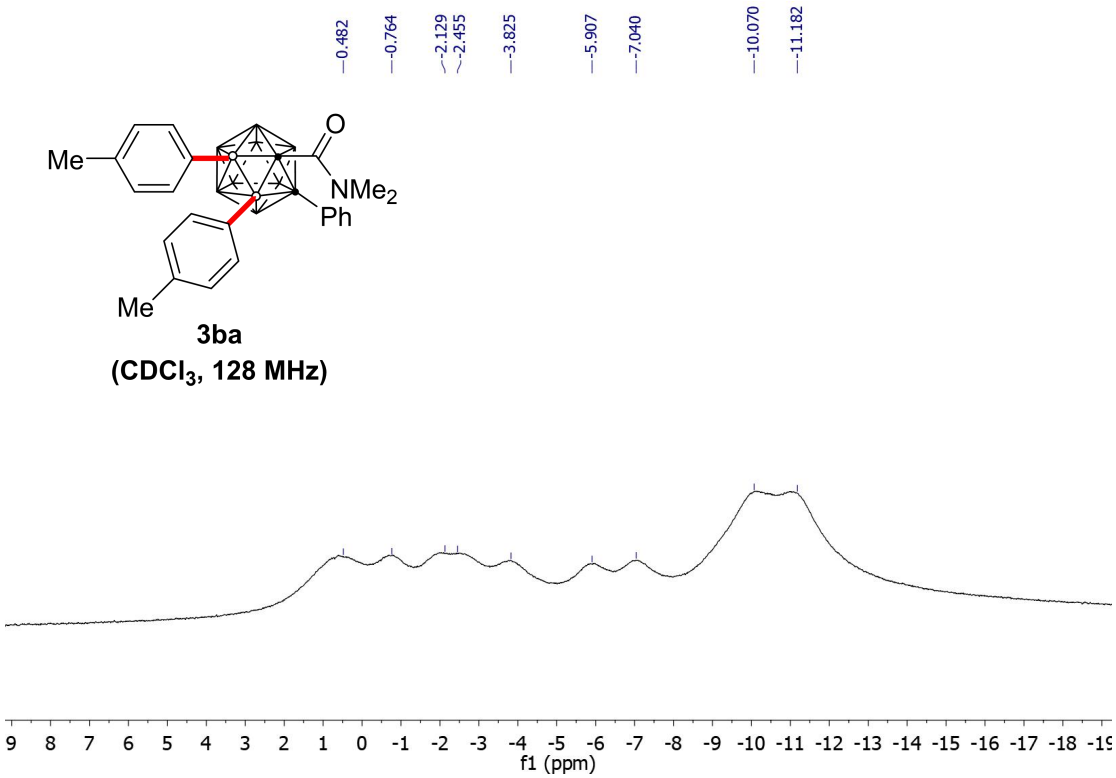


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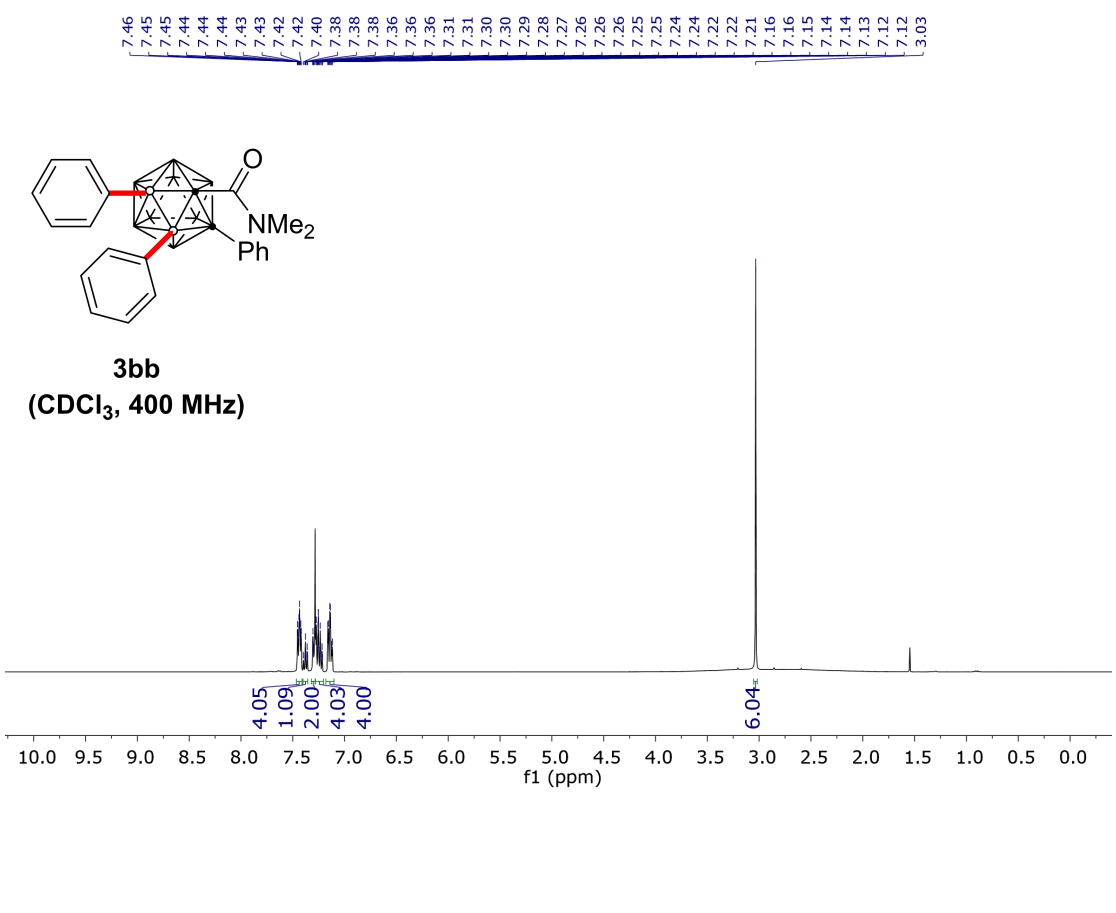


**3bb**

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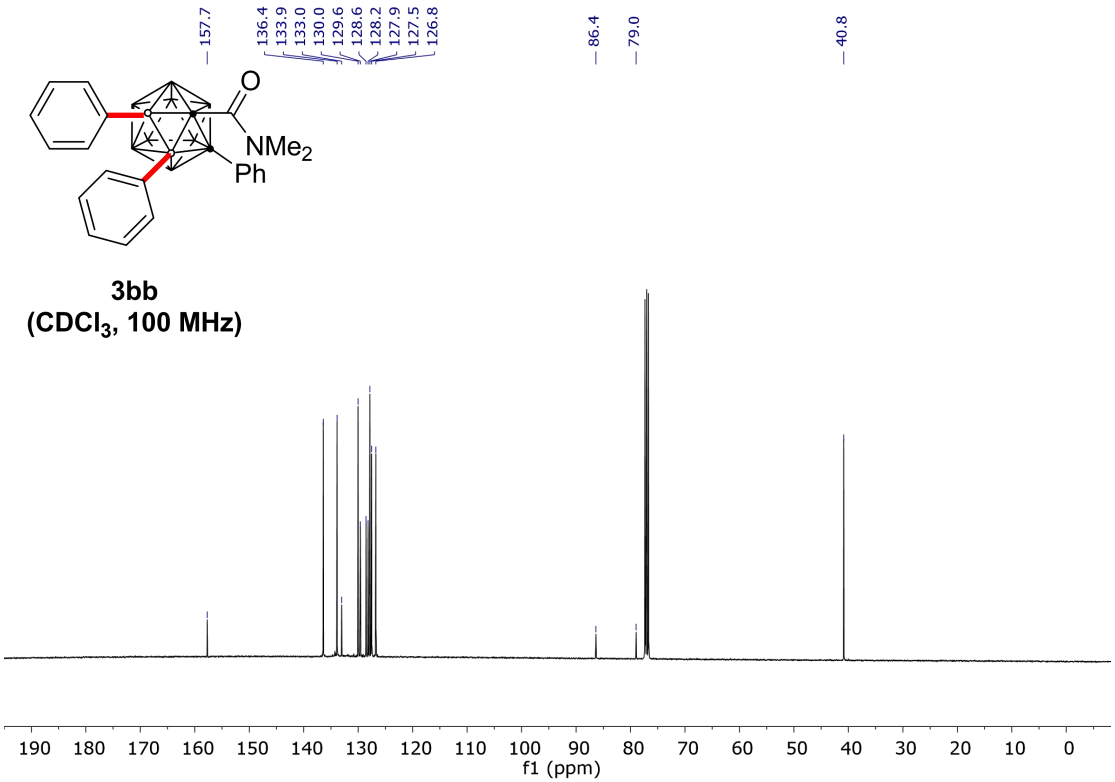


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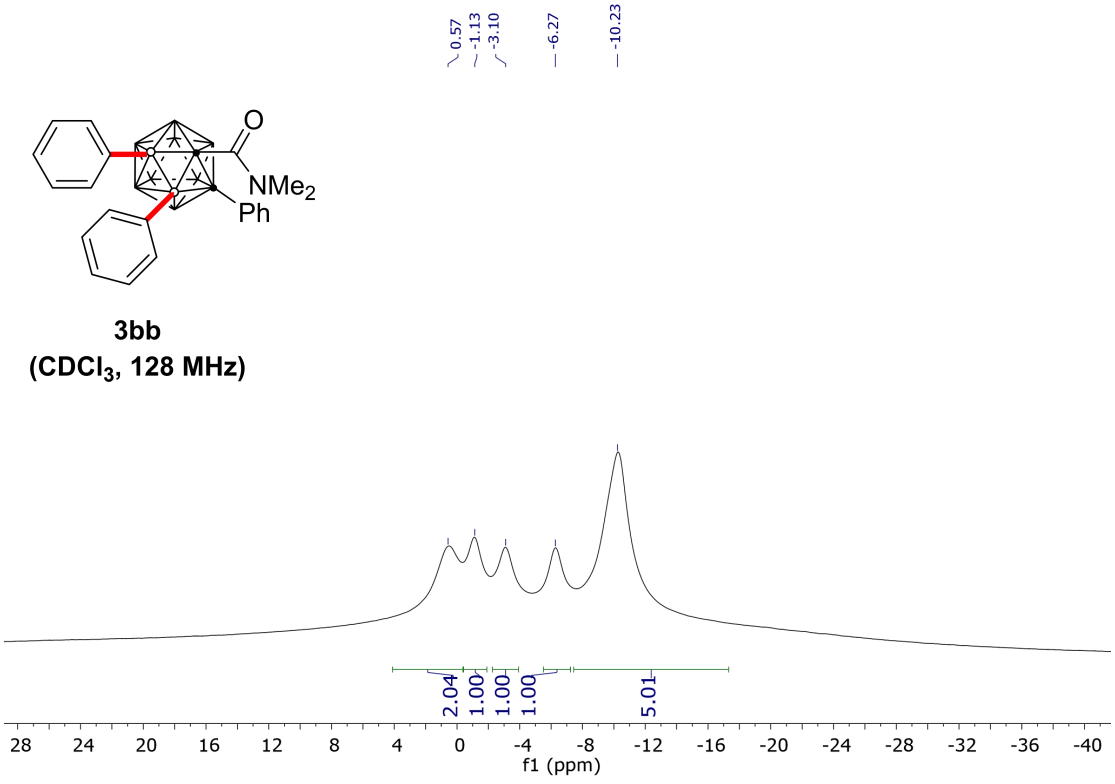


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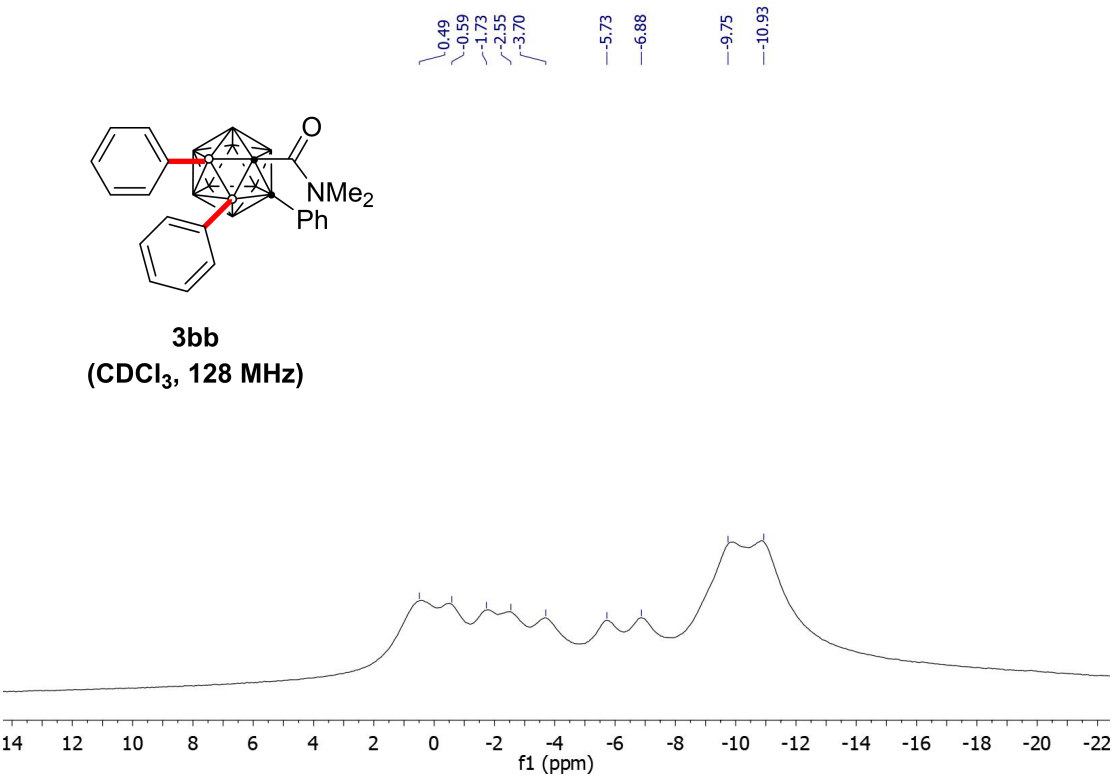


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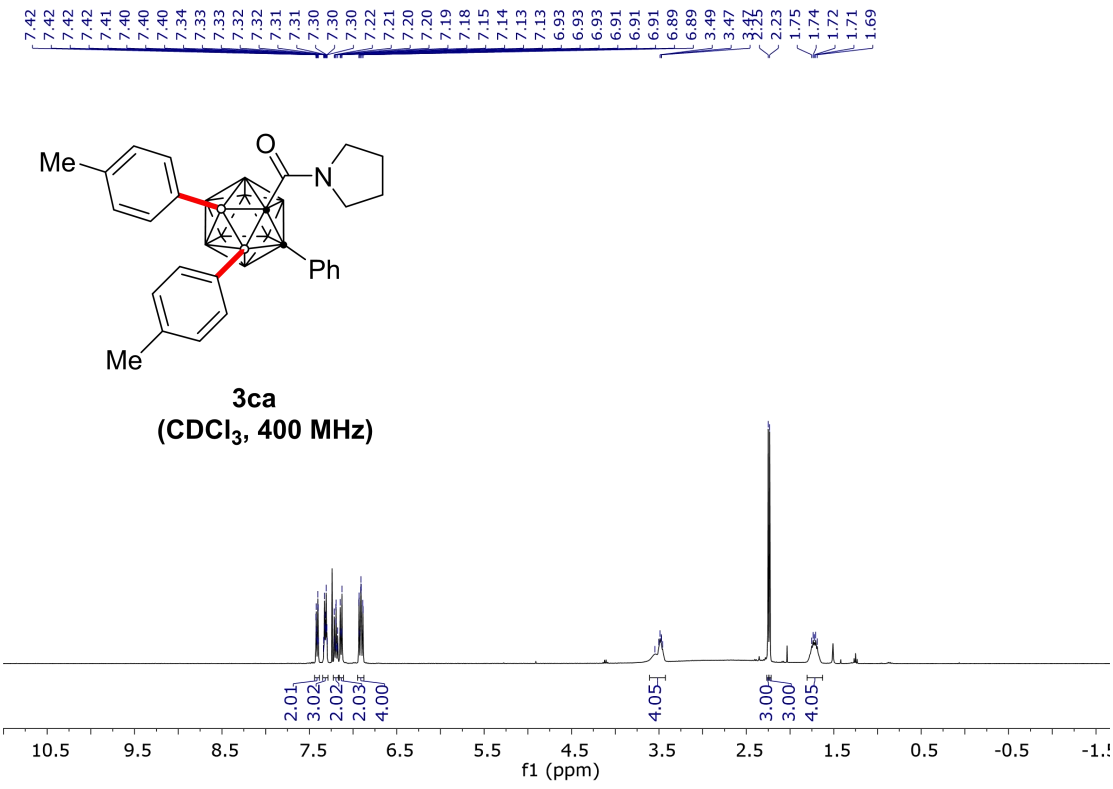


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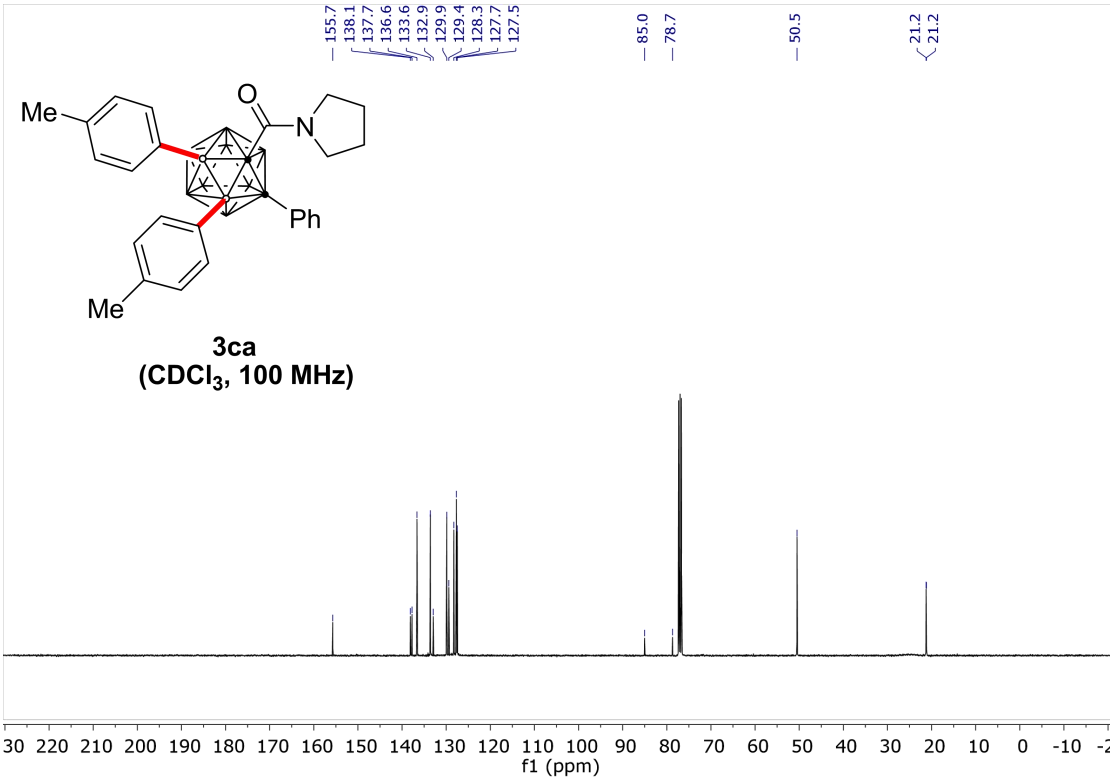


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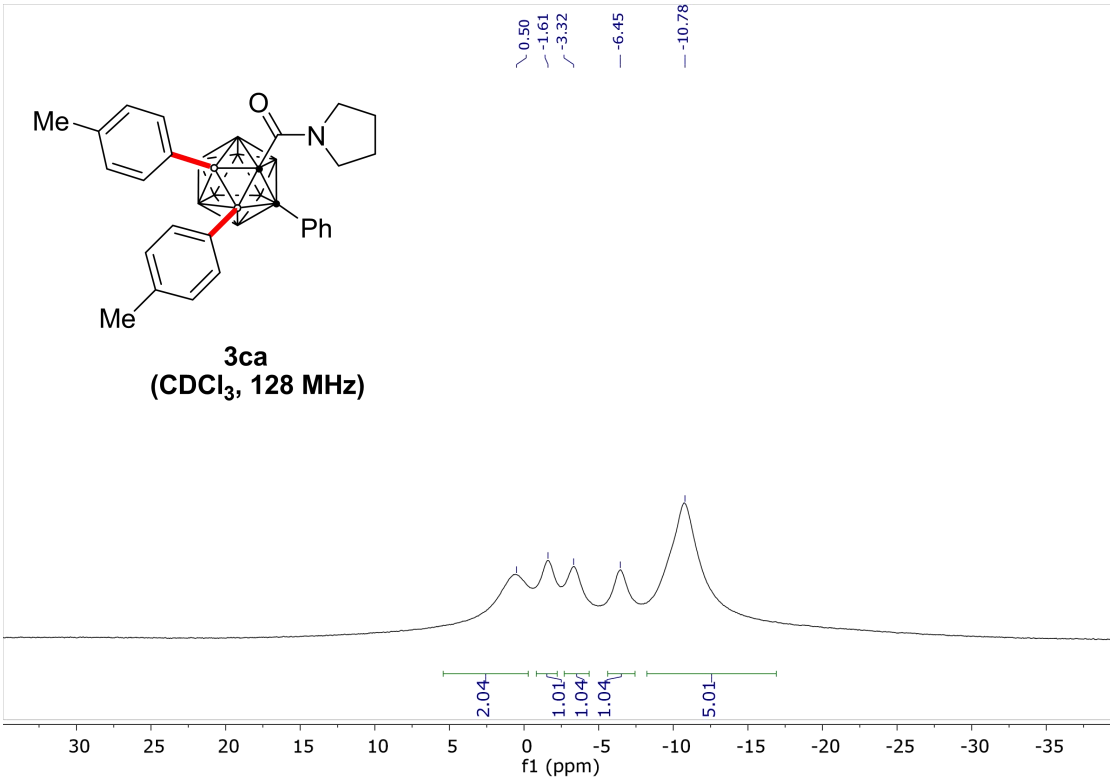


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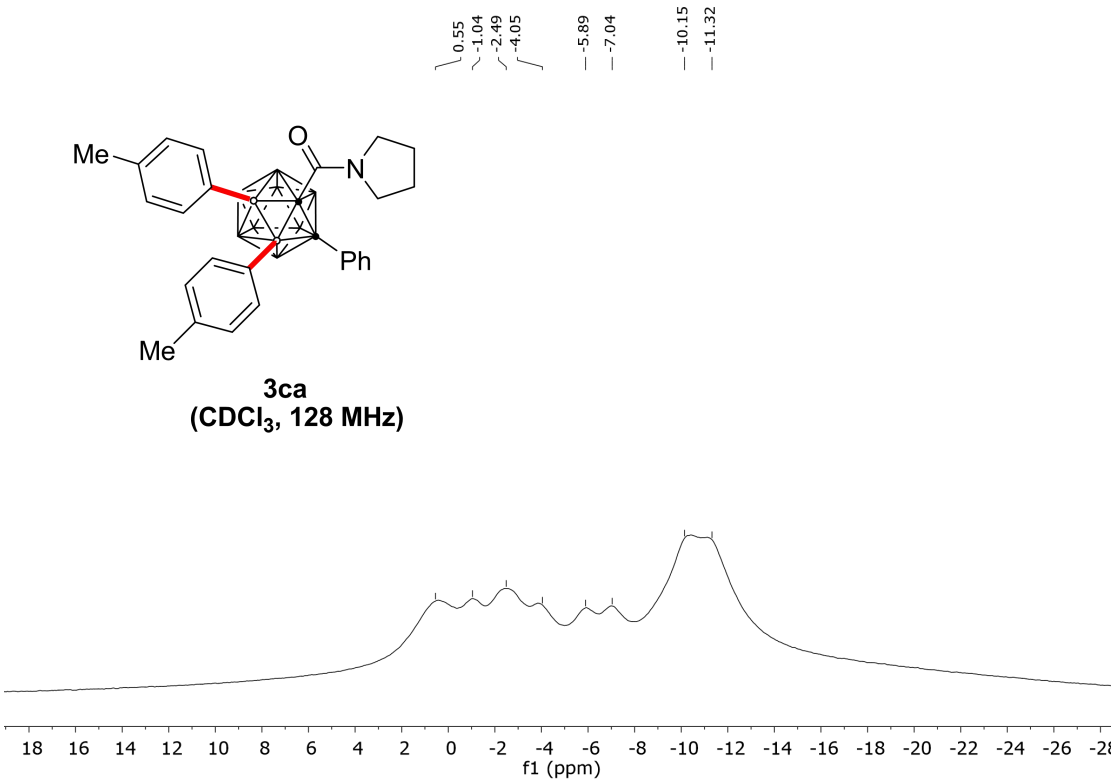


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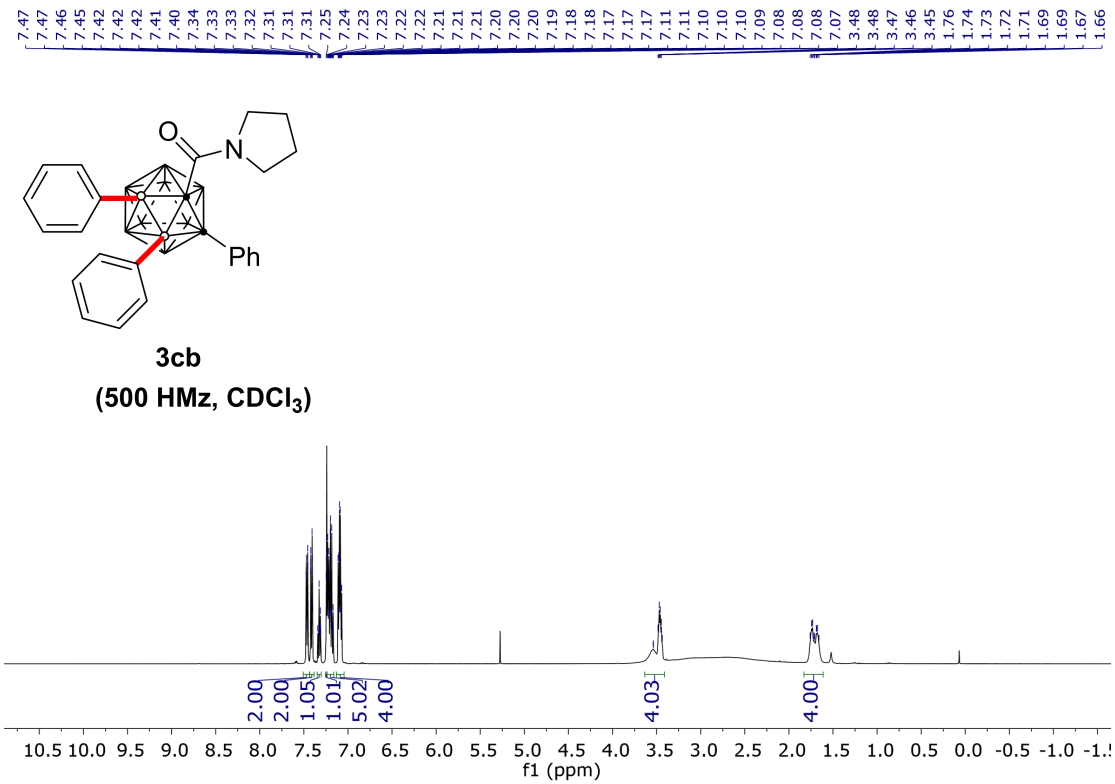
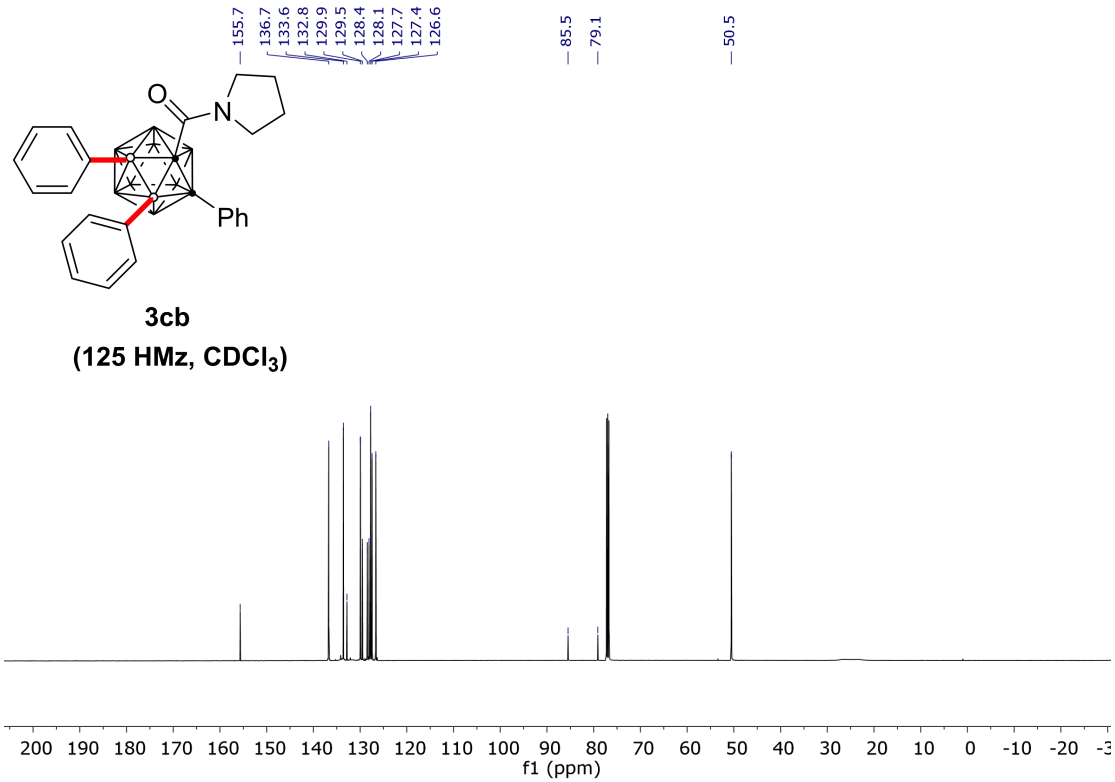



**3cb**
**(500 HMz, $CDCl_3$)**




**3cb**

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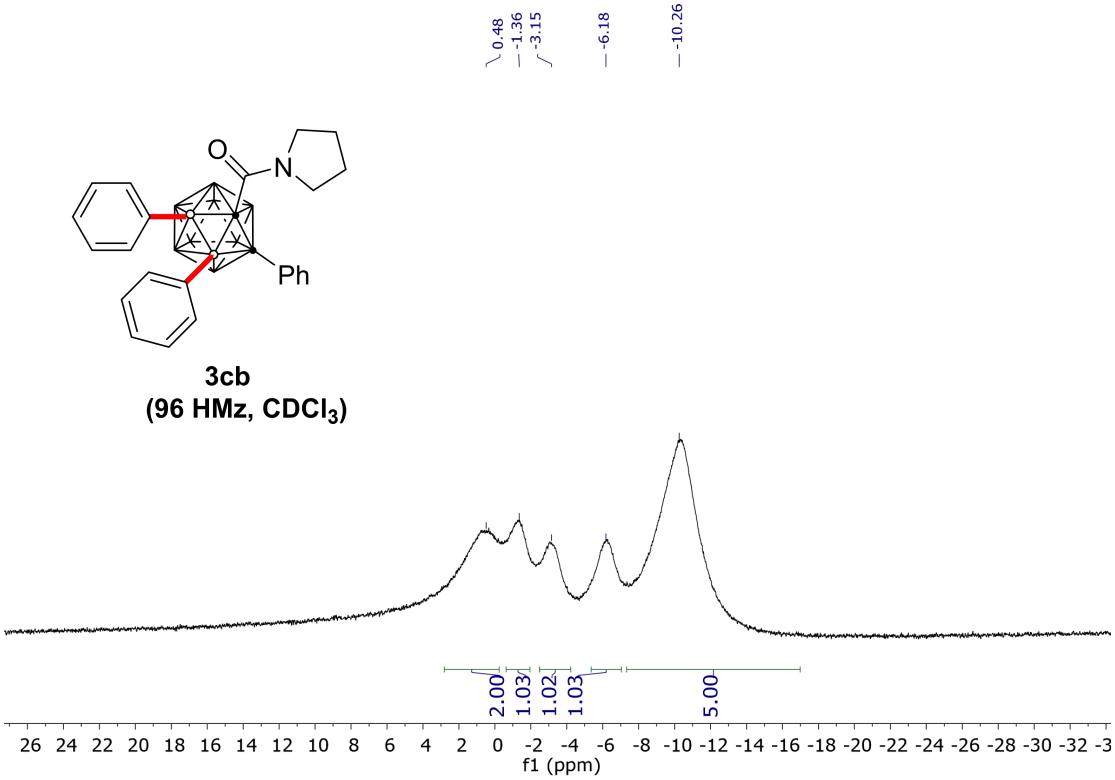
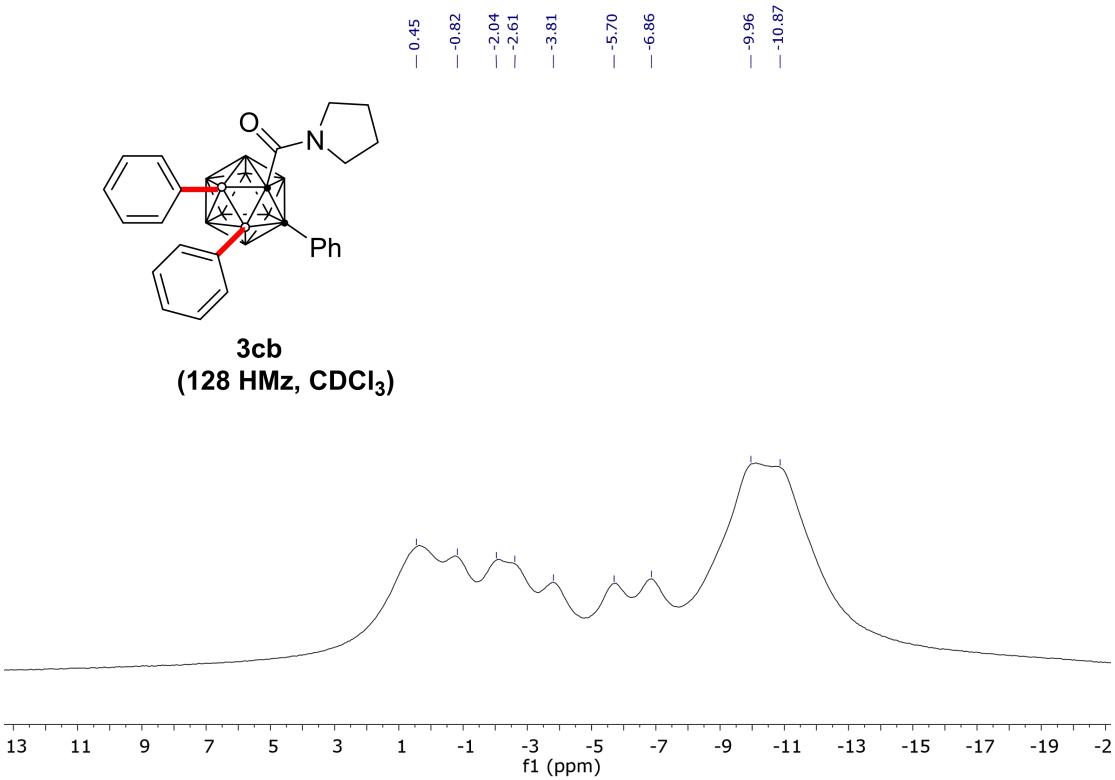



**3cb**

**(96 HMz, $CDCl_3$)**

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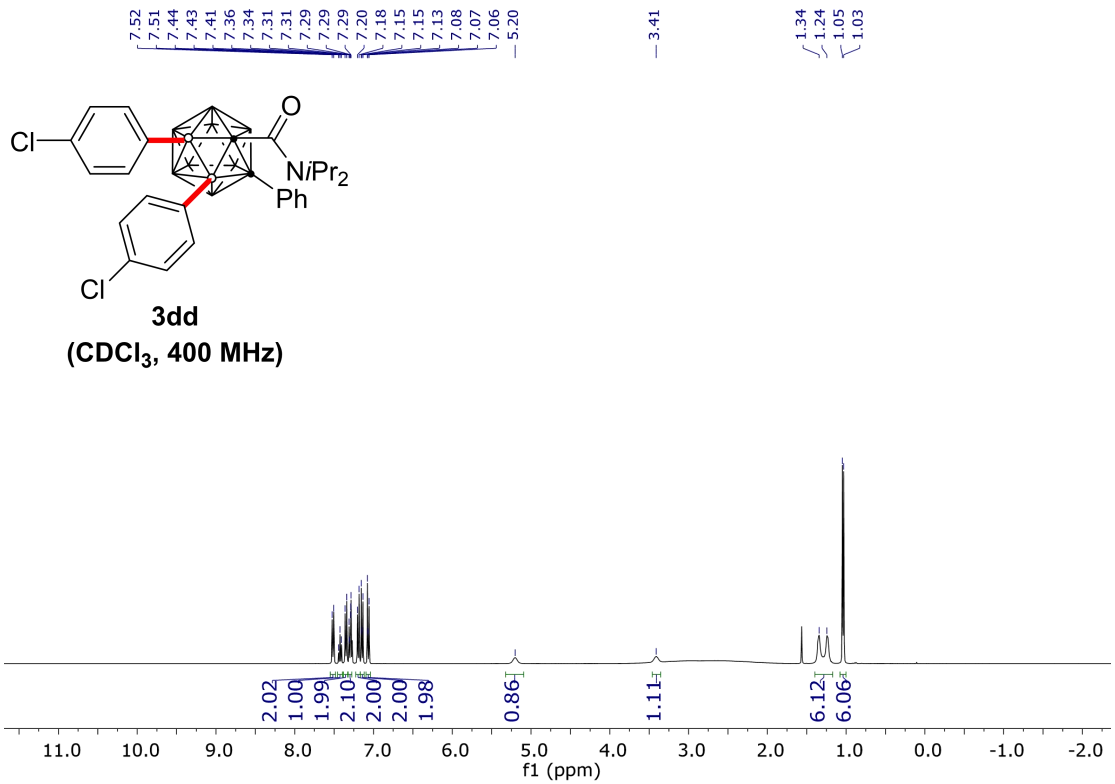


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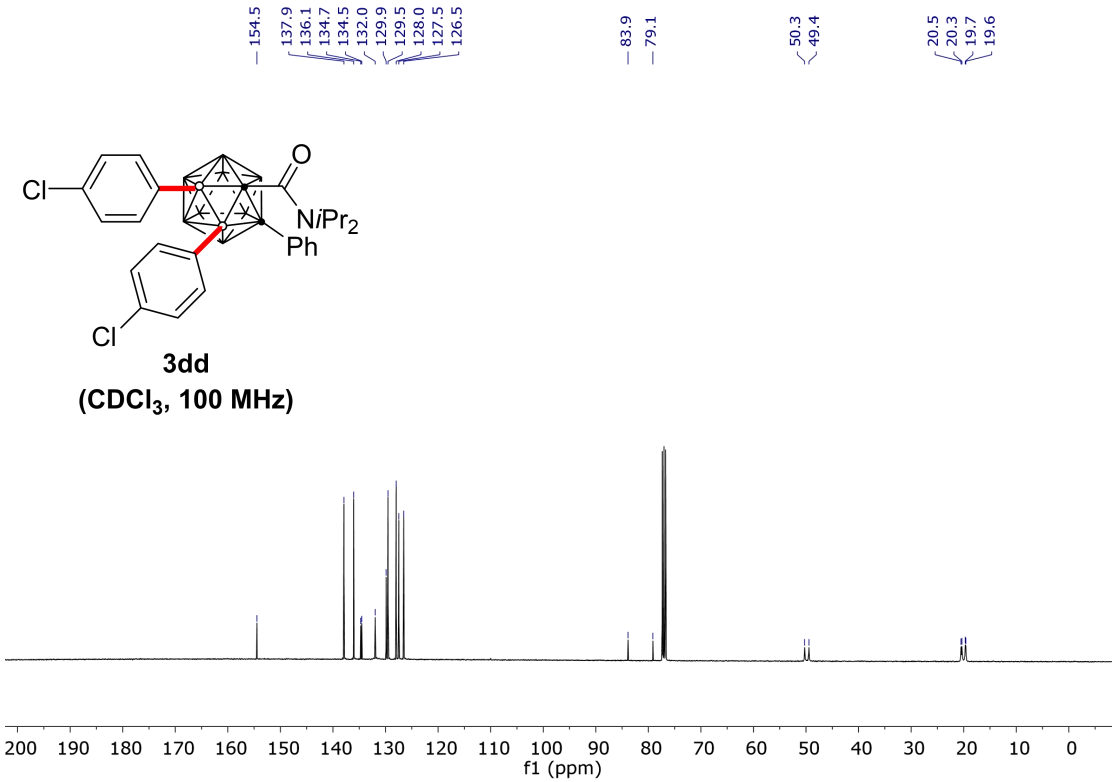
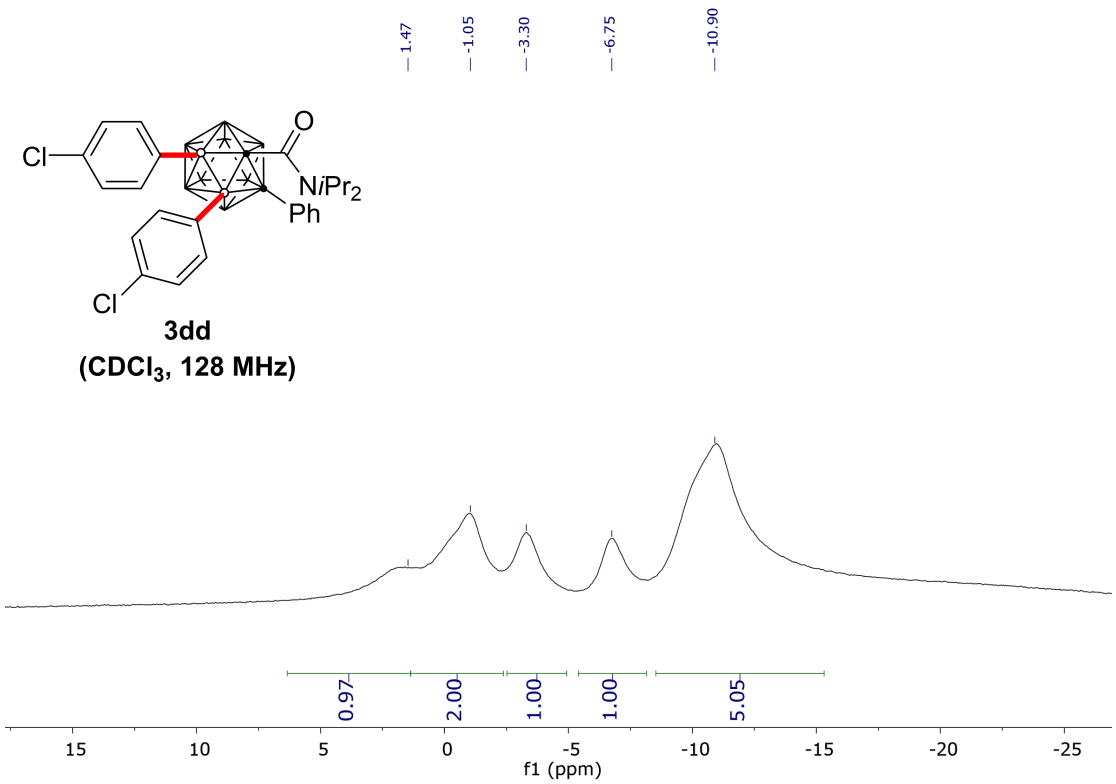


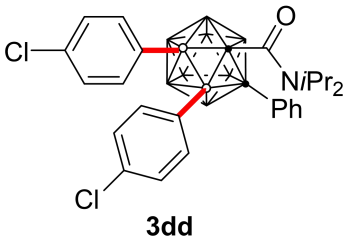

**3dd**

**($CDCl_3$, 100 MHz)**




**3dd**

**($CDCl_3$, 128 MHz)**

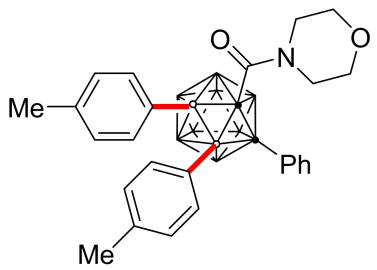



**3dd**

**($CDCl_3$, 128 MHz)**

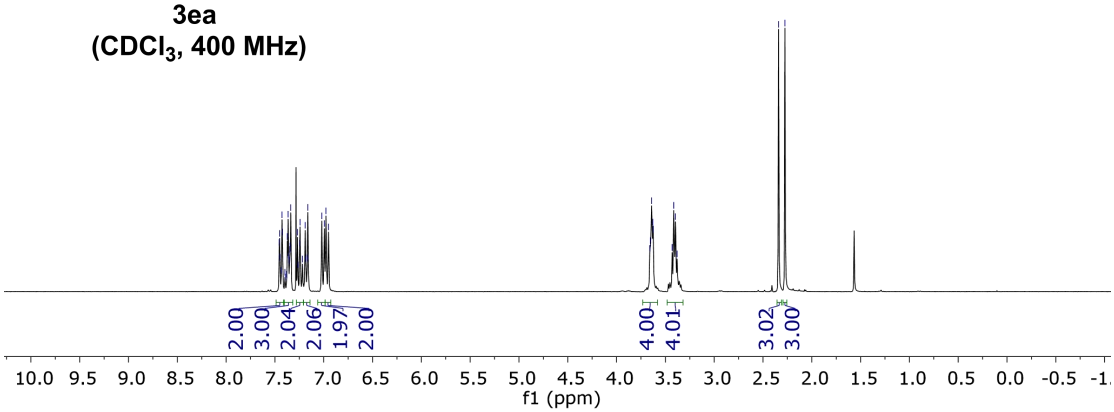


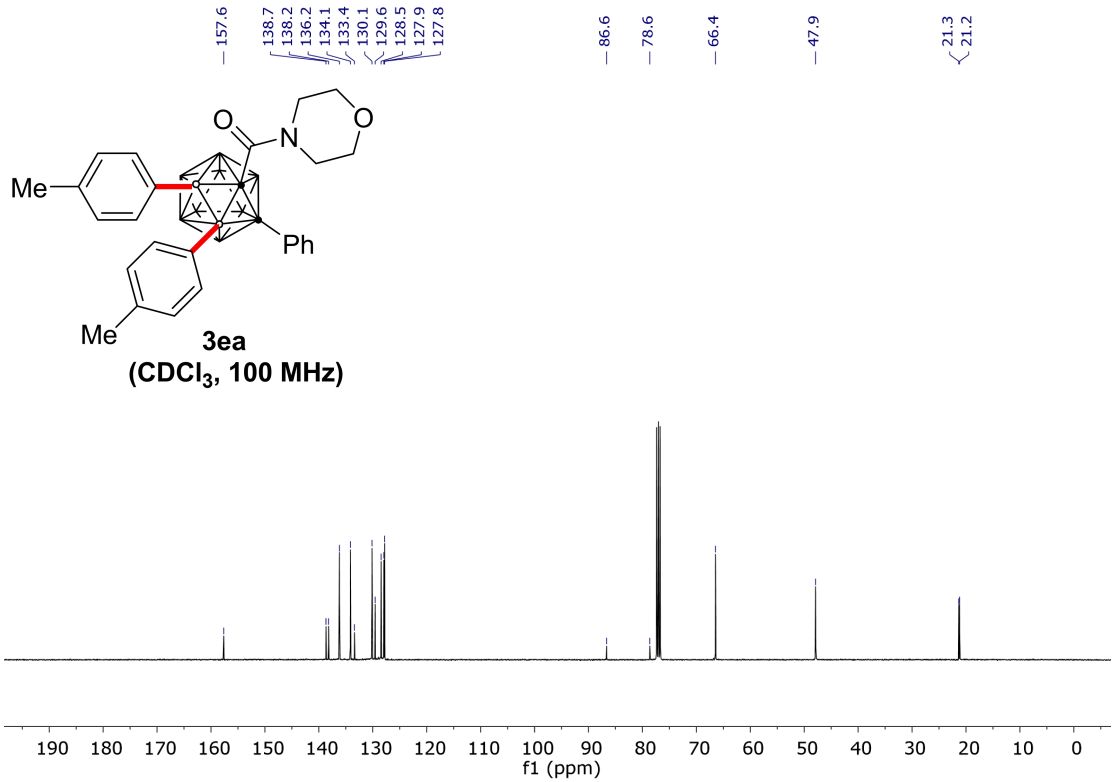




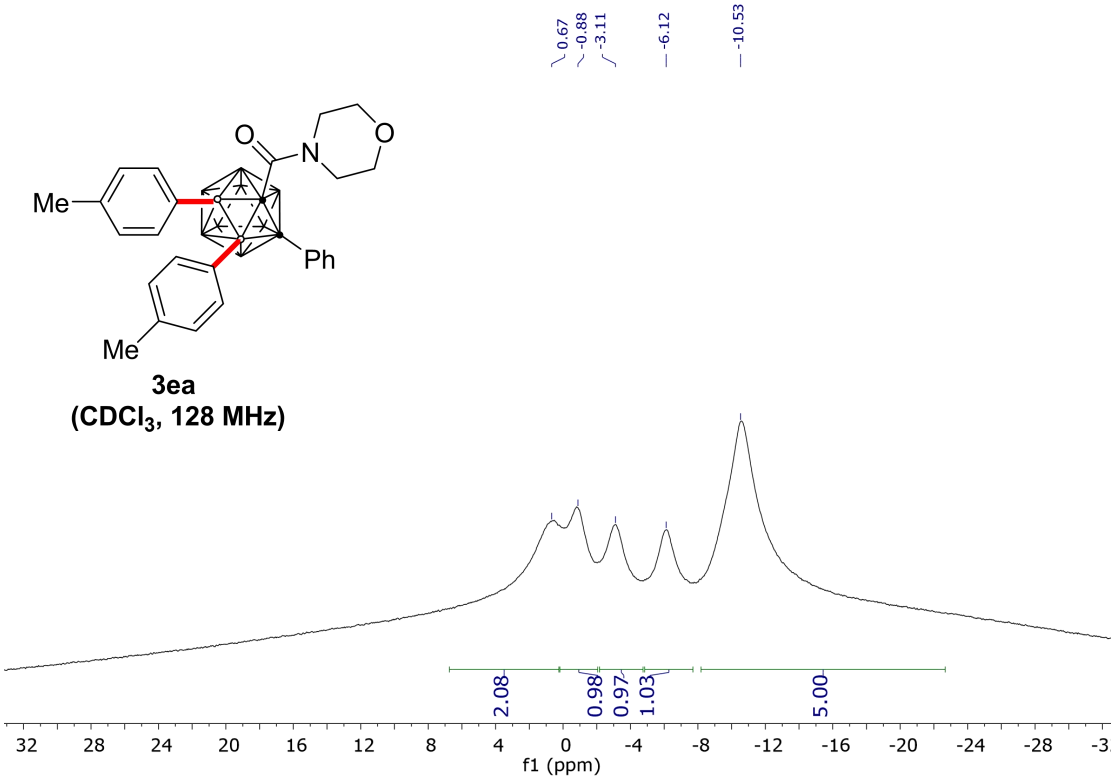

**3ea**

**($CDCl_3$, 400 MHz)**

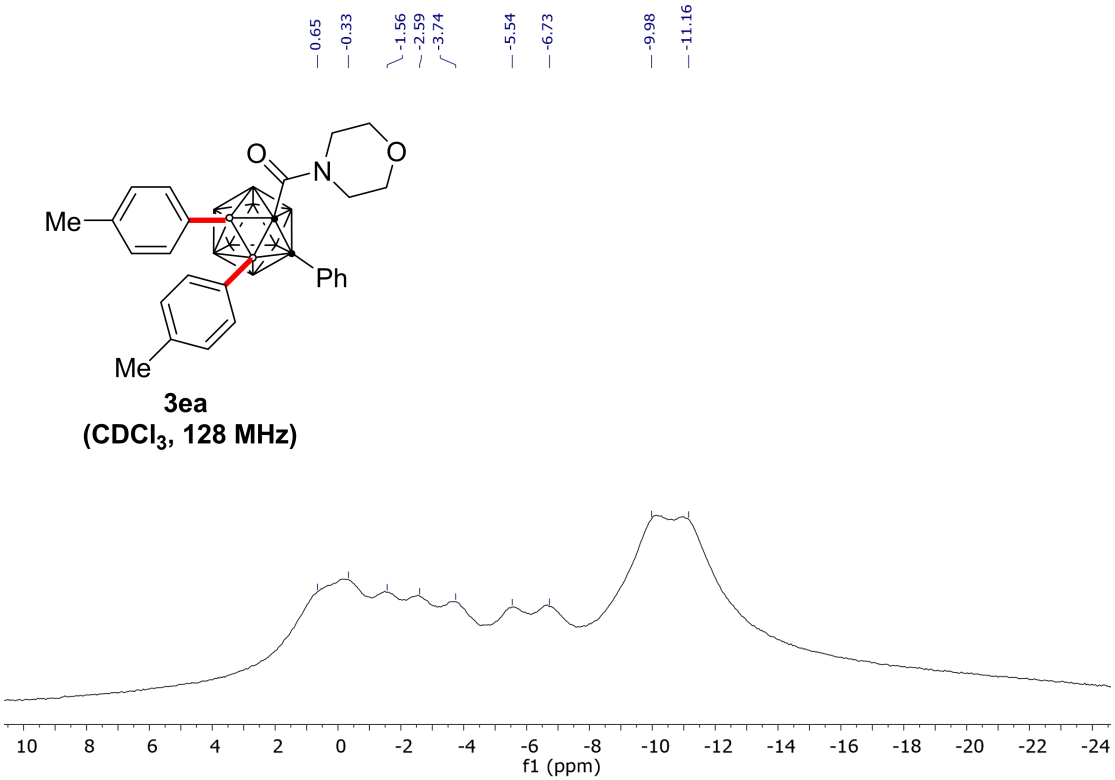




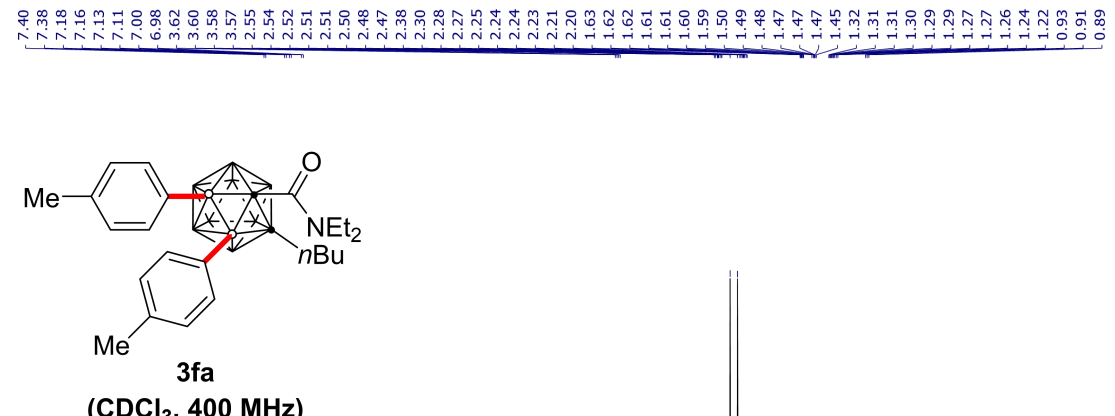

**3ea**
**($CDCl_3$, 100 MHz)**




**3ea**
**($CDCl_3$, 128 MHz)**



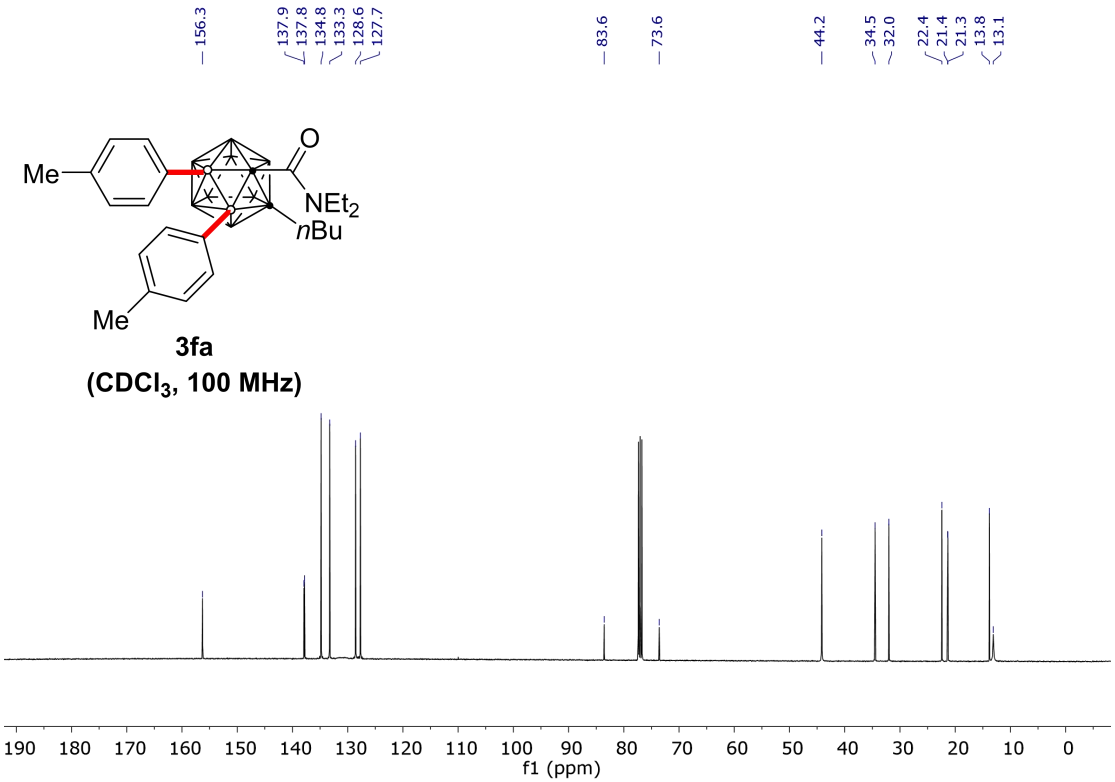

**3ea**
**($CDCl_3$, 128 MHz)**





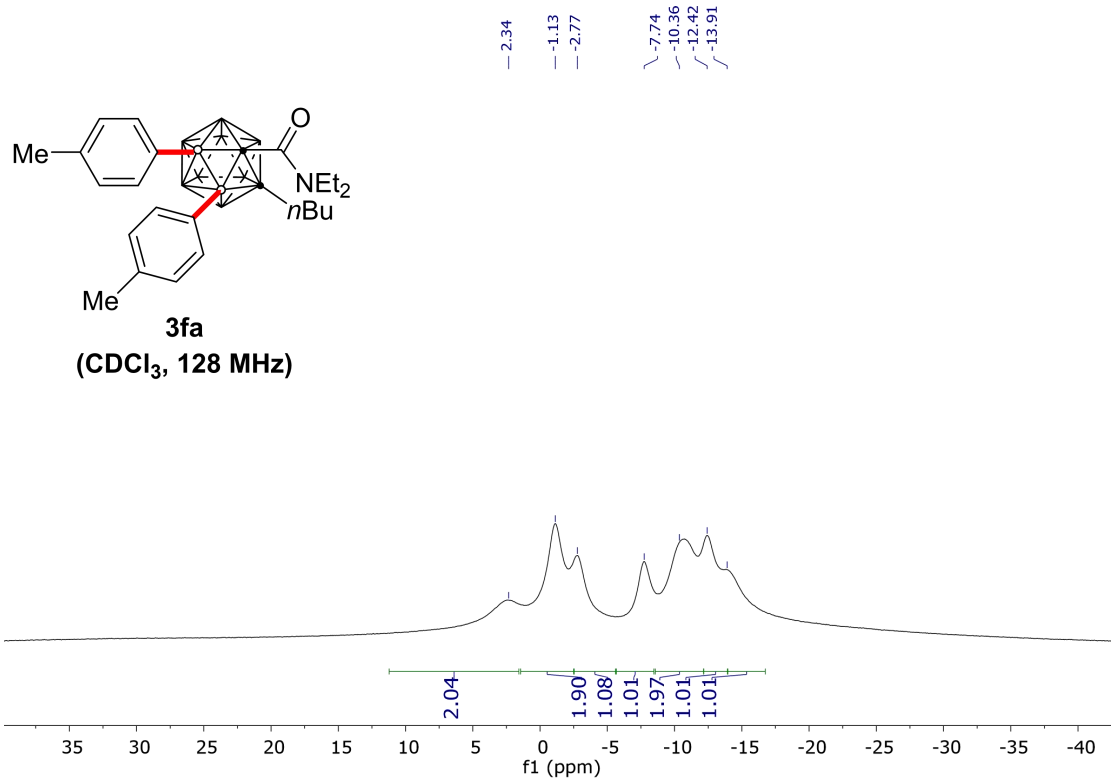


**3fa**
**($CDCl_3$, 400 MHz)**



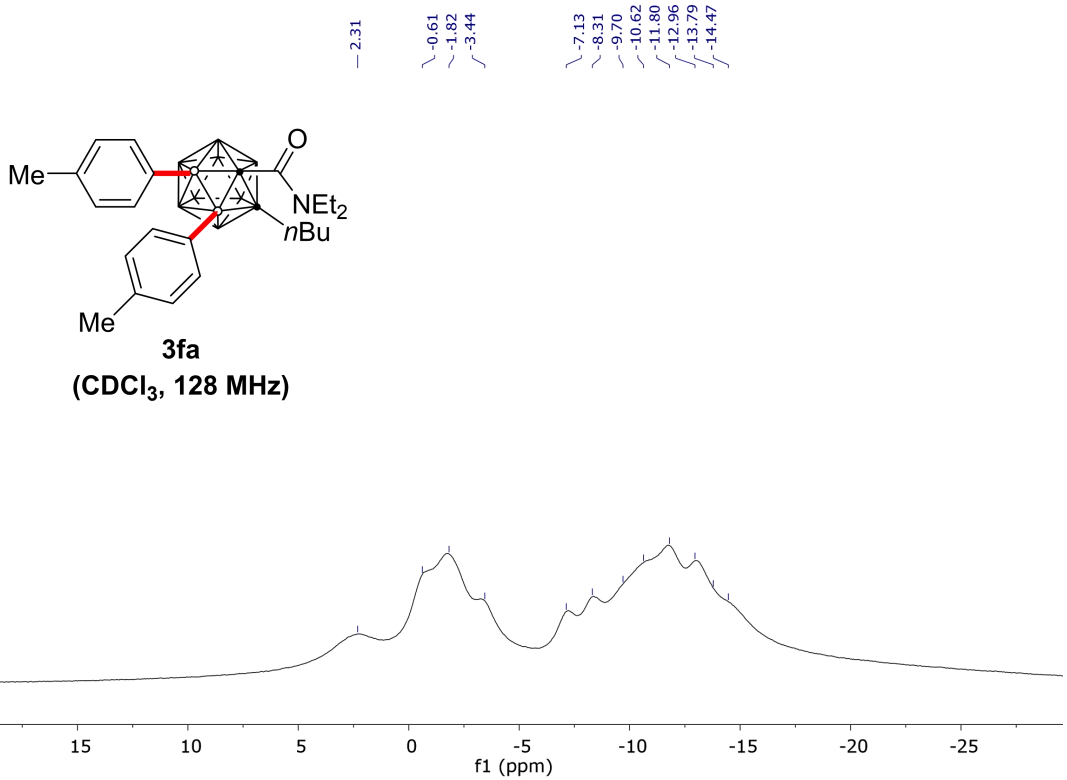

**3fa**

**($CDCl_3$, 100 MHz)**



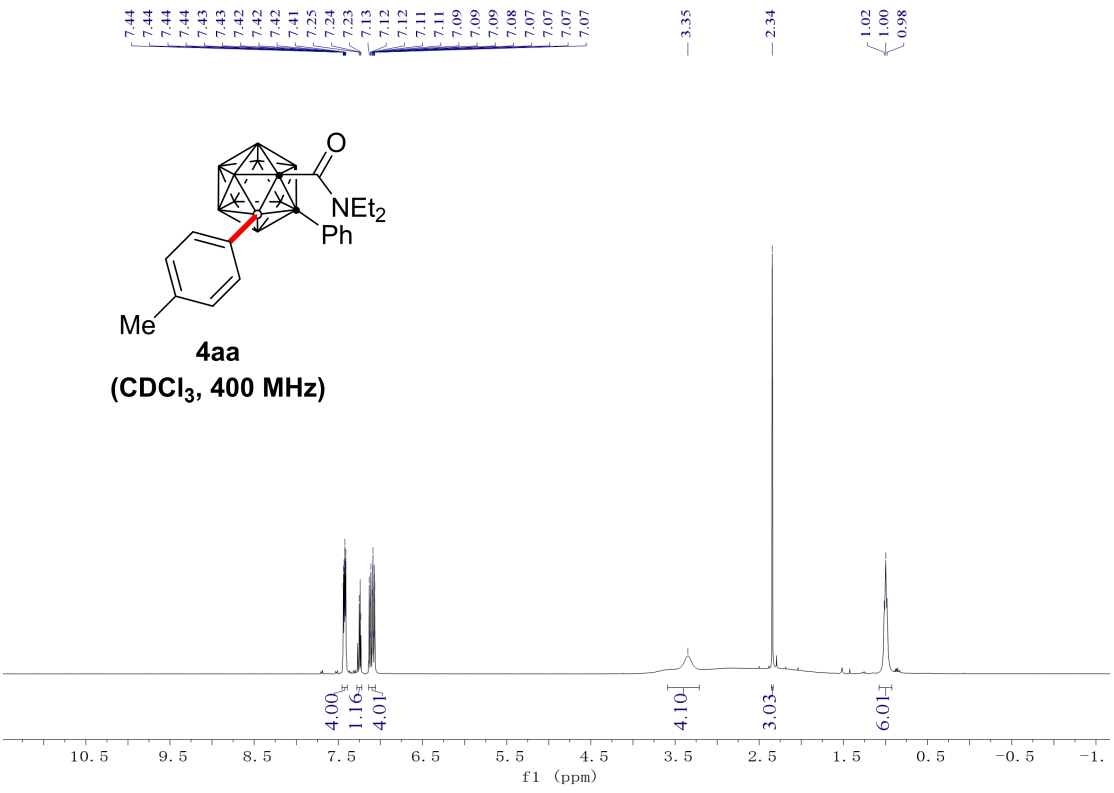

**3fa**

**($CDCl_3$, 128 MHz)**



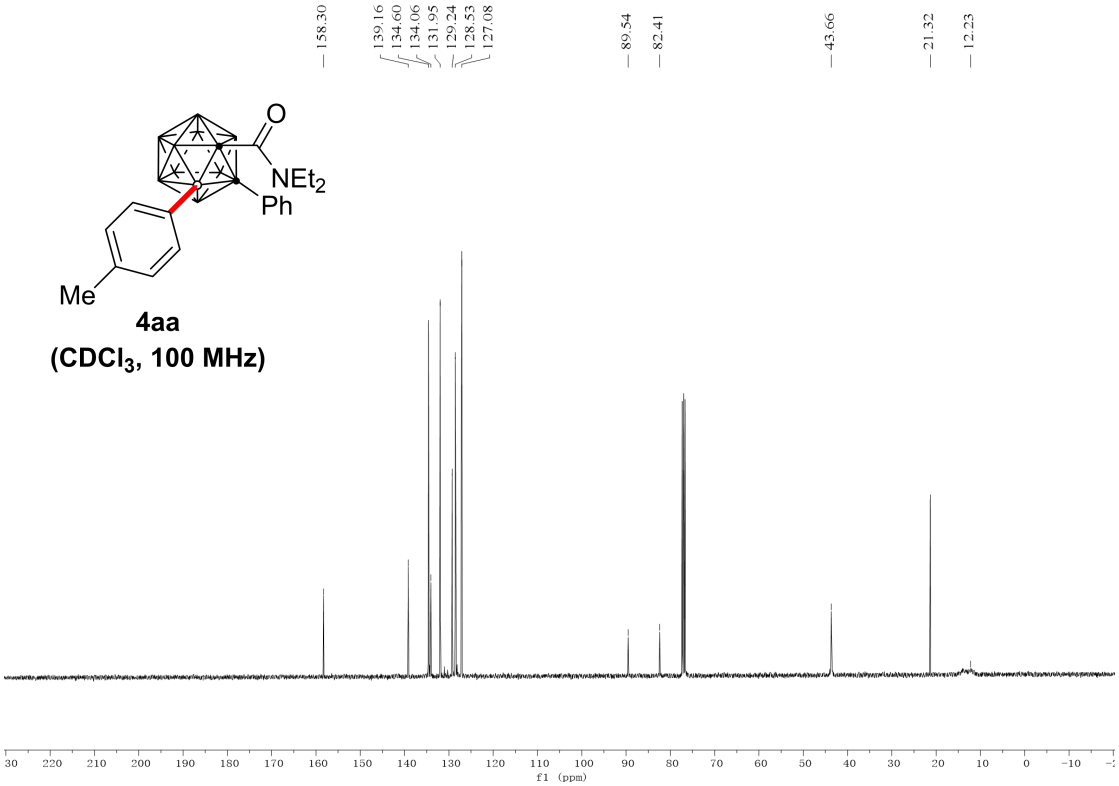

**3fa**

**($CDCl_3$, 128 MHz)**



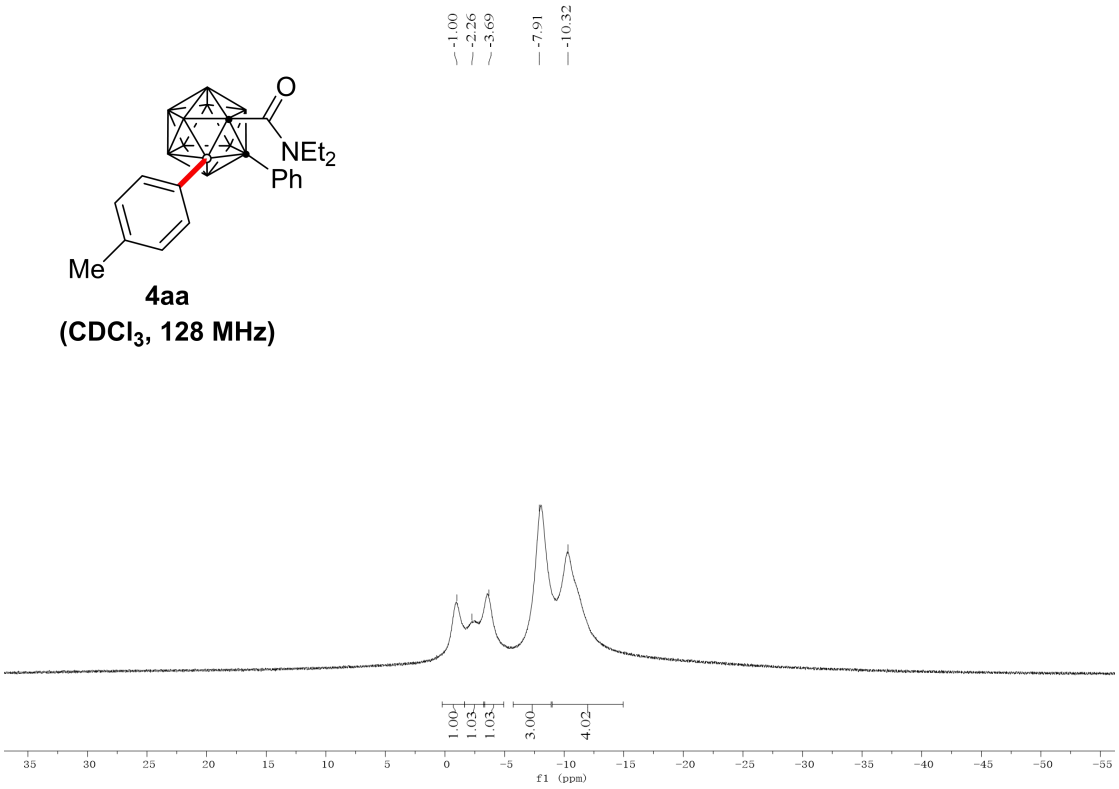

**4aa**

**($CDCl_3$, 400 MHz)**



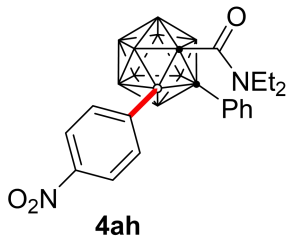

**4aa**

**($CDCl_3$, 100 MHz)**



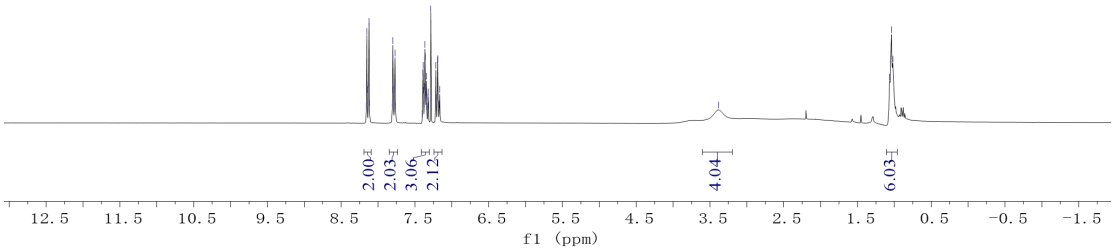

**4aa**

**($CDCl_3$, 128 MHz)**

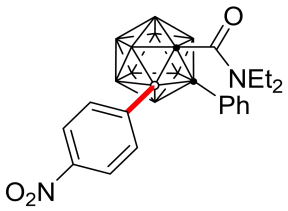




**4ah**

**($CDCl_3$, 300 MHz)**

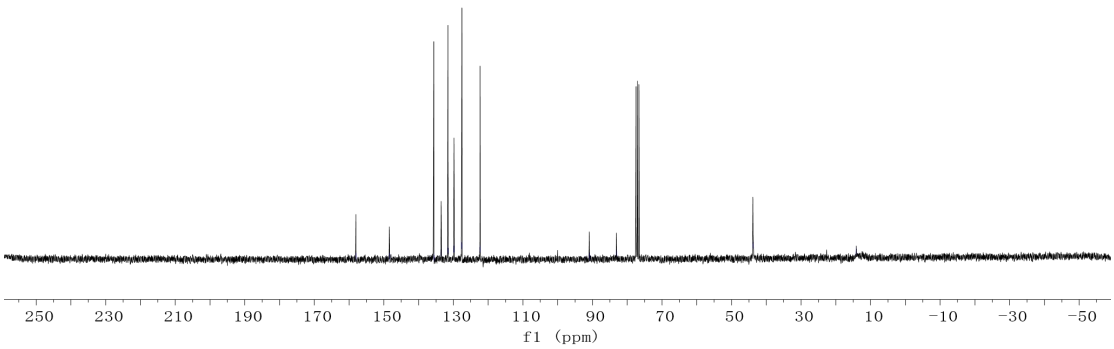


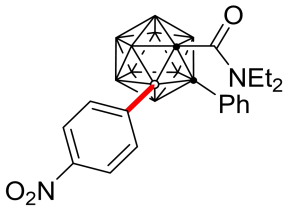





**4ah**

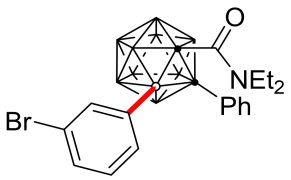
**($CDCl_3$, 75 MHz)**



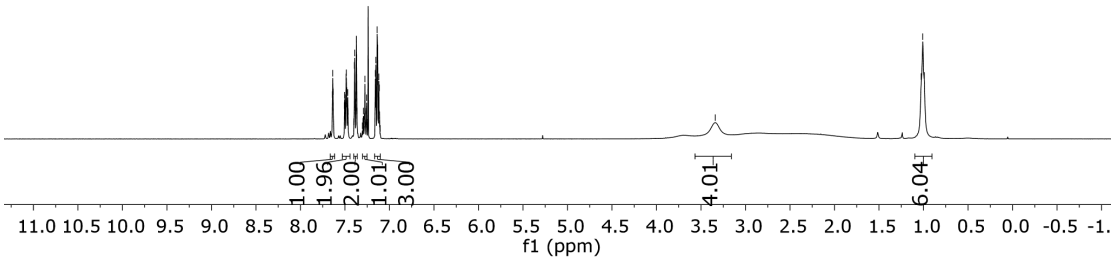


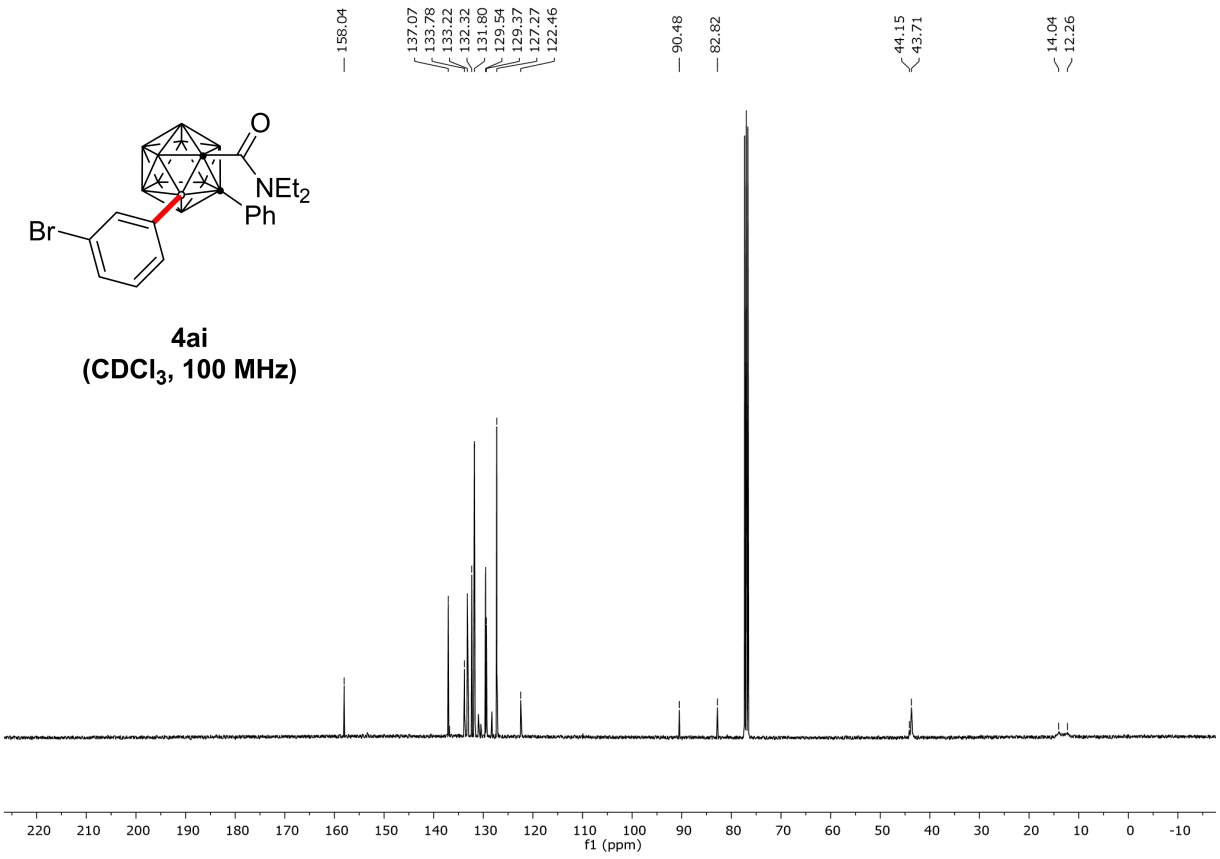

**4ah**
**($CDCl_3$, 96 MHz)**



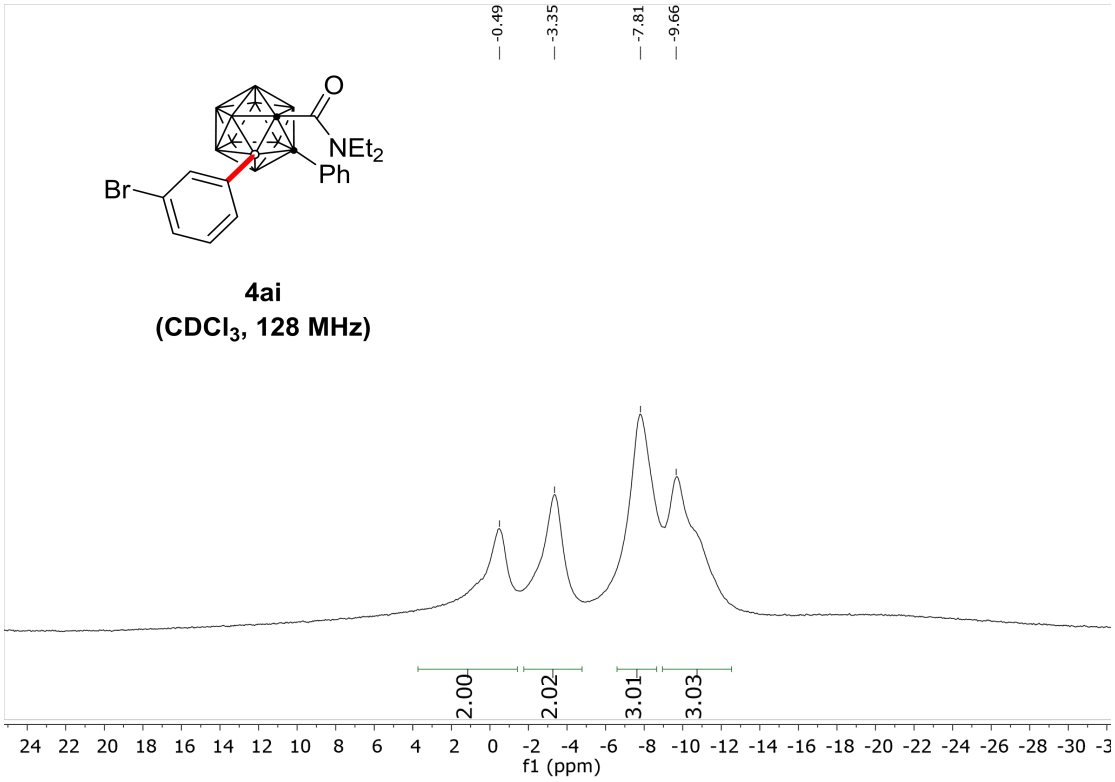




**4ai**
**($CDCl_3$, 400 MHz)**

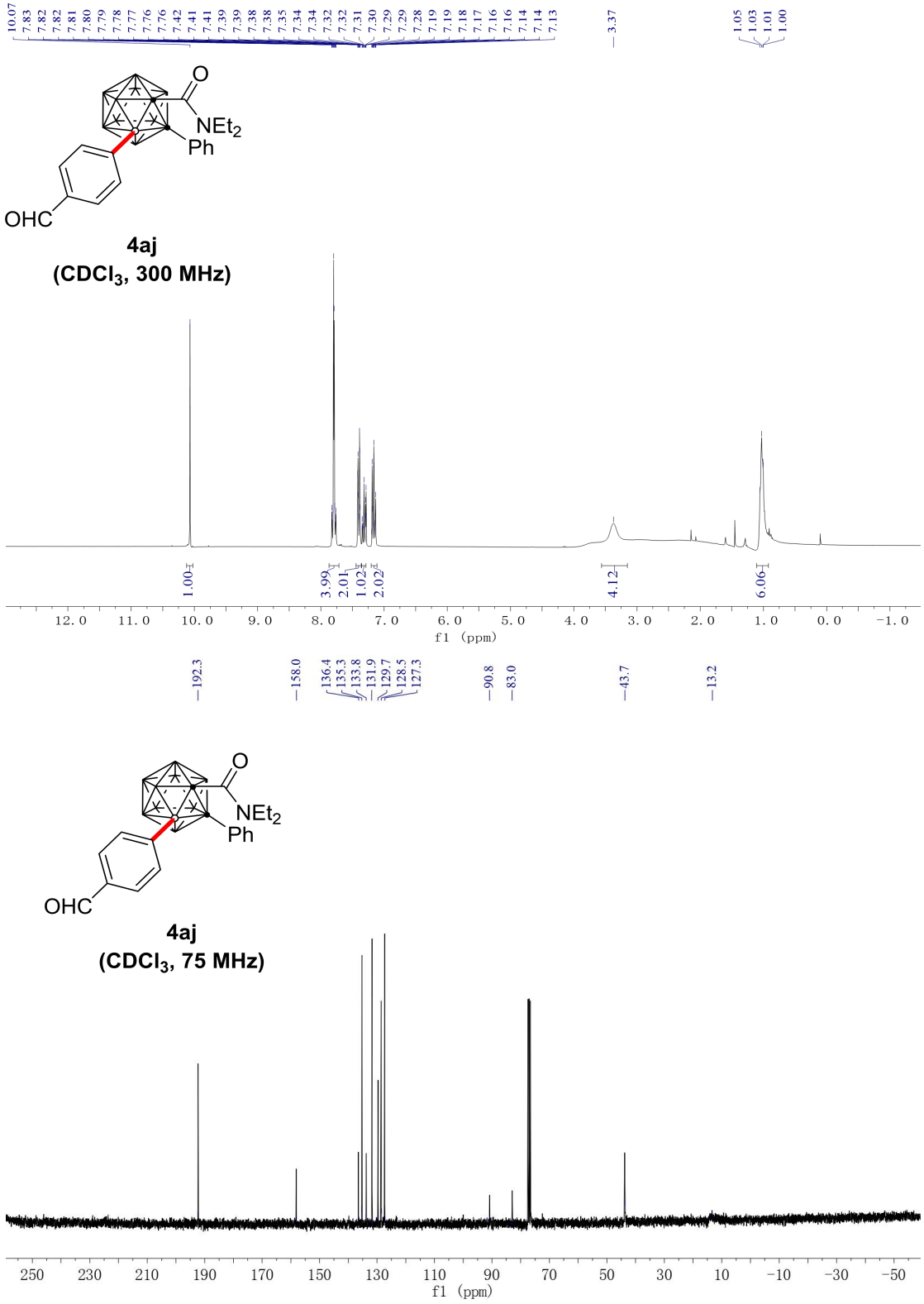


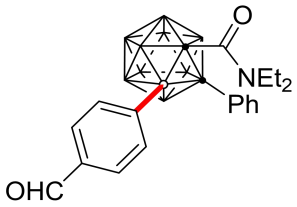



**4ai**
**($CDCl_3$, 100 MHz)**




**4ai**
**($CDCl_3$, 128 MHz)**


10.07
7.83
7.82
7.82
7.81
7.80
7.79
7.78
7.77
7.76
7.76
7.42
7.41
7.41
7.39
7.39
7.38
7.38
7.35
7.34
7.34
7.32
7.31
7.30
7.29
7.29
7.28
7.19
7.19
7.18
7.17
7.16
7.16
7.14
7.14
7.13
3.37
1.05
1.03
1.01
1.00
O
NEt2
Ph
OHC
4aj
(CDCl3, 300 MHz)
1.00
3.99
2.01
1.02
2.02
4.12
6.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
−1.0
f1 (ppm)
192.3
158.0
136.4
135.3
133.8
131.9
129.7
128.5
127.3
90.8
83.0
43.7
13.2
O
NEt2
Ph
OHC
4aj
(CDCl3, 75 MHz)
250
230
210
190
170
150
130
110
90
70
50
30
10
−10
−30
−50
f1 (ppm)




**4aj**
**($CDCl_3$, 96 MHz)**