

Electronic Supplementary Information

Naphthylaminoborane: From structural switches to frustrated Lewis pairs reactivity

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A. General Experimental Procedures, Materials and Instrumentation.

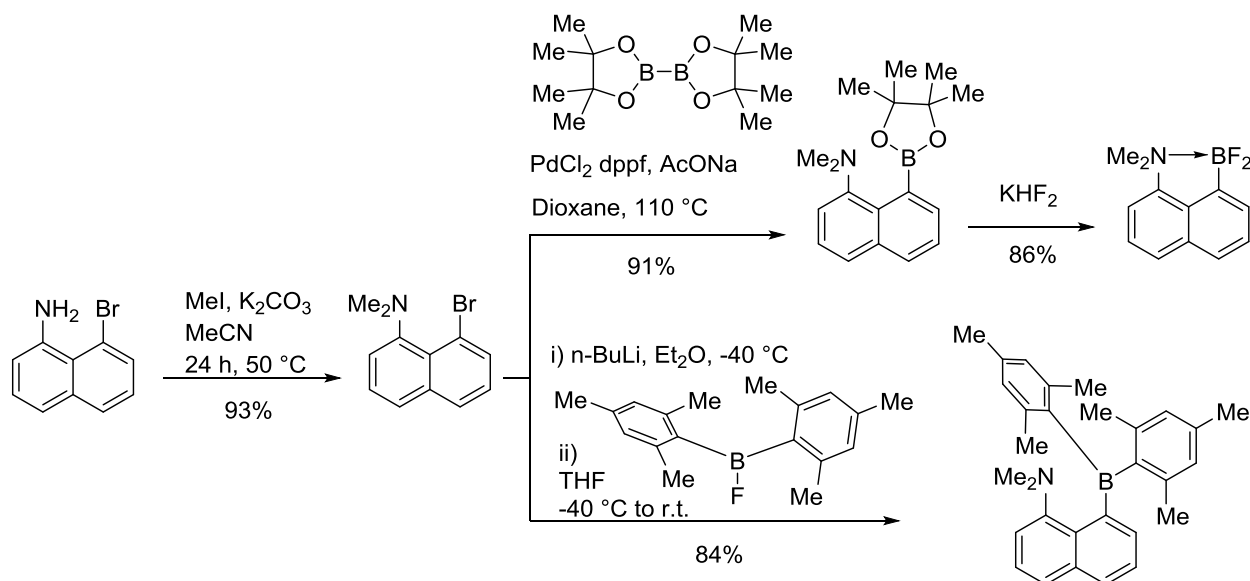
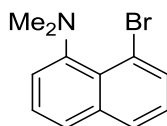
Instrumentation. Automated flash chromatography was performed with an Interchim Puriflash medium-pressure liquid chromatograph with prepacked C18 (15 μm) or silica gel (47-60 μm) columns. ^1H , ^{11}B , ^{13}C , and ^{19}F NMR spectra were recorded on a Bruker Avance 300 (300 MHz) spectrometer, and a Bruker Avance 400 (400 MHz) spectrometer. All spectra were recorded at ambient temperature (298 K). Chemical shifts (δ) are reported in ppm referenced to the appropriate residual solvent peaks (CD_3OD , $\text{d}_6\text{-DMSO}$, C_6D_6 , MeCN-d_3 or CDCl_3) and coupling constants are reported in Hz. The multiplicity of signals is indicated using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quadruplet, bs = broad singlet, bd = broad doublet, m = multiplet. Infrared (IR) spectra were recorded on a Perkin Elmer Spectrum One FT-IR spectrometer as thin films deposited in CHCl_3 . Vibration frequencies are expressed in cm^{-1} . High-resolution mass spectrometry (HRMS) were measured at the Mass Spectrometry Service at the University Paul Sabatier. Kugelrohr bulb-to-bulb distillations were carried out using a Büchi GKR-50 machine. Boiling points are the actual oven temperatures. X-ray crystallography was performed on single crystal diffractometers: Agilent Gemini, Bruker Nonius and Bruker Kappa Apex II.

Materials. Tetrahydrofuran (THF), toluene, pentane, Et_2O , CH_3CN and CH_2Cl_2 were dried and distilled using standard methods.¹ All reagents and other chemicals were purchased at the highest commercial quality and used without further purification unless noted otherwise. All reactions were monitored by TLC and or ^1H NMR spectra taken from reaction samples. Reactions were carried out under Ar atmosphere unless otherwise stated.

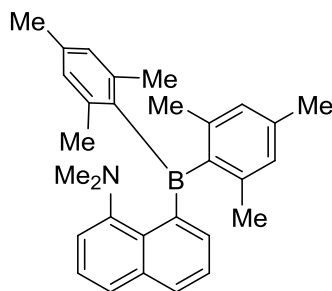
General Experimental Procedures. Reactions were performed in oven-dried borosilicate round bottom flasks fitted with a glass stopper, or in flame-dried borosilicate modified Schlenk (Kjeldahl shape) flasks fitted with a glass stopper under a positive pressure of Ar, unless otherwise noted. Air- and moisture-sensitive liquids and solutions were transferred via syringe. Double microfiber filters were prepared to carry out filtrations under rigorous inert conditions (no H_2O , no O_2) as follows: The filter consists of a glass microfiber filter (GF/A, $\varnothing = 25$ mm) adjusted to an extreme of a PTFE plastic tube ($\varnothing = 2$ mm) with a Teflon strip. A second glass microfiber filter (GF/A, $\varnothing = 25$ mm) is then mounted on top of the former. The other extreme of the PTFE plastic tube is placed through two threaded septa. Facile filtration can be carried out

¹ Perrin, D. D.; Armarego, W. L. F.; Purification of Laboratory Chemicals, Pergamon Press, Oxford, 1997.

by placing the double microfilter in the Schlenk flask containing the suspension of study and the other end is placed in another dried Schlenk flask under Ar. The transference is driven by a positive pressure of Ar applied to the flask containing the suspension. Organic solutions were concentrated by rotary evaporation below 30 °C. Analytical thin layer chromatography (TLC) was performed using pre-coated Merck glass backed silica gel plates (Silicagel 60 F254). Visualization was achieved using ultraviolet light (254 nm) and chemical staining with silica gel impregnated with iodine, or a ceric ammonium molybdate solution as appropriate. For each final product an X-ray structure was obtained.

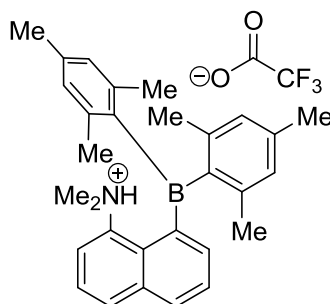
B. Synthesis of Naphthylamino Derivatives 1, 3, 5, 7, 9**8-Bromo-N,N-dimethylnaphthalen-1-amine**

K₂CO₃ (4.85 g, 31.5 mmol) was added to a solution of 8-bromonaphthalen-1-amine (0.78 g, 3.51 mmol) in distilled MeCN (20 mL). The resulting mixture was heated to 50 °C under stirring. MeI (6 mL, 91.26 mmol) was then added to the solution and stirred overnight at 50 °C. The solvent was then evaporated under vacuum to obtain a brown residue. The reaction residue was dissolved in CH₂Cl₂ (30 mL) and the organic phase was washed with H₂O (2 x 30 mL) and dried over anhydrous MgSO₄. After filtration, the solvent was evaporated under vacuum to yield a brown oil (819 mg, 93%). Characterization data matches literature reports.¹ ¹H NMR (400 MHz, DMSO-d₆) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 7.4 Hz, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 1H), 2.69 (s, 6H). ¹³C NMR (101 MHz, DMSO-d₆) δ 150.1 (C_q), 137.0 (C_q), 132.9 (CH), 128.9 (CH), 126.5 (CH), 126.2 (CH), 125.2 (C_q), 123.1 (CH), 117.1 (C_q), 116.5 (CH), 45.2 (CH₃). MS-Cl (m/z): 250 [M⁷⁹Br+H]⁺, 252 [M⁸¹Br+H]⁺.

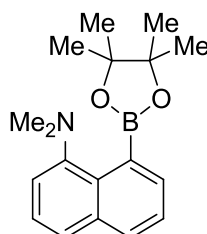
8-(Dimesitylboryl)-*N,N*-dimethylnaphthalen-1-amine (7).

8-Bromo-*N,N*-dimethylnaphthalen-1-amine (592.7 mg, 2.37 mmol) was dissolved in dry Et₂O (13 mL) in a Schlenk flask. The resulting solution was degassed (3 freeze-pump thaw cycles) and then cooled to -40 °C (MeCN-N₂ bath). ⁿBuLi (1.14 mL, 2.5 M in hexane, 2.84 mmol) was then added under Ar and stirred at -40 °C for 30 min. The supernatant was removed at -40 °C using a double microfiber filter and the resulting solid was kept under Ar.

Fluorodimesitylborane (762.6 mg, 2.84 mmol) was dissolved in dry THF (13 mL) in a separate Schlenk flask, degassed (3 freeze-pump thaw cycles) and cooled to -40 °C under Ar. The fluorodimesitylborane solution was cannulated dropwise to the Schlenk flask containing the organolithium derivative, and the resulting mixture was stirred at -40 °C and allowed to warm to rt overnight. The supernatant solution was transferred to a Schlenk flask using a double microfiber filter and solvent was then removed under vacuum. The residue was then triturated with dry pentane (3 x 10 mL), and supernatant fractions were discarded. The solid residue was then triturated with dry Et₂O, the supernatant was filtered out and evaporated under reduced pressure. The product was obtained as yellow foam (839 mg, 84%). An analytical portion of the solid was dissolved in a minimum amount of heptane (2 mL), sonicated and kept at -20 °C overnight to yield fine yellowish crystals which were suitable for X-ray analysis. IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 3026, 2985, 2950, 1605, 1453, 1417, 1243, 1205, 1151, 1031, 906, 846, 824, 777. ¹H NMR (400 MHz, CDCl₃) δ 7.84 (dd, *J* = 6.7, 2.8 Hz, 1H), 7.70 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.33 (m, 3H), 6.85 (s, 1H), 6.78 (s, 1H), 6.75 (s, 1H), 6.46 (s, 1H), 2.61 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H), 2.18 (s, 3H), 2.11 (s, 3H), 1.85 (s, 3H), 1.76 (s, 3H), 1.03 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 154.1 (C_q), 142.2 (C_q), 141.5 (C_q), 140.6 (C_q), 140.1 (C_q), 138.0 (C_q), 137.7 (C_q), 135.2 (C_q), 135.0 (C_q), 132.1 (CH), 130.5 (CH), 129.1 (CH), 128.5 (CH), 128.21 (CH), 128.19 (CH), 126.5 (CH), 125.9 (CH), 120.5 (CH), 51.3 (CH₃), 46.5 (CH₃), 24.2 (CH₃), 23.9 (CH₃), 23.3 (CH₃), 22.9 (CH₃), 21.3 (CH₃), 21.2 (CH₃). ¹¹B NMR (128 MHz, CDCl₃) δ 68.1. HRMS-ESI (*m/z*): found [M+H]⁺ 419.2899, calc'd ¹⁰BC₃₀H₃₅N requires 419.2880.

8-(Dimesitylboryl)-*N,N*-dimethylnaphthalen-1-ammonium trifluoroacetate (9).

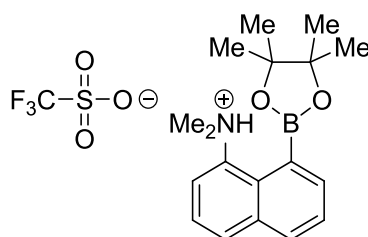
8-(Dimesitylboryl)-*N,N*-dimethylnaphthalen-1-amine **7** (27.4 mg, 0.07 mmol) was dissolved in CHCl_3 –TFA (10:1, 3 mL) in a round bottom flask. The mixture was stirred at rt for 15 min and solvents were then evaporated under reduced pressure to yield the desired salt as a yellow oil (34.8 mg, quant. yield). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 2925, 1778, 1604, 1450, 1203, 1151, 1031, 824, 772, 700. ^1H NMR (400 MHz, CDCl_3) δ 9.66 (bs, 1H), 8.22 (d, $J = 8.2$ Hz, 1H), 8.19 (d, $J = 7.9$ Hz, 1H), 8.05 (d, $J = 6.5$ Hz, 1H), 7.81 (d, $J = 7.5$ Hz, 1H), 7.74 (dd, $J = 7.9$ Hz, 1H), 7.67 (dd, $J = 7.7$ Hz, 1H), 7.13 (s, 1H), 6.94 (s, 1H), 6.89 (s, 1H), 6.88 (s, 1H), 3.28 (d, $J = 5.3$ Hz, 3H), 2.61 (d, $J = 4.9$ Hz, 3H), 2.35 (s, 3H), 2.31 (s, 3H), 2.19 (s, 3H), 2.17 (s, 3H), 1.83 (s, 3H), 1.33 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.2 (q, $J_{\text{C-F}} = 42.9$ Hz, C_q), 145.2 (C_q), 143.7 (C_q), 143.4 (C_q), 141.9 (C_q), 141.6 (CH), 141.3 (C_q), 140.2 (C_q), 139.0 (C_q), 136.0 (CH), 135.7 (C_q), 134.1 (CH), 131.6 (CH), 131.5 (CH), 129.5 (CH), 129.2 (CH), 128.0 (CH), 127.4 (C_q), 126.8 (CH), 120.4 (CH), 114.59 (q, $J_{\text{C-F}} = 285.0$ Hz, CF_3), 50.2 (CH_3), 45.2 (CH_3), 24.8 (CH_3), 23.8 (CH_3), 23.0 (CH_3), 22.8 (CH_3), 21.3 (CH_3), 21.2 (CH_3). ^{11}B NMR (128 MHz, CDCl_3) δ 74.0.

***N,N*-Dimethyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)naphthalen-1-amine (1)**

8-Bromo-*N,N*-dimethylnaphthalen-1-amine (100 mg, 0.40 mmol), AcONa (131 mg, 1.6 mmol), bispinacolatodiborane (203 mg, 0.80 mmol) and $\text{Pd}(\text{dppf})\text{Cl}_2$ (15 mg, 0.02 mmol) have been dissolved in degassed dioxane (4 mL). The mixture was stirred and heated to reflux at 110 °C overnight. Et_2O was added to the solution, filtered through a celite pad and the solvent was evaporated under vacuum. The product was purified by flash column chromatography (15 g pre-packed silica gel cartridge, crude loaded with a celite slurry, cyclohexane- Et_2O 8:2 as eluent) and a brown solid was obtained (108 mg, 91%). Characterization data matches literature

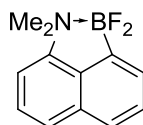
reports.² ^1H NMR (400 MHz, CDCl_3) δ 7.75 – 7.71 (m, 1H), 7.67 (d, J = 8.2 Hz, 1H), 7.63 (d, J = 6.5 Hz, 1H), 7.55 (dd, J = 8.1, 6.7 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.31 (d, J = 7.3 Hz, 1H), 2.84 (s, 6H), 1.41 (s, 12H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.3 (C_q), 134.5 (C_q), 132.6 (C_q), 129.0 (CH), 128.1 (CH), 125.9 (CH), 125.6 (CH), 114.9 (CH), 81.6 (C_q), 47.6 (CH_3), 26.5 (CH_3). ^{11}B NMR (128 MHz, CDCl_3) δ 22.0. HRMS-ESI (m/z): found $[\text{M}+\text{H}]^+$ 297.2013, calc'd $^{10}\text{BC}_{18}\text{H}_{25}\text{NO}_2$ requires 297.2015.

***N,N*-Dimethyl-8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)naphthalen-1-ammonium trifluoromethanesulfonate (3)**



Methyl triflate (80 μL , 0.72 mmol) was added to a solution of **1** (52.8 mg, 0.18 mmol) in CH_2Cl_2 (1.8 mL). The resulting mixture was stirred at rt for 5 h. *tert*-Butylmethyl ether (2 mL) was then added under Ar and the desired product precipitated as white flakes. The supernatant was discarded using a 0.20 μm PTFE filter and the white precipitate was washed with *tert*-butylmethyl ether (3 x 2 mL). The residue was then dried under vacuum and finally eluted with acetone to yield a yellow oil (72.3 mg, 91%). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 3480, 3059, 2980, 2932, 2743, 1466, 1356, 1275, 1259, 1155, 1138, 1031, 638. ^1H NMR (300 MHz, Acetone- d_6) δ 8.59 (dd, J = 7.1, 1.5 Hz, 1H), 8.41 (dt, J = 7.8, 0.9 Hz, 1H), 8.35 (dd, J = 8.3, 1.5 Hz, 1H), 8.26 (dd, J = 8.2, 1.2 Hz, 1H), 7.87 – 7.72 (m, 2H), 3.74 – 3.72 (m, 6H), 1.60 (s, 12H). ^{13}C NMR (75 MHz, Acetone) δ 142.3 (CH), 136.4 (C_q), 135.7 (CH), 133.8 (CH), 129.9 (C_q), 127.2 (q, J = 274 Hz, CF_3), 127.1 (CH), 126.8 (CH), 122.5 (CH), 115.5 (C_q), 87.8 (C_q), 48.4 (CH_3), 48.3 (CH_3), 25.0 (CH_3). ^{11}B NMR (96 MHz, Acetone- d_6) δ 30.50. HRMS-ESI (m/z): found $[\text{M}+\text{H}]^+$ 297.2011, calc'd $^{10}\text{BC}_{18}\text{H}_{25}\text{NO}_2$ requires 297.2015.

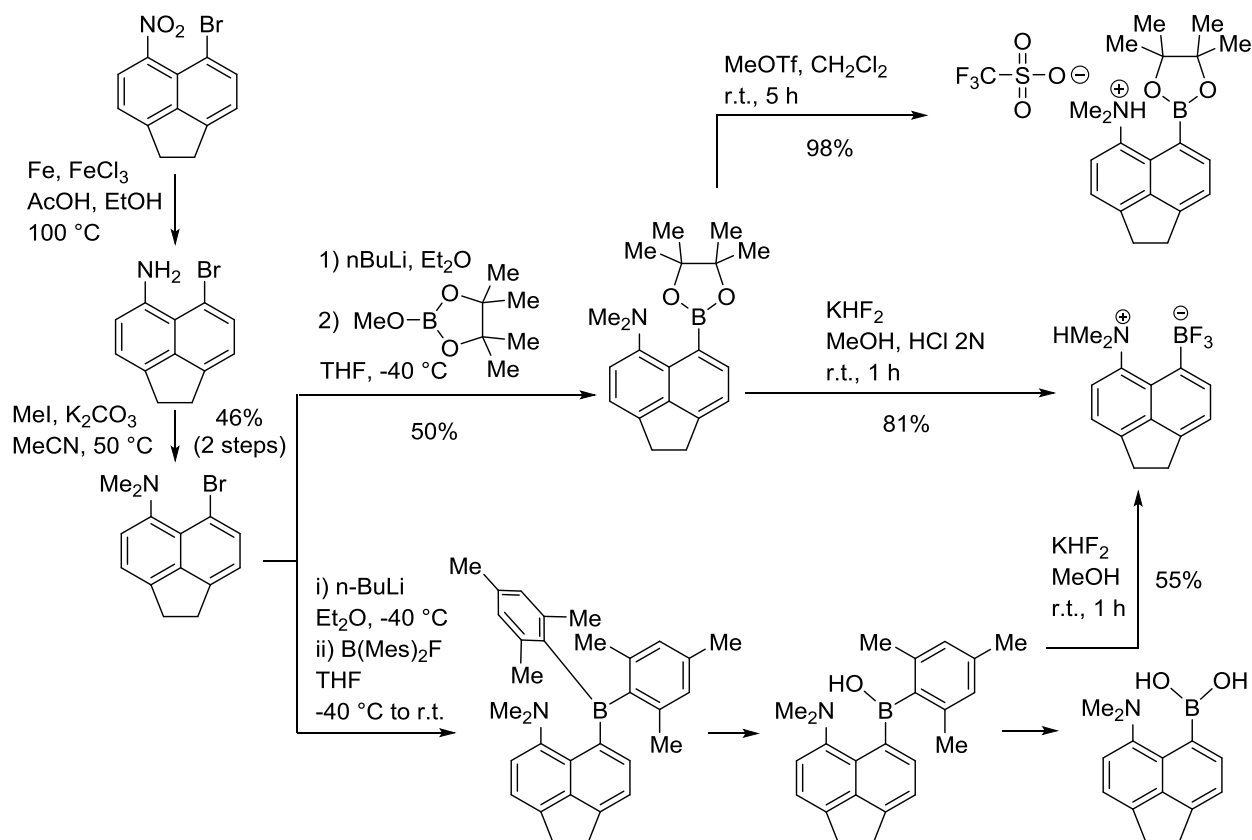
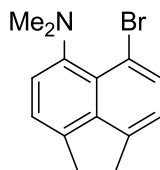
8-(Difluoroboryl)-*N,N*-dimethylnaphthalen-1-amine (5)



KHF_2 (53.1 mg, 0.68 mmol) was added in one solid portion to a solution of **1** in MeOH (1 mL). A solution of HCl 2 M (0.1 mL) was then added and the resulting mixture was sonicated for 5 min and then stirred for 1 h at rt. Solvents were removed under reduced pressure and the residue

was triturated in CHCl_3 (3x). The organic solution was filtered through a 0.20 μm PTFE filter and the solvent was evaporated under reduced pressure yielding a yellow oil (38.6 mg, 86%). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 2924, 2852, 1469, 1338, 1252, 1179, 1121, 826, 783. ^1H NMR (300 MHz, CDCl_3) δ 7.84 – 7.74 (m, 3H), 7.65 (dd, J = 8.1, 6.7 Hz, 1H), 7.54 – 7.47 (m, 1H), 7.34 (d, J = 7.4 Hz, 1H), 3.01 (t, J = 2.0 Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.6 (C_q), 134.3 (C_q), 131.8 (C_q), 129.4 (CH), 127.6 (CH), 126.6 (CH), 126.0 (CH), 125.3 (CH), 113.0 (CH), 48.2 (t, $J_{\text{C-F}}$ = 5.2 Hz, CH_3). ^{11}B NMR (96 MHz, CDCl_3) δ 9.79 (t, J = 56.4 Hz). ^{19}F NMR (282 MHz, CDCl_3) δ -147.77 – -148.98 (m). HRMS-ESI (m/z): found $[\text{M}+\text{H}]^+$ 220.1120, calc'd $\text{C}_{12}\text{H}_{13}\text{NBF}_2$ requires 220.1109.

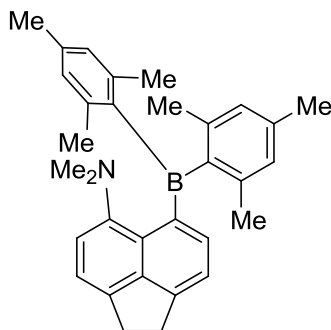
C. Synthesis of Acenaphthylamino Derivatives 2, 4, 6, 8, 10, 11

6-Bromo-*N,N*-dimethyl-1,2-dihydroacenaphthyl-5-amine

5-Bromo-6-nitro-1,2-dihydroacenaphthylene (5.02 g, 18 mmol) was dissolved in EtOH (50 mL) and AcOH (10 mL) and heated to 100°C under reflux. Fe (7.03 g, 125.8 mmol) and FeCl_3 (0.60 g, 3.6 mmol) were then added to the mixture and stirred at 100°C for 1 h. The solvent was evaporated under vacuum and the resulting liquid was filtered through a pad of celite. The cake was washed with Et_2O (4 x 100 mL), the combined organic fractions were concentrated under vacuum to yield a thick brown residue. This residue was dissolved in MeCN (100 mL), K_2CO_3 (12.42 g, 90 mmol) was added and the mixture was stirred at 50°C under reflux. Finally, MeI (9 mL, 144.6 mmol) was added and the solution was stirred overnight at 50°C . The reaction mixture was allowed to cool down to rt and Et_2O (50 mL) was added. The mixture was then filtered through a pad of silica gel and further eluted with Et_2O (200 mL). The solvent was then removed under vacuum to yield a thick brown oil (2.314 g, 46%). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 3273,

2932, 2821, 2772, 1667, 1631, 1574, 1449, 1416, 1337, 1034, 960, 835. ^1H NMR (300 MHz, CDCl_3) δ 7.68 (d, J = 7.4 Hz, 1H), 7.31 – 7.12 (m, 2H), 7.06 (dd, J = 7.4, 1.3 Hz, 1H), 3.31 (s, 4H), 2.78 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 147.9 (C_q), 146.4 (C_q), 142.4 (C_q), 141.0 (C_q), 134.0 (CH), 125.6 (C_q), 120.4 (CH), 120.1 (CH), 118.3 (CH), 113.1 (C_q), 46.4 (CH_3), 30.3 (CH_2), 29.9 (CH_2). MS-ESI (m/z): 276.0 [$\text{M}^{79}\text{Br}+\text{H}$] $^+$, 278.0 [$\text{M}^{81}\text{Br}+\text{H}$] $^+$.

6-(Dimesitylboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (8).



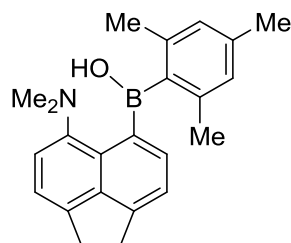
6-Bromo-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine was dissolved in dry Et_2O (22 mL) in a Schlenk flask. The resulting solution was degassed (3 freeze-pump thaw cycles) and then cooled to $-40\text{ }^\circ\text{C}$ (MeCN-N_2 bath). $n\text{BuLi}$ (1.89 mL, 2.5 M in hexane, 4.73 mmol) was then added under Ar and stirred at $-40\text{ }^\circ\text{C}$ for 2 h. The supernatant was removed at $-40\text{ }^\circ\text{C}$ using a double microfiber filter and the resulting solid was kept under Ar.

Fluorodimesitylborane (1.268 mg, 4.73 mmol) was dissolved in dry THF (22 mL) in a separate Schlenk flask, degassed (3 freeze-pump thaw cycles) and cooled to $-40\text{ }^\circ\text{C}$ under Ar. The fluorodimesitylborane solution was cannulated dropwise to the Schlenk flask containing the organolithium derivative, and the resulting mixture was stirred at $-40\text{ }^\circ\text{C}$ and allowed to warm to rt overnight. The supernatant solution was transferred to a Schlenk flask using a double microfiber filter and solvent was then removed under vacuum. The residue was then triturated with dry pentane (3 x 10 mL), and supernatant fractions were discarded. The solid residue was then triturated with dry Et_2O (10 mL), the supernatant was filtered out and concentrated under reduced pressure. The product was obtained as yellow foam (964 mg, 55%).

The product (**8**) was dissolved in dry CH_2Cl_2 (5 mL) under Ar, and kept at $-20\text{ }^\circ\text{C}$ to yield fine colorless crystals which were suitable for X-ray analysis. ^1H NMR (400 MHz, CDCl_3) δ 7.42 (d, J = 7.4 Hz, 1H), 7.36 (d, J = 6.9 Hz, 1H), 7.31 (d, J = 7.4 Hz, 1H), 7.21 (d, J = 6.9 Hz, 1H), 6.90 – 6.78 (m, 3H), 6.53 (s, 1H), 3.48 – 3.37 (m, 4H), 2.37 (s, 3H), 2.36 (s, 3H), 2.33 (s, 3H), 2.32 and 2.30 (2s, 3H), 2.23 (s, 3H), 2.17 (s, 3H), 1.97 (s, 3H), 1.25 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.8 (C_q), 148.9 (C_q), 143.8 (C_q), 142.1 (C_q), 141.6 (C_q), 140.6 (C_q), 140.2 (C_q), 140.1 (C_q), 137.9 (C_q), 137.6 (C_q), 134.1 (CH), 133.2 (C_q), 128.9 (CH), 128.3 (CH), 128.1 (CH),

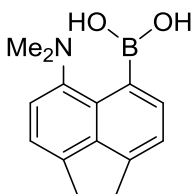
127.9 (CH), 127.1 (CH), 122.6 (CH), 119.8 (CH), 119.4 (CH), 50.1 (CH₃), 46.2 (CH₃), 30.7 (CH₂), 30.1 (CH₂), 24.0 (CH₃), 23.5 (CH₃), 23.3 (CH₃), 23.0 (CH₃), 21.4 (CH₃), 21.2 (CH₃). ¹¹B NMR (128 MHz, CDCl₃) δ 74.0. HRMS-ESI (m/z): found [M+H]⁺ 445.3049, calc'd ¹⁰BC₃₂H₃₇N requires 445.3055.

***N,N*-Dimethyl-6-(hydroxymesitylboryl)-1,2-dihydroacenaphthylen-5-amine (10)**



6-(Dimesitylboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine **8** (895 mg, 2.01 mmol) was dissolved in a minimum amount of heptane (10 mL), sonicated and kept at -20 °C to yield the semi-hydrolyzed *N,N*-dimethyl-6-(hydroxymesitylboryl)-1,2-dihydroacenaphthylen-5-amine product as yellow crystals (331 mg, 48%), which were suitable for X-ray analysis. ¹H NMR (400 MHz, CDCl₃) δ 7.86 (d, *J* = 7.1 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.21 (d, *J* = 7.1, 1H), 6.86 (s, 1H), 3.40 – 3.36 (m, 4H), 2.92 (s, 6H), 2.34 (s, 3H), 2.24 (s, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 151.3 (C_q), 146.3 (C_q), 145.3 (C_q), 145.0 (CH), 141.3 (C_q), 139.0 (C_q), 136.5 (C_q), 132.0 (C_q), 128.5 (C_q), 120.2 (CH), 120.1 (CH), 119.5 (CH), 46.2 (CH₃), 30.6 (CH₂), 29.7 (CH₂), 22.4 (CH₃), 21.4 (CH₃). ¹¹B NMR (128 MHz, CDCl₃) δ 47.3. HRMS-ESI (m/z): found [M+H]⁺ 344.2189, calc'd C₂₃H₂₇NOB requires 344.2186.

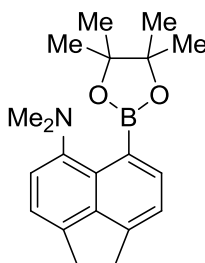
6-(Dihydroxyboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (11)



An analytical portion of 6-(dimesitylboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (**8**) was dissolved in CDCl₃ (1 mL). Colorless crystals were grown by vapour-diffusion crystallization from CDCl₃-cyclohexane at rt. X-ray analysis provided the fully hydrolyzed boronic acid derivative. IR ν_{max} /cm⁻¹ (neat film): 3267, 2982, 2945, 1503, 1460, 1403, 1377, 1125, 1036, 849. ¹H NMR (400 MHz, CDCl₃) δ 8.45 (d, *J* = 7.1 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.36 (dt, *J* = 7.1, 1.4 Hz, 1H), 7.29 (dt, *J* = 7.4, 1.4 Hz, 1H), 3.44 – 3.33 (m, 4H), 2.84 (s,

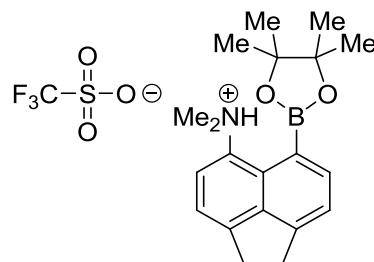
6H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.4 (C_q), 145.8 (C_q), 145.6 (C_q), 141.1 (C_q), 140.3 (CH), 131.8 (C_q), 120.4 (CH), 119.9 (CH), 119.1 (CH), 46.4 (CH_3), 30.6 (CH_2), 29.7 (CH_2). ^{11}B NMR (128 MHz, CDCl_3) δ 29.7. HRMS-ESI (m/z): found $[\text{M}+\text{H}]^+$ 241.1400, calc'd $^{10}\text{BC}_{14}\text{H}_{17}\text{NO}_2$ requires 241.1389.

***N,N*-Dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-dihydroacenaphthylen-5-amine (2)**



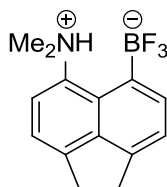
6-Bromo-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (515.9 mg, 1.87 mmol) was dissolved in dry Et_2O (11 mL) and stirred at -40°C . $n\text{BuLi}$ (2.1 mL, 1.05 M in hexane, 2.24 mmol) was then added under Ar and stirred at -40°C for 30 min. The solvent was removed at -40°C using a double microfiber filter and the resulting white solid was then dissolved in dry THF (11 mL). Methoxyphenyl borane (367 μL , 2.24 mmol) was added at -40°C under Ar and the resulting mixture was stirred at -40°C in a MeCN-N_2 bath and allowed to warm to rt overnight. The solvent was then removed under vacuum. The residue was then dissolved in CH_2Cl_2 and washed with sat. NaHCO_3 , brine, and the organic layer was dried with MgSO_4 . The solvent was evaporated under vacuum and the resulting residue was dissolved in a minimum amount of heptane (3 mL), sonicated and kept in the freezer overnight. The product was obtained as fine brown crystals (304 mg, 50%). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 2975, 2935, 2824, 2782, 1610, 1502, 1322, 1285, 1144, 1110, 1051, 960, 841. ^1H NMR (300 MHz, CDCl_3) δ 7.46 (d, $J = 6.8$ Hz, 1H), 7.28 (d, $J = 7.6$ Hz, 2H), 7.21 (tt, $J = 7.4, 1.4$ Hz, 1H), 3.44 – 3.25 (m, 4H), 2.71 (s, 6H), 1.42 (s, 12H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.8 (C_q), 146.6 (C_q), 142.7 (C_q), 140.1 (C_q), 132.0 (CH), 131.9 (CH), 119.4 (CH), 119.0 (CH), 118.6 (CH), 83.3 (C_q), 46.9 (CH_3), 30.9 (CH_2), 30.0 (CH_2), 25.4 (CH_3). ^{11}B NMR (128 MHz, CDCl_3) δ 31.9. HRMS-ESI (m/z): found $[\text{M}+\text{H}]^+$ 323.2177, calc'd $^{10}\text{BC}_{20}\text{H}_{27}\text{NO}_2$ requires 323.2171.

***N,N*-Dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-dihydroacenaphthylen-5-ammonium trifluoromethanesulfonate (4).**



Methyl triflate (143 μ L, 1.28 mmol) was added to a solution of *N,N*-dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-dihydroacenaphthylen-5-amine (102 mg, 0.32 mmol) in CH_2Cl_2 (3.2 mL). The resulting mixture was stirred at rt for 5 h. A solvent mixture of pentane-Et₂O (83:17, 24 mL) was then added under Ar and the desired product precipitated as white flakes. The supernatant was discarded using a double microfiber filter and the white precipitate was washed with dry pentane (3 x 5 mL). The residue was then dried under vacuum to yield a white powder (146 mg, 98%). IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 3499, 3062, 2981, 2926, 2751, 2696, 1602, 1518, 1376, 1310, 1257, 1137, 1029, 852, 636. ¹H NMR (300 MHz, Acetone-*d*₆) δ 12.17 (s, 1H), 8.46 (d, *J* = 7.1 Hz, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 7.65 – 7.52 (m, 2H), 3.70 (s, 3H), 3.69 (s, 3H), 3.53 – 3.42 (m, 4H), 1.59 (s, 12H). ¹³C NMR (75 MHz, Acetone) δ 154.1 (C_q), 151.5 (C_q), 143.6 (CH), 140.9 (C_q), 137.3 (C_q), 127.4 (C_q), 123.8 (CH), 121.5 (CH), 121.1 (CH), 87.4 (C_q), 48.3 (CH₃), 31.2 (CH₂), 30.3 (CH₂), 25.0 (CH₃). ¹¹B NMR (96 MHz, Acetone-*d*₆) δ 30.28. HRMS-ESI (*m/z*): found [M+H]⁺ 323.2175, calc'd ¹⁰BC₂₀H₂₇NO₂ requires 323.2171.

6-(Dimethylammonium)-1,2-dihydroacenaphthylen-5-yl)trifluoroborate (6)



Procedure A: KHF₂ (35.6 mg, 0.46 mmol) was added in one solid portion to a solution of *N,N*-dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-dihydroacenaphthylen-5-amine (44.7 mg) in MeOH (674 μ L). A solution of HCl 2 M (67 μ L) was then added and the resulting mixture was sonicated for 5 min and then stirred for 45 min at rt. Solvents were removed under reduced pressure and the residue was triturated in CHCl_3 (3x). The organic solution was filtered through a 0.20 μ m PTFE filter and the solvent was evaporated under reduced pressure yielding a yellow oil (29.7 mg, 81%).

Procedure B: KHF₂ (42.5 mg, 0.54 mmol) was added in one solid portion to a solution of *N,N*-dimethyl-6-(hydroxymesitylboryl)-1,2-dihydroacenaphthylen-5-amine **2** (56.5 mg, 0.17 mmol) in MeOH (1.6 mL). The resulting mixture was sonicated for 5 min and then stirred for 45 min at rt. Solvents were removed under reduced pressure and the residue was triturated in CHCl₃ (3x). Solids were filtered off using a 0.20 µm PTFE filter and the solvent was evaporated under reduced pressure. The residue was further triturated with Et₂O, the supernatant was discarded and the residue was dissolved in acetone, and filtered through a 0.20 µm PTFE filter. The solution was then evaporated under reduced pressure yielding a yellow oil (24.1 mg, 55%).

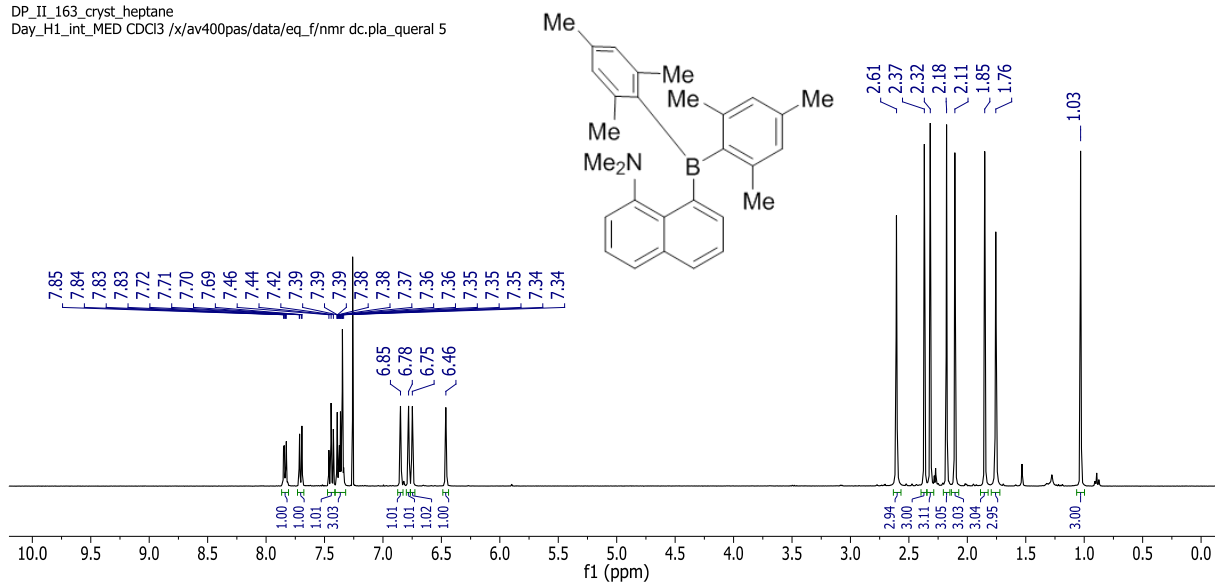
IR $\nu_{\text{max}}/\text{cm}^{-1}$ (neat film): 3358, 2924, 2853, 1600, 1502, 1458, 1439, 1372, 1259, 960, 837. ¹H NMR (300 MHz, Acetone-*d*₆) δ 11.13 (s, 1H), 7.96 (d, *J* = 7.4 Hz, 1H), 7.95 (d, *J* = 7.5 Hz, 1H), 7.40 – 7.30 (m, 2H), 3.53 (s, 3H), 3.51 (s, 3H), 3.37 (s, 4H), 2.82 (s, 1H). ¹³C NMR (75 MHz, Acetone) δ 150.3 (C_q), 145.7 (C_q), 141.2 (C_q), 138.5 (C_q), 135.1 (q, *J*_{CB} = 4.7 Hz, C_q), 121.4 (CH), 120.5 (CH), 118.7 (CH), 48.7 (CH₃), 30.5 (CH₂), 30.4 (CH₂). ¹¹B NMR (96 MHz, Acetone-*d*₆) δ 4.03 (q, *J* = 54.4 Hz). ¹⁹F NMR (282 MHz, Acetone-*d*₆) δ -134.66 – -135.81 (m). HRMS-ESI (m/z): found [M+H]⁺ 263.1221, calc'd ¹⁰BC₁₄H₁₄NF₃ requires 263.1208.

¹ a) Kiefl, C. *Eur. J. Org. Chem.* **2000**, 19, 3279-3286; b) Schiemenz, G. P.; Papageorgiu, E. *Phosphorus Sulfur*, **1982**, 13, 41-58.

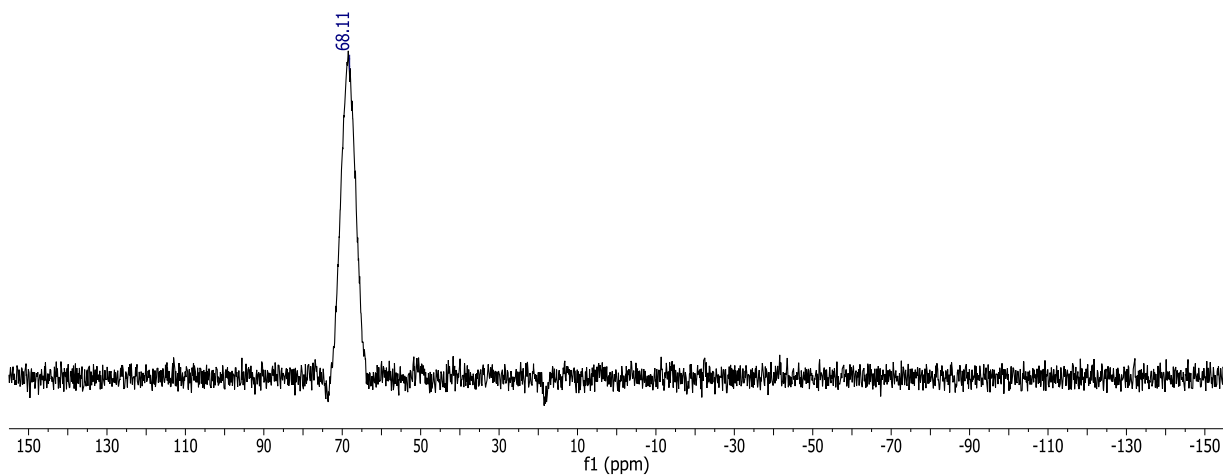
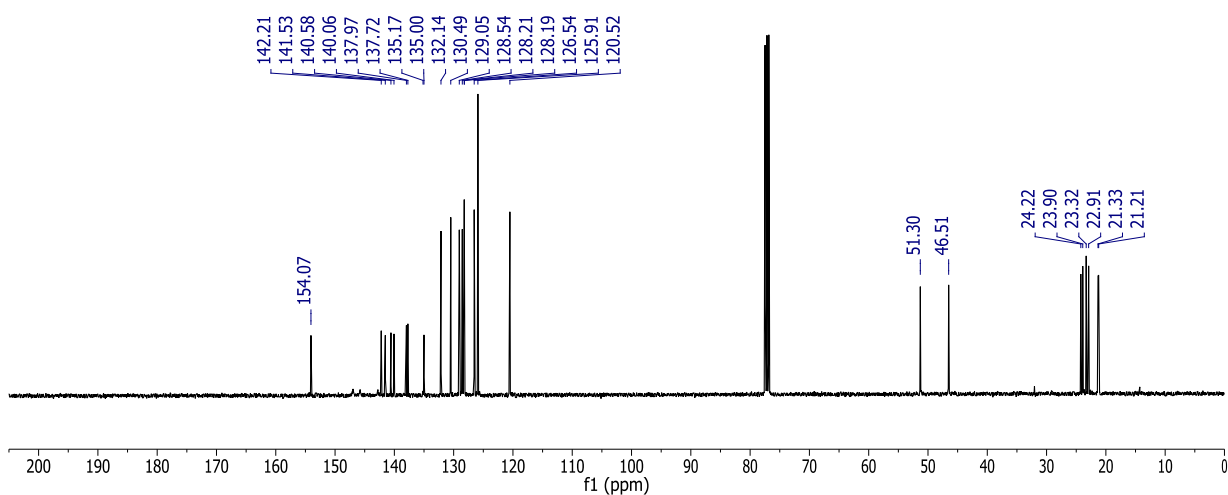
² Giles, R. L.; Howard, J. A.K.; Patrick, L. G. F.; Probert, M. R.; Smith, G. E.; Whiting, A. *J. Organomet. Chem.* **2003**, 680, 257-262

D. ^1H and ^{13}C -NMR Spectra of Selected Compounds

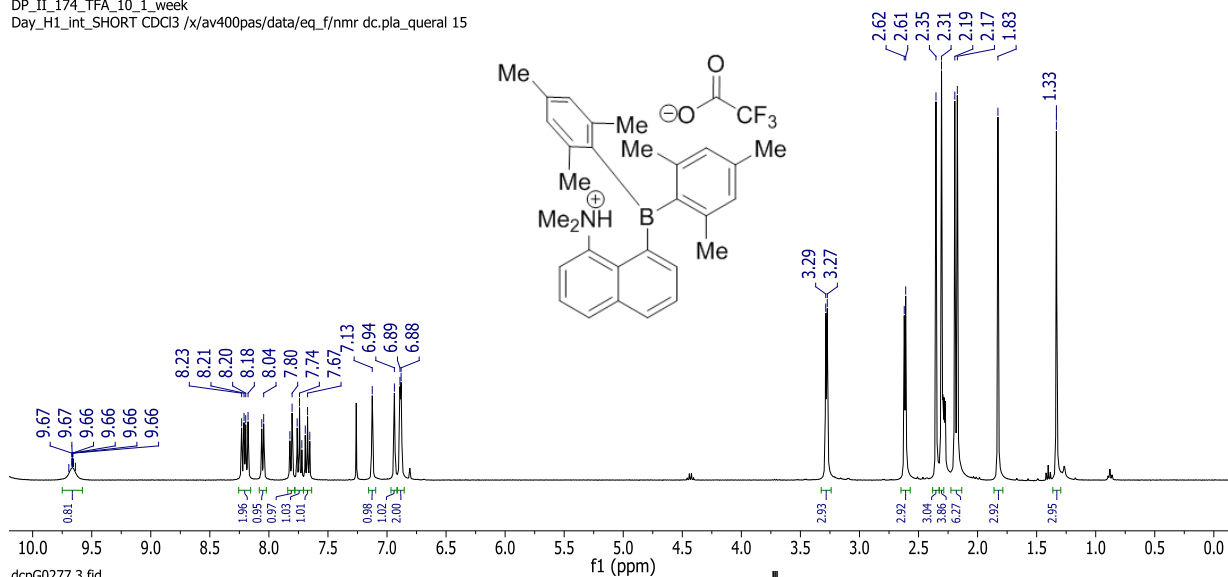
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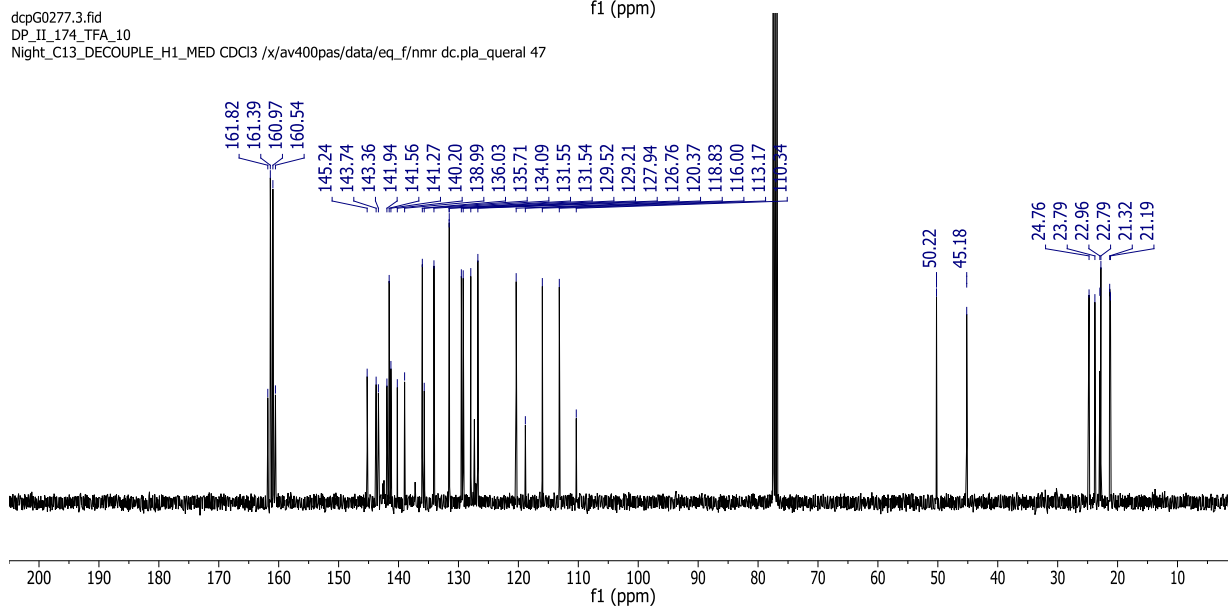
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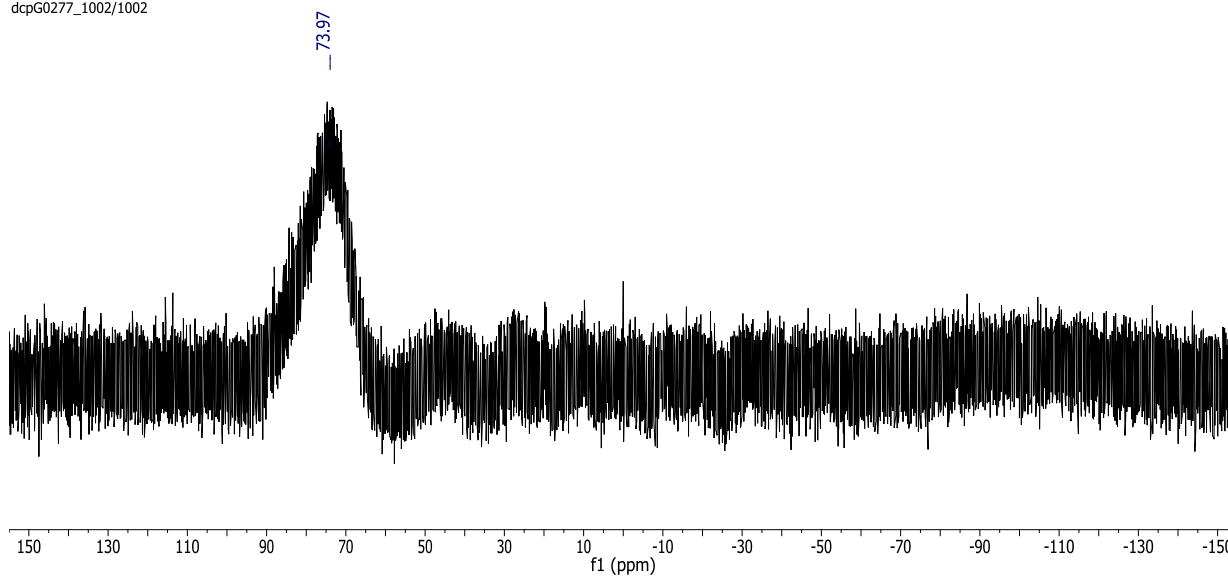
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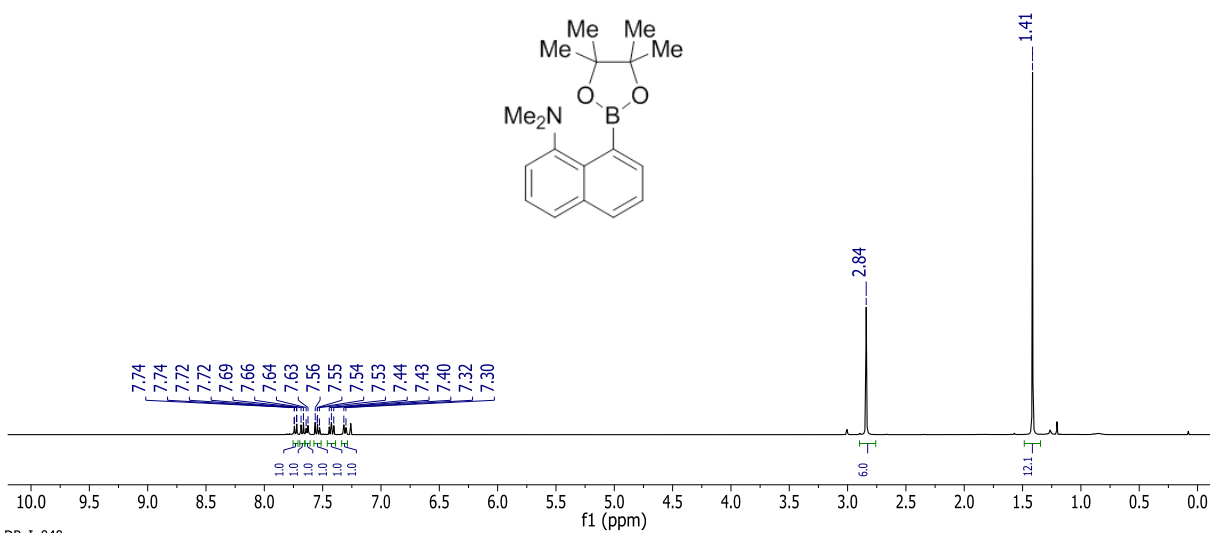
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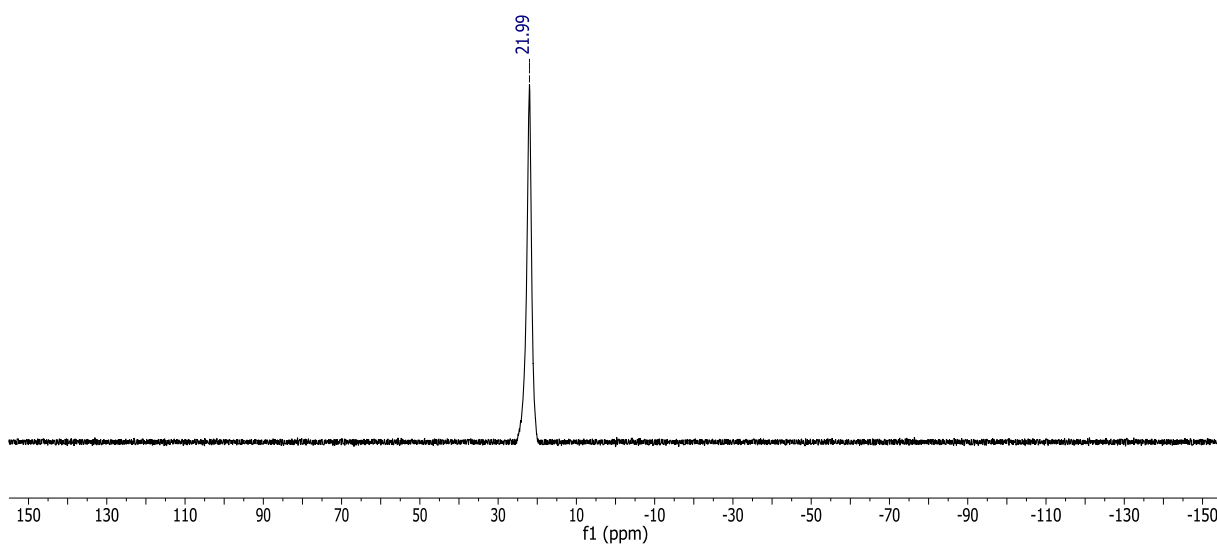
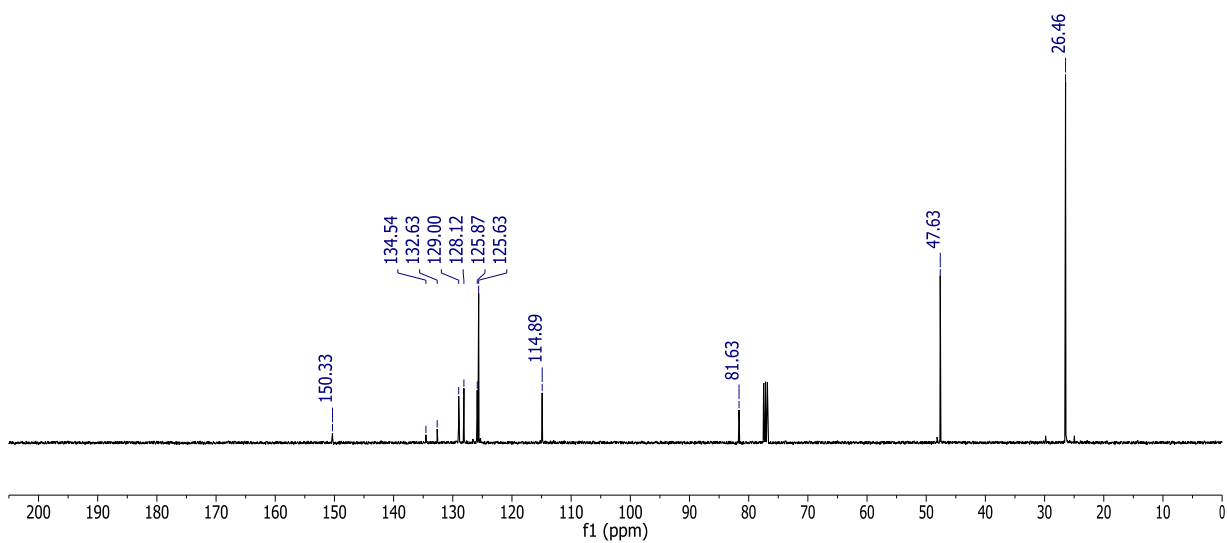
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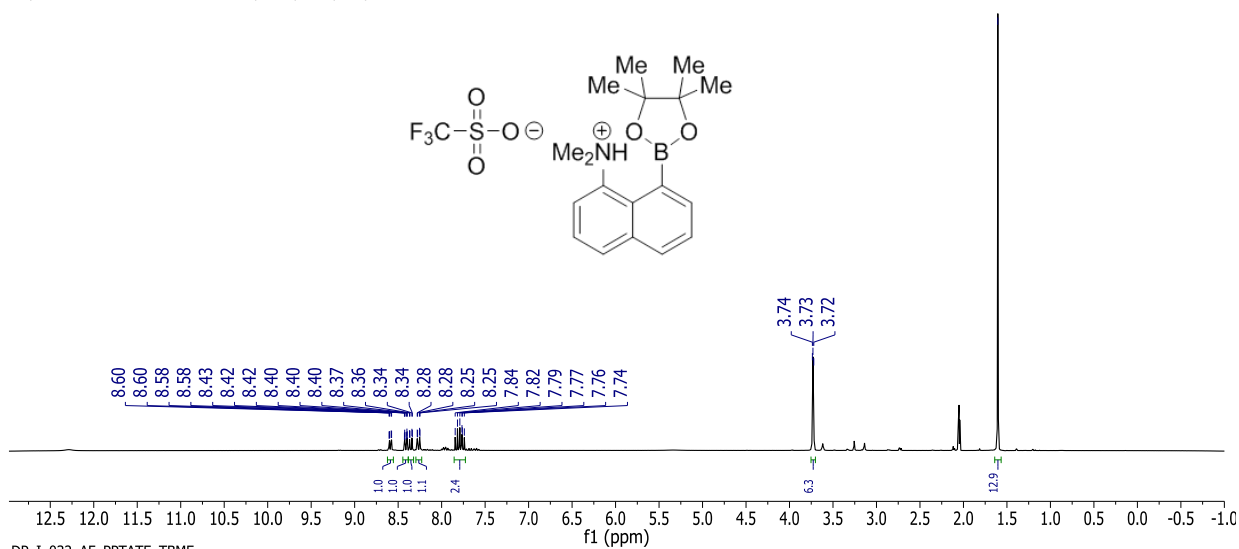
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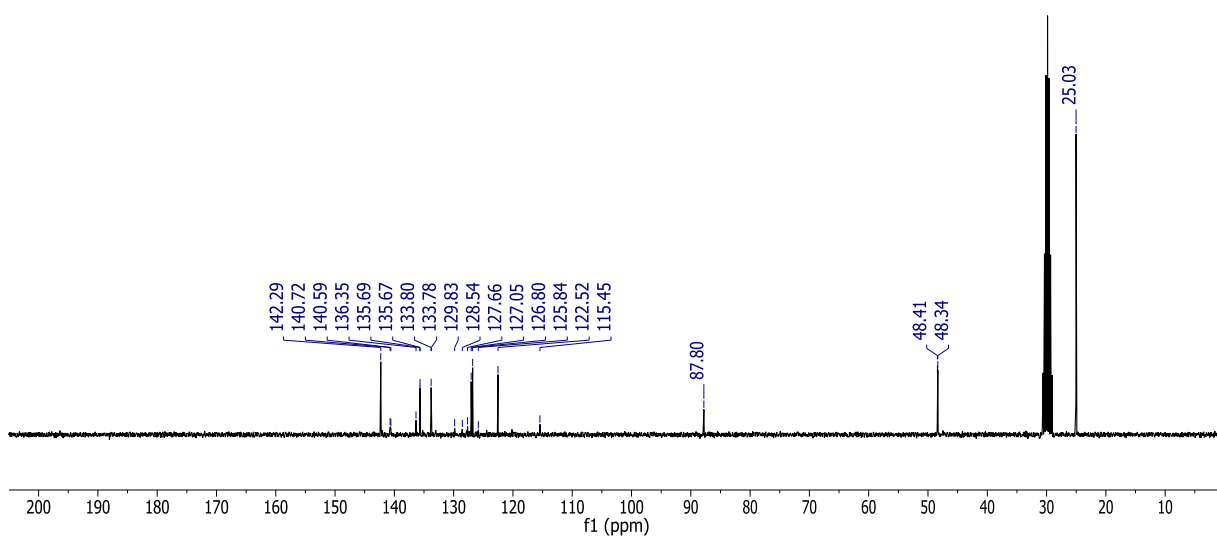
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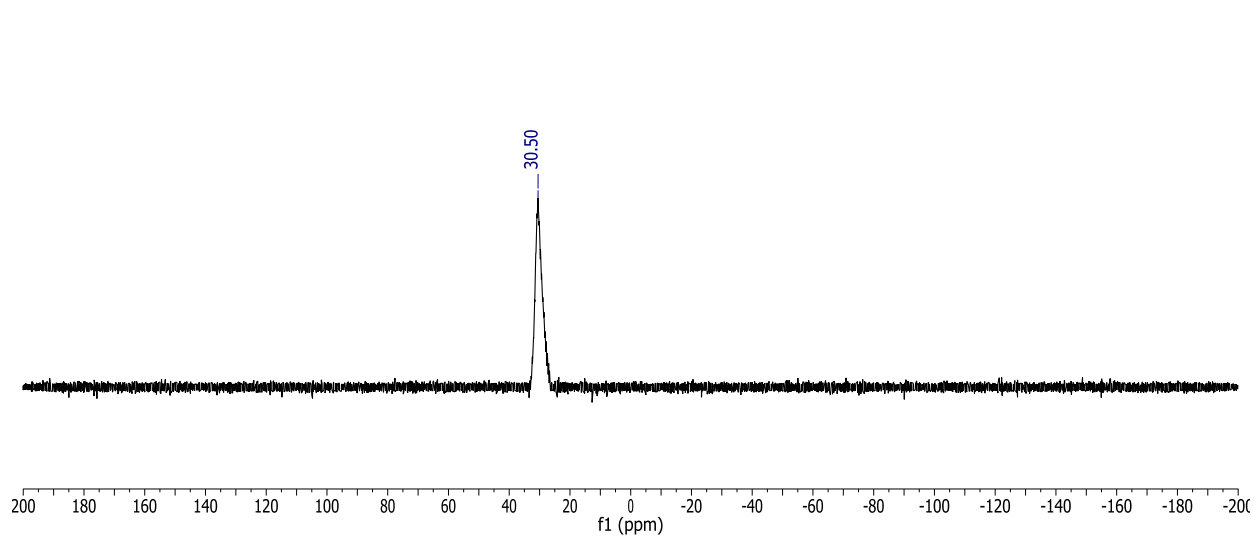
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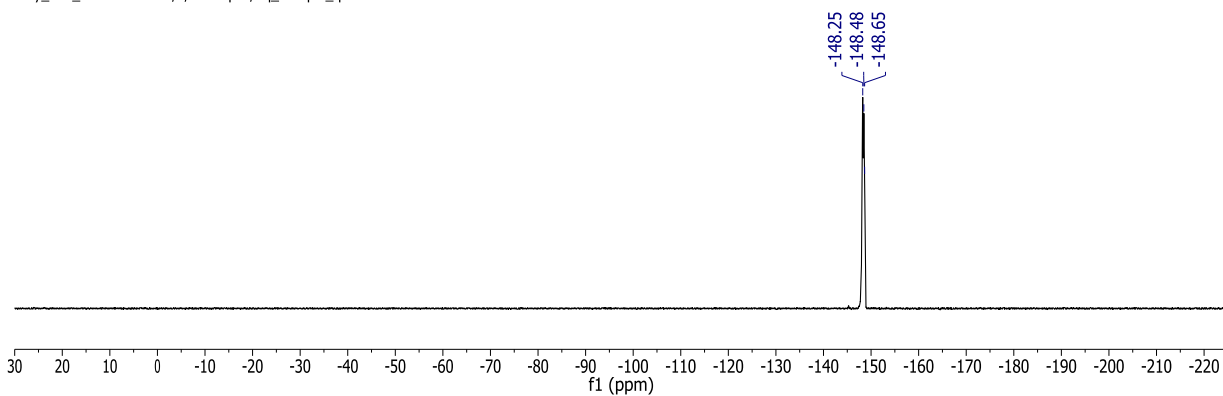
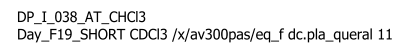
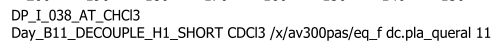


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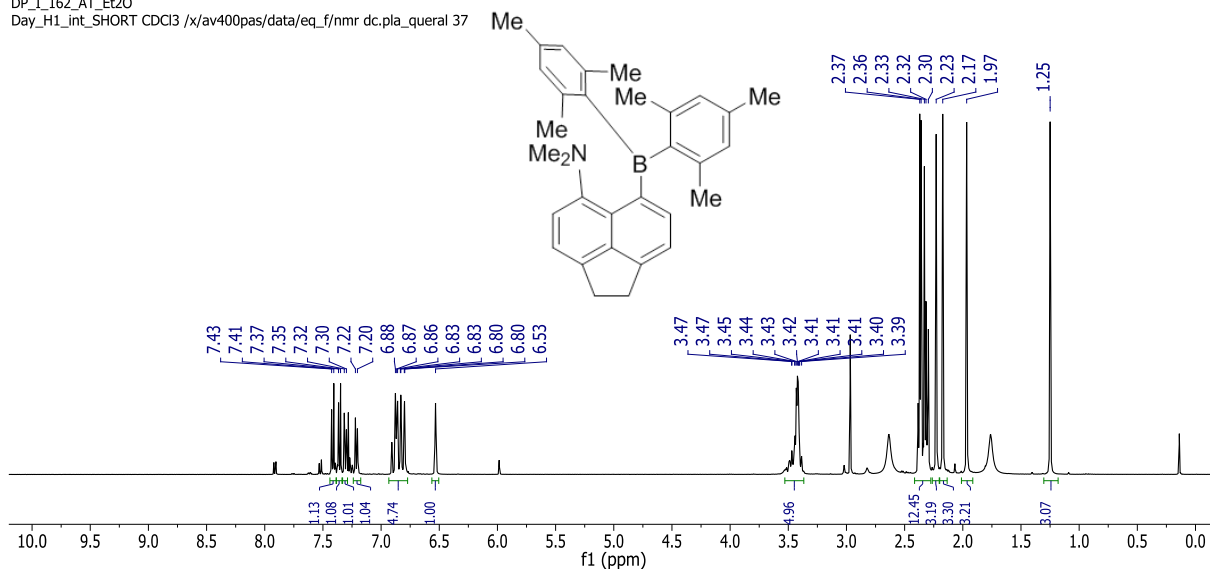


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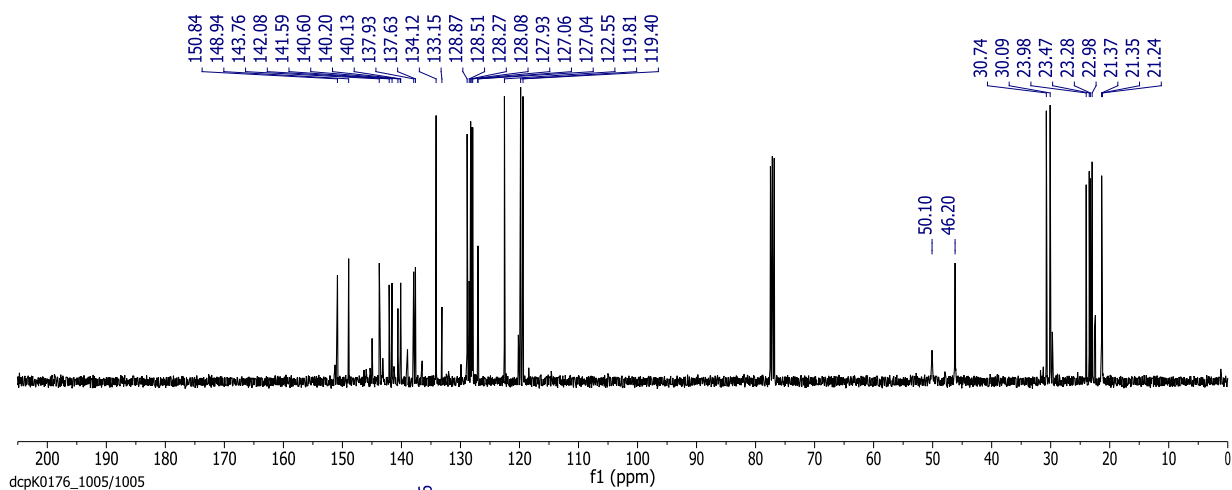


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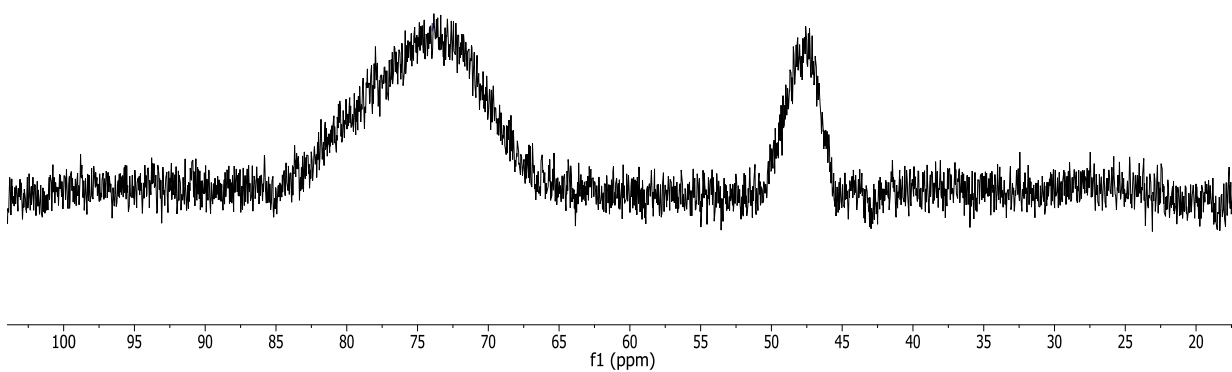
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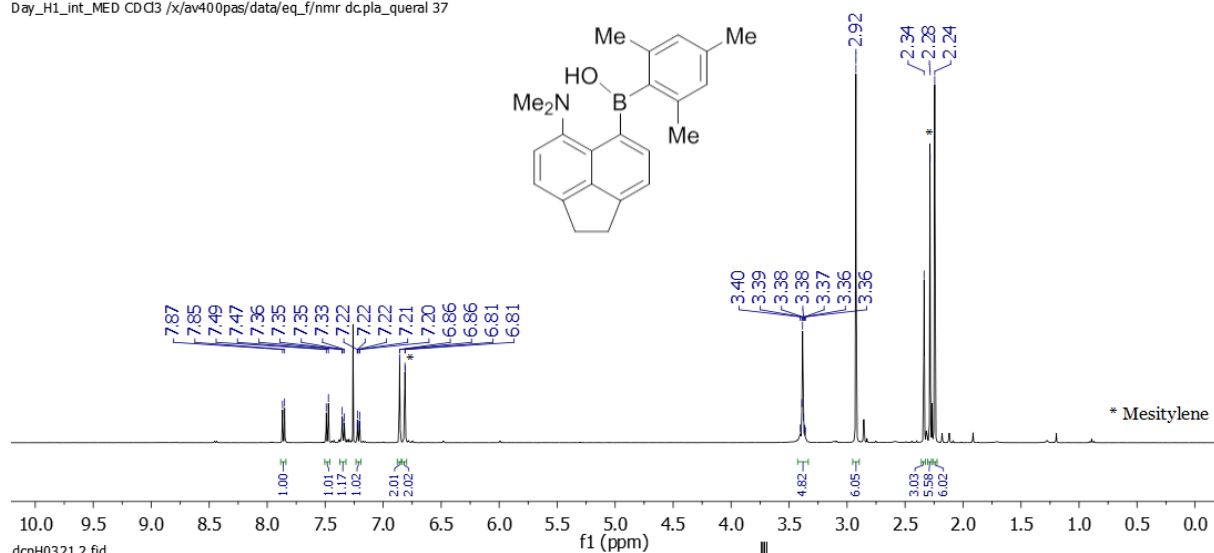
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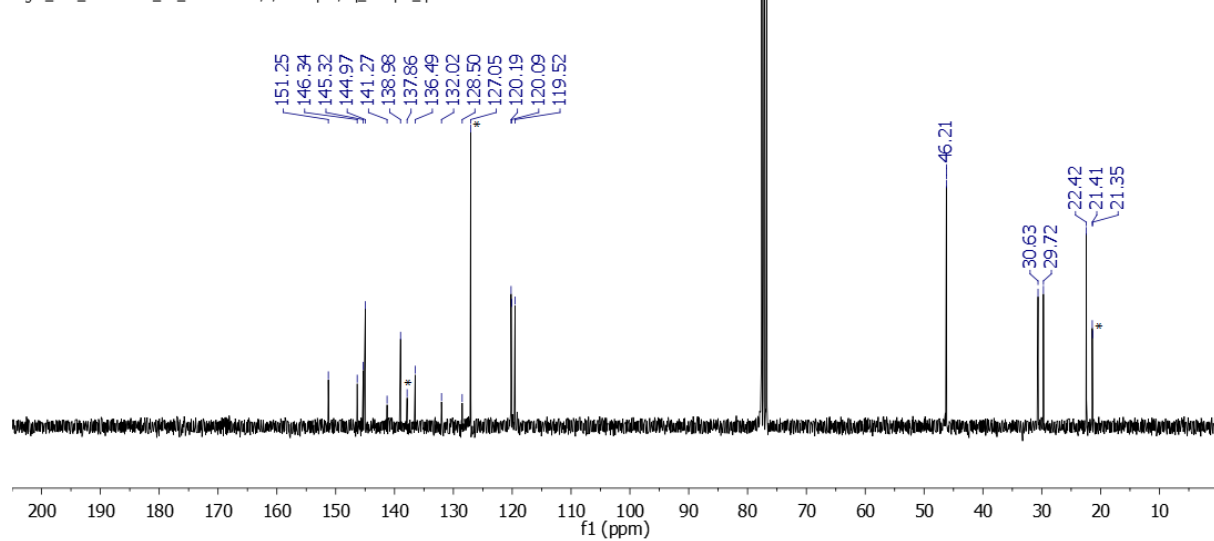
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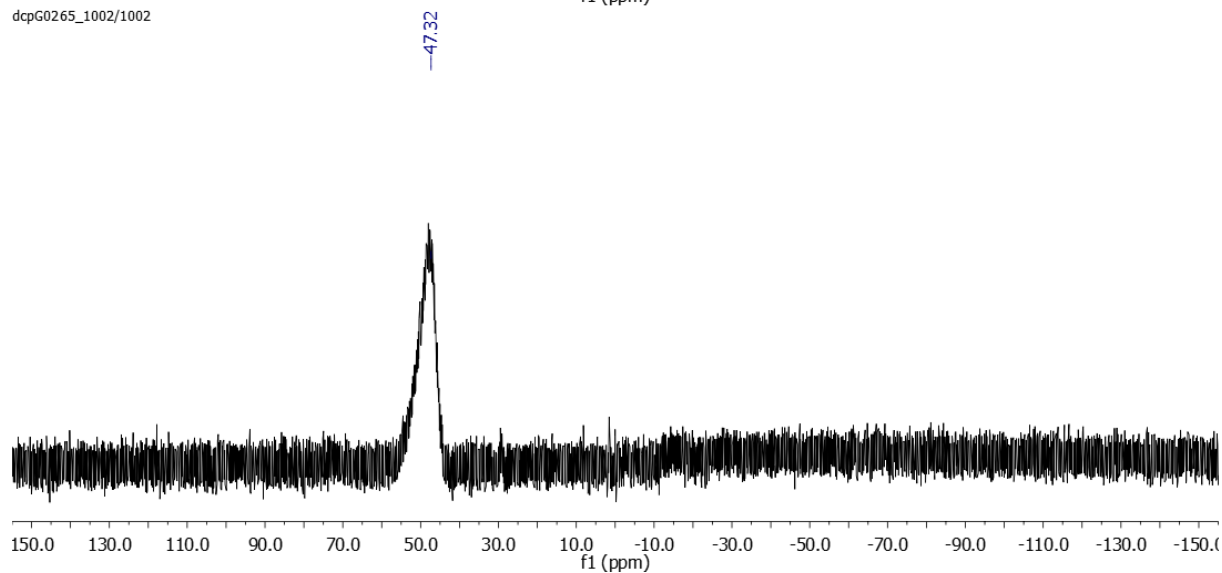
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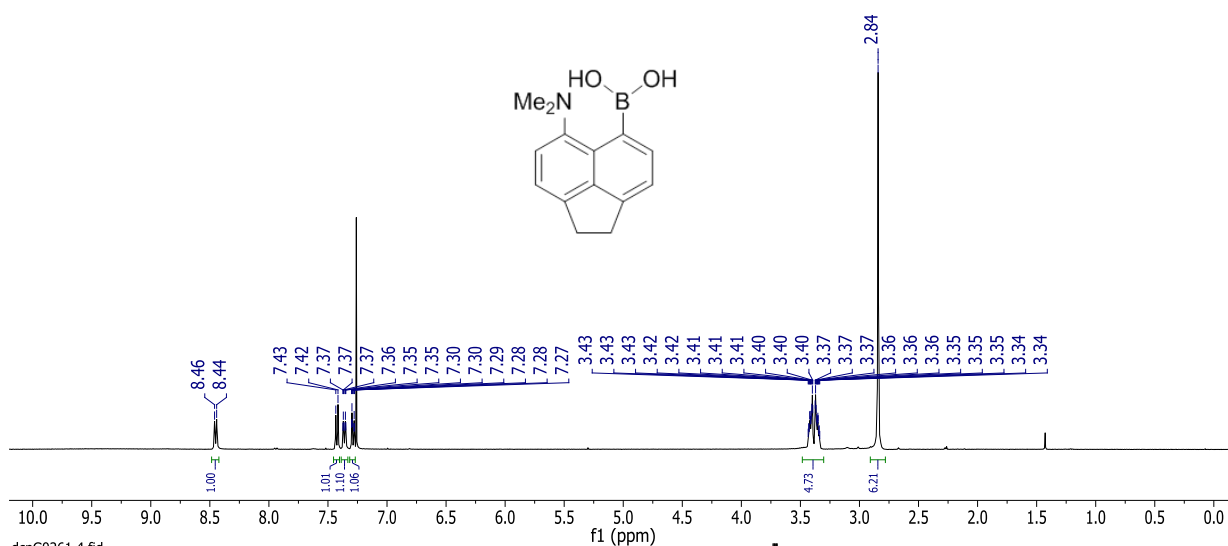
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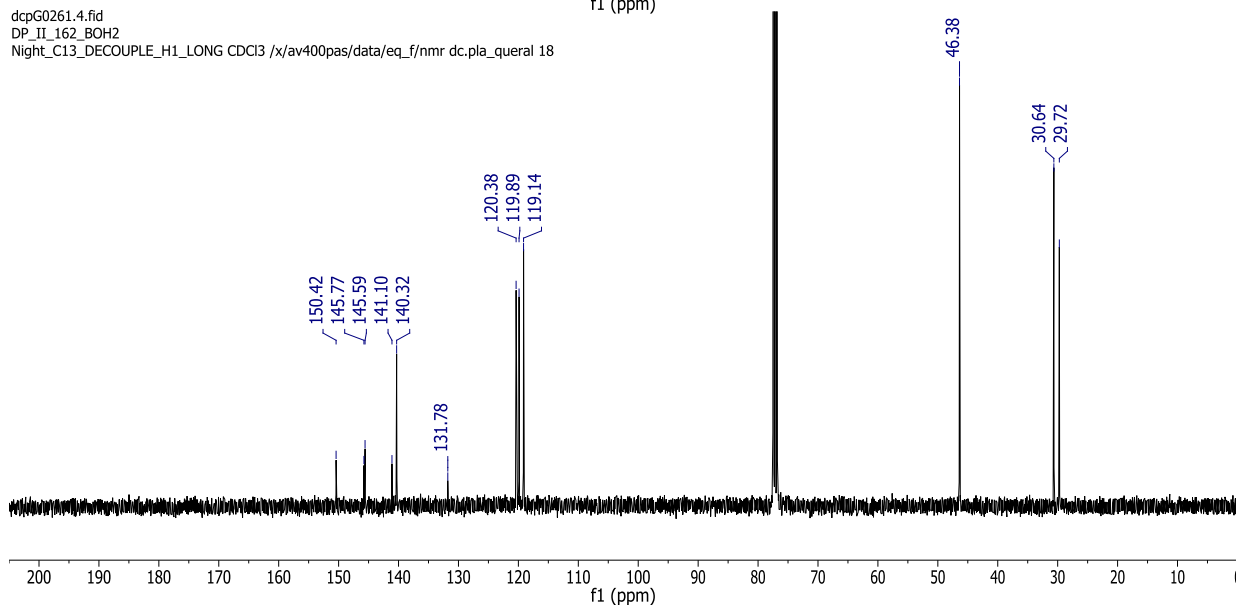
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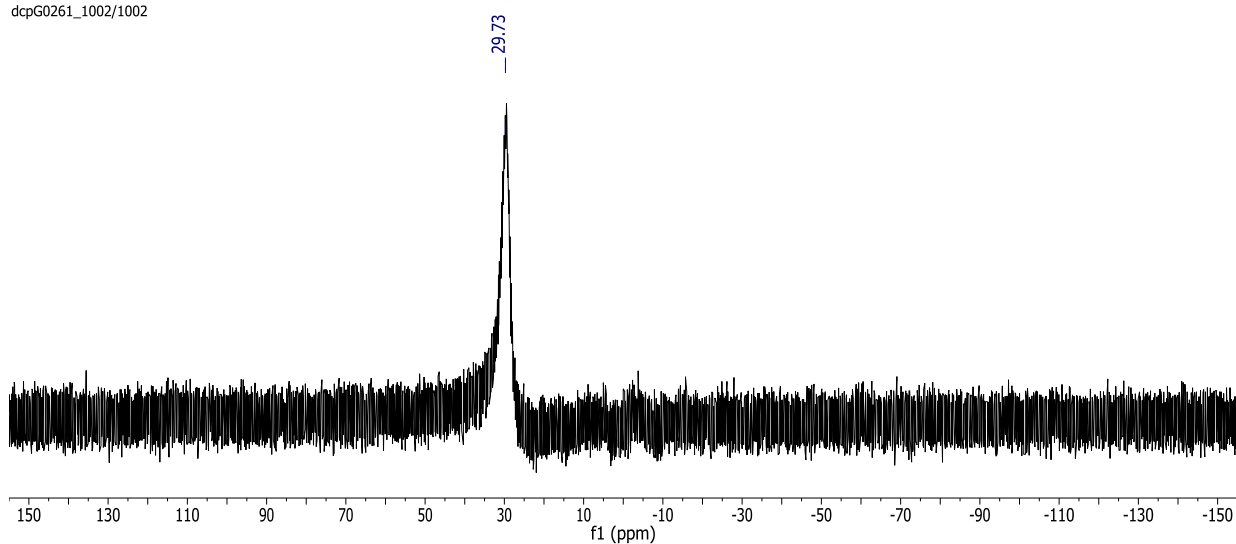
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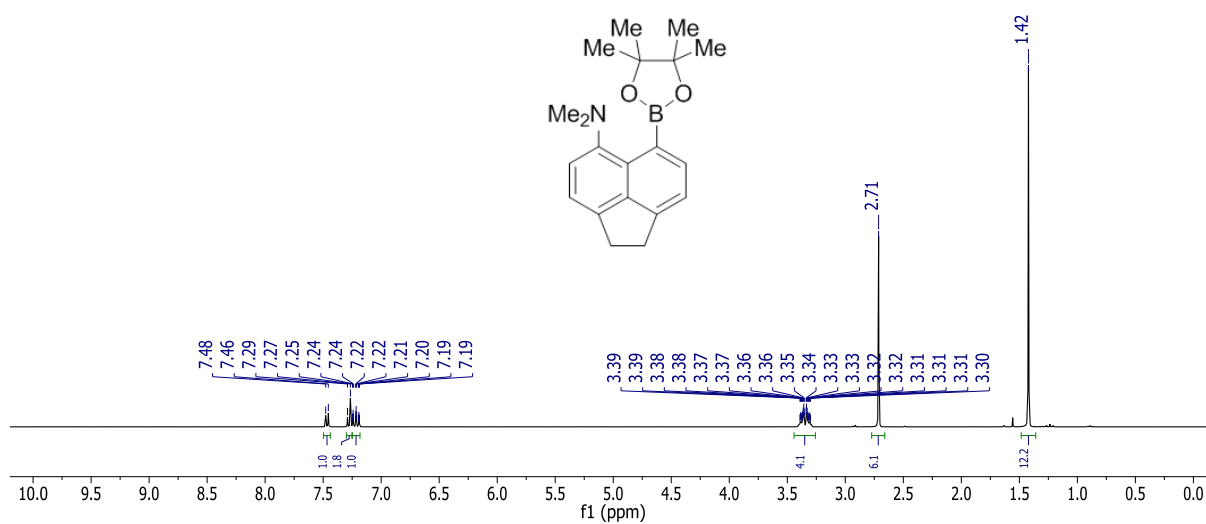
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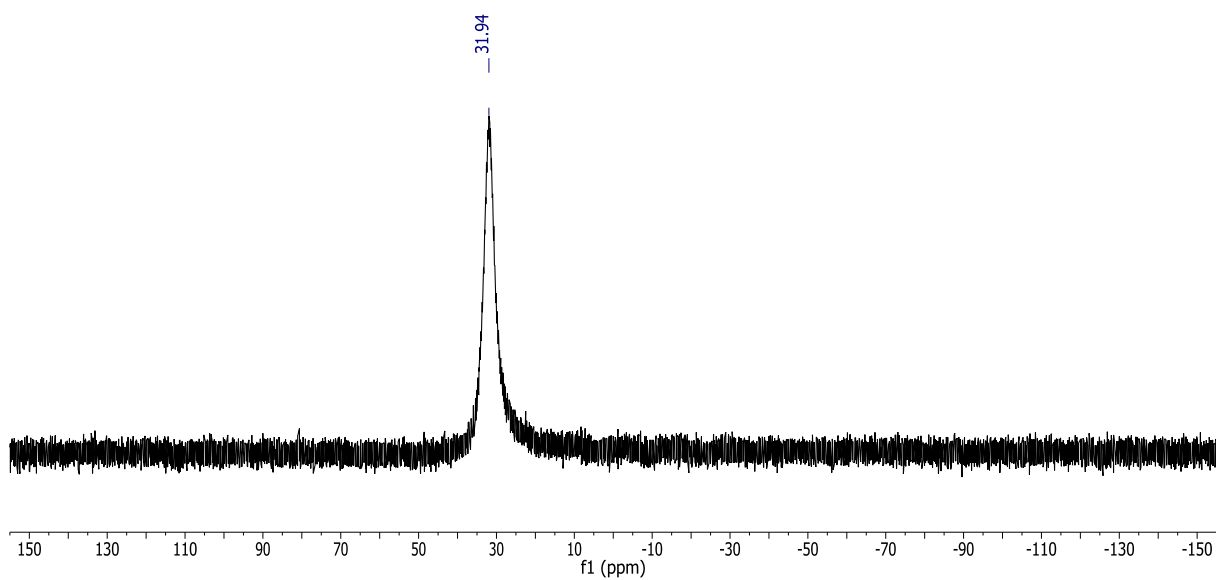
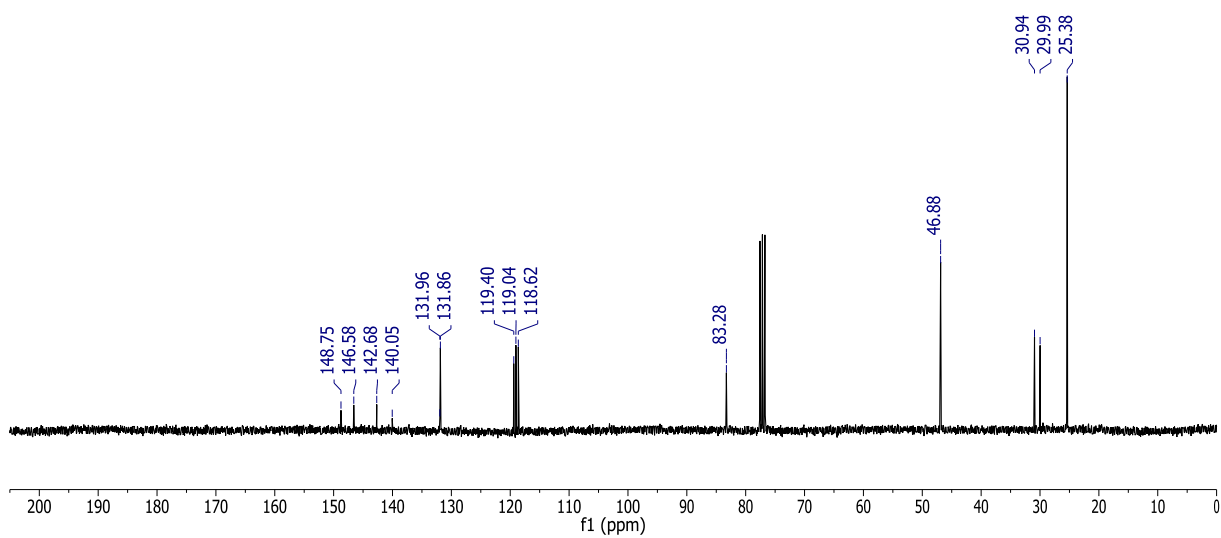
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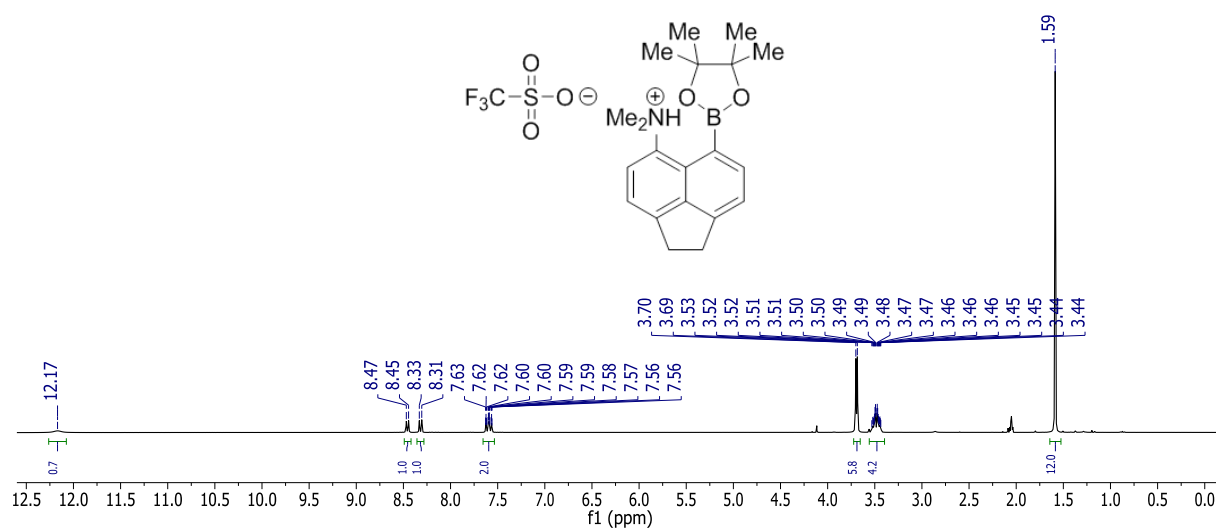
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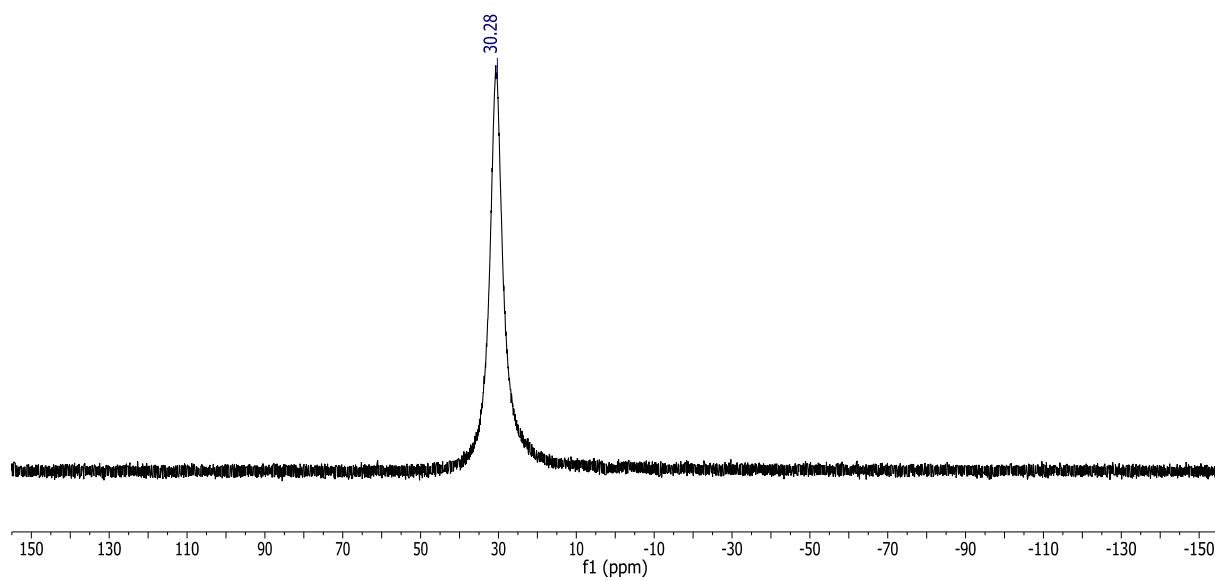
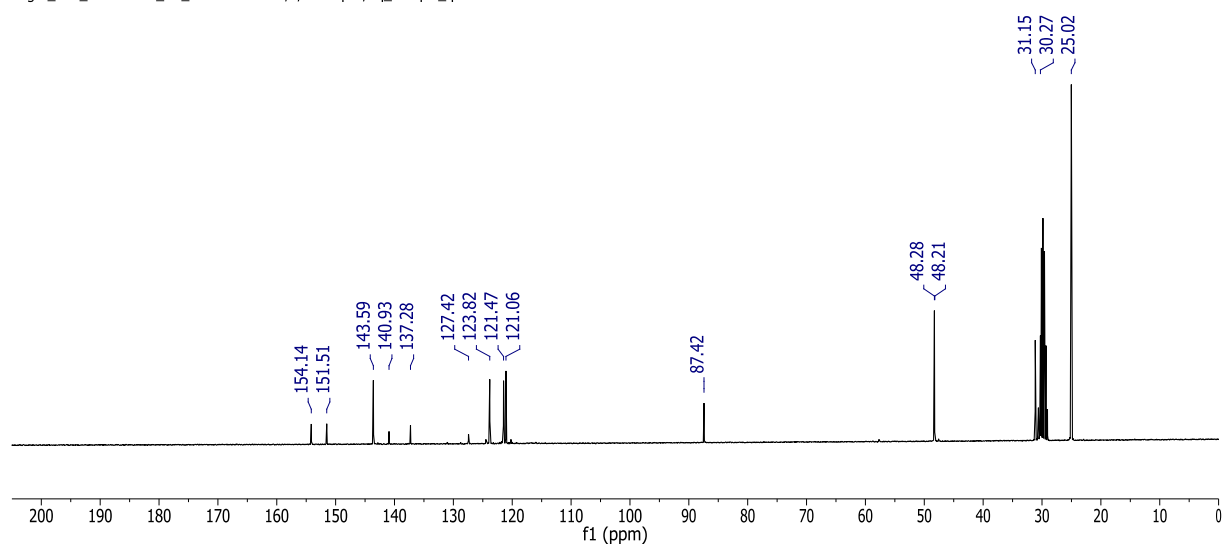
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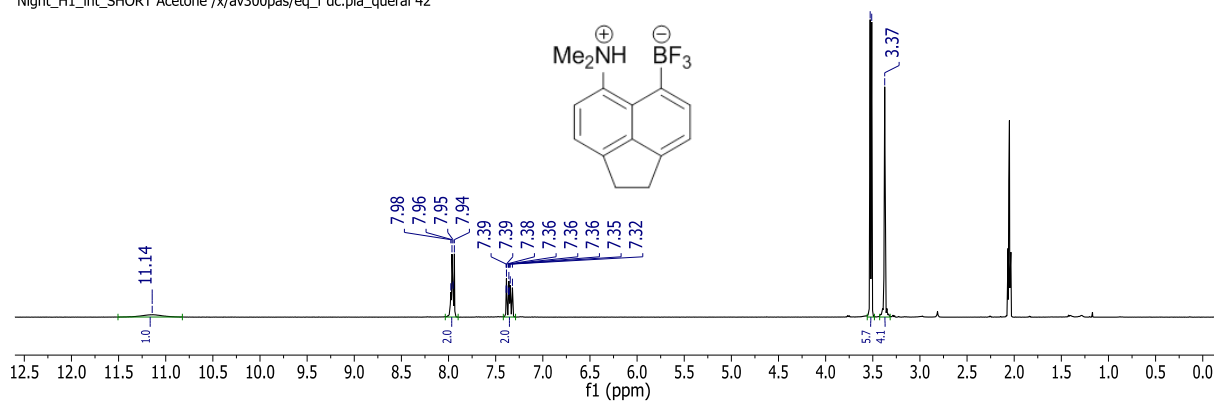
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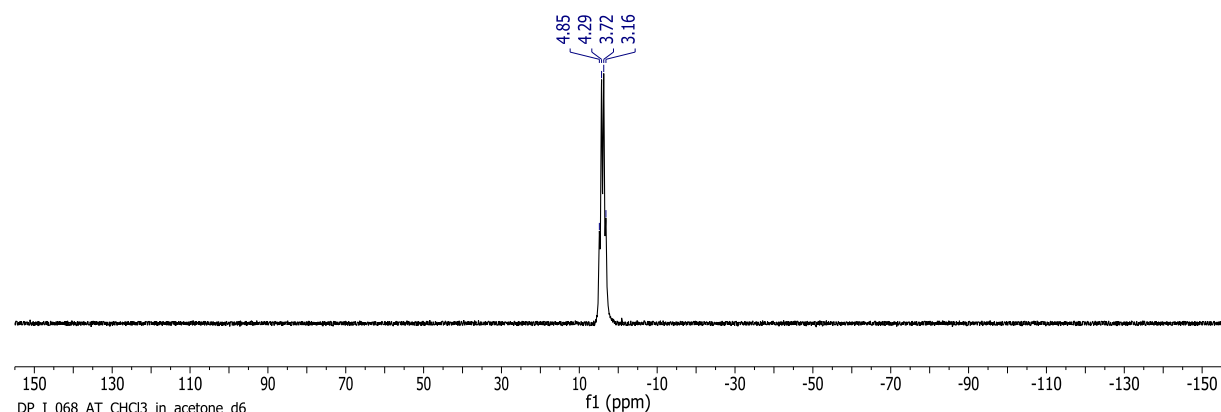
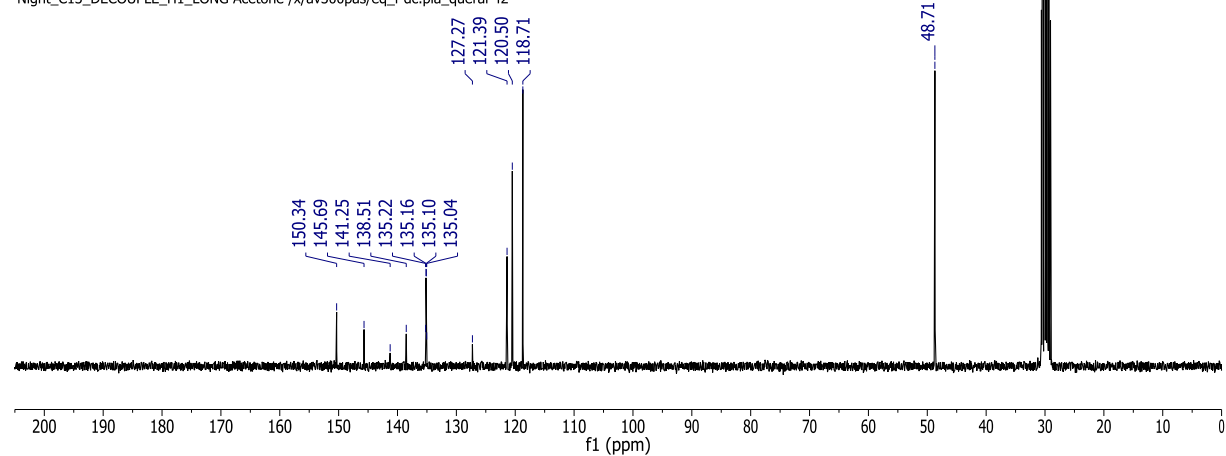
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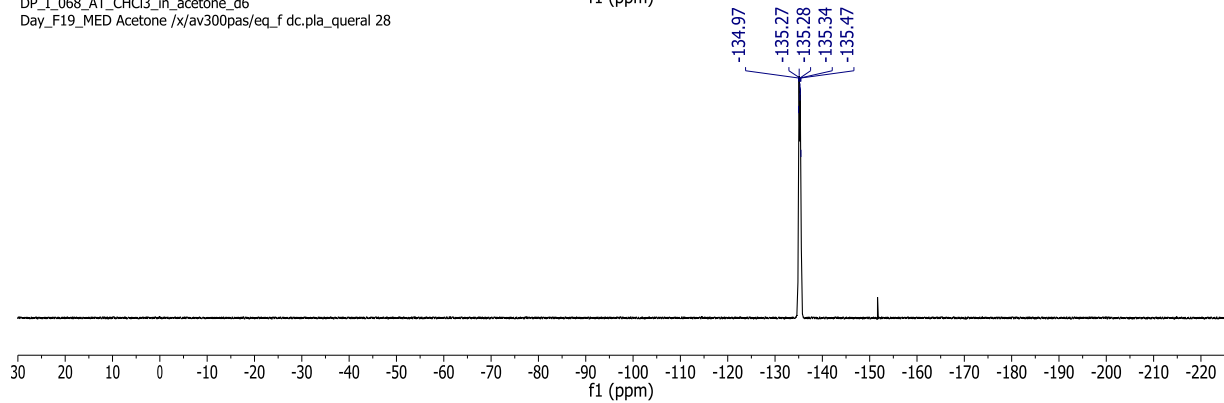
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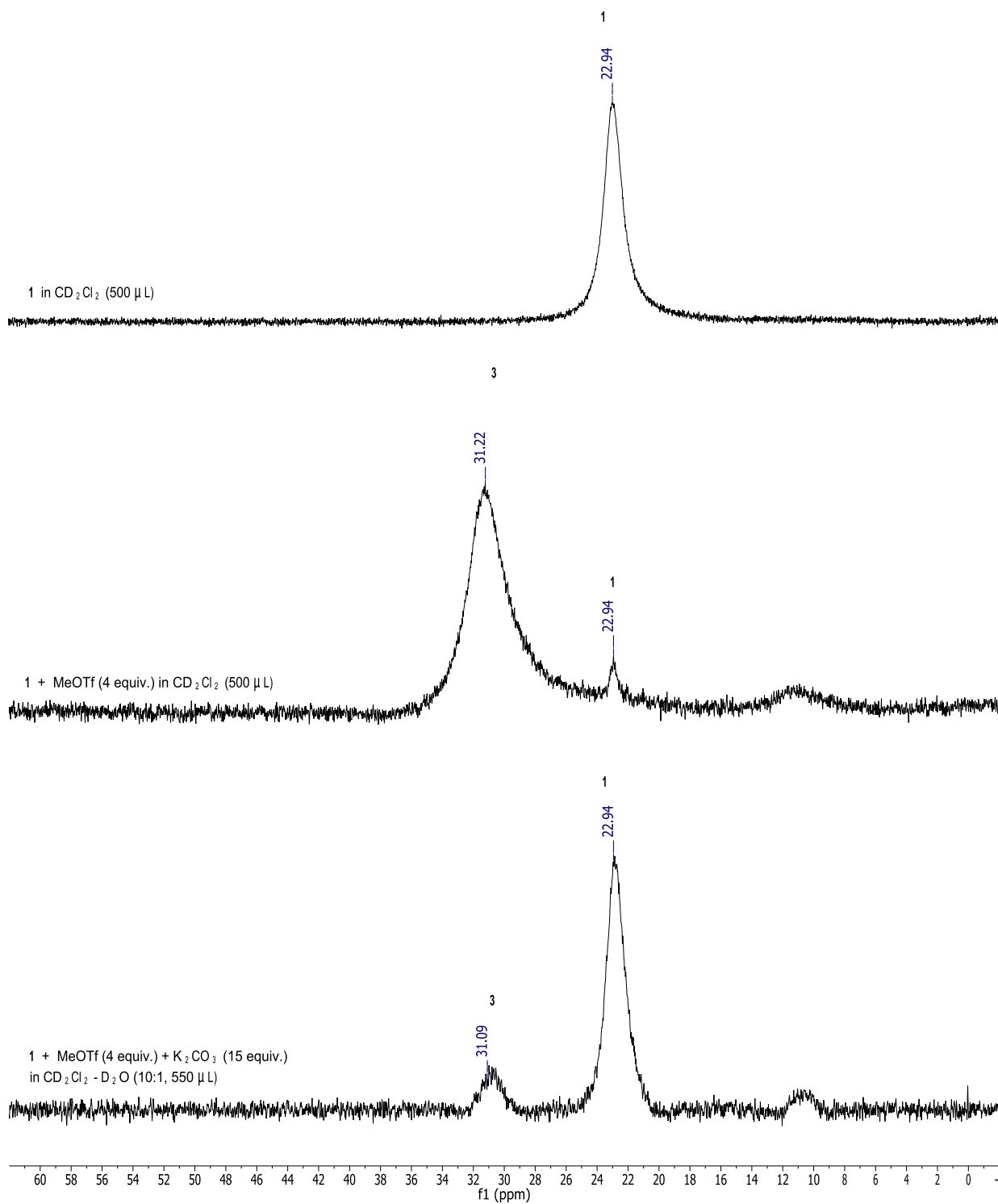
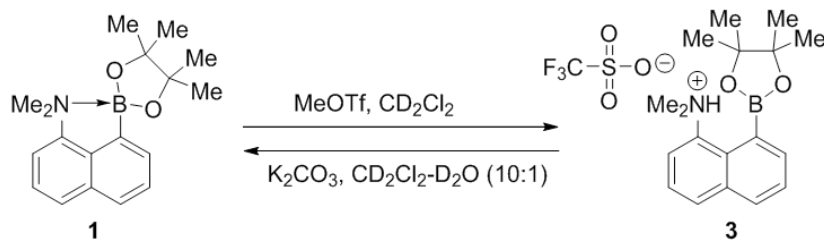


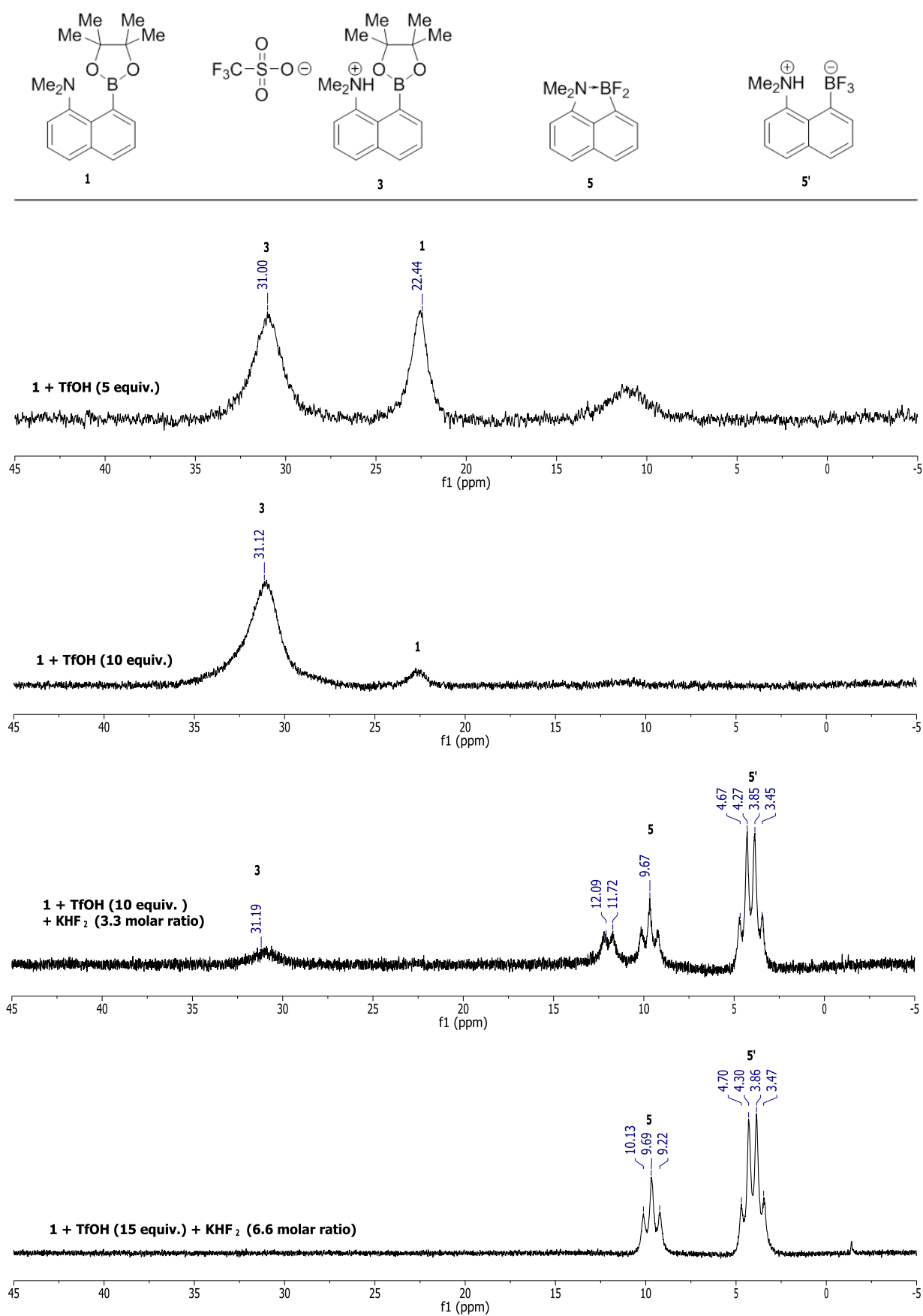
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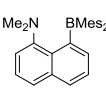
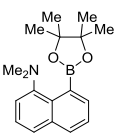
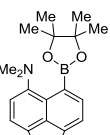
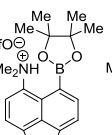
E. ^{11}B NMR study of the reversible protonation of 1

F. ^{11}B NMR timecourse of the fluorination of 1 with TfOH-KHF₂ in CD₂Cl₂

G. X-Ray Data Tables

CCDC 1403306-1403313 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

X-Ray Summary Table. Selected Interatomic Distances [Å] and Angles [deg].

										
Compound	7	1	5	<i>Peri-Region Distances</i>						
N1–B1	2.862	1.859(2)	1.726	N1–B1	3.025	3.139	3.171	2.774	3.236	3.075
N1–C1	1.454	1.461(2)	1.472	N1–C5	1.447	1.450	1.460	1.433	1.488	1.487
C8–B1	1.598	1.600(2)	1.591	C6–B1	1.569	1.584	1.583	1.563	1.555	1.615
				N1···H···O	---	2.541	2.536	---	2.675	---
<i>Peri-Region Bond Angles</i>										
α : (N1–C1–C9)	119.36	112.73(2)	108.99	(N1–C5–C10)	119.29	119.67	121.08	117.08	120.90	120.88
β : (C1–C9–C8)	124.39	114.72(2)	115.15	(C5–C10–C6)	127.38	129.71	130.47	125.94	131.95	129.86
γ : (C9–C8–B1)	126.49	112.50(2)	111.55	(C10–C6–B1)	128.88	129.37	129.03	125.38	130.14	126.29
Splay angle ^a	10.24	-20.00(2)	-24.31		15.55	18.75	20.58	8.40	22.99	17.03
δ : (C8–B1–X)	124.22	116.36(2)	109.59	(C6–B1–X)	123.87	122.36	117.04	123.86	125.89	112.85
δ' : (X–B1–X)	119.37	110.54(2)	109.10	(X–B1–X)	118.67	121.12	118.33	121.47	122.28	108.58
δ'' : (X–B1–X)	114.22	108.24(2)	109.04	(X–B1–X)	116.41	116.51	124.62	113.21	111.83	107.66
δ''' : (X–B1–X)	---	105.88(2)	106.80	(X–B1–X)	---	---	---	---	---	104.92
$\sum \delta_{X-B1-X}$	357.81	441.02(2)	434.53	$\sum \delta_{X-B1-X}$	358.95	359.99	359.99	358.54	360.00	434.01
<i>Central (Ace)Naphthyl Ring Torsion Angles</i>										
ϵ : C1–C9–C10–C5)	176.48	177.18(2)	-179.64	(C5–C10–C12–C11)	-175.76	177.75	-178.96	179.20	179.61	-179.84
η : C8–C9–C10–C4)	-179.64	177.92(2)	-179.01	(C6–C10–C12–C9)	178.89	179.75	177.75	177.08	177.07	178.66
<i>Out-of-Plane Displacement</i>										
N1	1.08	0.81(2)	0.38	N1	1.70	2.06	1.16	1.41	0.42	0.42
B1	6.18	2.82(2)	0.09	B1	5.13	3.29	0.42	2.84	0.14	1.81

^a Splay angle: $\sum$ of the three bay region angles ($\alpha + \beta + \gamma$) – 360°.

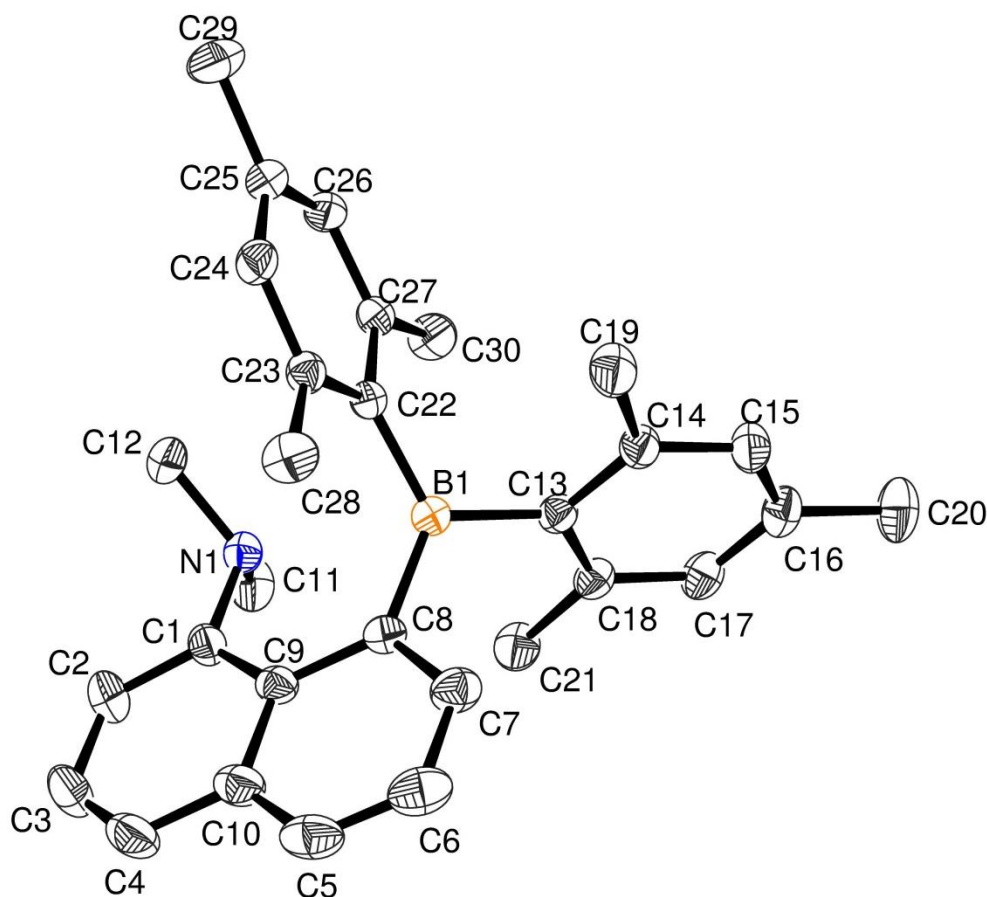
8-(Dimesitylboryl)-*N,N*-dimethylnaphthalen-1-amine (7).

Table. Crystal data and structure refinement for dp1163.

Identification code	DP-II-163
Empirical formula	C ₃₀ H ₃₄ B N
Formula weight	419.39
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, P -1
Unit cell dimensions	a = 8.8952(2) Å alpha = 100.1220(10) deg. b = 9.1463(2) Å beta = 97.4700(10) deg. c = 15.7704(4) Å gamma = 104.9290(10) deg.

Volume	1199.55(5) Å ³
Z, Calculated density	2, 1.161 Mg/m ³
Absorption coefficient	0.065 mm ⁻¹
F(000)	452
Crystal size	0.22 x 0.22 x 0.18 mm
Theta range for data collection	1.33 to 31.88 deg.
Limiting indices	-13 ≤ h ≤ 12, -13 ≤ k ≤ 13, -23 ≤ l ≤ 23
Reflections collected / unique	30766 / 8186 [R(int) = 0.0202]
Completeness to theta = 31.88	99.2 %
Max. and min. transmission	0.7463 and 0.7204
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8186 / 0 / 297
Goodness-of-fit on F ²	1.031
Final R indices [I > 2σ(I)]	R1 = 0.0528, wR2 = 0.1605
R indices (all data)	R1 = 0.0677, wR2 = 0.1760
Largest diff. peak and hole	0.390 and -0.316 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1163.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
B(1)	4318(1)	6906(1)	2854(1)	22(1)
C(9)	6513(1)	9300(1)	2513(1)	25(1)
C(8)	5972(1)	8169(1)	3018(1)	24(1)
C(1)	5473(1)	9702(1)	1888(1)	27(1)
C(10)	8164(1)	10122(1)	2662(1)	33(1)
C(2)	6059(2)	10821(2)	1437(1)	40(1)
C(7)	7074(1)	8008(1)	3676(1)	33(1)
C(12)	3200(2)	8072(2)	839(1)	34(1)
C(5)	9229(1)	9825(2)	3311(1)	40(1)
C(4)	8707(2)	11245(2)	2168(1)	42(1)
C(11)	2912(2)	10103(2)	1929(1)	38(1)
C(3)	7679(2)	11588(2)	1574(1)	45(1)
C(6)	8704(2)	8808(2)	3814(1)	41(1)
N(1)	3792(1)	8962(1)	1745(1)	25(1)
C(22)	3603(1)	5658(1)	1965(1)	22(1)
C(27)	1942(1)	5148(1)	1669(1)	25(1)
C(23)	4541(1)	4966(1)	1459(1)	24(1)
C(26)	1281(1)	3999(1)	906(1)	30(1)
C(24)	3821(1)	3796(1)	710(1)	29(1)
C(25)	2197(2)	3289(1)	423(1)	31(1)
C(28)	6318(1)	5369(2)	1699(1)	34(1)
C(30)	822(1)	5836(2)	2137(1)	34(1)
C(29)	1456(2)	2001(2)	-375(1)	47(1)
C(13)	3586(1)	6645(1)	3701(1)	24(1)
C(14)	3342(1)	5197(1)	3946(1)	27(1)
C(18)	3221(1)	7844(1)	4259(1)	26(1)
C(17)	2604(1)	7578(2)	5007(1)	32(1)
C(15)	2742(2)	4984(1)	4704(1)	32(1)
C(16)	2353(2)	6153(2)	5239(1)	34(1)
C(21)	3412(2)	9416(1)	4047(1)	34(1)
C(19)	3734(2)	3833(1)	3427(1)	37(1)
C(20)	1694(2)	5886(2)	6052(1)	48(1)

Table 3. Bond lengths [Å] and angles [deg] for dp1163.

B(1)-C(8)	1.5767(15)
B(1)-C(22)	1.5826(14)
B(1)-C(13)	1.5879(15)
C(9)-C(1)	1.4242(16)
C(9)-C(10)	1.4345(15)
C(9)-C(8)	1.4377(15)
C(8)-C(7)	1.3871(15)
C(1)-C(2)	1.3800(16)
C(1)-N(1)	1.4432(14)
C(10)-C(5)	1.413(2)
C(10)-C(4)	1.4202(18)
C(2)-C(3)	1.400(2)
C(2)-H(2)	0.9500
C(7)-C(6)	1.4149(18)
C(7)-H(7)	0.9500
C(12)-N(1)	1.4684(14)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(5)-C(6)	1.358(2)
C(5)-H(5)	0.9500
C(4)-C(3)	1.357(2)
C(4)-H(4)	0.9500
C(11)-N(1)	1.4696(15)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(3)-H(3)	0.9500
C(6)-H(6)	0.9500
C(22)-C(23)	1.4153(14)
C(22)-C(27)	1.4169(14)
C(27)-C(26)	1.3971(15)
C(27)-C(30)	1.5113(16)
C(23)-C(24)	1.3985(14)
C(23)-C(28)	1.5070(15)
C(26)-C(25)	1.3875(17)
C(26)-H(26)	0.9500
C(24)-C(25)	1.3850(17)
C(24)-H(24)	0.9500
C(25)-C(29)	1.5065(16)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(29)-H(29A)	0.9800

C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(13)-C(18)	1.4146(14)
C(13)-C(14)	1.4155(15)
C(14)-C(15)	1.3948(15)
C(14)-C(19)	1.5130(16)
C(18)-C(17)	1.3981(15)
C(18)-C(21)	1.5046(16)
C(17)-C(16)	1.3861(18)
C(17)-H(17)	0.9500
C(15)-C(16)	1.3877(17)
C(15)-H(15)	0.9500
C(16)-C(20)	1.5090(17)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(8)-B(1)-C(22)	123.25(9)
C(8)-B(1)-C(13)	116.05(8)
C(22)-B(1)-C(13)	118.91(8)
C(1)-C(9)-C(10)	117.44(10)
C(1)-C(9)-C(8)	123.09(9)
C(10)-C(9)-C(8)	119.42(10)
C(7)-C(8)-C(9)	117.58(10)
C(7)-C(8)-B(1)	113.38(9)
C(9)-C(8)-B(1)	128.55(9)
C(2)-C(1)-C(9)	120.42(11)
C(2)-C(1)-N(1)	119.94(11)
C(9)-C(1)-N(1)	119.62(9)
C(5)-C(10)-C(4)	120.74(11)
C(5)-C(10)-C(9)	119.49(11)
C(4)-C(10)-C(9)	119.76(12)
C(1)-C(2)-C(3)	121.45(13)
C(1)-C(2)-H(2)	119.3
C(3)-C(2)-H(2)	119.3
C(8)-C(7)-C(6)	122.60(12)
C(8)-C(7)-H(7)	118.7
C(6)-C(7)-H(7)	118.7
N(1)-C(12)-H(12A)	109.5
N(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
N(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

C(6)-C(5)-C(10)	120.93(11)
C(6)-C(5)-H(5)	119.5
C(10)-C(5)-H(5)	119.5
C(3)-C(4)-C(10)	120.97(12)
C(3)-C(4)-H(4)	119.5
C(10)-C(4)-H(4)	119.5
N(1)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(4)-C(3)-C(2)	119.91(12)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(6)-C(7)	119.75(12)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-H(6)	120.1
C(1)-N(1)-C(12)	111.00(9)
C(1)-N(1)-C(11)	111.40(9)
C(12)-N(1)-C(11)	108.84(10)
C(23)-C(22)-C(27)	117.50(9)
C(23)-C(22)-B(1)	123.07(9)
C(27)-C(22)-B(1)	119.37(9)
C(26)-C(27)-C(22)	120.28(10)
C(26)-C(27)-C(30)	117.32(10)
C(22)-C(27)-C(30)	122.38(9)
C(24)-C(23)-C(22)	120.06(10)
C(24)-C(23)-C(28)	116.34(9)
C(22)-C(23)-C(28)	123.54(9)
C(25)-C(26)-C(27)	122.22(10)
C(25)-C(26)-H(26)	118.9
C(27)-C(26)-H(26)	118.9
C(25)-C(24)-C(23)	122.48(10)
C(25)-C(24)-H(24)	118.8
C(23)-C(24)-H(24)	118.8
C(24)-C(25)-C(26)	117.42(10)
C(24)-C(25)-C(29)	121.17(12)
C(26)-C(25)-C(29)	121.40(11)
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5

H(30B)-C(30)-H(30C)	109.5
C(25)-C(29)-H(29A)	109.5
C(25)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(25)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(18)-C(13)-C(14)	117.33(9)
C(18)-C(13)-B(1)	122.26(9)
C(14)-C(13)-B(1)	120.34(9)
C(15)-C(14)-C(13)	120.29(10)
C(15)-C(14)-C(19)	116.81(10)
C(13)-C(14)-C(19)	122.89(10)
C(17)-C(18)-C(13)	120.61(10)
C(17)-C(18)-C(21)	117.96(10)
C(13)-C(18)-C(21)	121.37(10)
C(16)-C(17)-C(18)	121.76(11)
C(16)-C(17)-H(17)	119.1
C(18)-C(17)-H(17)	119.1
C(16)-C(15)-C(14)	122.19(11)
C(16)-C(15)-H(15)	118.9
C(14)-C(15)-H(15)	118.9
C(17)-C(16)-C(15)	117.79(10)
C(17)-C(16)-C(20)	121.13(12)
C(15)-C(16)-C(20)	121.08(12)
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

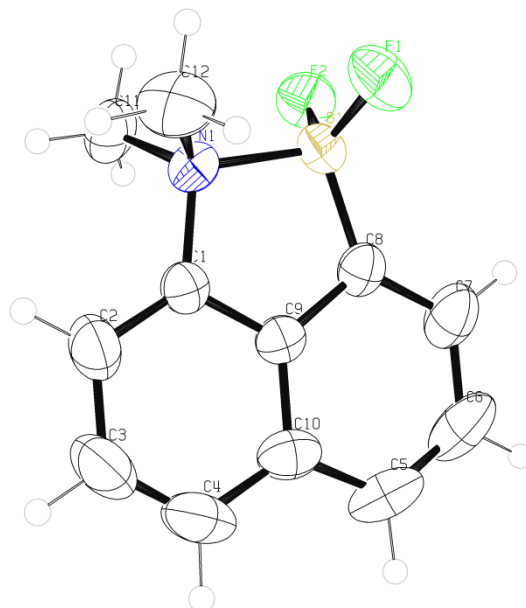
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1163.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
B(1)	22(1)	22(1)	23(1)	5(1)	4(1)	8(1)
C(9)	24(1)	22(1)	26(1)	1(1)	7(1)	5(1)
C(8)	24(1)	23(1)	24(1)	2(1)	3(1)	6(1)
C(1)	30(1)	25(1)	26(1)	6(1)	9(1)	6(1)
C(10)	27(1)	29(1)	37(1)	-2(1)	10(1)	3(1)
C(2)	46(1)	37(1)	39(1)	18(1)	13(1)	6(1)
C(7)	30(1)	33(1)	33(1)	6(1)	-2(1)	9(1)
C(12)	41(1)	37(1)	23(1)	8(1)	4(1)	8(1)
C(5)	23(1)	40(1)	49(1)	-2(1)	2(1)	4(1)
C(4)	35(1)	35(1)	48(1)	1(1)	19(1)	-4(1)
C(11)	46(1)	37(1)	41(1)	14(1)	14(1)	23(1)
C(3)	50(1)	38(1)	47(1)	15(1)	21(1)	-1(1)
C(6)	29(1)	44(1)	45(1)	2(1)	-7(1)	12(1)
N(1)	28(1)	26(1)	24(1)	7(1)	6(1)	10(1)
C(22)	21(1)	22(1)	21(1)	5(1)	5(1)	5(1)
C(27)	22(1)	27(1)	24(1)	6(1)	6(1)	3(1)
C(23)	25(1)	24(1)	24(1)	6(1)	7(1)	8(1)
C(26)	25(1)	33(1)	27(1)	4(1)	3(1)	-1(1)
C(24)	35(1)	27(1)	24(1)	4(1)	10(1)	10(1)
C(25)	37(1)	28(1)	23(1)	2(1)	5(1)	2(1)
C(28)	26(1)	39(1)	38(1)	1(1)	8(1)	14(1)
C(30)	22(1)	43(1)	36(1)	4(1)	8(1)	9(1)
C(29)	51(1)	41(1)	34(1)	-9(1)	3(1)	-1(1)
C(13)	26(1)	24(1)	21(1)	3(1)	4(1)	7(1)
C(14)	32(1)	26(1)	24(1)	6(1)	6(1)	10(1)
C(18)	30(1)	26(1)	23(1)	2(1)	4(1)	10(1)
C(17)	37(1)	36(1)	25(1)	3(1)	9(1)	15(1)
C(15)	41(1)	33(1)	28(1)	12(1)	10(1)	13(1)
C(16)	36(1)	43(1)	24(1)	9(1)	9(1)	14(1)
C(21)	46(1)	28(1)	33(1)	4(1)	10(1)	17(1)
C(19)	56(1)	27(1)	34(1)	9(1)	14(1)	19(1)
C(20)	58(1)	62(1)	33(1)	18(1)	23(1)	24(1)

8-(Difluoroboryl)-*N,N*-dimethylnaphthalen-1-amine (5)**Crystal Data DPla170414**a = 12.1467(5) Å $\alpha = 90^\circ$ b = 10.7629(5) Å $\beta = 90^\circ$ c = 16.8959(8) Å $\gamma = 90^\circ$ Volume 2208.86(17) Å³

Space group P b c a

Formula C₁₂ H₁₂ B₁ F₂ N₁

Cell determined from 9922 reflections

Temperature 295K

Shape block

Colour colorless

D_x 1.32 μ 0.099 mm⁻¹

Absorption correction multi-scan

T_{min} 0.95

Crystal Class orthorhombic

Z = 8

M_r 219.04Cell θ range = 2 - 29°

Size 0.15 × 0.20 × 0.20 mm

F000 912.000

T_{max} 0.99**Data Collection**

Diffractometer multi-scan

Scan type ϕ and ω scans

Reflections measured 42628

Independent reflections 2999

R_{int} 0.0221 $\theta_{\max}$ 29.8740

h = -16 → 16

k = -14 → 13

$l = -23 \rightarrow 23$

Refinement

$\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$

Reflections used 2416

Cutoff: $I > 3.00\sigma(I)$

Parameters refined 145

$S = 1.02$

R-factor 0.047

weighted R-factor 0.050

$\Delta/\sigma_{\max} = 0.0005$

Refinement on F

$w = w' \times [1 - (\Delta F_{\text{obs}} / 6 \times \Delta F_{\text{est}})^2]^2$

$w' = [P_0 T_0'(x) + P_1 T_1'(x) + \dots P_{n-1} T_{n-1}'(x)]^{-1}$,
where P_i are the coefficients of a Chebychev series in $t_i(x)$, and $x = F_{\text{calc}}/F_{\text{calcmax}}$.

$P_0 - P_{n-1} = 0.193 \ 0.164 \ 0.463\text{E-}01$

Parameters

Label	x	y	z	$U_{\text{iso/equiv}}$	Occupancy
C1	0.65790(8)	0.42511(10)	0.59909(7)	0.0378	1.0000
C2	0.71494(11)	0.52342(13)	0.56931(9)	0.0575	1.0000
C3	0.71366(14)	0.54106(17)	0.48629(10)	0.0725	1.0000
C4	0.65798(13)	0.46305(16)	0.43675(9)	0.0674	1.0000
C5	0.53688(14)	0.27370(15)	0.42298(8)	0.0667	1.0000
C6	0.48204(16)	0.18051(15)	0.46025(10)	0.0738	1.0000
C7	0.48417(13)	0.16660(13)	0.54328(10)	0.0612	1.0000
C8	0.54343(9)	0.24746(10)	0.58929(7)	0.0408	1.0000
C9	0.59963(9)	0.34364(10)	0.54989(6)	0.0367	1.0000
C10	0.59875(11)	0.36074(12)	0.46701(7)	0.0503	1.0000
C11	0.76037(11)	0.35963(14)	0.71520(9)	0.0577	1.0000
C12	0.59948(15)	0.49226(13)	0.72995(9)	0.0657	1.0000
N1	0.64846(7)	0.38921(8)	0.68290(5)	0.0375	1.0000
B1	0.56470(10)	0.25970(12)	0.68185(8)	0.0398	1.0000
F1	0.47466(6)	0.28688(9)	0.72790(5)	0.0667	1.0000
F2	0.62368(6)	0.16439(7)	0.71694(5)	0.0541	1.0000
H21	0.75453(11)	0.58256(13)	0.60349(9)	0.0715	1.0000
H31	0.75280(14)	0.61269(17)	0.46535(10)	0.0868	1.0000
H41	0.65815(13)	0.48001(16)	0.38065(9)	0.0818	1.0000
H51	0.53483(14)	0.28050(15)	0.36591(8)	0.0799	1.0000
H61	0.44305(16)	0.12372(15)	0.42881(10)	0.0913	1.0000
H71	0.44471(13)	0.09929(13)	0.56771(10)	0.0752	1.0000

H111	0.79260(11)	0.29360(14)	0.68038(9)	0.0865	1.0000
H112	0.80557(11)	0.43448(14)	0.71565(9)	0.0869	1.0000
H113	0.75120(11)	0.32551(14)	0.76835(9)	0.0872	1.0000
H121	0.52634(15)	0.51134(13)	0.70819(9)	0.0976	1.0000
H122	0.64667(15)	0.56491(13)	0.72626(9)	0.0978	1.0000
H123	0.59052(15)	0.46373(13)	0.78432(9)	0.0994	1.0000

Thermal Parameters

Label	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.0337(5)	0.0373(5)	0.0423(5)	0.0011(4)	-0.0002(4)	0.0020(4)
C2	0.0529(7)	0.0510(7)	0.0686(9)	0.0080(6)	-0.0002(6)	-0.0140(6)
C3	0.0685(9)	0.0737(10)	0.0752(10)	0.0294(8)	0.0108(8)	-0.0134(8)
C4	0.0712(9)	0.0829(10)	0.0481(7)	0.0229(7)	0.0091(7)	0.0080(8)
C5	0.0877(11)	0.0694(10)	0.0429(7)	-0.0085(6)	-0.0232(7)	0.0200(8)
C6	0.0932(12)	0.0575(8)	0.0706(10)	-0.0151(7)	-0.0415(9)	0.0021(8)
C7	0.0683(9)	0.0446(7)	0.0707(9)	0.0013(6)	-0.0221(7)	-0.0112(6)
C8	0.0400(5)	0.0357(5)	0.0467(6)	0.0009(4)	-0.0073(4)	0.0006(4)
C9	0.0362(5)	0.0363(5)	0.0376(5)	0.0008(4)	-0.0022(4)	0.0058(4)
C10	0.0549(7)	0.0560(7)	0.0401(6)	0.0034(5)	-0.0029(5)	0.0138(6)
C11	0.0471(7)	0.0604(8)	0.0657(8)	0.0069(6)	-0.0216(6)	-0.0032(6)
C12	0.0896(11)	0.0471(7)	0.0603(8)	-0.0160(6)	0.0130(8)	0.0117(7)
N1	0.0386(4)	0.0359(4)	0.0379(4)	-0.0041(3)	-0.0035(4)	0.0046(4)
B1	0.0358(5)	0.0397(6)	0.0439(6)	0.0041(5)	0.0045(5)	0.0003(5)
F1	0.0471(4)	0.0831(6)	0.0698(5)	-0.0010(4)	0.0224(4)	0.0021(4)
F2	0.0630(5)	0.0440(4)	0.0553(4)	0.0135(3)	-0.0056(3)	0.0042(3)

Distances

C1	C2	1.3611(16)Å	C1	C9	1.4004(15)Å
C1	N1	1.4722(14)Å	C2	C3	1.416(2)Å
C2	H21	0.985Å	C3	C4	1.365(2)Å
C3	H31	0.972Å	C4	C10	1.411(2)Å
C4	H41	0.965Å	C5	C6	1.359(2)Å
C5	C10	1.413(2)Å	C5	H51	0.967Å
C6	C7	1.411(2)Å	C6	H61	0.938Å
C7	C8	1.3711(17)Å	C7	H71	0.962Å
C8	C9	1.4074(15)Å	C8	B1	1.5905(17)Å
C9	C10	1.4125(16)Å	C11	N1	1.4990(15)Å
C11	H111	1.002Å	C11	H112	0.975Å
C11	H113	0.977Å	C12	N1	1.4887(15)Å
C12	H121	0.983Å	C12	H122	0.971Å
C12	H123	0.975Å	N1	B1	1.7259(16)Å
B1	F1	1.3736(14)Å	B1	F2	1.3846(14)Å

Angles

C2	C1	C9	121.64(11)°	C2	C1	N1	126.81(11)°
C9	C1	N1	111.55(9)°	C1	C2	C3	117.71(13)°
C1	C2	H21	122.293°	C3	C2	H21	119.980°
C2	C3	C4	122.05(13)°	C2	C3	H31	117.476°
C4	C3	H31	120.458°	C3	C4	C10	120.69(13)°
C3	C4	H41	119.004°	C10	C4	H41	120.286°
C6	C5	C10	120.42(13)°	C6	C5	H51	120.347°
C10	C5	H51	119.231°	C5	C6	C7	122.01(13)°
C5	C6	H61	117.772°	C7	C6	H61	120.211°
C6	C7	C8	120.40(14)°	C6	C7	H71	119.826°
C8	C7	H71	119.767°	C7	C8	C9	116.96(12)°
C7	C8	B1	134.05(12)°	C9	C8	B1	108.99(9)°
C1	C9	C8	115.14(10)°	C1	C9	C10	120.72(11)°
C8	C9	C10	124.13(11)°	C4	C10	C5	126.72(13)°
C4	C10	C9	117.19(12)°	C5	C10	C9	116.08(12)°
N1	C11	H111	106.921°	N1	C11	H112	109.758°
H111	C11	H112	111.755°	N1	C11	H113	108.128°
H111	C11	H113	108.527°	H112	C11	H113	111.577°
N1	C12	H121	108.482°	N1	C12	H122	109.243°
H121	C12	H122	109.941°	N1	C12	H123	108.254°
H121	C12	H123	108.497°	H122	C12	H123	112.335°
C1	N1	C11	109.59(9)°	C1	N1	C12	110.44(9)°
C11	N1	C12	109.04(11)°	C1	N1	B1	104.36(8)°
C11	N1	B1	111.52(9)°	C12	N1	B1	111.82(10)°
C8	B1	N1	99.95(8)°	C8	B1	F1	116.44(10)°
N1	B1	F1	106.95(9)°	C8	B1	F2	116.34(10)°
N1	B1	F2	106.79(9)°	F1	B1	F2	109.10(10)°

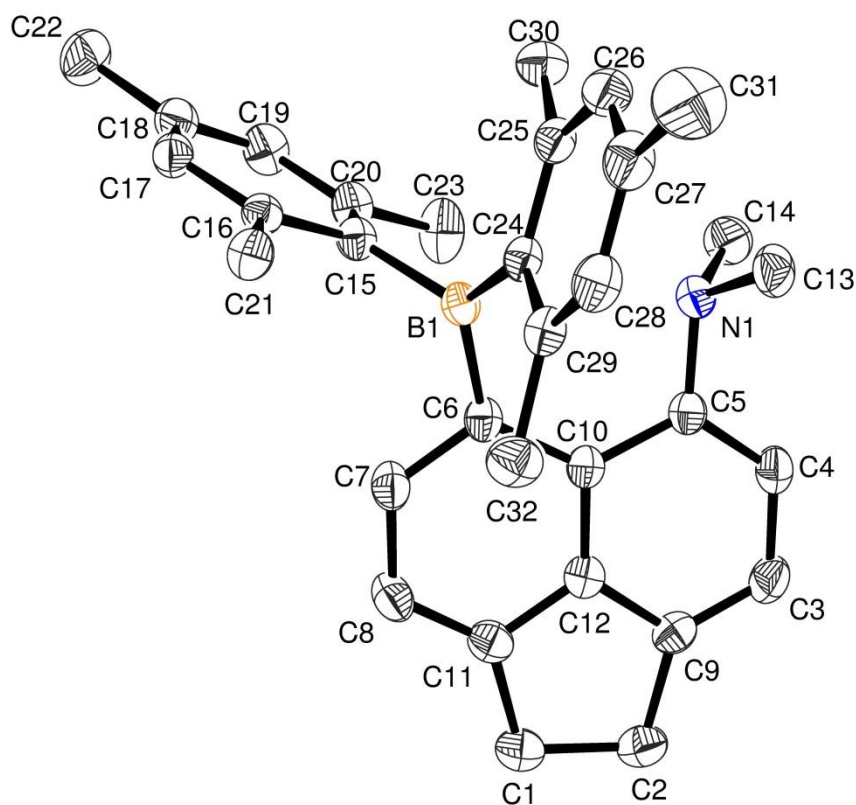
6-(Dimesitylboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (8).

Table 1. Crystal data and structure refinement for dp1162_a.

Identification code	DP-II-162
Empirical formula	C ₃₂ H ₃₆ B N
Formula weight	445.43
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, P -1
Unit cell dimensions	a = 9.2908(6) Å alpha = 97.351(2) deg. b = 9.5397(6) Å beta = 101.400(2) deg. c = 15.6546(10) Å gamma = 105.609(2) deg.
Volume	1285.62(14) Å ³
Z, Calculated density	2, 1.151 Mg/m ³
Absorption coefficient	0.065 mm ⁻¹

F(000)	480
Crystal size	0.24 x 0.10 x 0.08 mm
Theta range for data collection	1.35 to 28.35 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -20<=l<=20
Reflections collected / unique	34934 / 6369 [R(int) = 0.0270]
Completeness to theta = 28.35	99.4 %
Max. and min. transmission	0.9948 and 0.9846
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6369 / 0 / 315
Goodness-of-fit on F ²	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1249
R indices (all data)	R1 = 0.0637, wR2 = 0.1380
Largest diff. peak and hole	0.286 and -0.209 e.A ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1162_a.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	10998(2)	10310(2)	3352(1)	44(1)
C(2)	11792(2)	10045(2)	2593(1)	38(1)
C(3)	11524(2)	7484(2)	1618(1)	36(1)
C(4)	10727(2)	5952(2)	1435(1)	34(1)
C(5)	9588(2)	5323(2)	1842(1)	26(1)
C(6)	8071(2)	5777(2)	3000(1)	26(1)
C(7)	7999(2)	6852(2)	3669(1)	31(1)
C(8)	8851(2)	8373(2)	3833(1)	35(1)
C(9)	11166(2)	8390(2)	2238(1)	30(1)
C(10)	9176(1)	6240(1)	2488(1)	24(1)
C(11)	9860(2)	8824(2)	3324(1)	31(1)
C(12)	10024(2)	7757(2)	2667(1)	26(1)
C(13)	7925(2)	3215(2)	737(1)	37(1)
C(14)	9974(2)	2926(2)	1830(1)	39(1)
C(15)	6502(2)	3615(2)	3704(1)	26(1)
C(16)	5090(2)	3454(1)	3949(1)	25(1)
C(17)	4857(2)	2863(2)	4700(1)	29(1)
C(18)	5968(2)	2403(2)	5223(1)	33(1)
C(19)	7371(2)	2606(2)	4995(1)	35(1)
C(20)	7661(2)	3213(2)	4260(1)	31(1)
C(21)	3822(2)	3956(2)	3444(1)	31(1)
C(22)	5660(2)	1713(2)	6009(1)	47(1)
C(23)	9210(2)	3382(2)	4054(1)	45(1)
C(24)	5553(2)	3516(2)	1927(1)	25(1)
C(25)	5082(2)	1957(2)	1637(1)	28(1)
C(26)	3932(2)	1288(2)	861(1)	34(1)
C(27)	3199(2)	2103(2)	356(1)	37(1)
C(28)	3671(2)	3626(2)	633(1)	34(1)
C(29)	4834(2)	4350(2)	1398(1)	28(1)
C(30)	5836(2)	967(2)	2120(1)	36(1)
C(31)	1928(2)	1353(2)	-472(1)	58(1)
C(32)	5224(2)	6018(2)	1629(1)	38(1)
B(1)	6774(2)	4259(2)	2844(1)	25(1)
N(1)	8852(1)	3737(1)	1654(1)	27(1)

Table 3. Bond lengths [Å] and angles [deg] for dp1162_a.

C(1)-C(11)	1.513(2)
C(1)-C(2)	1.546(2)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(9)	1.514(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(9)	1.367(2)
C(3)-C(4)	1.411(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3811(19)
C(4)-H(4)	0.9500
C(5)-C(10)	1.4287(18)
C(5)-N(1)	1.4465(17)
C(6)-C(7)	1.3940(19)
C(6)-C(10)	1.4370(18)
C(6)-B(1)	1.569(2)
C(7)-C(8)	1.415(2)
C(7)-H(7)	0.9500
C(8)-C(11)	1.365(2)
C(8)-H(8)	0.9500
C(9)-C(12)	1.4078(19)
C(10)-C(12)	1.4100(19)
C(11)-C(12)	1.4122(19)
C(13)-N(1)	1.4653(18)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(1)	1.4624(18)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.4132(18)
C(15)-C(20)	1.4145(19)
C(15)-B(1)	1.586(2)
C(16)-C(17)	1.3960(19)
C(16)-C(21)	1.5080(19)
C(17)-C(18)	1.390(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.389(2)
C(18)-C(22)	1.509(2)
C(19)-C(20)	1.392(2)
C(19)-H(19)	0.9500
C(20)-C(23)	1.508(2)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(29)	1.4145(19)
C(24)-C(25)	1.4173(19)
C(24)-B(1)	1.5856(19)
C(25)-C(26)	1.3956(19)
C(25)-C(30)	1.510(2)
C(26)-C(27)	1.387(2)
C(26)-H(26)	0.9500
C(27)-C(28)	1.382(2)
C(27)-C(31)	1.513(2)
C(28)-C(29)	1.398(2)
C(28)-H(28)	0.9500
C(29)-C(32)	1.512(2)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(11)-C(1)-C(2)	105.34(12)
C(11)-C(1)-H(1A)	110.7
C(2)-C(1)-H(1A)	110.7
C(11)-C(1)-H(1B)	110.7
C(2)-C(1)-H(1B)	110.7
H(1A)-C(1)-H(1B)	108.8
C(9)-C(2)-C(1)	104.60(12)
C(9)-C(2)-H(2A)	110.8
C(1)-C(2)-H(2A)	110.8
C(9)-C(2)-H(2B)	110.8
C(1)-C(2)-H(2B)	110.8
H(2A)-C(2)-H(2B)	108.9
C(9)-C(3)-C(4)	118.37(13)
C(9)-C(3)-H(3)	120.8
C(4)-C(3)-H(3)	120.8
C(5)-C(4)-C(3)	123.41(13)
C(5)-C(4)-H(4)	118.3
C(3)-C(4)-H(4)	118.3
C(4)-C(5)-C(10)	119.67(13)
C(4)-C(5)-N(1)	120.97(12)
C(10)-C(5)-N(1)	119.30(11)
C(7)-C(6)-C(10)	116.91(12)

C(7)-C(6)-B(1)	113.78(12)
C(10)-C(6)-B(1)	128.88(11)
C(6)-C(7)-C(8)	124.74(13)
C(6)-C(7)-H(7)	117.6
C(8)-C(7)-H(7)	117.6
C(11)-C(8)-C(7)	118.22(13)
C(11)-C(8)-H(8)	120.9
C(7)-C(8)-H(8)	120.9
C(3)-C(9)-C(12)	118.68(13)
C(3)-C(9)-C(2)	131.97(13)
C(12)-C(9)-C(2)	109.34(13)
C(12)-C(10)-C(5)	115.18(12)
C(12)-C(10)-C(6)	117.35(12)
C(5)-C(10)-C(6)	127.37(12)
C(8)-C(11)-C(12)	118.89(13)
C(8)-C(11)-C(1)	132.15(14)
C(12)-C(11)-C(1)	108.82(13)
C(9)-C(12)-C(10)	124.65(12)
C(9)-C(12)-C(11)	111.59(13)
C(10)-C(12)-C(11)	123.74(12)
N(1)-C(13)-H(13A)	109.5
N(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-H(14A)	109.5
N(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-C(20)	117.77(12)
C(16)-C(15)-B(1)	120.55(12)
C(20)-C(15)-B(1)	121.67(12)
C(17)-C(16)-C(15)	119.94(12)
C(17)-C(16)-C(21)	117.88(12)
C(15)-C(16)-C(21)	122.13(12)
C(18)-C(17)-C(16)	122.31(13)
C(18)-C(17)-H(17)	118.8
C(16)-C(17)-H(17)	118.8
C(19)-C(18)-C(17)	117.47(13)
C(19)-C(18)-C(22)	121.42(14)
C(17)-C(18)-C(22)	121.11(14)
C(18)-C(19)-C(20)	122.07(13)
C(18)-C(19)-H(19)	119.0
C(20)-C(19)-H(19)	119.0
C(19)-C(20)-C(15)	120.33(13)
C(19)-C(20)-C(23)	118.67(13)
C(15)-C(20)-C(23)	120.96(13)

C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-H(22A)	109.5
C(18)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(18)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(29)-C(24)-C(25)	117.70(12)
C(29)-C(24)-B(1)	122.19(12)
C(25)-C(24)-B(1)	120.01(12)
C(26)-C(25)-C(24)	120.23(13)
C(26)-C(25)-C(30)	117.48(13)
C(24)-C(25)-C(30)	122.23(12)
C(27)-C(26)-C(25)	121.96(14)
C(27)-C(26)-H(26)	119.0
C(25)-C(26)-H(26)	119.0
C(28)-C(27)-C(26)	117.80(13)
C(28)-C(27)-C(31)	121.03(15)
C(26)-C(27)-C(31)	121.17(15)
C(27)-C(28)-C(29)	122.39(14)
C(27)-C(28)-H(28)	118.8
C(29)-C(28)-H(28)	118.8
C(28)-C(29)-C(24)	119.88(13)
C(28)-C(29)-C(32)	116.86(13)
C(24)-C(29)-C(32)	123.23(12)
C(25)-C(30)-H(30A)	109.5
C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-H(31A)	109.5
C(27)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(27)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(6)-B(1)-C(24)	123.87(12)
C(6)-B(1)-C(15)	116.41(11)
C(24)-B(1)-C(15)	118.67(11)
C(5)-N(1)-C(14)	111.68(11)
C(5)-N(1)-C(13)	111.67(11)
C(14)-N(1)-C(13)	109.88(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1162_a.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	53(1)	27(1)	47(1)	3(1)	19(1)	5(1)
C(2)	38(1)	30(1)	44(1)	11(1)	11(1)	7(1)
C(3)	35(1)	39(1)	35(1)	9(1)	17(1)	6(1)
C(4)	38(1)	37(1)	30(1)	4(1)	16(1)	10(1)
C(5)	26(1)	30(1)	23(1)	5(1)	6(1)	9(1)
C(6)	23(1)	31(1)	22(1)	4(1)	5(1)	8(1)
C(7)	28(1)	37(1)	28(1)	0(1)	10(1)	6(1)
C(8)	35(1)	34(1)	33(1)	-4(1)	10(1)	10(1)
C(9)	28(1)	31(1)	29(1)	10(1)	6(1)	7(1)
C(10)	22(1)	29(1)	20(1)	4(1)	3(1)	8(1)
C(11)	30(1)	28(1)	31(1)	3(1)	4(1)	9(1)
C(12)	23(1)	30(1)	25(1)	6(1)	4(1)	9(1)
C(13)	39(1)	42(1)	24(1)	0(1)	7(1)	5(1)
C(14)	37(1)	38(1)	47(1)	10(1)	15(1)	18(1)
C(15)	24(1)	29(1)	22(1)	3(1)	3(1)	7(1)
C(16)	24(1)	24(1)	23(1)	1(1)	4(1)	5(1)
C(17)	28(1)	31(1)	26(1)	3(1)	8(1)	6(1)
C(18)	43(1)	34(1)	23(1)	6(1)	7(1)	12(1)
C(19)	38(1)	44(1)	26(1)	9(1)	3(1)	20(1)
C(20)	29(1)	40(1)	25(1)	4(1)	4(1)	14(1)
C(21)	24(1)	38(1)	31(1)	8(1)	6(1)	11(1)
C(22)	61(1)	53(1)	35(1)	21(1)	15(1)	22(1)
C(23)	34(1)	73(1)	35(1)	14(1)	8(1)	29(1)
C(24)	22(1)	30(1)	22(1)	6(1)	7(1)	6(1)
C(25)	26(1)	31(1)	26(1)	6(1)	8(1)	6(1)
C(26)	33(1)	32(1)	31(1)	2(1)	5(1)	1(1)
C(27)	31(1)	47(1)	27(1)	4(1)	2(1)	4(1)
C(28)	32(1)	45(1)	26(1)	11(1)	4(1)	13(1)
C(29)	27(1)	34(1)	24(1)	7(1)	8(1)	9(1)
C(30)	38(1)	31(1)	39(1)	8(1)	7(1)	10(1)
C(31)	50(1)	62(1)	39(1)	0(1)	-13(1)	2(1)
C(32)	43(1)	36(1)	35(1)	10(1)	4(1)	15(1)
B(1)	22(1)	28(1)	25(1)	4(1)	7(1)	11(1)
N(1)	27(1)	28(1)	24(1)	3(1)	6(1)	8(1)

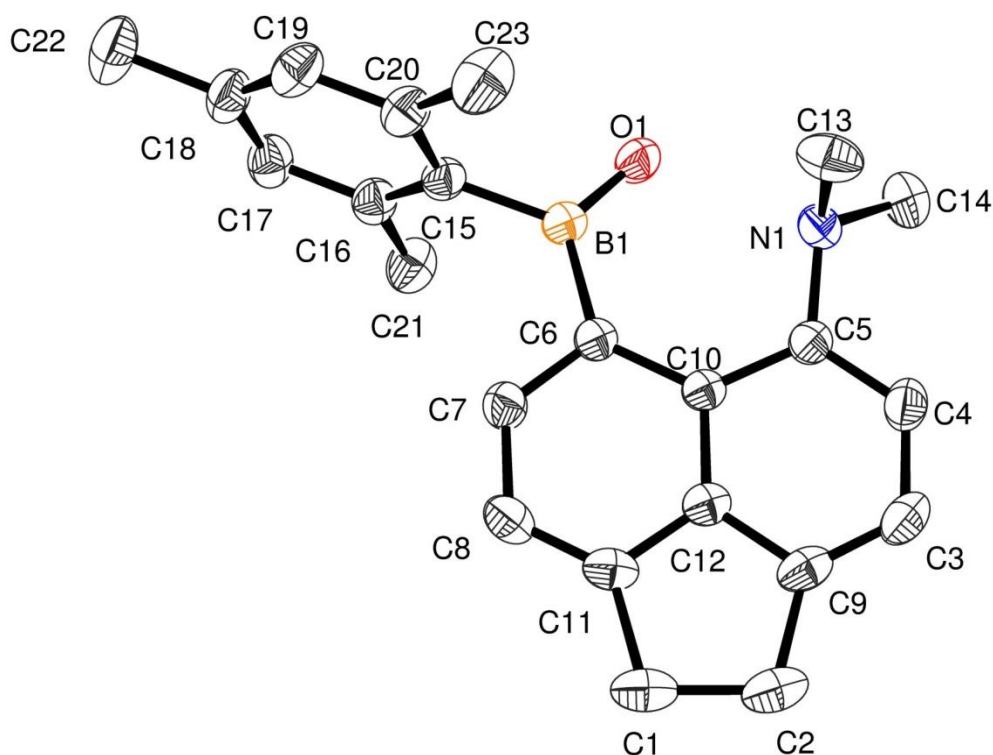
***N,N*-dimethyl-6-(hydroxymesitylboryl)-1,2-dihydroacenaphthylen-5-amine (10)**

Table 1. Crystal data and structure refinement for exp_3058.

Identification code	DP-II-162-BMesOH
Empirical formula	C ₂₃ H ₂₆ B N O, C ₁₈ H ₂₃ B O
Formula weight	609.43
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P 2 ₁ /n
Unit cell dimensions	a = 10.4501(8) Å alpha = 90 deg. b = 29.6982(17) Å beta = 97.774(6) deg. c = 11.6740(6) Å gamma = 90 deg.
Volume	3589.7(4) Å ³
Z, Calculated density	4, 1.128 Mg/m ³
Absorption coefficient	0.067 mm ⁻¹

F(000)	1312
Crystal size	0.2 x 0.18 x 0.12 mm
Theta range for data collection	3.13 to 27.48 deg.
Limiting indices	-13<=h<=13, -37<=k<=38, -15<=l<=15
Reflections collected / unique	60154 / 8202 [R(int) = 0.0422]
Completeness to theta = 27.48	99.6 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8202 / 2 / 432
Goodness-of-fit on F ²	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.1225
R indices (all data)	R1 = 0.0764, wR2 = 0.1335
Largest diff. peak and hole	0.306 and -0.200 e.A ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (A² x 10³) for exp_3058.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(22)	10186(2)	2430(1)	-591(2)	58(1)
C(1)	10036(2)	494(1)	6570(2)	43(1)
C(2)	9161(2)	89(1)	6762(2)	44(1)
C(3)	7253(2)	-241(1)	5318(2)	41(1)
C(4)	6548(2)	-193(1)	4211(2)	39(1)
C(5)	6794(2)	145(1)	3455(1)	30(1)
C(6)	8215(2)	842(1)	3105(1)	28(1)
C(7)	9276(2)	1085(1)	3620(2)	34(1)
C(8)	9948(2)	1004(1)	4734(2)	38(1)
C(9)	8219(2)	55(1)	5659(2)	35(1)
C(10)	7796(2)	468(1)	3769(1)	26(1)
C(11)	9538(2)	665(1)	5370(1)	33(1)

C(12)	8484(2)	399(1)	4889(1)	29(1)
C(13)	6719(2)	-126(1)	1507(2)	51(1)
C(14)	4703(2)	30(1)	2233(2)	47(1)
C(15)	8285(2)	1417(1)	1256(1)	31(1)
C(16)	8104(2)	1877(1)	1460(2)	35(1)
C(17)	8734(2)	2198(1)	865(2)	40(1)
C(18)	9531(2)	2077(1)	60(2)	41(1)
C(19)	9688(2)	1622(1)	-149(2)	42(1)
C(20)	9085(2)	1292(1)	437(2)	37(1)
C(21)	7223(2)	2030(1)	2306(2)	45(1)
C(23)	9291(2)	800(1)	185(2)	55(1)
C(24)	4816(2)	1357(1)	-2755(1)	28(1)
C(25)	3630(2)	1483(1)	-3388(1)	30(1)
C(26)	3473(2)	1476(1)	-4595(2)	36(1)
C(27)	4459(2)	1345(1)	-5207(2)	39(1)
C(28)	5619(2)	1220(1)	-4586(2)	38(1)
C(29)	5823(2)	1224(1)	-3382(2)	31(1)
C(30)	2480(2)	1615(1)	-2801(2)	40(1)
C(31)	4257(3)	1342(1)	-6516(2)	55(1)
C(32)	7138(2)	1093(1)	-2781(2)	39(1)
C(33)	4728(2)	1791(1)	-649(1)	27(1)
C(34)	5252(2)	2218(1)	-820(1)	30(1)
C(35)	4894(2)	2587(1)	-205(2)	35(1)
C(36)	4012(2)	2551(1)	580(2)	37(1)
C(37)	3507(2)	2129(1)	754(2)	35(1)
C(38)	3851(2)	1750(1)	166(1)	30(1)
C(39)	6215(2)	2285(1)	-1660(2)	39(1)
C(40)	3608(2)	2961(1)	1204(2)	53(1)
C(41)	3243(2)	1303(1)	397(2)	38(1)
B(1)	7571(2)	1045(1)	1905(2)	30(1)
B(2)	5064(2)	1369(1)	-1382(2)	27(1)
N(1)	6074(1)	154(1)	2302(1)	33(1)
O(1)	6390(1)	917(1)	1406(1)	39(1)
O(2)	5590(1)	994(1)	-868(1)	36(1)

Table 3. Bond lengths [Å] and angles [deg] for exp_3058.

C(22)-C(18)	1.512(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(1)-C(11)	1.514(2)
C(1)-C(2)	1.546(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(9)	1.514(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(9)	1.358(3)
C(3)-C(4)	1.405(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(2)
C(4)-H(4)	0.9500
C(5)-C(10)	1.431(2)
C(5)-N(1)	1.451(2)
C(6)-C(7)	1.390(2)
C(6)-C(10)	1.455(2)
C(6)-B(1)	1.589(2)
C(7)-C(8)	1.412(2)
C(7)-H(7)	0.9500
C(8)-C(11)	1.356(3)
C(8)-H(8)	0.9500
C(9)-C(12)	1.412(2)
C(10)-C(12)	1.418(2)
C(11)-C(12)	1.408(2)
C(13)-N(1)	1.476(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(1)	1.471(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(20)	1.403(2)
C(15)-C(16)	1.404(2)
C(15)-B(1)	1.583(3)
C(16)-C(17)	1.394(2)
C(16)-C(21)	1.508(3)
C(17)-C(18)	1.385(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(3)
C(19)-C(20)	1.394(3)
C(19)-H(19)	0.9500
C(20)-C(23)	1.512(3)

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.405(2)
C(24)-C(29)	1.416(2)
C(24)-B(2)	1.589(2)
C(25)-C(26)	1.396(2)
C(25)-C(30)	1.513(2)
C(26)-C(27)	1.386(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.377(3)
C(27)-C(31)	1.514(3)
C(28)-C(29)	1.393(2)
C(28)-H(28)	0.9500
C(29)-C(32)	1.508(3)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.406(2)
C(33)-C(38)	1.413(2)
C(33)-B(2)	1.582(2)
C(34)-C(35)	1.390(2)
C(34)-C(39)	1.511(2)
C(35)-C(36)	1.389(2)
C(35)-H(35)	0.9500
C(36)-C(37)	1.386(3)
C(36)-C(40)	1.508(3)
C(37)-C(38)	1.390(2)
C(37)-H(37)	0.9500
C(38)-C(41)	1.512(2)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
B(1)-O(1)	1.346(2)
B(2)-O(2)	1.348(2)

O(1)-H(1)	0.855(10)
O(2)-H(2)	0.851(9)
C(18)-C(22)-H(22A)	109.5
C(18)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(18)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(11)-C(1)-C(2)	104.94(15)
C(11)-C(1)-H(1A)	110.8
C(2)-C(1)-H(1A)	110.8
C(11)-C(1)-H(1B)	110.8
C(2)-C(1)-H(1B)	110.8
H(1A)-C(1)-H(1B)	108.8
C(9)-C(2)-C(1)	104.92(15)
C(9)-C(2)-H(2A)	110.8
C(1)-C(2)-H(2A)	110.8
C(9)-C(2)-H(2B)	110.8
C(1)-C(2)-H(2B)	110.8
H(2A)-C(2)-H(2B)	108.8
C(9)-C(3)-C(4)	118.74(17)
C(9)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(5)-C(4)-C(3)	122.71(17)
C(5)-C(4)-H(4)	118.6
C(3)-C(4)-H(4)	118.6
C(4)-C(5)-C(10)	121.00(16)
C(4)-C(5)-N(1)	119.19(15)
C(10)-C(5)-N(1)	119.70(14)
C(7)-C(6)-C(10)	116.50(15)
C(7)-C(6)-B(1)	113.68(15)
C(10)-C(6)-B(1)	129.61(15)
C(6)-C(7)-C(8)	125.33(17)
C(6)-C(7)-H(7)	117.3
C(8)-C(7)-H(7)	117.3
C(11)-C(8)-C(7)	118.37(17)
C(11)-C(8)-H(8)	120.8
C(7)-C(8)-H(8)	120.8
C(3)-C(9)-C(12)	118.93(17)
C(3)-C(9)-C(2)	131.62(17)
C(12)-C(9)-C(2)	109.43(17)
C(12)-C(10)-C(5)	113.69(14)
C(12)-C(10)-C(6)	116.71(15)
C(5)-C(10)-C(6)	129.59(15)
C(8)-C(11)-C(12)	119.11(16)
C(8)-C(11)-C(1)	131.31(17)
C(12)-C(11)-C(1)	109.56(16)
C(11)-C(12)-C(9)	111.15(15)
C(11)-C(12)-C(10)	123.94(16)

C(9)-C(12)-C(10)	124.90(16)
N(1)-C(13)-H(13A)	109.5
N(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-H(14A)	109.5
N(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	118.71(16)
C(20)-C(15)-B(1)	120.21(15)
C(16)-C(15)-B(1)	121.05(15)
C(17)-C(16)-C(15)	119.73(17)
C(17)-C(16)-C(21)	119.51(17)
C(15)-C(16)-C(21)	120.75(16)
C(18)-C(17)-C(16)	121.98(18)
C(18)-C(17)-H(17)	119.0
C(16)-C(17)-H(17)	119.0
C(17)-C(18)-C(19)	117.86(17)
C(17)-C(18)-C(22)	121.12(19)
C(19)-C(18)-C(22)	121.01(19)
C(18)-C(19)-C(20)	121.83(18)
C(18)-C(19)-H(19)	119.1
C(20)-C(19)-H(19)	119.1
C(19)-C(20)-C(15)	119.88(17)
C(19)-C(20)-C(23)	119.90(17)
C(15)-C(20)-C(23)	120.22(16)
C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(29)	117.78(15)
C(25)-C(24)-B(2)	122.48(14)
C(29)-C(24)-B(2)	119.73(15)
C(26)-C(25)-C(24)	120.12(16)
C(26)-C(25)-C(30)	117.97(16)
C(24)-C(25)-C(30)	121.89(15)
C(27)-C(26)-C(25)	122.02(17)

C(27)-C(26)-H(26)	119.0
C(25)-C(26)-H(26)	119.0
C(28)-C(27)-C(26)	117.84(16)
C(28)-C(27)-C(31)	121.49(18)
C(26)-C(27)-C(31)	120.67(19)
C(27)-C(28)-C(29)	122.15(17)
C(27)-C(28)-H(28)	118.9
C(29)-C(28)-H(28)	118.9
C(28)-C(29)-C(24)	120.09(17)
C(28)-C(29)-C(32)	118.16(16)
C(24)-C(29)-C(32)	121.74(15)
C(25)-C(30)-H(30A)	109.5
C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-H(31A)	109.5
C(27)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(27)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(38)	118.21(15)
C(34)-C(33)-B(2)	121.14(14)
C(38)-C(33)-B(2)	120.60(15)
C(35)-C(34)-C(33)	120.09(15)
C(35)-C(34)-C(39)	118.69(16)
C(33)-C(34)-C(39)	121.22(15)
C(36)-C(35)-C(34)	121.94(17)
C(36)-C(35)-H(35)	119.0
C(34)-C(35)-H(35)	119.0
C(37)-C(36)-C(35)	117.81(16)
C(37)-C(36)-C(40)	121.48(17)
C(35)-C(36)-C(40)	120.70(18)
C(36)-C(37)-C(38)	122.04(16)
C(36)-C(37)-H(37)	119.0
C(38)-C(37)-H(37)	119.0
C(37)-C(38)-C(33)	119.90(16)
C(37)-C(38)-C(41)	118.71(15)
C(33)-C(38)-C(41)	121.38(15)
C(34)-C(39)-H(39A)	109.5
C(34)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5

C(34)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(36)-C(40)-H(40A)	109.5
C(36)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(36)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(38)-C(41)-H(41A)	109.5
C(38)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(38)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
O(1)-B(1)-C(15)	117.00(15)
O(1)-B(1)-C(6)	121.88(16)
C(15)-B(1)-C(6)	121.10(15)
O(2)-B(2)-C(33)	121.32(15)
O(2)-B(2)-C(24)	115.62(15)
C(33)-B(2)-C(24)	123.06(14)
C(5)-N(1)-C(14)	115.15(15)
C(5)-N(1)-C(13)	110.44(14)
C(14)-N(1)-C(13)	110.42(15)
B(1)-O(1)-H(1)	107.9(19)
B(2)-O(2)-H(2)	116.5(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for exp_3058.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(22)	52(1)	55(1)	70(2)	24(1)	15(1)	-6(1)
C(1)	48(1)	49(1)	29(1)	-4(1)	-2(1)	18(1)
C(2)	59(1)	45(1)	28(1)	3(1)	7(1)	21(1)
C(3)	59(1)	33(1)	36(1)	8(1)	18(1)	3(1)
C(4)	49(1)	30(1)	40(1)	-1(1)	14(1)	-6(1)
C(5)	36(1)	25(1)	28(1)	-2(1)	8(1)	2(1)
C(6)	31(1)	24(1)	28(1)	-1(1)	5(1)	3(1)
C(7)	37(1)	28(1)	36(1)	2(1)	2(1)	-1(1)
C(8)	36(1)	35(1)	41(1)	-5(1)	-5(1)	-1(1)
C(9)	50(1)	31(1)	26(1)	2(1)	12(1)	14(1)
C(10)	32(1)	23(1)	25(1)	-2(1)	6(1)	5(1)

C(11)	37(1)	32(1)	28(1)	-5(1)	-1(1)	12(1)
C(12)	35(1)	25(1)	26(1)	-3(1)	7(1)	8(1)
C(13)	55(1)	61(1)	37(1)	-15(1)	4(1)	3(1)
C(14)	42(1)	46(1)	53(1)	-2(1)	4(1)	-11(1)
C(15)	32(1)	32(1)	30(1)	5(1)	1(1)	1(1)
C(16)	34(1)	33(1)	37(1)	4(1)	2(1)	1(1)
C(17)	39(1)	30(1)	48(1)	8(1)	2(1)	0(1)
C(18)	34(1)	43(1)	45(1)	17(1)	2(1)	-3(1)
C(19)	38(1)	49(1)	42(1)	11(1)	13(1)	4(1)
C(20)	38(1)	36(1)	38(1)	6(1)	7(1)	4(1)
C(21)	52(1)	36(1)	51(1)	2(1)	15(1)	5(1)
C(23)	71(2)	42(1)	58(1)	2(1)	29(1)	10(1)
C(24)	35(1)	22(1)	26(1)	-2(1)	7(1)	-2(1)
C(25)	36(1)	28(1)	28(1)	-1(1)	5(1)	-4(1)
C(26)	42(1)	35(1)	29(1)	2(1)	1(1)	-7(1)
C(27)	58(1)	33(1)	27(1)	-2(1)	12(1)	-13(1)
C(28)	52(1)	30(1)	35(1)	-5(1)	21(1)	-6(1)
C(29)	40(1)	22(1)	34(1)	-2(1)	12(1)	-2(1)
C(30)	34(1)	52(1)	33(1)	-1(1)	2(1)	5(1)
C(31)	84(2)	55(1)	28(1)	-2(1)	13(1)	-16(1)
C(32)	38(1)	35(1)	48(1)	2(1)	17(1)	4(1)
C(33)	26(1)	31(1)	22(1)	0(1)	1(1)	2(1)
C(34)	29(1)	33(1)	26(1)	-1(1)	3(1)	2(1)
C(35)	39(1)	31(1)	35(1)	-3(1)	7(1)	-1(1)
C(36)	39(1)	37(1)	34(1)	-6(1)	7(1)	7(1)
C(37)	35(1)	43(1)	29(1)	-1(1)	10(1)	5(1)
C(38)	30(1)	35(1)	24(1)	0(1)	3(1)	2(1)
C(39)	42(1)	37(1)	40(1)	-3(1)	16(1)	-5(1)
C(40)	62(1)	42(1)	57(1)	-12(1)	23(1)	6(1)
C(41)	40(1)	42(1)	33(1)	2(1)	11(1)	-3(1)
B(1)	33(1)	27(1)	28(1)	0(1)	5(1)	4(1)
B(2)	26(1)	30(1)	26(1)	0(1)	4(1)	-1(1)
N(1)	34(1)	32(1)	32(1)	-4(1)	4(1)	-4(1)
O(1)	39(1)	43(1)	33(1)	11(1)	-1(1)	-5(1)
O(2)	47(1)	32(1)	28(1)	-1(1)	2(1)	5(1)

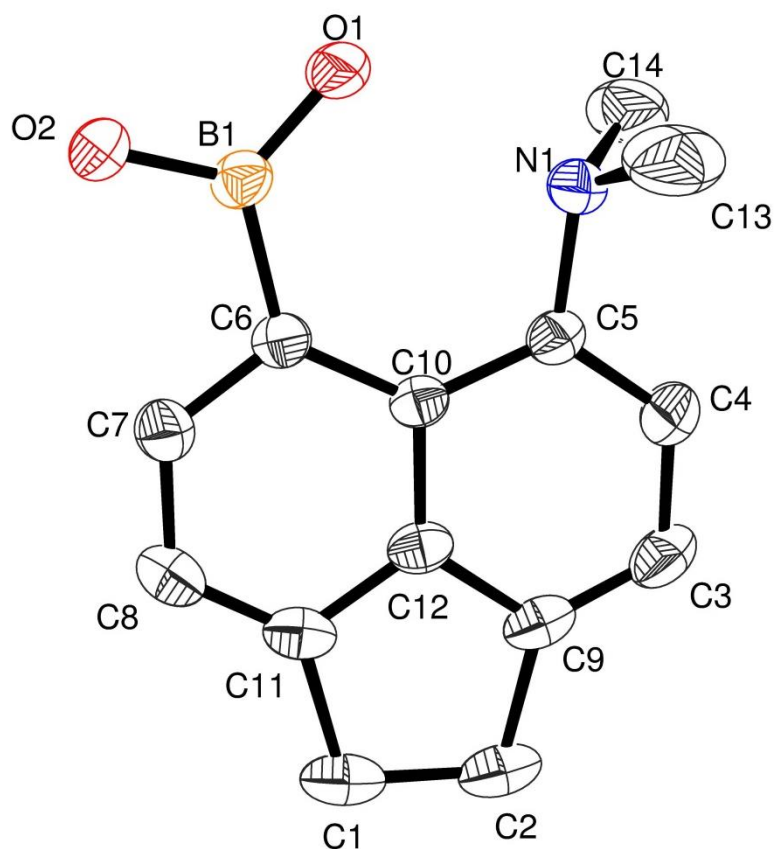
6-(Dihydroxyboryl)-*N,N*-dimethyl-1,2-dihydroacenaphthylen-5-amine (11)

Table 1. Crystal data and structure refinement for dp1162bis.

Identification code	DP-II-162-B(OH) ₂
Empirical formula	C ₁₄ H ₁₆ B N O ₂
Formula weight	241.09
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P 2 ₁ /c
Unit cell dimensions	a = 11.5658(12) Å alpha = 90 deg. b = 10.1745(10) Å beta = 117.252(3) deg. c = 12.0844(12) Å gamma = 90 deg.
Volume	1264.2(2) Å ³
Z, Calculated density	2, 1.267 Mg/m ³

Absorption coefficient	0.083 mm ⁻¹
F(000)	512
Crystal size	0.18 x 0.14 x 0.08 mm
Theta range for data collection	2.76 to 30.69 deg.
Limiting indices	-16 ≤ h ≤ 16, -14 ≤ k ≤ 13, -17 ≤ l ≤ 17
Reflections collected / unique	30829 / 3915 [R(int) = 0.0356]
Completeness to theta = 30.69	99.8 %
Max. and min. transmission	0.7461 and 0.6726
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3915 / 2 / 173
Goodness-of-fit on F ²	1.041
Final R indices [I > 2σ(I)]	R1 = 0.0510, wR2 = 0.1390
R indices (all data)	R1 = 0.0698, wR2 = 0.1540
Largest diff. peak and hole	0.368 and -0.172 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1162bis.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	-2327(1)	3913(2)	-108(2)	48(1)
C(2)	-2147(1)	2743(2)	-823(1)	45(1)
C(3)	16(2)	1576(2)	-423(1)	44(1)
C(4)	1370(2)	1558(2)	349(1)	41(1)
C(5)	1998(1)	2424(1)	1319(1)	32(1)
C(6)	1751(1)	4471(1)	2505(1)	30(1)
C(7)	828(1)	5343(1)	2506(1)	37(1)
C(8)	-521(1)	5278(2)	1702(1)	42(1)
C(9)	-699(1)	2480(1)	-182(1)	37(1)
C(10)	1294(1)	3429(1)	1586(1)	28(1)
C(11)	-968(1)	4283(2)	860(1)	36(1)
C(12)	-70(1)	3387(1)	795(1)	31(1)
C(13)	3746(2)	1041(2)	2769(2)	77(1)
C(14)	4126(2)	2427(2)	1351(2)	62(1)
B(1)	3185(1)	4775(2)	3537(1)	33(1)
N(1)	3402(1)	2280(1)	2072(1)	37(1)
O(1)	4248(1)	4084(1)	3699(1)	48(1)
O(2)	3339(1)	5789(1)	4324(1)	48(1)

Table 3. Bond lengths [Å] and angles [deg] for dp1162bis.

C(1)-C(11)	1.5157(19)
C(1)-C(2)	1.539(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(9)	1.5132(19)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(9)	1.355(2)
C(3)-C(4)	1.408(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3783(18)
C(4)-H(4)	0.9500
C(5)-C(10)	1.4334(18)
C(5)-N(1)	1.4602(16)
C(6)-C(7)	1.3877(18)
C(6)-C(10)	1.4485(17)
C(6)-B(1)	1.5838(18)
C(7)-C(8)	1.4125(19)
C(7)-H(7)	0.9500
C(8)-C(11)	1.359(2)
C(8)-H(8)	0.9500
C(9)-C(12)	1.4097(19)
C(10)-C(12)	1.4222(16)
C(11)-C(12)	1.4108(19)
C(13)-N(1)	1.466(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(1)	1.465(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
B(1)-O(1)	1.3506(19)
B(1)-O(2)	1.3584(18)
O(1)-H(1)	0.859(10)
O(2)-H(2)	0.846(10)
C(11)-C(1)-C(2)	105.45(12)
C(11)-C(1)-H(1A)	110.7
C(2)-C(1)-H(1A)	110.7
C(11)-C(1)-H(1B)	110.7
C(2)-C(1)-H(1B)	110.7
H(1A)-C(1)-H(1B)	108.8
C(9)-C(2)-C(1)	104.58(12)
C(9)-C(2)-H(2A)	110.8
C(1)-C(2)-H(2A)	110.8
C(9)-C(2)-H(2B)	110.8

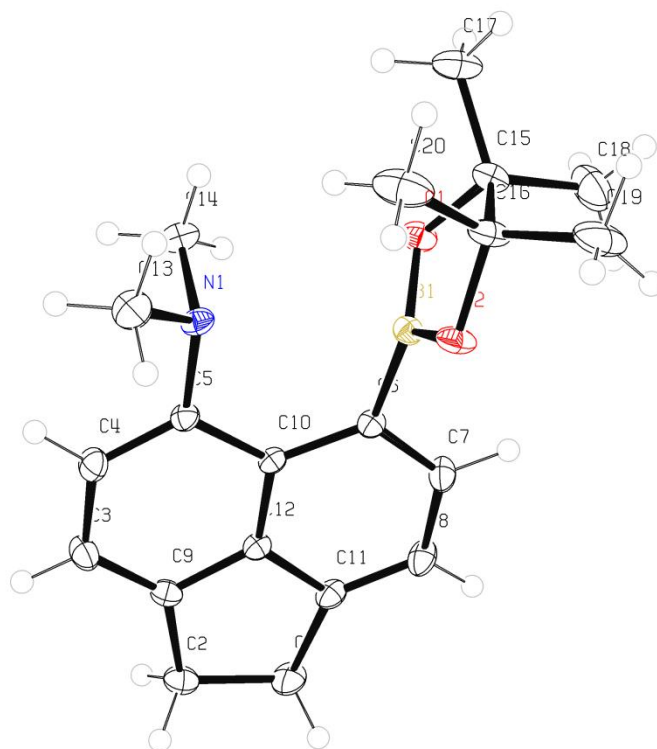
C(1)-C(2)-H(2B)	110.8
H(2A)-C(2)-H(2B)	108.9
C(9)-C(3)-C(4)	117.99(13)
C(9)-C(3)-H(3)	121.0
C(4)-C(3)-H(3)	121.0
C(5)-C(4)-C(3)	123.26(14)
C(5)-C(4)-H(4)	118.4
C(3)-C(4)-H(4)	118.4
C(4)-C(5)-C(10)	120.99(12)
C(4)-C(5)-N(1)	117.94(12)
C(10)-C(5)-N(1)	121.07(11)
C(7)-C(6)-C(10)	117.24(11)
C(7)-C(6)-B(1)	113.74(11)
C(10)-C(6)-B(1)	129.02(11)
C(6)-C(7)-C(8)	125.25(13)
C(6)-C(7)-H(7)	117.4
C(8)-C(7)-H(7)	117.4
C(11)-C(8)-C(7)	118.14(13)
C(11)-C(8)-H(8)	120.9
C(7)-C(8)-H(8)	120.9
C(3)-C(9)-C(12)	119.53(12)
C(3)-C(9)-C(2)	130.66(13)
C(12)-C(9)-C(2)	109.80(13)
C(12)-C(10)-C(5)	113.39(11)
C(12)-C(10)-C(6)	116.12(11)
C(5)-C(10)-C(6)	130.48(11)
C(8)-C(11)-C(12)	119.07(12)
C(8)-C(11)-C(1)	131.90(14)
C(12)-C(11)-C(1)	109.03(13)
C(9)-C(12)-C(11)	111.03(12)
C(9)-C(12)-C(10)	124.80(12)
C(11)-C(12)-C(10)	124.14(12)
N(1)-C(13)-H(13A)	109.5
N(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-H(14A)	109.5
N(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
N(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(1)-B(1)-O(2)	118.37(12)
O(1)-B(1)-C(6)	124.61(12)
O(2)-B(1)-C(6)	117.01(12)
C(5)-N(1)-C(14)	113.23(12)
C(5)-N(1)-C(13)	112.08(12)
C(14)-N(1)-C(13)	110.52(16)

B(1)-O(1)-H(1)	109.1(19)
B(1)-O(2)-H(2)	113.2(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for dp1162bis.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	26(1)	62(1)	50(1)	11(1)	11(1)	-3(1)
C(2)	30(1)	55(1)	39(1)	8(1)	6(1)	-12(1)
C(3)	41(1)	43(1)	36(1)	-8(1)	7(1)	-11(1)
C(4)	40(1)	40(1)	38(1)	-10(1)	13(1)	-2(1)
C(5)	29(1)	35(1)	30(1)	-3(1)	10(1)	-3(1)
C(6)	29(1)	36(1)	26(1)	-2(1)	13(1)	-2(1)
C(7)	36(1)	41(1)	36(1)	-5(1)	19(1)	1(1)
C(8)	34(1)	50(1)	45(1)	3(1)	22(1)	7(1)
C(9)	31(1)	41(1)	30(1)	4(1)	7(1)	-10(1)
C(10)	26(1)	32(1)	26(1)	1(1)	11(1)	-3(1)
C(11)	26(1)	46(1)	36(1)	9(1)	14(1)	0(1)
C(12)	27(1)	36(1)	29(1)	4(1)	11(1)	-5(1)
C(13)	43(1)	67(1)	89(2)	24(1)	2(1)	6(1)
C(14)	40(1)	93(2)	57(1)	-24(1)	27(1)	-5(1)
B(1)	32(1)	40(1)	29(1)	-5(1)	15(1)	-5(1)
N(1)	28(1)	42(1)	36(1)	-8(1)	11(1)	2(1)
O(1)	29(1)	66(1)	43(1)	-27(1)	10(1)	-2(1)
O(2)	36(1)	54(1)	45(1)	-23(1)	10(1)	-1(1)

***N,N*-Dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-dihydroacenaphthylen-5-amine (2)****Crystal Data DPLA130514**a = 10.38334(18) Å $\alpha = 90^\circ$ b = 11.57825(19) Å $\beta = 90^\circ$ c = 14.9187(3) Å $\gamma = 90^\circ$ Volume 1793.54(5) Å³Space group P 2₁ 2₁ 2₁Formula C₂₀ H₂₆ B₁ N₁ O₂

Cell determined from 17066 reflections

Temperature 100K

Shape block

Colour colorless

D_x 1.20 μ 0.075 mm⁻¹

Absorption correction multi-scan

T_{min} 0.94

Crystal Class orthorhombic

Z = 4

M_r 323.24Cell θ range = 4 - 31°

Size 0.15 × 0.20 × 0.20 mm

F000 696.000

T_{max} 0.99**Data Collection**

Diffractometer multi-scan

Scan type ϕ and ω scans

Reflections measured 46361

Independent reflections 3008

R _{int}	0.0294
$\theta_{\max}$	30.7259
h =	-14 $\rightarrow$ 14
k =	-15 $\rightarrow$ 15
l =	-21 $\rightarrow$ 20

Refinement

$\Delta\rho_{\min}$ =	-0.14 e Å ⁻³
$\Delta\rho_{\max}$ =	0.26 e Å ⁻³
Reflections used	2761
Cutoff: I >	3.00 σ (I)
Parameters refined	217
S =	1.13
R-factor	0.031
weighted R-factor	0.034
$\Delta/\sigma_{\max}$	0.0006
Refinement on	F
w =	$w' \times [1 - (\Delta F_{\text{obs}} / 6 \times \Delta F_{\text{est}})^2]^2$
w' =	$[P_0 T_0'(x) + P_1 T_1'(x) + \dots P_{n-1} T_{n-1}'(x)]^{-1}$, where P_i are the coefficients of a Chebychev series in $t_i(x)$, and $x = F_{\text{calc}}/F_{\text{calcmax}}$.
$P_0 - P_{n-1}$ =	6.60 -2.13 4.08

Parameters

Label	x	y	z	U _{iso/equiv}	Occupancy
C1	0.55735(13)	0.71878(11)	0.62411(9)	0.0241	1.0000
C2	0.49590(12)	0.65685(11)	0.70622(8)	0.0208	1.0000
C3	0.59634(12)	0.48582(10)	0.80004(8)	0.0209	1.0000
C4	0.70317(12)	0.41029(10)	0.80660(8)	0.0196	1.0000
C5	0.80586(11)	0.41382(9)	0.74798(7)	0.0145	1.0000
C6	0.90114(11)	0.50753(9)	0.60940(7)	0.0143	1.0000
C7	0.88535(12)	0.59508(10)	0.54682(8)	0.0197	1.0000
C8	0.77874(13)	0.67167(10)	0.54570(8)	0.0215	1.0000
C9	0.59375(11)	0.56608(9)	0.73291(8)	0.0167	1.0000
C10	0.80543(10)	0.49629(9)	0.67705(7)	0.0131	1.0000
C11	0.68382(12)	0.65731(10)	0.60837(7)	0.0173	1.0000
C12	0.69856(11)	0.57029(9)	0.67325(7)	0.0143	1.0000
C13	0.88521(14)	0.22088(10)	0.77977(9)	0.0244	1.0000
C14	1.01233(12)	0.38802(11)	0.81653(8)	0.0231	1.0000
C15	1.23155(11)	0.38248(10)	0.57672(9)	0.0197	1.0000
C16	1.14616(11)	0.28403(11)	0.53774(9)	0.0209	1.0000
C17	1.33881(12)	0.34020(12)	0.63737(10)	0.0288	1.0000
C18	1.28421(15)	0.46420(14)	0.50574(12)	0.0367	1.0000

C19	1.18176(14)	0.24832(16)	0.44297(11)	0.0392	1.0000
C20	1.13765(14)	0.17940(12)	0.59823(13)	0.0354	1.0000
O1	1.14041(8)	0.45006(7)	0.62916(6)	0.0193	1.0000
O2	1.01843(8)	0.33720(7)	0.53626(6)	0.0197	1.0000
B1	1.01987(12)	0.42601(11)	0.59709(8)	0.0154	1.0000
N1	0.91621(9)	0.33998(8)	0.75481(6)	0.0165	1.0000
H11	0.57103(13)	0.80236(11)	0.63731(9)	0.0291	1.0000
H12	0.50182(13)	0.71211(11)	0.57311(9)	0.0307	1.0000
H21	0.47808(12)	0.70952(11)	0.75633(8)	0.0256	1.0000
H22	0.41293(12)	0.61837(11)	0.69191(8)	0.0269	1.0000
H31	0.52905(12)	0.48213(10)	0.84171(8)	0.0262	1.0000
H41	0.70866(12)	0.35601(10)	0.85364(8)	0.0240	1.0000
H71	0.94997(12)	0.60658(10)	0.50158(8)	0.0252	1.0000
H81	0.77427(13)	0.73255(10)	0.50117(8)	0.0271	1.0000
H131	0.96346(14)	0.17682(10)	0.77347(9)	0.0354	1.0000
H132	0.85477(14)	0.21480(10)	0.84255(9)	0.0367	1.0000
H133	0.81845(14)	0.19349(10)	0.73731(9)	0.0366	1.0000
H141	1.08801(12)	0.34099(11)	0.81098(8)	0.0334	1.0000
H142	0.98160(12)	0.38777(11)	0.88014(8)	0.0344	1.0000
H143	1.03160(12)	0.46642(11)	0.79764(8)	0.0334	1.0000
H172	1.38964(12)	0.40459(12)	0.65601(10)	0.0433	1.0000
H171	1.39242(12)	0.28458(12)	0.60505(10)	0.0420	1.0000
H173	1.30135(12)	0.30340(12)	0.69145(10)	0.0423	1.0000
H182	1.32341(15)	0.53075(14)	0.53694(12)	0.0542	1.0000
H181	1.34798(15)	0.42188(14)	0.47028(12)	0.0533	1.0000
H183	1.21420(15)	0.48828(14)	0.46546(12)	0.0553	1.0000
H192	1.12899(14)	0.18286(16)	0.42641(11)	0.0591	1.0000
H191	1.27008(14)	0.22441(16)	0.44175(11)	0.0573	1.0000
H193	1.16745(14)	0.31130(16)	0.39834(11)	0.0587	1.0000
H202	1.06995(14)	0.12905(12)	0.57687(13)	0.0527	1.0000
H201	1.21832(14)	0.13664(12)	0.59792(13)	0.0523	1.0000
H203	1.11772(14)	0.20311(12)	0.65970(13)	0.0510	1.0000

Thermal Parameters

Label	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.0258(6)	0.0227(5)	0.0237(5)	0.0033(5)	-0.0008(5)	0.0112(5)
C2	0.0168(5)	0.0205(5)	0.0253(5)	-0.0012(4)	-0.0007(4)	0.0050(4)
C3	0.0183(5)	0.0200(5)	0.0244(5)	0.0037(4)	0.0057(4)	-0.0007(4)
C4	0.0211(5)	0.0174(5)	0.0204(5)	0.0058(4)	0.0025(4)	0.0006(4)
C5	0.0156(5)	0.0122(4)	0.0157(4)	0.0020(3)	-0.0011(4)	-0.0001(4)
C6	0.0166(5)	0.0121(4)	0.0141(4)	-0.0006(3)	-0.0002(4)	0.0024(4)
C7	0.0247(5)	0.0178(5)	0.0165(5)	0.0025(4)	0.0055(4)	0.0050(4)

C8	0.0305(6)	0.0170(5)	0.0169(5)	0.0041(4)	0.0023(5)	0.0073(5)
C9	0.0139(4)	0.0156(5)	0.0205(5)	-0.0017(4)	-0.0007(4)	0.0015(4)
C10	0.0151(4)	0.0111(4)	0.0129(4)	-0.0001(3)	-0.0017(4)	0.0006(4)
C11	0.0213(5)	0.0146(4)	0.0160(4)	-0.0001(4)	-0.0020(4)	0.0052(4)
C12	0.0159(5)	0.0128(4)	0.0141(4)	-0.0005(3)	-0.0013(4)	0.0012(4)
C13	0.0275(6)	0.0148(5)	0.0309(6)	0.0057(4)	0.0008(5)	0.0036(5)
C14	0.0222(5)	0.0237(5)	0.0234(6)	0.0006(5)	-0.0073(5)	0.0025(5)
C15	0.0135(4)	0.0199(5)	0.0256(5)	-0.0021(4)	0.0000(4)	0.0006(4)
C16	0.0127(4)	0.0221(5)	0.0278(6)	-0.0075(5)	-0.0037(4)	0.0049(4)
C17	0.0171(5)	0.0299(6)	0.0396(7)	-0.0067(6)	-0.0099(5)	0.0031(5)
C18	0.0292(7)	0.0351(7)	0.0458(8)	0.0099(7)	0.0143(7)	0.0002(6)
C19	0.0210(6)	0.0602(10)	0.0365(8)	-0.0274(7)	-0.0056(6)	0.0168(7)
C20	0.0219(6)	0.0185(6)	0.0658(11)	0.0029(6)	-0.0058(7)	0.0008(5)
O1	0.0158(4)	0.0177(4)	0.0243(4)	-0.0045(3)	-0.0012(3)	0.0008(3)
O2	0.0129(3)	0.0209(4)	0.0251(4)	-0.0079(3)	-0.0030(3)	0.0051(3)
B1	0.0151(5)	0.0140(5)	0.0170(5)	0.0001(4)	0.0008(4)	0.0008(4)
N1	0.0173(4)	0.0139(4)	0.0184(4)	0.0028(3)	-0.0029(4)	0.0028(3)

Distances

C1 C2	1.5562(18)Å	C1 C11	1.5120(16)Å
C1 H11	0.998Å	C1 H12	0.958Å
C2 C9	1.5150(16)Å	C2 H21	0.982Å
C2 H22	0.993Å	C3 C4	1.4159(17)Å
C3 C9	1.3666(16)Å	C3 H31	0.936Å
C4 C5	1.3796(16)Å	C4 H41	0.944Å
C5 C10	1.4254(14)Å	C5 N1	1.4332(14)Å
C6 C7	1.3877(15)Å	C6 C10	1.4223(15)Å
C6 B1	1.5635(16)Å	C7 C8	1.4185(16)Å
C7 H71	0.961Å	C8 C11	1.3686(17)Å
C8 H81	0.970Å	C9 C12	1.4067(15)Å
C10 C12	1.4031(14)Å	C11 C12	1.4055(15)Å
C13 N1	1.4641(15)Å	C13 H131	0.964Å
C13 H132	0.991Å	C13 H133	0.991Å
C14 N1	1.4674(15)Å	C14 H141	0.960Å
C14 H142	1.001Å	C14 H143	0.971Å
C15 C16	1.5569(17)Å	C15 C17	1.5162(17)Å
C15 C18	1.5217(19)Å	C15 O1	1.4560(14)Å
C16 C19	1.5187(18)Å	C16 C20	1.513(2)Å
C16 O2	1.4623(13)Å	C17 H172	0.955Å
C17 H171	0.978Å	C17 H173	0.992Å
C18 H182	0.988Å	C18 H181	0.979Å
C18 H183	0.983Å	C19 H192	0.967Å

C19 H191 0.958Å

C20 H202 0.967Å

C20 H203 0.979Å

O2 B1 1.3716(15)Å

C19 H193 0.999Å

C20 H201 0.973Å

O1 B1 1.3687(15)Å

Angles

C2 C1 C11 105.15(9)°

C11 C1 H11 111.317°

C11 C1 H12 111.197°

C1 C2 C9 104.57(10)°

C9 C2 H21 110.912°

C9 C2 H22 109.090°

C4 C3 C9 119.08(11)°

C9 C3 H31 120.201°

C3 C4 H41 120.660°

C4 C5 C10 119.21(10)°

C10 C5 N1 117.06(9)°

C7 C6 B1 117.07(10)°

C6 C7 C8 123.83(11)°

C8 C7 H71 116.741°

C7 C8 H81 119.989°

C2 C9 C3 132.65(11)°

C3 C9 C12 118.17(10)°

C5 C10 C12 116.20(10)°

C1 C11 C8 132.40(10)°

C8 C11 C12 118.63(10)°

C9 C12 C11 112.10(10)°

N1 C13 H131 106.760°

H131 C13 H132 108.873°

H131 C13 H133 110.964°

N1 C14 H141 106.726°

H141 C14 H142 109.944°

H141 C14 H143 109.664°

C16 C15 C17 113.88(10)°

C17 C15 C18 110.62(11)°

C17 C15 O1 109.29(10)°

C15 C16 C19 114.11(12)°

C19 C16 C20 110.58(12)°

C19 C16 O2 108.75(10)°

C15 C17 H172 109.130°

H172 C17 H171 110.059°

H172 C17 H173 108.376°

C2 C1 H11 110.478°

C2 C1 H12 109.957°

H11 C1 H12 108.713°

C1 C2 H21 112.971°

C1 C2 H22 113.150°

H21 C2 H22 106.181°

C4 C3 H31 120.708°

C3 C4 C5 122.92(10)°

C5 C4 H41 116.383°

C4 C5 N1 123.72(10)°

C7 C6 C10 117.49(10)°

C10 C6 B1 125.38(9)°

C6 C7 H71 119.419°

C7 C8 C11 118.55(10)°

C11 C8 H81 121.459°

C2 C9 C12 109.18(10)°

C5 C10 C6 125.87(10)°

C6 C10 C12 117.91(9)°

C1 C11 C12 108.97(10)°

C9 C12 C10 124.42(10)°

C10 C12 C11 123.48(10)°

N1 C13 H132 112.176°

N1 C13 H133 107.013°

H132 C13 H133 110.983°

N1 C14 H142 112.141°

N1 C14 H143 108.205°

H142 C14 H143 110.077°

C16 C15 C18 113.57(12)°

C16 C15 O1 102.95(9)°

C18 C15 O1 105.87(10)°

C15 C16 C20 113.36(11)°

C15 C16 O2 102.35(9)°

C20 C16 O2 107.04(10)°

C15 C17 H171 109.654°

C15 C17 H173 109.639°

H171 C17 H173 109.959°

C15 C18 H182 107.758°
H182 C18 H181 111.488°
H182 C18 H183 111.793°
C16 C19 H192 108.246°
H192 C19 H191 108.117°
H192 C19 H193 108.515°
C16 C20 H202 109.170°
H202 C20 H201 108.507°
H202 C20 H203 108.898°
C15 O1 B1 107.29(9)°
C6 B1 O1 123.86(10)°
O1 B1 O2 113.19(10)°
C5 N1 C14 111.24(9)°

C15 C18 H181 107.936°
C15 C18 H183 109.621°
H181 C18 H183 108.166°
C16 C19 H191 109.229°
C16 C19 H193 112.691°
H191 C19 H193 109.924°
C16 C20 H201 110.748°
C16 C20 H203 110.264°
H201 C20 H203 109.210°
C16 O2 B1 107.20(9)°
C6 B1 O2 121.45(10)°
C5 N1 C13 113.84(10)°
C13 N1 C14 110.30(10)°

[illegible]
$$T_{\max} \quad 1.00$$

Data Collection

Diffractometer	multi-scan
Scan type	φ and ω scans
Reflections measured	64803
Independent reflections	16467
R _{int}	0.0677
$\theta_{\max}$	29.2926
h =	-15 $\rightarrow$ 14
k =	-19 $\rightarrow$ 18
l =	-31 $\rightarrow$ 31

Refinement

$\Delta\rho_{\min}$ =	-0.97 e Å ⁻³
$\Delta\rho_{\max}$ =	2.48 e Å ⁻³
Reflections used	8778
Cutoff: I >	2.50 σ (I)
Parameters refined	865
S =	1.07
R-factor	0.074
weighted R-factor	0.083
$\Delta/\sigma_{\max}$	0.0006
Refinement on	F
w =	$w' \times [1 - (\Delta F_{\text{obs}} / 6 \times \Delta F_{\text{est}})^2]^2$
w' =	$[P_0 T_0'(x) + P_1 T_1'(x) + \dots P_{n-1} T_{n-1}'(x)]^{-1}$, where P_i are the coefficients of a Chebychev series in $t_i(x)$, and $x = F_{\text{calc}}/F_{\text{calcmax}}$.
$P_0 - P_{n-1}$ =	21.5 9.43 16.5 8.42

Parameters

Label	x	y	z	U _{iso/equiv}	Occupancy
C1	0.6033(4)	0.5917(3)	0.86511(16)	0.0238	1.0000
C2	0.6159(4)	0.5410(3)	0.80806(16)	0.0225	1.0000
C3	0.6311(4)	0.3546(3)	0.79806(16)	0.0239	1.0000
C4	0.6493(4)	0.2591(3)	0.82885(16)	0.0235	1.0000
C5	0.6650(4)	0.2425(3)	0.88801(16)	0.0196	1.0000
C6	0.6814(3)	0.3184(3)	0.98345(15)	0.0196	1.0000
C7	0.6766(4)	0.4079(3)	1.00374(15)	0.0226	1.0000
C8	0.6536(4)	0.5020(3)	0.96973(16)	0.0232	1.0000
C9	0.6277(3)	0.4322(3)	0.82804(15)	0.0189	1.0000
C10	0.6634(3)	0.3198(3)	0.92215(16)	0.0183	1.0000
C11	0.6351(4)	0.5045(3)	0.91229(16)	0.0198	1.0000
C12	0.6419(3)	0.4151(3)	0.88898(15)	0.0171	1.0000
C13	0.5811(5)	0.1008(4)	0.9119(2)	0.0405	1.0000

C14	0.8127(5)	0.0653(4)	0.8901(2)	0.0431	1.0000
C15	0.7244(4)	0.0746(3)	1.08299(18)	0.0284	1.0000
C16	0.7318(5)	0.1496(3)	1.12546(18)	0.0333	1.0000
C17	0.5962(5)	0.0609(4)	1.0852(3)	0.0501	1.0000
C18	0.8271(5)	-0.0263(3)	1.0860(2)	0.0386	1.0000
C19	0.6400(7)	0.1553(4)	1.1801(2)	0.0632	1.0000
C20	0.8635(6)	0.1324(4)	1.1397(2)	0.0483	1.0000
C21	0.2741(4)	0.4329(3)	0.88210(16)	0.0235	1.0000
C22	0.2725(4)	0.5303(3)	0.84292(16)	0.0240	1.0000
C23	0.3251(3)	0.5508(3)	0.72917(16)	0.0197	1.0000
C24	0.3615(4)	0.4982(3)	0.67805(16)	0.0206	1.0000
C25	0.3744(3)	0.3976(3)	0.67908(15)	0.0175	1.0000
C26	0.3568(3)	0.2353(3)	0.74136(15)	0.0172	1.0000
C27	0.3348(3)	0.1985(3)	0.79874(16)	0.0200	1.0000
C28	0.3062(4)	0.2549(3)	0.84808(15)	0.0211	1.0000
C29	0.3047(3)	0.4991(3)	0.78096(15)	0.0182	1.0000
C30	0.3501(3)	0.3396(3)	0.73175(14)	0.0149	1.0000
C31	0.2981(3)	0.3533(3)	0.83922(15)	0.0186	1.0000
C32	0.3169(3)	0.3959(3)	0.78172(15)	0.0170	1.0000
C33	0.5675(5)	0.3212(4)	0.6157(2)	0.0413	1.0000
C34	0.3674(5)	0.4073(3)	0.57036(17)	0.0389	1.0000
C35	0.4202(4)	0.0796(3)	0.60933(16)	0.0232	1.0000
C36	0.4046(4)	0.0029(3)	0.66233(16)	0.0220	1.0000
C41	0.0120(4)	0.2380(3)	0.77944(19)	0.0284	1.0000
C42	-0.0176(4)	0.2849(3)	0.83918(18)	0.0248	1.0000
C43	-0.0642(4)	0.4735(3)	0.85867(16)	0.0234	1.0000
C44	-0.0765(4)	0.5709(3)	0.83103(16)	0.0224	1.0000
C45	-0.0578(3)	0.5886(3)	0.77126(15)	0.0188	1.0000
C46	0.0128(4)	0.5106(3)	0.67046(16)	0.0213	1.0000
C47	0.0442(4)	0.4195(3)	0.64527(17)	0.0291	1.0000
C48	0.0446(4)	0.3273(3)	0.67534(18)	0.0303	1.0000
C49	-0.0327(3)	0.3951(3)	0.82430(16)	0.0212	1.0000
C50	-0.0193(3)	0.5090(3)	0.73314(15)	0.0186	1.0000
C51	0.0175(4)	0.3243(3)	0.73476(18)	0.0237	1.0000
C52	-0.0121(3)	0.4136(3)	0.76295(16)	0.0199	1.0000
C53	-0.2276(4)	0.7561(3)	0.75807(17)	0.0247	1.0000
C54	-0.0104(4)	0.7477(3)	0.77182(16)	0.0228	1.0000
C55	0.0089(4)	0.7586(3)	0.58118(16)	0.0249	1.0000
C56	0.0646(4)	0.6772(3)	0.53563(17)	0.0305	1.0000
C61	0.8781(5)	0.1097(4)	0.6433(2)	0.0415	1.0000
C69	0.6715(5)	0.5991(4)	0.6171(2)	0.0418	1.0000

C77	0.0910(6)	0.2973(5)	1.0204(2)	0.0637	1.0000
F62	0.8641(4)	0.2052(3)	0.65130(17)	0.0759	1.0000
F63	0.8152(3)	0.1138(2)	0.59733(11)	0.0411	1.0000
F64	0.9984(3)	0.0603(4)	0.62854(18)	0.0836	1.0000
F70	0.7137(3)	0.6558(2)	0.64564(15)	0.0607	1.0000
F71	0.6630(4)	0.5209(2)	0.65476(15)	0.0627	1.0000
F72	0.7616(3)	0.5608(3)	0.57443(17)	0.0685	1.0000
F78	0.0836(4)	0.4011(3)	1.02723(17)	0.0842	1.0000
F79	0.0022(4)	0.2960(5)	1.05613(17)	0.1115	1.0000
F80	0.0765(3)	0.3053(2)	0.96560(11)	0.0468	1.0000
S65	0.81663(12)	0.04972(8)	0.70925(4)	0.0321	1.0000
S73	0.52017(11)	0.67183(8)	0.58865(4)	0.0306	1.0000
S81	0.24837(12)	0.21705(7)	1.03962(4)	0.0316	1.0000
O1	0.7408(3)	0.1288(2)	1.02508(12)	0.0266	1.0000
O2	0.6881(3)	0.2469(2)	1.09072(12)	0.0306	1.0000
O66	0.6870(4)	0.1177(3)	0.71896(15)	0.0498	1.0000
O67	0.8289(3)	-0.0469(2)	0.69107(13)	0.0368	1.0000
O68	0.9005(4)	0.0458(3)	0.75174(16)	0.0603	1.0000
O74	0.4940(4)	0.5969(3)	0.56033(13)	0.0438	1.0000
O75	0.4372(4)	0.7056(3)	0.64013(16)	0.0476	1.0000
O76	0.5491(4)	0.7493(3)	0.54943(15)	0.0457	1.0000
O82	0.2481(5)	0.2208(4)	1.09977(17)	0.1036	1.0000
O83	0.2668(5)	0.1257(3)	1.0187(2)	0.0709	1.0000
O84	0.3377(5)	0.2610(4)	1.0025(2)	0.0798	1.0000
B1	0.7041(4)	0.2303(3)	1.03293(19)	0.0234	1.0000
B21	0.3806(4)	0.1552(3)	0.69632(18)	0.0198	1.0000
B41	0.0224(4)	0.5997(3)	0.62503(18)	0.0227	1.0000
N10	0.6894(3)	0.1366(2)	0.91437(14)	0.0227	1.0000
N21	0.4259(3)	0.3491(2)	0.62381(13)	0.0210	1.0000
N41	-0.0878(3)	0.6965(2)	0.74864(13)	0.0193	1.0000
O210	0.3670(6)	0.1793(5)	0.6376(3)	0.0210	0.5000
O21	0.4223(6)	0.1631(5)	0.6387(3)	0.0210	0.5000
O22	0.3528(6)	0.0666(5)	0.7101(3)	0.0210	0.5000
O220	0.4126(6)	0.0552(5)	0.7142(3)	0.0210	0.5000
C37	0.5453(9)	0.0402(8)	0.5696(4)	0.0304	0.5000
C370	0.5567(9)	0.0658(8)	0.5875(4)	0.0304	0.5000
C390	0.5138(10)	-0.0971(7)	0.6632(4)	0.0294	0.5000
C39	0.5305(10)	-0.0758(7)	0.6786(4)	0.0294	0.5000
C38	0.3090(10)	0.1199(8)	0.5721(4)	0.0304	0.5000
C380	0.3398(10)	0.0916(8)	0.5591(4)	0.0304	0.5000
C400	0.2749(9)	-0.0083(7)	0.6708(4)	0.0294	0.5000

C40	0.3089(9)	-0.0489(7)	0.6543(4)	0.0294	0.5000
O42	0.0926(4)	0.5781(4)	0.57354(19)	0.0236	0.7000
O410	0.0063(11)	0.6974(11)	0.6343(6)	0.0236	0.3000
C60	0.1869(8)	0.6732(6)	0.5009(3)	0.0359	0.7000
C600	0.2102(19)	0.6651(14)	0.5207(7)	0.0359	0.3000
C580	0.0802(17)	0.8316(13)	0.5860(7)	0.0361	0.3000
C58	0.1152(7)	0.7840(5)	0.6042(3)	0.0361	0.7000
C59	-0.0359(8)	0.6748(6)	0.4976(3)	0.0456	0.7000
C590	-0.002(2)	0.7042(14)	0.4786(7)	0.0456	0.3000
C570	-0.1385(16)	0.8296(13)	0.5730(7)	0.0278	0.3000
C57	-0.0981(7)	0.8478(5)	0.5631(3)	0.0278	0.7000
O420	0.0482(11)	0.5921(9)	0.5643(5)	0.0236	0.3000
O41	-0.0385(4)	0.7014(4)	0.6326(2)	0.0236	0.7000
H11	0.6623(4)	0.6288(3)	0.86257(16)	0.0303	1.0000
H12	0.5157(4)	0.6371(3)	0.87308(16)	0.0301	1.0000
H22	0.6924(4)	0.5426(3)	0.78376(16)	0.0281	1.0000
H21	0.5410(4)	0.5749(3)	0.78596(16)	0.0281	1.0000
H31	0.6213(4)	0.3643(3)	0.75765(16)	0.0312	1.0000
H41	0.6519(4)	0.2045(3)	0.80878(16)	0.0291	1.0000
H71	0.6891(4)	0.4066(3)	1.04361(15)	0.0278	1.0000
H81	0.6526(4)	0.5598(3)	0.98600(16)	0.0283	1.0000
H132	0.6012(5)	0.0337(4)	0.9327(2)	0.0660	1.0000
H131	0.5041(5)	0.1478(4)	0.9307(2)	0.0660	1.0000
H133	0.5726(5)	0.0973(4)	0.8707(2)	0.0659	1.0000
H142	0.8282(5)	-0.0003(4)	0.9114(2)	0.0720	1.0000
H141	0.8805(5)	0.0905(4)	0.8947(2)	0.0721	1.0000
H143	0.8082(5)	0.0611(4)	0.8490(2)	0.0722	1.0000
H173	0.5945(5)	0.0248(4)	1.0525(3)	0.0811	1.0000
H172	0.5826(5)	0.0232(4)	1.1215(3)	0.0810	1.0000
H171	0.5287(5)	0.1266(4)	1.0840(3)	0.0809	1.0000
H183	0.8155(5)	-0.0675(3)	1.0594(2)	0.0581	1.0000
H182	0.8241(5)	-0.0576(3)	1.1249(2)	0.0579	1.0000
H181	0.9080(5)	-0.0175(3)	1.0762(2)	0.0579	1.0000
H193	0.6448(7)	0.2065(4)	1.2027(2)	0.0980	1.0000
H192	0.6660(7)	0.0902(4)	1.2018(2)	0.0980	1.0000
H191	0.5549(7)	0.1723(4)	1.1680(2)	0.0981	1.0000
H203	0.8616(6)	0.1898(4)	1.1584(2)	0.0770	1.0000
H202	0.8913(6)	0.0722(4)	1.1665(2)	0.0767	1.0000
H201	0.9203(6)	0.1247(4)	1.1042(2)	0.0770	1.0000
H211	0.3429(4)	0.4114(3)	0.90757(16)	0.0310	1.0000
H212	0.1920(4)	0.4431(3)	0.90552(16)	0.0311	1.0000

H222	0.3358(4)	0.5556(3)	0.85300(16)	0.0312	1.0000
H221	0.1885(4)	0.5828(3)	0.84728(16)	0.0311	1.0000
H231	0.3164(3)	0.6197(3)	0.72720(16)	0.0240	1.0000
H241	0.3790(4)	0.5322(3)	0.64234(16)	0.0260	1.0000
H271	0.3396(3)	0.1308(3)	0.80551(16)	0.0251	1.0000
H281	0.2932(4)	0.2255(3)	0.88575(15)	0.0262	1.0000
H333	0.5997(5)	0.2844(4)	0.5818(2)	0.0639	1.0000
H332	0.6045(5)	0.2803(4)	0.6498(2)	0.0641	1.0000
H331	0.5872(5)	0.3822(4)	0.6107(2)	0.0642	1.0000
H343	0.3922(5)	0.3638(3)	0.53883(17)	0.0599	1.0000
H342	0.3980(5)	0.4635(3)	0.56025(17)	0.0601	1.0000
H341	0.2758(5)	0.4319(3)	0.57837(17)	0.0600	1.0000
H411	0.0941(4)	0.1825(3)	0.77783(19)	0.0350	1.0000
H412	-0.0552(4)	0.2137(3)	0.77238(19)	0.0351	1.0000
H422	0.0536(4)	0.2519(3)	0.86334(18)	0.0299	1.0000
H421	-0.0959(4)	0.2779(3)	0.85970(18)	0.0302	1.0000
H431	-0.0767(4)	0.4631(3)	0.89967(16)	0.0289	1.0000
H441	-0.0997(4)	0.6259(3)	0.85407(16)	0.0270	1.0000
H471	0.0653(4)	0.4209(3)	0.60455(17)	0.0373	1.0000
H481	0.0645(4)	0.2693(3)	0.65553(18)	0.0371	1.0000
H532	-0.2426(4)	0.8227(3)	0.73858(17)	0.0409	1.0000
H531	-0.2504(4)	0.7598(3)	0.79954(17)	0.0409	1.0000
H533	-0.2751(4)	0.7224(3)	0.74184(17)	0.0408	1.0000
H542	-0.0279(4)	0.8147(3)	0.75240(16)	0.0380	1.0000
H541	-0.0345(4)	0.7526(3)	0.81318(16)	0.0381	1.0000
H543	0.0790(4)	0.7089(3)	0.76474(16)	0.0378	1.0000
H5701	-0.1420(16)	0.8706(13)	0.5370(7)	0.0420	0.3000
H5702	-0.1685(16)	0.8717(13)	0.6046(7)	0.0420	0.3000
H5703	-0.1906(16)	0.7895(13)	0.5732(7)	0.0420	0.3000
H571	-0.0700(7)	0.8851(5)	0.5305(3)	0.0420	0.7000
H572	-0.1323(7)	0.8900(5)	0.5945(3)	0.0420	0.7000
H573	-0.1620(7)	0.8258(5)	0.5523(3)	0.0420	0.7000
H5801	0.0850(17)	0.8748(13)	0.5515(7)	0.0520	0.3000
H5802	0.0497(17)	0.8710(13)	0.6187(7)	0.0520	0.3000
H5803	0.1626(17)	0.7834(13)	0.5918(7)	0.0520	0.3000
H581	0.1513(7)	0.8211(5)	0.5745(3)	0.0520	0.7000
H582	0.0789(7)	0.8238(5)	0.6365(3)	0.0520	0.7000
H583	0.1798(7)	0.7231(5)	0.6168(3)	0.0520	0.7000
H6001	0.2532(19)	0.6503(14)	0.5552(7)	0.0600	0.3000
H6002	0.2269(19)	0.7201(14)	0.4975(7)	0.0600	0.3000
H6003	0.2397(19)	0.6070(14)	0.4990(7)	0.0600	0.3000

H601	0.2447(8)	0.6731(6)	0.5275(3)	0.0600	0.7000
H603	0.2226(8)	0.6143(6)	0.4799(3)	0.0600	0.7000
H5901	0.007(2)	0.7629(14)	0.4564(7)	0.0785	0.3000
H5902	-0.089(2)	0.7167(14)	0.4914(7)	0.0785	0.3000
H5903	0.029(2)	0.6487(14)	0.4549(7)	0.0785	0.3000
H591	-0.0586(8)	0.7360(6)	0.4727(3)	0.0785	0.7000
H592	-0.1096(8)	0.6700(6)	0.5212(3)	0.0785	0.7000
H593	-0.0010(8)	0.6185(6)	0.4745(3)	0.0785	0.7000
H4001	0.2666(9)	-0.0406(7)	0.6387(4)	0.0382	0.5000
H4002	0.2674(9)	-0.0486(7)	0.7063(4)	0.0382	0.5000
H4003	0.2096(9)	0.0565(7)	0.6722(4)	0.0382	0.5000
H401	0.3402(9)	-0.0920(7)	0.6232(4)	0.0382	0.5000
H402	0.2957(9)	-0.0877(7)	0.6896(4)	0.0382	0.5000
H403	0.2304(9)	0.0024(7)	0.6454(4)	0.0382	0.5000
H3901	0.5930(10)	-0.0860(7)	0.6585(4)	0.0382	0.5000
H3902	0.5071(10)	-0.1356(7)	0.6994(4)	0.0382	0.5000
H3903	0.5093(10)	-0.1331(7)	0.6320(4)	0.0382	0.5000
H391	0.5882(10)	-0.0424(7)	0.6828(4)	0.0382	0.5000
H392	0.5165(10)	-0.1124(7)	0.7146(4)	0.0382	0.5000
H393	0.5655(10)	-0.1216(7)	0.6489(4)	0.0382	0.5000
H3701	0.5933(9)	0.0038(8)	0.5694(4)	0.0387	0.5000
H3702	0.6039(9)	0.0640(8)	0.6191(4)	0.0387	0.5000
H3703	0.5588(9)	0.1206(8)	0.5595(4)	0.0387	0.5000
H371	0.6141(9)	0.0141(8)	0.5936(4)	0.0387	0.5000
H372	0.5553(9)	0.0951(8)	0.5437(4)	0.0387	0.5000
H373	0.5445(9)	-0.0118(8)	0.5474(4)	0.0387	0.5000
H381	0.3257(10)	0.1657(8)	0.5412(4)	0.0387	0.5000
H382	0.2344(10)	0.1546(8)	0.5959(4)	0.0387	0.5000
H383	0.2964(10)	0.0658(8)	0.5562(4)	0.0387	0.5000
H3801	0.3703(10)	0.0303(8)	0.5403(4)	0.0387	0.5000
H3802	0.2535(10)	0.1047(8)	0.5743(4)	0.0387	0.5000
H3803	0.3453(10)	0.1461(8)	0.5316(4)	0.0387	0.5000
H101	0.6966(3)	0.1374(2)	0.95091(14)	0.0275	1.0000
H213	0.4107(3)	0.2931(2)	0.62770(13)	0.0256	1.0000
H413	-0.0686(3)	0.6970(2)	0.71137(13)	0.0231	1.0000
H602	0.1726(8)	0.7319(6)	0.4740(3)	0.0600	0.7000

Thermal Parameters

Label	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C1	0.025(2)	0.0180(18)	0.0259(19)	0.0019(15)	-0.0020(15)	-0.0054(15)
C2	0.022(2)	0.0212(19)	0.0235(18)	0.0034(14)	-0.0052(15)	-0.0071(15)
C3	0.027(2)	0.032(2)	0.0150(16)	-0.0015(15)	-0.0045(14)	-0.0117(17)

C4	0.023(2)	0.027(2)	0.0238(19)	-0.0099(15)	-0.0024(15)	-0.0097(16)
C5	0.0212(19)	0.0164(17)	0.0204(17)	-0.0025(14)	-0.0011(14)	-0.0053(14)
C6	0.0203(19)	0.0192(18)	0.0195(17)	-0.0031(14)	-0.0022(14)	-0.0064(15)
C7	0.029(2)	0.027(2)	0.0127(16)	-0.0005(14)	-0.0017(14)	-0.0110(16)
C8	0.034(2)	0.0153(17)	0.0235(18)	-0.0059(14)	-0.0008(16)	-0.0108(16)
C9	0.0156(18)	0.0213(18)	0.0170(16)	0.0032(13)	-0.0039(13)	-0.0036(14)
C10	0.0123(17)	0.0200(18)	0.0224(17)	-0.0004(14)	-0.0025(13)	-0.0055(14)
C11	0.0217(19)	0.0180(17)	0.0195(17)	0.0000(13)	-0.0023(14)	-0.0071(15)
C12	0.0155(17)	0.0182(17)	0.0177(16)	-0.0001(13)	-0.0029(13)	-0.0062(14)
C13	0.039(3)	0.035(2)	0.053(3)	0.009(2)	-0.020(2)	-0.020(2)
C14	0.036(3)	0.027(2)	0.055(3)	-0.004(2)	0.006(2)	-0.001(2)
C15	0.032(2)	0.028(2)	0.027(2)	0.0079(16)	-0.0105(17)	-0.0143(18)
C16	0.049(3)	0.020(2)	0.026(2)	0.0079(16)	-0.0041(18)	-0.0085(19)
C17	0.045(3)	0.053(3)	0.057(3)	0.021(3)	-0.020(2)	-0.027(3)
C18	0.064(3)	0.019(2)	0.037(2)	0.0078(17)	-0.025(2)	-0.017(2)
C19	0.102(5)	0.034(3)	0.033(3)	0.009(2)	0.010(3)	-0.009(3)
C20	0.075(4)	0.029(2)	0.051(3)	0.002(2)	-0.034(3)	-0.022(2)
C21	0.031(2)	0.0234(19)	0.0161(17)	-0.0047(14)	-0.0010(15)	-0.0088(16)
C22	0.027(2)	0.030(2)	0.0179(17)	-0.0069(15)	-0.0024(15)	-0.0109(16)
C23	0.0208(19)	0.0152(17)	0.0218(17)	-0.0051(13)	-0.0018(14)	-0.0036(14)
C24	0.025(2)	0.0194(18)	0.0173(17)	0.0002(14)	-0.0030(14)	-0.0075(15)
C25	0.0195(18)	0.0180(17)	0.0156(16)	-0.0045(13)	-0.0003(13)	-0.0067(14)
C26	0.0163(18)	0.0207(17)	0.0150(16)	-0.0008(13)	-0.0028(13)	-0.0065(14)
C27	0.0188(18)	0.0192(18)	0.0207(17)	-0.0017(14)	-0.0018(14)	-0.0050(14)
C28	0.0221(19)	0.0241(19)	0.0153(16)	0.0022(14)	-0.0024(14)	-0.0068(15)
C29	0.0149(18)	0.0232(18)	0.0179(16)	-0.0076(14)	-0.0030(13)	-0.0059(14)
C30	0.0116(16)	0.0192(17)	0.0148(15)	-0.0026(13)	-0.0035(12)	-0.0052(13)
C31	0.0145(17)	0.0253(19)	0.0154(16)	-0.0033(13)	-0.0033(13)	-0.0050(14)
C32	0.0156(17)	0.0198(18)	0.0159(16)	-0.0012(13)	-0.0031(13)	-0.0059(14)
C33	0.036(3)	0.042(3)	0.044(3)	-0.023(2)	0.010(2)	-0.009(2)
C34	0.059(3)	0.034(2)	0.0161(19)	-0.0041(17)	-0.0070(19)	-0.005(2)
C35	0.031(2)	0.0199(18)	0.0193(17)	-0.0040(14)	-0.0080(15)	-0.0062(16)
C36	0.025(2)	0.0220(18)	0.0191(17)	-0.0051(14)	-0.0058(14)	-0.0056(15)
C41	0.025(2)	0.0214(19)	0.040(2)	0.0018(17)	-0.0072(17)	-0.0097(16)
C42	0.0185(19)	0.0202(19)	0.034(2)	0.0037(15)	-0.0033(15)	-0.0057(15)
C43	0.026(2)	0.0233(19)	0.0176(17)	0.0050(14)	-0.0036(15)	-0.0069(16)
C44	0.024(2)	0.0240(19)	0.0183(17)	-0.0020(14)	-0.0056(14)	-0.0060(16)
C45	0.0216(19)	0.0154(17)	0.0178(16)	0.0024(13)	-0.0045(14)	-0.0046(14)
C46	0.023(2)	0.0248(19)	0.0181(17)	-0.0057(14)	-0.0033(14)	-0.0090(15)
C47	0.039(2)	0.033(2)	0.0188(18)	-0.0070(16)	-0.0012(16)	-0.0145(19)
C48	0.036(2)	0.027(2)	0.032(2)	-0.0114(17)	-0.0045(18)	-0.0128(18)

C49	0.0139(18)	0.0253(19)	0.0220(18)	0.0015(14)	-0.0041(14)	-0.0042(15)
C50	0.0167(18)	0.0211(18)	0.0194(17)	-0.0026(14)	-0.0071(13)	-0.0062(14)
C51	0.0175(19)	0.0193(18)	0.035(2)	-0.0004(15)	-0.0064(15)	-0.0069(15)
C52	0.0161(18)	0.0201(18)	0.0243(18)	-0.0005(14)	-0.0076(14)	-0.0059(14)
C53	0.024(2)	0.0221(19)	0.0269(19)	0.0030(15)	-0.0086(15)	-0.0057(16)
C54	0.028(2)	0.0212(18)	0.0225(18)	0.0013(14)	-0.0088(15)	-0.0114(16)
C55	0.035(2)	0.025(2)	0.0136(16)	0.0015(14)	-0.0005(15)	-0.0118(17)
C56	0.040(2)	0.028(2)	0.0158(18)	-0.0002(15)	-0.0008(16)	-0.0025(18)
C61	0.047(3)	0.042(3)	0.045(3)	0.015(2)	-0.021(2)	-0.029(2)
C69	0.050(3)	0.035(3)	0.043(3)	-0.009(2)	-0.009(2)	-0.014(2)
C77	0.055(3)	0.071(4)	0.019(2)	0.003(2)	0.004(2)	0.030(3)
F62	0.126(3)	0.056(2)	0.077(2)	0.0228(18)	-0.044(2)	-0.069(2)
F63	0.0528(17)	0.0421(15)	0.0289(13)	0.0090(11)	-0.0128(12)	-0.0181(13)
F64	0.0362(19)	0.124(4)	0.084(3)	0.041(2)	-0.0072(17)	-0.035(2)
F70	0.069(2)	0.0548(19)	0.072(2)	-0.0152(17)	-0.0268(18)	-0.0289(17)
F71	0.090(3)	0.0407(17)	0.059(2)	0.0131(15)	-0.0339(18)	-0.0213(17)
F72	0.049(2)	0.060(2)	0.087(3)	-0.0343(19)	0.0139(18)	-0.0063(16)
F78	0.105(3)	0.052(2)	0.070(2)	-0.0165(18)	-0.028(2)	0.015(2)
F79	0.042(2)	0.228(6)	0.054(2)	0.025(3)	-0.0042(18)	-0.046(3)
F80	0.0548(18)	0.0524(17)	0.0278(13)	-0.0034(12)	-0.0180(12)	-0.0073(14)
S65	0.0534(7)	0.0271(5)	0.0212(5)	-0.0019(4)	-0.0079(4)	-0.0191(5)
S73	0.0399(6)	0.0305(5)	0.0234(5)	0.0004(4)	0.0024(4)	-0.0175(5)
S81	0.0514(7)	0.0168(5)	0.0218(5)	-0.0043(4)	-0.0141(4)	-0.0015(4)
O1	0.0366(16)	0.0214(14)	0.0237(13)	0.0039(11)	-0.0079(12)	-0.0125(12)
O2	0.0460(18)	0.0212(14)	0.0206(14)	0.0017(11)	-0.0032(12)	-0.0079(13)
O66	0.061(2)	0.043(2)	0.0419(19)	-0.0211(16)	0.0071(17)	-0.0127(18)
O67	0.062(2)	0.0226(15)	0.0269(15)	-0.0003(12)	0.0004(14)	-0.0181(15)
O68	0.095(3)	0.060(2)	0.040(2)	0.0046(17)	-0.035(2)	-0.037(2)
O74	0.065(2)	0.056(2)	0.0260(16)	-0.0012(14)	-0.0057(15)	-0.0400(19)
O75	0.057(2)	0.0352(18)	0.052(2)	-0.0134(15)	0.0226(17)	-0.0235(17)
O76	0.063(2)	0.0407(19)	0.0353(17)	0.0076(14)	0.0028(16)	-0.0271(17)
O82	0.099(4)	0.116(4)	0.0250(19)	-0.020(2)	-0.021(2)	0.059(3)
O83	0.096(3)	0.0251(18)	0.089(3)	-0.0179(19)	-0.059(3)	0.0035(19)
O84	0.087(3)	0.072(3)	0.088(3)	0.034(3)	-0.034(3)	-0.041(3)
B1	0.022(2)	0.025(2)	0.025(2)	-0.0023(17)	-0.0046(17)	-0.0083(17)
B21	0.018(2)	0.019(2)	0.0200(19)	0.0009(15)	-0.0044(15)	-0.0044(16)
B41	0.024(2)	0.027(2)	0.0181(19)	-0.0055(16)	-0.0034(16)	-0.0075(18)
N10	0.0280(18)	0.0169(15)	0.0236(16)	-0.0049(12)	-0.0062(13)	-0.0059(13)
N21	0.0282(17)	0.0197(15)	0.0143(14)	-0.0009(12)	0.0008(12)	-0.0086(13)
N41	0.0240(17)	0.0204(15)	0.0127(13)	-0.0015(11)	-0.0051(12)	-0.0055(13)
O210	0.029(3)	0.0192(16)	0.0165(11)	-0.0028(11)	-0.006(2)	-0.009(2)

O21	0.029(3)	0.0192(16)	0.0165(11)	-0.0028(11)	-0.006(2)	-0.009(2)
O22	0.029(3)	0.0192(16)	0.0165(11)	-0.0028(11)	-0.006(2)	-0.009(2)
O220	0.029(3)	0.0192(16)	0.0165(11)	-0.0028(11)	-0.006(2)	-0.009(2)
C37	0.036(3)	0.036(4)	0.018(3)	-0.002(2)	-0.008(2)	-0.010(2)
C370	0.036(3)	0.036(4)	0.018(3)	-0.002(2)	-0.008(2)	-0.010(2)
C390	0.039(3)	0.022(3)	0.029(3)	-0.004(2)	-0.008(2)	-0.010(2)
C39	0.039(3)	0.022(3)	0.029(3)	-0.004(2)	-0.008(2)	-0.010(2)
C38	0.036(3)	0.036(4)	0.018(3)	-0.002(2)	-0.008(2)	-0.010(2)
C380	0.036(3)	0.036(4)	0.018(3)	-0.002(2)	-0.008(2)	-0.010(2)
C400	0.039(3)	0.022(3)	0.029(3)	-0.004(2)	-0.008(2)	-0.010(2)
C40	0.039(3)	0.022(3)	0.029(3)	-0.004(2)	-0.008(2)	-0.010(2)
O42	0.028(2)	0.0222(13)	0.0147(12)	-0.0001(9)	-0.0021(15)	-0.0014(19)
O410	0.028(2)	0.0222(13)	0.0147(12)	-0.0001(9)	-0.0021(15)	-0.0014(19)
C60	0.052(3)	0.032(2)	0.015(3)	-0.002(2)	-0.003(2)	-0.004(2)
C600	0.052(3)	0.032(2)	0.015(3)	-0.002(2)	-0.003(2)	-0.004(2)
C580	0.046(3)	0.035(2)	0.026(2)	0.0016(17)	-0.0011(17)	-0.0146(19)
C58	0.046(3)	0.035(2)	0.026(2)	0.0016(17)	-0.0011(17)	-0.0146(19)
C59	0.064(3)	0.044(2)	0.022(3)	-0.001(2)	0.003(2)	-0.015(2)
C590	0.064(3)	0.044(2)	0.022(3)	-0.001(2)	0.003(2)	-0.015(2)
C570	0.037(3)	0.027(2)	0.018(2)	0.0023(17)	-0.0003(17)	-0.0117(19)
C57	0.037(3)	0.027(2)	0.018(2)	0.0023(17)	-0.0003(17)	-0.0117(19)
O420	0.028(2)	0.0222(13)	0.0147(12)	-0.0001(9)	-0.0021(15)	-0.0014(19)
O41	0.028(2)	0.0222(13)	0.0147(12)	-0.0001(9)	-0.0021(15)	-0.0014(19)

Distances

C1	C2	1.545(5)Å	C1	C11	1.513(5)Å
C1	H11	0.975Å	C1	H12	0.975Å
C2	C9	1.516(5)Å	C2	H22	0.972Å
C2	H21	0.982Å	C3	C4	1.406(6)Å
C3	C9	1.356(5)Å	C3	H31	0.942Å
C4	C5	1.381(5)Å	C4	H41	0.940Å
C5	C10	1.421(5)Å	C5	N10	1.488(5)Å
C6	C7	1.387(5)Å	C6	C10	1.453(5)Å
C6	B1	1.555(6)Å	C7	C8	1.415(5)Å
C7	H71	0.946Å	C8	C11	1.364(5)Å
C8	H81	0.938Å	C9	C12	1.418(5)Å
C10	C12	1.422(5)Å	C11	C12	1.410(5)Å
C13	N10	1.489(5)Å	C13	H132	0.973Å
C13	H131	0.974Å	C13	H133	0.978Å
C14	N10	1.484(6)Å	C14	H142	0.963Å
C14	H141	0.972Å	C14	H143	0.969Å
C15	C16	1.563(6)Å	C15	C17	1.518(6)Å

C15	C18	1.484(6)Å	C15	O1	1.481(5)Å
C16	C19	1.516(7)Å	C16	C20	1.489(7)Å
C16	O2	1.459(5)Å	C17	H173	0.970Å
C17	H172	0.961Å	C17	H171	0.969Å
C18	H183	0.949Å	C18	H182	0.953Å
C18	H181	0.958Å	C19	H193	0.964Å
C19	H192	0.957Å	C19	H191	0.971Å
C20	H203	0.960Å	C20	H202	0.968Å
C20	H201	0.965Å	C21	C22	1.548(5)Å
C21	C31	1.521(5)Å	C21	H211	0.972Å
C21	H212	0.981Å	C22	C29	1.511(5)Å
C22	H222	0.968Å	C22	H221	0.975Å
C23	C24	1.412(5)Å	C23	C29	1.360(5)Å
C23	H231	0.941Å	C24	C25	1.376(5)Å
C24	H241	0.937Å	C25	C30	1.433(5)Å
C25	N21	1.477(4)Å	C26	C27	1.387(5)Å
C26	C30	1.442(5)Å	C26	B21	1.564(5)Å
C27	C28	1.410(5)Å	C27	H271	0.935Å
C28	C31	1.354(5)Å	C28	H281	0.934Å
C29	C32	1.415(5)Å	C30	C32	1.419(5)Å
C31	C32	1.411(5)Å	C33	N21	1.492(6)Å
C33	H333	0.956Å	C33	H332	0.963Å
C33	H331	0.956Å	C34	N21	1.486(5)Å
C34	H343	0.962Å	C34	H342	0.966Å
C34	H341	0.965Å	C35	C36	1.567(5)Å
C35	O210	1.518(8)Å	C35	O21	1.443(8)Å
C35	C37	1.540(10)Å	C35	C370	1.505(11)Å
C35	C38	1.511(11)Å	C35	C380	1.520(11)Å
C36	O22	1.441(7)Å	C36	O220	1.512(7)Å
C36	C390	1.508(10)Å	C36	C39	1.517(10)Å
C36	C400	1.510(10)Å	C36	C40	1.543(10)Å
C41	C42	1.552(6)Å	C41	C51	1.511(5)Å
C41	H411	0.976Å	C41	H412	0.974Å
C42	C49	1.508(5)Å	C42	H422	0.978Å
C42	H421	0.976Å	C43	C44	1.413(5)Å
C43	C49	1.361(6)Å	C43	H431	0.940Å
C44	C45	1.374(5)Å	C44	H441	0.938Å
C45	C50	1.425(5)Å	C45	N41	1.483(4)Å
C46	C47	1.391(6)Å	C46	C50	1.446(5)Å
C46	B41	1.562(6)Å	C47	C48	1.399(6)Å
C47	H471	0.940Å	C48	C51	1.366(6)Å

C48	H481	0.933Å	C49	C52	1.413(5)Å
C50	C52	1.418(5)Å	C51	C52	1.408(5)Å
C53	N41	1.500(5)Å	C53	H532	0.959Å
C53	H531	0.962Å	C53	H533	0.965Å
C54	N41	1.496(5)Å	C54	H542	0.960Å
C54	H541	0.963Å	C54	H543	0.964Å
C55	C56	1.564(6)Å	C55	O410	1.415(14)Å
C55	C580	1.539(17)Å	C55	C58	1.538(8)Å
C55	C570	1.626(17)Å	C55	C57	1.461(8)Å
C55	O41	1.502(6)Å	C56	O42	1.511(6)Å
C56	C60	1.489(9)Å	C56	C600	1.58(2)Å
C56	C59	1.531(9)Å	C56	C590	1.537(18)Å
C56	O420	1.361(13)Å	C61	F62	1.338(6)Å
C61	F63	1.335(5)Å	C61	F64	1.306(6)Å
C61	S65	1.829(5)Å	C69	F70	1.339(5)Å
C69	F71	1.343(6)Å	C69	F72	1.333(6)Å
C69	S73	1.807(5)Å	C77	F78	1.470(8)Å
C77	F79	1.216(7)Å	C77	F80	1.283(5)Å
C77	S81	1.809(5)Å	S65	O66	1.440(4)Å
S65	O67	1.435(3)Å	S65	O68	1.431(4)Å
S73	O74	1.444(3)Å	S73	O75	1.432(3)Å
S73	O76	1.435(3)Å	S81	O82	1.397(4)Å
S81	O83	1.374(4)Å	S81	O84	1.491(5)Å
O1	B1	1.375(5)Å	O2	B1	1.362(5)Å
B21	O210	1.371(8)Å	B21	O21	1.358(8)Å
B21	O22	1.389(8)Å	B21	O220	1.354(8)Å
B41	O42	1.345(6)Å	B41	O410	1.370(15)Å
B41	O420	1.405(12)Å	B41	O41	1.378(7)Å
N10	H101	0.860Å	N21	H213	0.860Å
N41	H413	0.860Å	O210	O21	0.585(7)Å
O22	O220	0.651(6)Å	C37	C370	0.635(10)Å
C37	H3701	0.600Å	C37	H3703	1.191Å
C37	H371	0.950Å	C37	H372	0.950Å
C37	H373	0.950Å	C370	H3701	0.950Å
C370	H3702	0.950Å	C370	H3703	0.950Å
C370	H371	0.796Å	C370	H372	1.043Å
C390	C39	0.579(10)Å	C390	H3901	0.950Å
C390	H3902	0.950Å	C390	H3903	0.950Å
C390	H392	1.183Å	C390	H393	0.635Å
C39	H3901	0.770Å	C39	H3902	1.020Å
C39	H391	0.950Å	C39	H392	0.950Å

C39	H393	0.950Å	C38	C380	0.524(12)Å
C38	H381	0.950Å	C38	H382	0.950Å
C38	H383	0.950Å	C38	H3802	0.724Å
C38	H3803	1.050Å	C380	H381	1.041Å
C380	H383	0.721Å	C380	H3801	0.950Å
C380	H3802	0.950Å	C380	H3803	0.950Å
C400	C40	0.695(10)Å	C400	H4001	0.950Å
C400	H4002	0.950Å	C400	H4003	0.950Å
C400	H402	1.105Å	C400	H403	0.786Å
C40	H4001	0.604Å	C40	H4002	1.231Å
C40	H401	0.950Å	C40	H402	0.950Å
C40	H403	0.950Å	O42	O420	0.531(10)Å
O410	O41	0.493(12)Å	C60	C600	0.537(15)Å
C60	H6002	0.916Å	C60	H6003	0.917Å
C60	H601	0.950Å	C60	H603	0.950Å
C60	H602	0.950Å	C600	H6001	0.950Å
C600	H6002	0.950Å	C600	H6003	0.950Å
C600	H601	0.489Å	C600	H603	1.219Å
C580	C58	0.755(16)Å	C580	H5801	0.950Å
C580	H5802	0.950Å	C580	H5803	0.950Å
C580	H581	0.776Å	C580	H582	1.157Å
C58	H5802	1.251Å	C58	H5803	0.571Å
C58	H581	0.950Å	C58	H582	0.950Å
C58	H583	0.950Å	C59	C590	0.736(18)Å
C59	H5902	0.692Å	C59	H5903	1.165Å
C59	H591	0.950Å	C59	H592	0.950Å
C59	H593	0.950Å	C590	H5901	0.950Å
C590	H5902	0.950Å	C590	H5903	0.950Å
C590	H591	0.659Å	C590	H593	1.226Å
C570	C57	0.607(15)Å	C570	H5701	0.950Å
C570	H5702	0.950Å	C570	H5703	0.950Å
C570	H572	1.067Å	C570	H573	0.592Å
C57	H5701	0.792Å	C57	H5702	1.164Å
C57	H571	0.950Å	C57	H572	0.950Å
C57	H573	0.950Å	H5701	H573	0.776Å
H5702	H572	0.567Å	H5703	H573	0.785Å
H5802	H582	0.730Å	H5803	H581	0.609Å
H6001	H601	0.684Å	H6002	H602	0.830Å
H6003	H603	0.488Å	H5902	H591	0.614Å
H5903	H593	0.718Å	H4001	H403	0.625Å
H4002	H402	0.672Å	H3901	H393	0.745Å

H3902 H392 0.553Å

H3703 H372 0.558Å

H383 H3802 0.726Å

H3701 H371 0.683Å

H381 H3803 0.365Å

Angles

C2	C1	C11	104.6(3)°	C2	C1	H11	111.174°
C11	C1	H11	110.971°	C2	C1	H12	109.747°
C11	C1	H12	109.846°	H11	C1	H12	110.359°
C1	C2	C9	104.9(3)°	C1	C2	H22	110.108°
C9	C2	H22	109.816°	C1	C2	H21	111.312°
C9	C2	H21	111.015°	H22	C2	H21	109.605°
C4	C3	C9	118.4(3)°	C4	C3	H31	120.594°
C9	C3	H31	121.035°	C3	C4	C5	121.8(3)°
C3	C4	H41	119.522°	C5	C4	H41	118.627°
C4	C5	C10	122.9(3)°	C4	C5	N10	116.1(3)°
C10	C5	N10	120.9(3)°	C7	C6	C10	117.9(3)°
C7	C6	B1	111.9(3)°	C10	C6	B1	130.2(3)°
C6	C7	C8	125.3(3)°	C6	C7	H71	117.728°
C8	C7	H71	116.968°	C7	C8	C11	117.3(3)°
C7	C8	H81	121.147°	C11	C8	H81	121.588°
C2	C9	C3	131.6(3)°	C2	C9	C12	108.8(3)°
C3	C9	C12	119.5(3)°	C5	C10	C6	131.9(3)°
C5	C10	C12	112.7(3)°	C6	C10	C12	115.4(3)°
C1	C11	C8	130.9(3)°	C1	C11	C12	109.3(3)°
C8	C11	C12	119.8(3)°	C9	C12	C10	124.6(3)°
C9	C12	C11	111.1(3)°	C10	C12	C11	124.2(3)°
N10	C13	H132	107.989°	N10	C13	H131	108.820°
H132	C13	H131	110.092°	N10	C13	H133	107.891°
H132	C13	H133	110.228°	H131	C13	H133	111.711°
N10	C14	H142	108.722°	N10	C14	H141	108.935°
H142	C14	H141	109.656°	N10	C14	H143	108.965°
H142	C14	H143	110.508°	H141	C14	H143	110.021°
C16	C15	C17	115.7(4)°	C16	C15	C18	114.8(3)°
C17	C15	C18	109.5(4)°	C16	C15	O1	101.6(3)°
C17	C15	O1	105.6(3)°	C18	C15	O1	108.8(4)°
C15	C16	C19	112.5(4)°	C15	C16	C20	114.1(4)°
C19	C16	C20	111.9(5)°	C15	C16	O2	102.2(3)°
C19	C16	O2	107.9(4)°	C20	C16	O2	107.5(4)°
C15	C17	H173	110.179°	C15	C17	H172	108.817°
H173	C17	H172	109.878°	C15	C17	H171	109.735°
H173	C17	H171	109.860°	H172	C17	H171	108.338°
C15	C18	H183	109.732°	C15	C18	H182	109.092°

H183	C18	H182	109.890°	C15	C18	H181	108.988°
H183	C18	H181	109.853°	H182	C18	H181	109.265°
C16	C19	H193	108.059°	C16	C19	H192	107.775°
H193	C19	H192	110.624°	C16	C19	H191	108.026°
H193	C19	H191	111.479°	H192	C19	H191	110.732°
C16	C20	H203	108.204°	C16	C20	H202	109.344°
H203	C20	H202	108.981°	C16	C20	H201	109.586°
H203	C20	H201	110.377°	H202	C20	H201	110.311°
C22	C21	C31	104.6(3)°	C22	C21	H211	111.000°
C31	C21	H211	109.583°	C22	C21	H212	111.030°
C31	C21	H212	110.390°	H211	C21	H212	110.113°
C21	C22	C29	105.5(3)°	C21	C22	H222	110.870°
C29	C22	H222	109.847°	C21	C22	H221	110.352°
C29	C22	H221	111.007°	H222	C22	H221	109.196°
C24	C23	C29	118.4(3)°	C24	C23	H231	120.355°
C29	C23	H231	121.268°	C23	C24	C25	122.1(3)°
C23	C24	H241	119.222°	C25	C24	H241	118.684°
C24	C25	C30	122.4(3)°	C24	C25	N21	116.4(3)°
C30	C25	N21	120.9(3)°	C27	C26	C30	117.0(3)°
C27	C26	B21	113.0(3)°	C30	C26	B21	130.0(3)°
C26	C27	C28	125.3(3)°	C26	C27	H271	117.695°
C28	C27	H271	116.978°	C27	C28	C31	117.9(3)°
C27	C28	H281	121.262°	C31	C28	H281	120.796°
C22	C29	C23	131.7(3)°	C22	C29	C32	108.9(3)°
C23	C29	C32	119.3(3)°	C25	C30	C26	130.5(3)°
C25	C30	C32	112.8(3)°	C26	C30	C32	116.7(3)°
C21	C31	C28	131.3(3)°	C21	C31	C32	109.2(3)°
C28	C31	C32	119.5(3)°	C29	C32	C30	125.0(3)°
C29	C32	C31	111.6(3)°	C30	C32	C31	123.4(3)°
N21	C33	H333	108.935°	N21	C33	H332	109.787°
H333	C33	H332	110.106°	N21	C33	H331	108.441°
H333	C33	H331	110.080°	H332	C33	H331	109.466°
N21	C34	H343	109.321°	N21	C34	H342	108.243°
H343	C34	H342	109.861°	N21	C34	H341	109.085°
H343	C34	H341	110.069°	H342	C34	H341	110.227°
C36	C35	O210	101.3(4)°	C36	C35	O21	101.8(4)°
O210	C35	O21	22.6(3)°	C36	C35	C37	114.3(4)°
O210	C35	C37	127.4(5)°	O21	C35	C37	109.0(5)°
C36	C35	C370	114.2(4)°	O210	C35	C370	106.5(5)°
O21	C35	C370	86.0(5)°	C37	C35	C370	24.0(4)°
C36	C35	C38	114.4(5)°	O210	C35	C38	87.5(5)°

O21	C35	C38	107.4(5)°	C37	C35	C38	109.4(5)°
C370	C35	C38	125.1(6)°	C36	C35	C380	115.9(5)°
O210	C35	C380	106.2(5)°	O21	C35	C380	124.0(5)°
C37	C35	C380	92.0(6)°	C370	C35	C380	111.5(6)°
C38	C35	C380	19.9(4)°	C35	C36	O22	103.2(4)°
C35	C36	O220	102.3(4)°	O22	C36	O220	25.3(3)°
C35	C36	C390	113.2(5)°	O22	C36	C390	126.7(5)°
O220	C36	C390	106.6(5)°	C35	C36	C39	113.2(5)°
O22	C36	C39	107.8(5)°	O220	C36	C39	85.4(5)°
C390	C36	C39	22.1(4)°	C35	C36	C400	113.9(4)°
O22	C36	C400	83.0(5)°	O220	C36	C400	106.1(5)°
C390	C36	C400	113.5(6)°	C39	C36	C400	127.4(6)°
C35	C36	C40	113.6(4)°	O22	C36	C40	108.1(5)°
O220	C36	C40	128.9(5)°	C390	C36	C40	91.8(6)°
C39	C36	C40	110.5(5)°	C400	C36	C40	26.3(4)°
C42	C41	C51	104.4(3)°	C42	C41	H411	110.909°
C51	C41	H411	110.132°	C42	C41	H412	110.902°
C51	C41	H412	110.526°	H411	C41	H412	109.836°
C41	C42	C49	105.3(3)°	C41	C42	H422	110.148°
C49	C42	H422	109.866°	C41	C42	H421	110.510°
C49	C42	H421	110.902°	H422	C42	H421	110.043°
C44	C43	C49	118.1(3)°	C44	C43	H431	120.848°
C49	C43	H431	121.048°	C43	C44	C45	122.3(4)°
C43	C44	H441	119.102°	C45	C44	H441	118.597°
C44	C45	C50	122.3(3)°	C44	C45	N41	115.7(3)°
C50	C45	N41	122.0(3)°	C47	C46	C50	117.1(3)°
C47	C46	B41	112.9(3)°	C50	C46	B41	129.9(3)°
C46	C47	C48	125.4(4)°	C46	C47	H471	116.754°
C48	C47	H471	117.805°	C47	C48	C51	118.0(4)°
C47	C48	H481	121.026°	C51	C48	H481	120.991°
C42	C49	C43	131.4(3)°	C42	C49	C52	109.2(3)°
C43	C49	C52	119.3(3)°	C45	C50	C46	130.7(3)°
C45	C50	C52	113.0(3)°	C46	C50	C52	116.3(3)°
C41	C51	C48	131.0(4)°	C41	C51	C52	109.8(3)°
C48	C51	C52	119.2(4)°	C49	C52	C50	124.9(3)°
C49	C52	C51	111.2(3)°	C50	C52	C51	123.9(3)°
N41	C53	H532	108.160°	N41	C53	H531	108.153°
H532	C53	H531	110.515°	N41	C53	H533	109.168°
H532	C53	H533	110.143°	H531	C53	H533	110.633°
N41	C54	H542	109.419°	N41	C54	H541	108.451°
H542	C54	H541	109.340°	N41	C54	H543	109.508°

H542	C54	H543	109.544°	H541	C54	H543	110.557°
C56	C55	O410	101.8(7)°	C56	C55	C580	118.7(7)°
O410	C55	C580	110.6(8)°	C56	C55	C58	111.4(4)°
O410	C55	C58	86.8(6)°	C580	C55	C58	28.4(6)°
C56	C55	C570	112.9(6)°	O410	C55	C570	106.1(8)°
C580	C55	C570	106.1(9)°	C58	C55	C570	129.7(7)°
C56	C55	C57	115.1(4)°	O410	C55	C57	124.3(6)°
C580	C55	C57	87.2(7)°	C58	C55	C57	113.9(5)°
C570	C55	C57	21.9(5)°	C56	C55	O41	102.5(3)°
O410	C55	O41	19.2(5)°	C580	C55	O41	124.4(7)°
C58	C55	O41	104.1(4)°	C570	C55	O41	88.5(6)°
C57	C55	O41	108.5(4)°	C55	C56	O42	103.1(3)°
C55	C56	C60	117.3(4)°	O42	C56	C60	106.1(4)°
C55	C56	C600	106.4(7)°	O42	C56	C600	94.0(7)°
C60	C56	C600	19.8(5)°	C55	C56	C59	112.7(4)°
O42	C56	C59	103.2(4)°	C60	C56	C59	112.6(5)°
C600	C56	C59	131.7(7)°	C55	C56	C590	114.7(7)°
O42	C56	C590	126.3(8)°	C60	C56	C590	89.4(8)°
C600	C56	C590	109.2(10)°	C59	C56	C590	27.7(7)°
C55	C56	O420	104.3(6)°	O42	C56	O420	20.5(5)°
C60	C56	O420	121.3(7)°	C600	C56	O420	112.7(9)°
C59	C56	O420	84.2(6)°	C590	C56	O420	109.6(9)°
F62	C61	F63	107.0(4)°	F62	C61	F64	108.8(4)°
F63	C61	F64	106.7(5)°	F62	C61	S65	110.3(4)°
F63	C61	S65	111.6(3)°	F64	C61	S65	112.2(3)°
F70	C69	F71	107.2(4)°	F70	C69	F72	107.0(4)°
F71	C69	F72	107.3(4)°	F70	C69	S73	111.8(3)°
F71	C69	S73	111.6(4)°	F72	C69	S73	111.7(4)°
F78	C77	F79	96.8(5)°	F78	C77	F80	100.0(4)°
F79	C77	F80	119.2(6)°	F78	C77	S81	105.1(5)°
F79	C77	S81	116.4(4)°	F80	C77	S81	114.4(3)°
C61	S65	O66	103.0(2)°	C61	S65	O67	102.5(2)°
O66	S65	O67	114.6(2)°	C61	S65	O68	103.3(2)°
O66	S65	O68	115.9(2)°	O67	S65	O68	115.0(2)°
C69	S73	O74	102.1(2)°	C69	S73	O75	103.4(2)°
O74	S73	O75	114.8(2)°	C69	S73	O76	103.1(2)°
O74	S73	O76	114.7(2)°	O75	S73	O76	115.9(2)°
C77	S81	O82	106.4(2)°	C77	S81	O83	104.4(3)°
O82	S81	O83	118.8(3)°	C77	S81	O84	105.0(3)°
O82	S81	O84	114.4(4)°	O83	S81	O84	106.5(3)°
C15	O1	B1	107.7(3)°	C16	O2	B1	109.0(3)°

C6	B1	O1	125.9(4)°	C6	B1	O2	122.3(4)°
O1	B1	O2	111.8(3)°	C26	B21	O210	124.0(4)°
C26	B21	O21	126.7(4)°	O210	B21	O21	24.7(3)°
C26	B21	O22	123.1(4)°	O210	B21	O22	105.4(5)°
O21	B21	O22	110.0(5)°	C26	B21	O220	120.8(4)°
O210	B21	O220	115.2(5)°	O21	B21	O220	107.6(5)°
O22	B21	O220	27.4(3)°	C46	B41	O42	119.1(4)°
C46	B41	O410	129.2(6)°	O42	B41	O410	108.2(7)°
C46	B41	O420	124.0(6)°	O42	B41	O420	22.1(5)°
O410	B41	O420	106.8(8)°	C46	B41	O41	125.2(4)°
O42	B41	O41	115.8(4)°	O410	B41	O41	20.7(5)°
O420	B41	O41	106.4(6)°	C5	N10	C13	113.0(3)°
C5	N10	C14	112.1(3)°	C13	N10	C14	112.4(4)°
C5	N10	H101	106.231°	C13	N10	H101	106.276°
C14	N10	H101	106.250°	C25	N21	C33	110.3(3)°
C25	N21	C34	115.7(3)°	C33	N21	C34	110.7(4)°
C25	N21	H213	106.542°	C33	N21	H213	106.586°
C34	N21	H213	106.537°	C45	N41	C53	111.9(3)°
C45	N41	C54	113.7(3)°	C53	N41	C54	110.8(3)°
C45	N41	H413	106.576°	C53	N41	H413	106.612°
C54	N41	H413	106.666°	C35	O210	B21	106.2(5)°
C35	O210	O21	71.5(12)°	B21	O210	O21	76.4(13)°
C35	O21	B21	111.3(5)°	C35	O21	O210	85.9(13)°
B21	O21	O210	78.9(13)°	C36	O22	B21	108.7(5)°
C36	O22	O220	83.5(10)°	B21	O22	O220	73.3(10)°
C36	O220	B21	106.6(5)°	C36	O220	O22	71.2(9)°
B21	O220	O22	79.3(10)°	C35	C37	C370	74.9(14)°
C35	C37	H3701	137.476°	C370	C37	H3701	100.589°
C35	C37	H3703	94.987°	C370	C37	H3703	52.541°
H3701	C37	H3703	116.033°	C35	C37	H371	108.407°
C370	C37	H371	56.170°	H3701	C37	H371	45.750°
H3703	C37	H371	92.971°	C35	C37	H372	108.836°
C370	C37	H372	79.630°	H3701	C37	H372	111.852°
H3703	C37	H372	27.359°	H371	C37	H372	109.476°
C35	C37	H373	111.146°	C370	C37	H373	165.516°
H3701	C37	H373	65.838°	H3703	C37	H373	136.729°
H371	C37	H373	109.476°	H372	C37	H373	109.473°
C35	C370	C37	81.0(15)°	C35	C370	H3701	108.862°
C37	C370	H3701	38.371°	C35	C370	H3702	110.313°
C37	C370	H3702	146.153°	H3701	C370	H3702	109.476°
C35	C370	H3703	109.221°	C37	C370	H3703	95.440°

H3701 C370	H3703 109.475°	H3702 C370	H3703 109.476°
C35 C370	H371 122.788°	C37 C370	H371 82.372°
H3701 C370	H371 45.014°	H3702 C370	H371 64.512°
H3703 C370	H371 126.641°	C35 C370	H372 105.980°
C37 C370	H372 63.617°	H3701 C370	H372 81.179°
H3702 C370	H372 135.574°	H3703 C370	H372 32.089°
H371 C370	H372 114.343°	C36 C390	C39 79.8(16)°
C36 C390	H3901 110.295°	C39 C390	H3901 54.075°
C36 C390	H3902 109.499°	C39 C390	H3902 79.674°
H3901 C390	H3902 109.477°	C36 C390	H3903 108.602°
C39 C390	H3903 163.542°	H3901 C390	H3903 109.475°
H3902 C390	H3903 109.475°	C36 C390	H392 97.613°
C39 C390	H392 52.574°	H3901 C390	H392 92.105°
H3902 C390	H392 27.375°	H3903 C390	H392 136.600°
C36 C390	H393 142.709°	C39 C390	H393 102.879°
H3901 C390	H393 51.557°	H3902 C390	H393 107.540°
H3903 C390	H393 61.708°	H392 C390	H393 113.688°
C36 C39	C390 78.1(16)°	C36 C39	H3901 123.167°
C390 C39	H3901 88.377°	C36 C39	H3902 104.819°
C390 C39	H3902 66.371°	H3901 C39	H3902 119.527°
C36 C39	H391 109.037°	C390 C39	H391 146.072°
H3901 C39	H391 59.510°	H3902 C39	H391 137.033°
C36 C39	H392 109.111°	C390 C39	H392 98.470°
H3901 C39	H392 127.507°	H3902 C39	H392 32.373°
H391 C39	H392 109.476°	C36 C39	H393 110.250°
C390 C39	H393 40.657°	H3901 C39	H393 50.036°
H3902 C39	H393 81.873°	H391 C39	H393 109.476°
H392 C39	H393 109.475°	C35 C38	C380 81(2)°
C35 C38	H381 109.184°	C380 C38	H381 84.657°
C35 C38	H382 108.754°	C380 C38	H382 157.897°
H381 C38	H382 109.476°	C35 C38	H383 110.457°
C380 C38	H383 48.650°	H381 C38	H383 109.476°
H382 C38	H383 109.476°	C35 C38	H3802 128.090°
C380 C38	H3802 97.837°	H381 C38	H3802 122.449°
H382 C38	H3802 60.376°	H383 C38	H3802 49.187°
C35 C38	H3803 105.409°	C380 C38	H3803 64.444°
H381 C38	H3803 20.268°	H382 C38	H3803 128.073°
H383 C38	H3803 93.279°	H3802 C38	H3803 120.857°
C35 C380	C38 79(2)°	C35 C380	H381 103.429°
C38 C380	H381 65.267°	C35 C380	H383 128.397°
C38 C380	H383 98.255°	H381 C380	H383 122.344°

C35	C380	H3801	108.659°	C38	C380	H3801	157.969°
H381	C380	H3801	129.397°	H383	C380	H3801	60.499°
C35	C380	H3802	109.110°	C38	C380	H3802	49.030°
H381	C380	H3802	95.158°	H383	C380	H3802	49.226°
H3801	C380	H3802	109.475°	C35	C380	H3803	110.624°
C38	C380	H3803	85.704°	H381	C380	H3803	20.490°
H383	C380	H3803	120.625°	H3801	C380	H3803	109.477°
H3802	C380	H3803	109.476°	C36	C400	C40	79.5(13)°
C36	C400	H4001	108.208°	C40	C400	H4001	39.370°
C36	C400	H4002	109.931°	C40	C400	H4002	95.600°
H4001	C400	H4002	109.475°	C36	C400	H4003	110.254°
C40	C400	H4003	146.801°	H4001	C400	H4003	109.475°
H4002	C400	H4003	109.477°	C36	C400	H402	103.115°
C40	C400	H402	58.538°	H4001	C400	H402	77.812°
H4002	C400	H402	37.195°	H4003	C400	H402	140.764°
C36	C400	H403	123.533°	C40	C400	H403	79.522°
H4001	C400	H403	40.880°	H4002	C400	H403	123.861°
H4003	C400	H403	68.595°	H402	C400	H403	109.055°
C36	C40	C400	74.2(12)°	C36	C40	H4001	135.679°
C400	C40	H4001	93.742°	C36	C40	H4002	94.008°
C400	C40	H4002	50.201°	H4001	C40	H4002	110.797°
C36	C40	H401	110.540°	C400	C40	H401	163.230°
H4001	C40	H401	71.483°	H4002	C40	H401	141.901°
C36	C40	H402	109.426°	C400	C40	H402	82.852°
H4001	C40	H402	111.111°	H4002	C40	H402	32.784°
H401	C40	H402	109.476°	C36	C40	H403	108.428°
C400	C40	H403	54.475°	H4001	C40	H403	40.231°
H4002	C40	H403	88.437°	H401	C40	H403	109.476°
H402	C40	H403	109.476°	C56	O42	B41	106.5(4)°
C56	O42	O420	63.6(17)°	B41	O42	O420	85.3(17)°
C55	O410	B41	112.1(10)°	C55	O410	O41	90(2)°
B41	O410	O41	81(2)°	C56	C60	C600	90(3)°
C56	C60	H6002	127.733°	C600	C60	H6002	76.778°
C56	C60	H6003	109.683°	C600	C60	H6003	76.739°
H6002	C60	H6003	115.669°	C56	C60	H601	107.535°
C600	C60	H601	21.137°	H6002	C60	H601	56.760°
H6003	C60	H601	82.358°	C56	C60	H603	112.053°
C600	C60	H603	106.880°	H6002	C60	H603	120.197°
H6003	C60	H603	30.275°	H601	C60	H603	109.476°
C56	C60	H602	109.254°	C600	C60	H602	127.812°
H6002	C60	H602	52.751°	H6003	C60	H602	133.225°

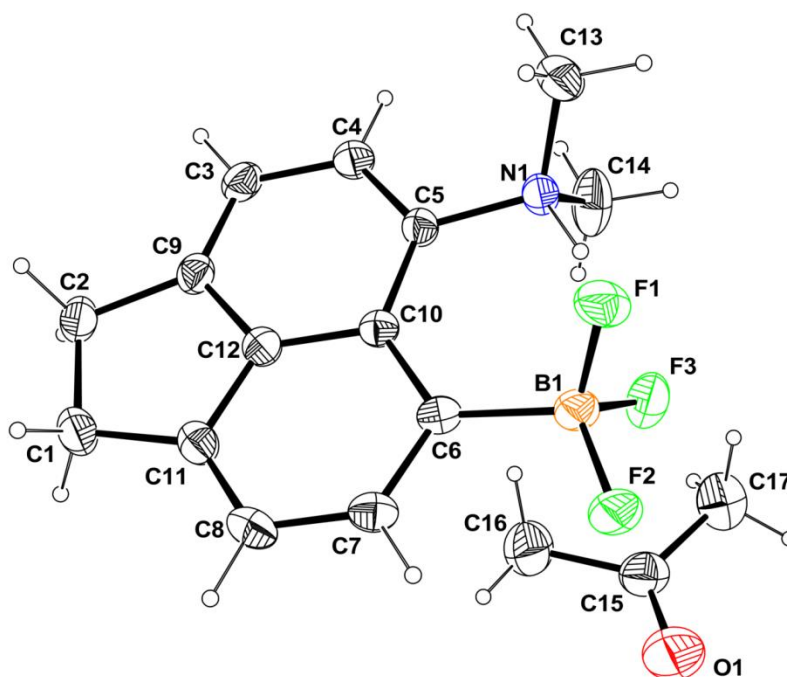
H601	C60	H602	109.238°	H603	C60	H602	109.236°
C56	C600	C60	70(3)°	C56	C600	H6001	111.174°
C60	C600	H6001	178.686°	C56	C600	H6002	115.959°
C60	C600	H6002	69.849°	H6001	C600	H6002	109.476°
C56	C600	H6003	100.868°	C60	C600	H6003	69.894°
H6001	C600	H6003	109.476°	H6002	C600	H6003	109.476°
C56	C600	H601	142.317°	C60	C600	H601	135.553°
H6001	C600	H601	43.474°	H6002	C600	H601	67.602°
H6003	C600	H601	113.397°	C56	C600	H603	92.793°
C60	C600	H603	48.205°	H6001	C600	H603	131.102°
H6002	C600	H603	95.647°	H6003	C600	H603	21.826°
H601	C600	H603	124.784°	C55	C580	C58	75.8(14)°
C55	C580	H5801	114.451°	C58	C580	H5801	145.708°
C55	C580	H5802	114.038°	C58	C580	H5802	93.692°
H5801	C580	H5802	109.476°	C55	C580	H5803	99.384°
C58	C580	H5803	36.973°	H5801	C580	H5803	109.475°
H5802	C580	H5803	109.477°	C55	C580	H581	123.516°
C58	C580	H581	76.688°	H5801	C580	H581	70.574°
H5802	C580	H581	116.059°	H5803	C580	H581	39.750°
C55	C580	H582	97.657°	C58	C580	H582	54.831°
H5801	C580	H582	144.366°	H5802	C580	H582	39.005°
H5803	C580	H582	78.308°	H581	C580	H582	105.004°
C55	C58	C580	75.9(14)°	C55	C58	H5802	97.933°
C580	C58	H5802	49.284°	C55	C58	H5803	126.880°
C580	C58	H5803	90.427°	H5802	C58	H5803	111.158°
C55	C58	H581	110.462°	C580	C58	H581	52.681°
H5802	C58	H581	82.415°	H5803	C58	H581	37.796°
C55	C58	H582	108.206°	C580	C58	H582	84.671°
H5802	C58	H582	35.532°	H5803	C58	H582	121.481°
H581	C58	H582	109.476°	C55	C58	H583	109.724°
C580	C58	H583	161.184°	H5802	C58	H583	142.578°
H5803	C58	H583	71.741°	H581	C58	H583	109.476°
H582	C58	H583	109.476°	C56	C59	C590	76.6(17)°
C56	C59	H5902	122.943°	C590	C59	H5902	83.356°
C56	C59	H5903	99.632°	C590	C59	H5903	54.485°
H5902	C59	H5903	110.722°	C56	C59	H591	107.592°
C590	C59	H591	43.749°	H5902	C59	H591	40.218°
H5903	C59	H591	78.635°	C56	C59	H592	111.040°
C590	C59	H592	151.380°	H5902	C59	H592	69.257°
H5903	C59	H592	143.135°	H591	C59	H592	109.475°
C56	C59	H593	109.750°	C590	C59	H593	92.435°

H5902 C59	H593	124.121°	H5903 C59	H593	38.034°
H591 C59	H593	109.475°	H592 C59	H593	109.477°
C56 C590	C59	75.7(15)°	C56 C590	H5901	113.477°
C59 C590	H5901	155.527°	C56 C590	H5902	104.075°
C59 C590	H5902	46.366°	H5901 C590	H5902	109.476°
C56 C590	H5903	110.697°	C59 C590	H5903	86.444°
H5901 C590	H5903	109.475°	H5902 C590	H5903	109.475°
C56 C590	H591	130.997°	C59 C590	H591	85.701°
H5901 C590	H591	71.160°	H5902 C590	H591	39.980°
H5903 C590	H591	112.888°	C56 C590	H593	95.533°
C59 C590	H593	50.731°	H5901 C590	H593	143.308°
H5902 C590	H593	82.944°	H5903 C590	H593	35.797°
H591 C590	H593	106.906°	C55 C570	C57	63.5(18)°
C55 C570	H5701	109.244°	C57 C570	H5701	56.044°
C55 C570	H5702	107.995°	C57 C570	H5702	94.107°
H5701 C570	H5702	109.475°	C55 C570	H5703	111.146°
C57 C570	H5703	155.979°	H5701 C570	H5703	109.475°
H5702 C570	H5703	109.476°	C55 C570	H572	93.380°
C57 C570	H572	62.147°	H5701 C570	H572	88.815°
H5702 C570	H572	31.999°	H5703 C570	H572	141.096°
C55 C570	H573	118.719°	C57 C570	H573	104.772°
H5701 C570	H573	54.692°	H5702 C570	H573	133.265°
H5703 C570	H573	55.568°	H572 C570	H573	136.535°
C55 C57	C570	94.6(19)°	C55 C57	H5701	141.303°
C570 C57	H5701	84.438°	C55 C57	H5702	107.358°
C570 C57	H5702	54.520°	H5701 C57	H5702	103.366°
C55 C57	H571	109.747°	C570 C57	H571	145.241°
H5701 C57	H571	60.998°	H5702 C57	H571	133.245°
C55 C57	H572	110.077°	C570 C57	H572	83.433°
H5701 C57	H572	108.232°	H5702 C57	H572	28.952°
H571 C57	H572	109.475°	C55 C57	H573	108.573°
C570 C57	H573	37.043°	H5701 C57	H573	51.983°
H5702 C57	H573	83.951°	H571 C57	H573	109.476°
H572 C57	H573	109.475°	C56 O420	B41	111.8(9)°
C56 O420	O42	95.9(19)°	B41 O420	O42	72.5(16)°
C55 O41	B41	106.6(4)°	C55 O41	O410	70.4(19)°
B41 O41	O410	79(2)°	C570 H5701	C57	39.518°
C570 H5701	H573	38.467°	C57 H5701	H573	74.567°
C570 H5702	C57	31.373°	C570 H5702	H572	85.475°
C57 H5702	H572	54.144°	C570 H5703	H573	38.425°
C570 H572	C57	34.420°	C570 H572	H5702	62.525°

C57	H572	H5702	96.904°	C570	H573	C57	38.185°
C570	H573	H5701	86.841°	C57	H573	H5701	53.450°
C570	H573	H5703	86.006°	C57	H573	H5703	122.688°
H5701	H573	H5703	166.693°	C580	H5802	C58	37.024°
C580	H5802	H582	86.009°	C58	H5802	H582	49.134°
C580	H5803	C58	52.601°	C580	H5803	H581	54.578°
C58	H5803	H581	107.118°	C580	H581	C58	50.632°
C580	H581	H5803	85.671°	C58	H581	H5803	35.085°
C580	H582	C58	40.498°	C580	H582	H5802	54.986°
C58	H582	H5802	95.335°	C600	H6001	H601	29.498°
C60	H6002	C600	33.373°	C60	H6002	H602	65.720°
C600	H6002	H602	98.217°	C60	H6003	C600	33.367°
C60	H6003	H603	78.653°	C600	H6003	H603	111.868°
C60	H601	C600	23.309°	C60	H601	H6001	130.331°
C600	H601	H6001	107.028°	C60	H603	C600	24.915°
C60	H603	H6003	71.071°	C600	H603	H6003	46.306°
C59	H5902	C590	50.278°	C59	H5902	H591	93.097°
C590	H5902	H591	43.553°	C59	H5903	C590	39.071°
C59	H5903	H593	54.556°	C590	H5903	H593	93.542°
C59	H591	C590	50.550°	C59	H591	H5902	46.685°
C590	H591	H5902	96.466°	C59	H593	C590	36.834°
C59	H593	H5903	87.410°	C590	H593	H5903	50.662°
C400	H4001	C40	46.888°	C400	H4001	H403	55.361°
C40	H4001	H403	101.190°	C400	H4002	C40	34.200°
C400	H4002	H402	84.045°	C40	H4002	H402	49.982°
C400	H402	C40	38.611°	C400	H402	H4002	58.761°
C40	H402	H4002	97.233°	C400	H403	C40	46.004°
C400	H403	H4001	83.759°	C40	H403	H4001	38.579°
C390	H3901	C39	37.547°	C390	H3901	H393	41.849°
C39	H3901	H393	77.651°	C390	H3902	C39	33.955°
C390	H3902	H392	100.490°	C39	H3902	H392	66.823°
C390	H392	C39	28.956°	C390	H392	H3902	52.135°
C39	H392	H3902	80.803°	C390	H393	C39	36.464°
C390	H393	H3901	86.594°	C39	H393	H3901	52.313°
C37	H3701	C370	41.040°	C37	H3701	H371	95.286°
C370	H3701	H371	55.491°	C37	H3703	C370	32.020°
C37	H3703	H372	51.469°	C370	H3703	H372	83.185°
C37	H371	C370	41.458°	C37	H371	H3701	38.964°
C370	H371	H3701	79.495°	C37	H372	C370	36.754°
C37	H372	H3703	101.172°	C370	H372	H3703	64.726°
C38	H381	C380	30.076°	C38	H381	H3803	95.505°

C380	H381	H3803	65.507°
C38	H383	H3802	48.977°
C38	H3802	C380	33.133°
C380	H3802	H383	48.703°
C38	H3803	H381	64.227°
C60	H602	H6002	61.529°

C38	H383	C380	33.095°
C380	H383	H3802	82.071°
C38	H3802	H383	81.836°
C38	H3803	C380	29.853°
C380	H3803	H381	94.003°

(6-(Dimethylammonium)-1,2-dihydroacenaphthylen-5-yl)trifluoroborate (6)**Refinement**

Crystal data, data collection and structure refinement details are summarized in Table 1.

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996); *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Crystal data

$C_{14}H_{15}BF_3N \cdot C_3H_6O$

$M_r = 323.16$

Triclinic, $P\bar{1}$

$a = 7.7848$ (9) Å

$b = 8.3548$ (10) Å

$c = 13.5437$ (14) Å

$\alpha = 101.869$ (2)°

$\beta = 103.288$ (3)°

$\gamma = 99.358$ (3)°

$V = 818.35$ (16) Å³

$Z = 2$

$F(000) = 340$

$D_x = 1.311$ Mg m⁻³

Mo K α radiation, $\lambda = 0.71073$ Å

Cell parameters from 4959 reflections

$q = 2.6\text{--}30.0^\circ$

$\mu = 0.10$ mm⁻¹

$T = 173$ K

Platelet, colorless

$0.27 \times 0.17 \times 0.07$ mm

Data collection

Bruker diffractometer Radiation source: fine-focus sealed tube Graphite monochromator f and w scans Absorption correction: multi-scan SADABS (Sheldrick, 2008) $T_{\min} = 0.712$, $T_{\max} = 0.746$ 15726 measured reflections	APEX-II CCD 3327 independent reflections 2739 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.030$ $q_{\max} = 26.4^\circ$, $q_{\min} = 1.6^\circ$ $h = -9 \text{--} 9$ $k = -10 \text{--} 10$ $l = -15 \text{--} 16$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.265P]$
	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(D/s)_{\max} < 0.001$
3327 reflections	$D\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$
212 parameters	$D\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.08093 (16)	0.33482 (13)	0.15169 (8)	0.0250 (3)
H1	0.0376	0.4335	0.1323	0.030*
B1	-0.0122 (2)	0.68221 (19)	0.17771 (12)	0.0268 (3)
F1	-0.16971 (11)	0.55194 (10)	0.13136 (7)	0.0364 (2)
F2	-0.05857 (12)	0.83461 (10)	0.17113 (7)	0.0377 (2)
F3	0.10487 (12)	0.65171 (11)	0.11192 (6)	0.0368 (2)
C1	0.2832 (2)	0.67373 (19)	0.62358 (11)	0.0312 (3)
H1A	0.1930	0.6837	0.6642	0.037*
H1B	0.3969	0.7568	0.6630	0.037*
C2	0.3172 (2)	0.49394 (18)	0.60305 (10)	0.0303 (3)
H2A	0.4463	0.4956	0.6327	0.036*

H2B	0.2429	0.4226	0.6347	0.036*
C3	0.26254 (19)	0.27941 (17)	0.42177 (11)	0.0274 (3)
H3	0.3032	0.1937	0.4510	0.033*
C4	0.20086 (19)	0.25471 (16)	0.31229 (10)	0.0263 (3)
H4	0.2007	0.1508	0.2677	0.032*
C5	0.14097 (17)	0.37654 (16)	0.26817 (10)	0.0216 (3)
C6	0.07828 (17)	0.67723 (15)	0.29662 (10)	0.0221 (3)
C7	0.09191 (18)	0.81802 (17)	0.37548 (11)	0.0272 (3)
H7	0.0540	0.9115	0.3548	0.033*
C8	0.15771 (19)	0.83324 (17)	0.48403 (11)	0.0302 (3)
H8	0.1635	0.9338	0.5338	0.036*
C9	0.26243 (17)	0.42963 (16)	0.48487 (10)	0.0245 (3)
C10	0.13783 (16)	0.53694 (15)	0.32959 (10)	0.0201 (3)
C11	0.21268 (18)	0.70081 (17)	0.51598 (10)	0.0257 (3)
C12	0.20257 (17)	0.55472 (16)	0.43891 (10)	0.0220 (3)
C13	-0.0752 (2)	0.1875 (2)	0.10557 (12)	0.0431 (4)
H13A	-0.0378	0.0868	0.1210	0.065*
H13B	-0.1154	0.1716	0.0294	0.065*
H13C	-0.1749	0.2074	0.1360	0.065*
C14	0.2335 (2)	0.3132 (2)	0.10401 (12)	0.0451 (4)
H14A	0.3333	0.4119	0.1354	0.068*
H14B	0.1919	0.3004	0.0282	0.068*
H14C	0.2753	0.2131	0.1172	0.068*
O1	0.4255 (2)	1.01019 (17)	0.15244 (11)	0.0706 (5)
C15	0.4771 (2)	0.88255 (19)	0.15696 (13)	0.0368 (4)
C16	0.5279 (2)	0.8354 (2)	0.25869 (13)	0.0473 (4)
H16A	0.4983	0.9142	0.3132	0.071*
H16B	0.6581	0.8393	0.2785	0.071*
H16C	0.4608	0.7216	0.2510	0.071*
C17	0.4915 (2)	0.7652 (2)	0.06159 (13)	0.0428 (4)
H17A	0.3837	0.6733	0.0350	0.064*
H17B	0.5995	0.7194	0.0795	0.064*
H17C	0.5008	0.8256	0.0076	0.064*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0353 (6)	0.0210 (5)	0.0199 (5)	0.0127 (5)	0.0059 (5)	0.0050 (4)
B1	0.0301 (8)	0.0210 (7)	0.0288 (8)	0.0095 (6)	0.0039 (6)	0.0072 (6)
F1	0.0336 (5)	0.0276 (4)	0.0385 (5)	0.0057 (4)	-0.0055 (4)	0.0058 (4)
F2	0.0493 (5)	0.0240 (4)	0.0387 (5)	0.0161 (4)	0.0021 (4)	0.0105 (4)
F3	0.0472 (5)	0.0418 (5)	0.0310 (5)	0.0190 (4)	0.0161 (4)	0.0169 (4)
C1	0.0326 (8)	0.0355 (8)	0.0219 (7)	0.0031 (6)	0.0073 (6)	0.0029 (6)
C2	0.0315 (7)	0.0353 (8)	0.0225 (7)	0.0006 (6)	0.0069 (6)	0.0098 (6)
C3	0.0311 (7)	0.0240 (7)	0.0284 (7)	0.0062 (6)	0.0052 (6)	0.0126 (5)
C4	0.0322 (7)	0.0207 (6)	0.0263 (7)	0.0082 (6)	0.0071 (6)	0.0059 (5)
C5	0.0238 (6)	0.0214 (6)	0.0196 (6)	0.0059 (5)	0.0049 (5)	0.0054 (5)
C6	0.0195 (6)	0.0197 (6)	0.0277 (7)	0.0046 (5)	0.0070 (5)	0.0063 (5)
C7	0.0278 (7)	0.0205 (6)	0.0329 (7)	0.0069 (5)	0.0076 (6)	0.0051 (5)
C8	0.0326 (8)	0.0236 (7)	0.0302 (7)	0.0054 (6)	0.0089 (6)	-0.0022 (6)

C9	0.0229 (6)	0.0274 (7)	0.0228 (6)	0.0015 (5)	0.0061 (5)	0.0088 (5)
C10	0.0177 (6)	0.0201 (6)	0.0229 (6)	0.0034 (5)	0.0068 (5)	0.0052 (5)
C11	0.0230 (7)	0.0282 (7)	0.0233 (7)	0.0016 (5)	0.0077 (5)	0.0028 (5)
C12	0.0190 (6)	0.0235 (6)	0.0232 (6)	0.0023 (5)	0.0077 (5)	0.0052 (5)
C13	0.0549 (10)	0.0306 (8)	0.0296 (8)	-0.0001 (7)	-0.0066 (7)	0.0046 (6)
C14	0.0528 (10)	0.0675 (12)	0.0297 (8)	0.0328 (9)	0.0203 (7)	0.0189 (8)
O1	0.1088 (13)	0.0408 (7)	0.0610 (9)	0.0355 (8)	0.0079 (8)	0.0124 (6)
C15	0.0328 (8)	0.0317 (8)	0.0417 (9)	0.0073 (6)	0.0019 (6)	0.0095 (7)
C16	0.0461 (10)	0.0505 (10)	0.0410 (9)	0.0089 (8)	0.0026 (8)	0.0141 (8)
C17	0.0343 (8)	0.0546 (10)	0.0423 (9)	0.0189 (8)	0.0101 (7)	0.0121 (8)

Geometric parameters (Å, °) for (shelx)

N1—C5	1.4868 (16)	C4—C5	1.3737 (18)
N1—C13	1.4937 (19)	C5—C10	1.4317 (17)
N1—C14	1.4948 (19)	C6—C7	1.3879 (18)
B1—F2	1.3933 (17)	C6—C10	1.4439 (17)
B1—F1	1.4191 (18)	C7—C8	1.413 (2)
B1—F3	1.4298 (18)	C8—C11	1.364 (2)
B1—C6	1.615 (2)	C9—C12	1.4105 (18)
C1—C11	1.5115 (19)	C10—C12	1.4178 (18)
C1—C2	1.547 (2)	C11—C12	1.4116 (18)
C2—C9	1.5134 (18)	O1—C15	1.2072 (19)
C3—C9	1.3656 (19)	C15—C17	1.491 (2)
C3—C4	1.4095 (19)	C15—C16	1.495 (2)
C5—N1—C13	113.02 (11)	C10—C6—B1	126.29 (11)
C5—N1—C14	112.11 (11)	C6—C7—C8	125.15 (13)
C13—N1—C14	111.34 (13)	C11—C8—C7	118.71 (12)
F2—B1—F1	108.56 (11)	C3—C9—C12	119.33 (12)
F2—B1—F3	107.66 (11)	C3—C9—C2	131.30 (12)
F1—B1—F3	104.92 (11)	C12—C9—C2	109.37 (11)
F2—B1—C6	112.85 (11)	C12—C10—C5	112.83 (11)
F1—B1—C6	110.50 (11)	C12—C10—C6	117.31 (11)
F3—B1—C6	111.98 (11)	C5—C10—C6	129.85 (12)
C11—C1—C2	105.05 (11)	C8—C11—C12	118.46 (12)
C9—C2—C1	104.93 (11)	C8—C11—C1	132.18 (12)
C9—C3—C4	118.38 (12)	C12—C11—C1	109.35 (12)
C5—C4—C3	121.93 (12)	C9—C12—C11	111.30 (12)
C4—C5—C10	122.62 (12)	C9—C12—C10	124.90 (12)
C4—C5—N1	116.49 (11)	C11—C12—C10	123.79 (12)
C10—C5—N1	120.89 (11)	O1—C15—C17	121.55 (15)
C7—C6—C10	116.57 (12)	O1—C15—C16	121.12 (16)
C7—C6—B1	117.06 (11)	C17—C15—C16	117.33 (14)

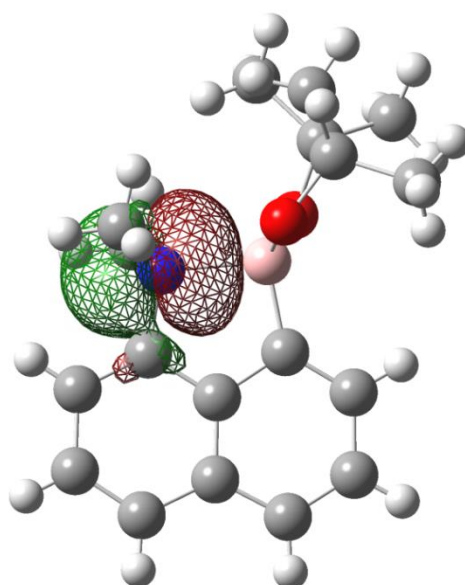
Document origin: *publCIF* [Westrip, S. P. (2010). *J. Apply. Cryst.*, **43**, 920-925].

H. Natural Bond Orbitals Data Tables

DFT calculations: Calculations have been performed with the Gaussian09 package at the B3LYP/6-31G** level unless otherwise stated.²

Natural bonding orbital (NBO) analysis: NBOs are transformed molecular orbitals, calculated to provide the ideal Lewis structure of a molecule. The NBO approach provides insights into the interaction between a filled (bonding or lone pair) Lewis type NBO (that act as a donor) and an empty (antibonding or Rydberg) non-Lewis NBO (that act as an acceptor).

1



Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. O	0.0000	0.0284	0.0209	0.0130	0.0044	0.0017	0.0043	0.0004	0.0014
2. O	0.0284	0.0000	0.0174	0.0162	0.0059	0.0013	0.0073	0.0002	0.0031
3. N	0.0209	0.0174	0.0000	0.0096	0.0105	0.9360	0.0036	0.0004	0.0003
4. C	0.0130	0.0162	0.0096	0.0000	1.2432	0.0132	1.5142	0.0076	0.1082
5. C	0.0044	0.0059	0.0105	1.2432	0.0000	1.2528	0.0115	0.0091	0.0103
6. C	0.0017	0.0013	0.9360	0.0132	1.2528	0.0000	0.0349	0.0001	0.0084
7. C	0.0043	0.0073	0.0036	1.5142	0.0115	0.0349	0.0000	0.9293	0.0103
8. H	0.0004	0.0002	0.0004	0.0076	0.0091	0.0001	0.9293	0.0000	0.0061
9. C	0.0014	0.0031	0.0003	0.1082	0.0103	0.0084	0.0103	0.0061	0.0000
10. H	0.0000	0.0000	0.0003	0.0003	0.0074	0.0001	0.0089	0.0001	0.9284

² Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian, Inc.*, Wallingford CT, **2009**.

	Atom	10	11	12	13	14	15	16	17	18
1.	O	0.0000	0.0200	0.0002	0.0038	0.0012	0.0003	0.0012	0.0003	0.0000
2.	O	0.0000	0.8811	0.0003	0.0015	0.0007	0.0002	0.0002	0.0005	0.0000
3.	N	0.0003	0.0032	0.0070	0.9174	0.0050	0.0016	0.0029	0.0004	0.0002
4.	C	0.0003	0.0055	0.0147	0.0011	0.0003	0.0002	0.0003	0.0128	0.0062
5.	C	0.0074	0.0006	1.2368	0.0078	0.0001	0.0001	0.0005	0.0554	0.0003
6.	C	0.0001	0.0004	0.0112	0.0088	0.0004	0.0005	0.0061	0.0020	0.0003
7.	C	0.0089	0.0007	0.0650	0.0005	0.0001	0.0000	0.0001	1.3049	0.0040
8.	H	0.0001	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0034	0.0012
9.	C	0.9284	0.0003	1.2665	0.0001	0.0000	0.0000	0.0000	1.5488	0.0053
10.	H	0.0000	0.0000	0.0044	0.0000	0.0000	0.0000	0.0000	0.0060	0.0018
11.	C	0.0000	0.0000	0.0001	0.0003	0.0001	0.0000	0.0001	0.0001	0.0000
12.	C	0.0044	0.0001	0.0000	0.0003	0.0000	0.0000	0.0001	0.0117	0.0083
13.	C	0.0000	0.0003	0.0003	0.0000	0.9431	0.9324	0.9326	0.0002	0.0000
14.	H	0.0000	0.0001	0.0000	0.9431	0.0000	0.0017	0.0015	0.0000	0.0000
15.	H	0.0000	0.0000	0.0000	0.9324	0.0017	0.0000	0.0023	0.0000	0.0000
16.	H	0.0000	0.0001	0.0001	0.9326	0.0015	0.0023	0.0000	0.0000	0.0000
17.	C	0.0060	0.0001	0.0117	0.0002	0.0000	0.0000	0.0000	0.0000	0.9315
18.	H	0.0018	0.0000	0.0083	0.0000	0.0000	0.0000	0.0000	0.9315	0.0000
19.	C	0.0000	0.9509	0.0002	0.0002	0.0001	0.0000	0.0002	0.0001	0.0000
20.	B	0.0004	0.0095	0.0080	0.0047	0.0052	0.0003	0.0002	0.0082	0.0001
21.	C	0.0000	0.0002	0.0003	0.0096	0.0004	0.0063	0.0002	0.0002	0.0000
22.	H	0.0000	0.0000	0.0000	0.0006	0.0005	0.0001	0.0001	0.0000	0.0000
23.	H	0.0000	0.0000	0.0002	0.0004	0.0001	0.0001	0.0001	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0091	0.0000	0.0004	0.0001	0.0000	0.0000
25.	C	0.0000	0.9880	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
26.	H	0.0000	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0010	0.0000	1.2700	0.0031	0.0000	0.0000	0.0008	0.0365	0.0001
30.	H	0.0002	0.0000	0.0045	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
31.	C	0.0000	0.0002	0.0624	0.0071	0.0003	0.0002	0.0015	0.0312	0.0000
32.	H	0.0000	0.0000	0.0003	0.0002	0.0001	0.0000	0.0001	0.0000	0.0000
33.	C	0.0001	0.0000	0.0106	0.0004	0.0000	0.0000	0.0001	0.0004	0.0002
34.	H	0.0000	0.0000	0.0077	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
35.	C	0.0000	0.0066	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

39.	C	0.0000	0.0054	0.0000	0.0009	0.0001	0.0000	0.0007	0.0000	0.0000
40.	H	0.0000	0.0076	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0007	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0004	0.0000	0.0001	0.0000	0.0000	0.0006	0.0000	0.0000
43.	C	0.0000	1.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0039	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0039	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0060	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		19	20	21	22	23	24	25	26	27
1.	O	0.8789	0.7848	0.0009	0.0009	0.0002	0.0002	0.0013	0.0003	0.0002
2.	O	0.0223	0.7540	0.0047	0.0015	0.0007	0.0012	0.0251	0.0012	0.0112
3.	N	0.0018	0.4028	0.9360	0.0054	0.0033	0.0025	0.0008	0.0000	0.0004
4.	C	0.0088	0.7963	0.0021	0.0004	0.0004	0.0001	0.0009	0.0000	0.0000
5.	C	0.0006	0.0143	0.0076	0.0001	0.0003	0.0002	0.0001	0.0000	0.0000
6.	C	0.0004	0.0054	0.0087	0.0005	0.0079	0.0004	0.0001	0.0000	0.0000
7.	C	0.0007	0.0162	0.0003	0.0002	0.0001	0.0000	0.0003	0.0000	0.0000
8.	H	0.0001	0.0007	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
9.	C	0.0003	0.0029	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
10.	H	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.9509	0.0095	0.0002	0.0000	0.0000	0.0000	0.9880	0.0034	0.0053
12.	C	0.0002	0.0080	0.0003	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
13.	C	0.0002	0.0047	0.0096	0.0006	0.0004	0.0091	0.0001	0.0000	0.0000
14.	H	0.0001	0.0052	0.0004	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000
15.	H	0.0000	0.0003	0.0063	0.0001	0.0001	0.0004	0.0000	0.0000	0.0000
16.	H	0.0002	0.0002	0.0002	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
17.	C	0.0001	0.0082	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
18.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0092	0.0003	0.0001	0.0001	0.0001	0.0059	0.0079	0.0007
20.	B	0.0092	0.0000	0.0049	0.0065	0.0002	0.0002	0.0045	0.0001	0.0004
21.	C	0.0003	0.0049	0.0000	0.9413	0.9322	0.9260	0.0002	0.0000	0.0000
22.	H	0.0001	0.0065	0.9413	0.0000	0.0015	0.0016	0.0001	0.0000	0.0000
23.	H	0.0001	0.0002	0.9322	0.0015	0.0000	0.0024	0.0001	0.0000	0.0000
24.	H	0.0001	0.0002	0.9260	0.0016	0.0024	0.0000	0.0000	0.0000	0.0000
25.	C	0.0059	0.0045	0.0002	0.0001	0.0001	0.0000	0.0000	0.9318	0.9336
26.	H	0.0079	0.0001	0.0000	0.0000	0.0000	0.0000	0.9318	0.0000	0.0021
27.	H	0.0007	0.0004	0.0000	0.0000	0.0000	0.0000	0.9336	0.0021	0.0000
28.	H	0.0004	0.0008	0.0000	0.0000	0.0000	0.0000	0.9313	0.0021	0.0020
29.	C	0.0000	0.0002	0.0017	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0001	0.0062	0.0041	0.0002	0.0012	0.0001	0.0000	0.0000	0.0000
32.	H	0.0000	0.0001	0.0003	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
33.	C	0.0000	0.0002	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	1.0010	0.0072	0.0001	0.0000	0.0001	0.0000	0.0029	0.0005	0.0005
36.	H	0.0038	0.0001	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001
37.	H	0.0039	0.0002	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.0001
38.	H	0.0061	0.0004	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001
39.	C	0.9849	0.0051	0.0012	0.0001	0.0003	0.0000	0.0078	0.0002	0.0001
40.	H	0.0032	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	0.0000
41.	H	0.0053	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
42.	H	0.0034	0.0005	0.0002	0.0000	0.0010	0.0000	0.0002	0.0000	0.0000
43.	C	0.0065	0.0077	0.0002	0.0000	0.0001	0.0000	0.0068	0.0013	0.0002
44.	H	0.0091	0.0001	0.0000	0.0000	0.0000	0.0000	0.0015	0.0001	0.0000
45.	H	0.0008	0.0002	0.0001	0.0000	0.0001	0.0000	0.0099	0.0001	0.0001
46.	H	0.0005	0.0004	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000

	Atom	28	29	30	31	32	33	34	35	36
1.	O	0.0005	0.0001	0.0000	0.0009	0.0000	0.0002	0.0000	0.0184	0.0014
2.	O	0.0017	0.0002	0.0000	0.0010	0.0000	0.0001	0.0000	0.0056	0.0009
3.	N	0.0001	0.0009	0.0004	0.0123	0.0025	0.0103	0.0004	0.0005	0.0000
4.	C	0.0002	0.0097	0.0003	0.0369	0.0002	0.0009	0.0002	0.0006	0.0000
5.	C	0.0001	0.0102	0.0072	0.0144	0.0083	0.0603	0.0003	0.0001	0.0000
6.	C	0.0000	0.1045	0.0003	1.5192	0.0058	0.0160	0.0058	0.0000	0.0000
7.	C	0.0002	0.0005	0.0000	0.0004	0.0003	0.0329	0.0000	0.0002	0.0000
8.	H	0.0002	0.0003	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0097	0.0010	0.0011	0.0003	0.0353	0.0002	0.0000	0.0000
10.	H	0.0000	0.0010	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
11.	C	0.0035	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0066	0.0090
12.	C	0.0000	1.2700	0.0045	0.0624	0.0003	0.0106	0.0077	0.0000	0.0000
13.	C	0.0000	0.0031	0.0000	0.0071	0.0002	0.0004	0.0000	0.0001	0.0000
14.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
15.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0008	0.0000	0.0015	0.0001	0.0001	0.0000	0.0000	0.0000
17.	C	0.0000	0.0365	0.0001	0.0312	0.0000	0.0004	0.0002	0.0000	0.0000

18.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
19.	C	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	1.0010	0.0038
20.	B	0.0008	0.0002	0.0003	0.0062	0.0001	0.0002	0.0002	0.0072	0.0001
21.	C	0.0000	0.0017	0.0000	0.0041	0.0003	0.0004	0.0000	0.0001	0.0000
22.	H	0.0000	0.0000	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0005	0.0000	0.0012	0.0001	0.0001	0.0000	0.0001	0.0000
24.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.9313	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0005
26.	H	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
27.	H	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
29.	C	0.0000	0.0000	0.9292	0.0099	0.0065	1.5497	0.0052	0.0000	0.0000
30.	H	0.0000	0.9292	0.0000	0.0080	0.0001	0.0053	0.0015	0.0000	0.0000
31.	C	0.0000	0.0099	0.0080	0.0000	0.9259	1.2947	0.0038	0.0000	0.0000
32.	H	0.0000	0.0065	0.0001	0.9259	0.0000	0.0052	0.0013	0.0000	0.0000
33.	C	0.0000	1.5497	0.0053	1.2947	0.0052	0.0000	0.9314	0.0000	0.0000
34.	H	0.0000	0.0052	0.0015	0.0038	0.0013	0.9314	0.0000	0.0000	0.0000
35.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9289
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9289	0.0000
37.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9279	0.0020
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9310	0.0021
39.	C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0065	0.0015
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013	0.0001
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0073	0.0001
43.	C	0.0074	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013	0.0001
44.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002
45.	H	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
46.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000

Atom		37	38	39	40	41	42	43	44	45
1.	O	0.0019	0.0107	0.0245	0.0012	0.0103	0.0014	0.0055	0.0009	0.0001
2.	O	0.0001	0.0005	0.0011	0.0003	0.0003	0.0004	0.0180	0.0016	0.0021
3.	N	0.0000	0.0002	0.0009	0.0000	0.0001	0.0003	0.0004	0.0000	0.0001
4.	C	0.0001	0.0001	0.0006	0.0000	0.0004	0.0001	0.0004	0.0000	0.0000
5.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
6.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0008	0.0005	0.0054	0.0076	0.0007	0.0004	1.0005	0.0039	0.0039
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0009	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
14.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0000	0.0007	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0039	0.0061	0.9849	0.0032	0.0053	0.0034	0.0065	0.0091	0.0008
20.	B	0.0002	0.0004	0.0051	0.0001	0.0003	0.0005	0.0077	0.0001	0.0002
21.	C	0.0000	0.0000	0.0012	0.0000	0.0000	0.0002	0.0002	0.0000	0.0001
22.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0010	0.0001	0.0000	0.0001
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0005	0.0001	0.0078	0.0003	0.0001	0.0002	0.0068	0.0015	0.0099
26.	H	0.0001	0.0000	0.0002	0.0003	0.0000	0.0000	0.0013	0.0001	0.0001
27.	H	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
28.	H	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0074	0.0001	0.0006
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.9279	0.9310	0.0065	0.0013	0.0002	0.0073	0.0013	0.0001	0.0001
36.	H	0.0020	0.0021	0.0015	0.0001	0.0000	0.0001	0.0001	0.0002	0.0000
37.	H	0.0000	0.0021	0.0097	0.0001	0.0001	0.0005	0.0001	0.0000	0.0000
38.	H	0.0021	0.0000	0.0002	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000
39.	C	0.0097	0.0002	0.0000	0.9330	0.9307	0.9372	0.0027	0.0004	0.0004
40.	H	0.0001	0.0000	0.9330	0.0000	0.0022	0.0020	0.0005	0.0000	0.0001
41.	H	0.0001	0.0000	0.9307	0.0022	0.0000	0.0022	0.0005	0.0001	0.0001
42.	H	0.0005	0.0001	0.9372	0.0020	0.0022	0.0000	0.0001	0.0000	0.0001
43.	C	0.0001	0.0001	0.0027	0.0005	0.0005	0.0001	0.0000	0.9276	0.9314
44.	H	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.9276	0.0000	0.0020
45.	H	0.0000	0.0000	0.0004	0.0001	0.0001	0.0001	0.9314	0.0020	0.0000

46. H 0.0000 0.0001 0.0001 0.0000 0.0001 0.0000 0.9307 0.0021 0.0020

	Atom	46
1.	O	0.0005
2.	O	0.0113
3.	N	0.0000
4.	C	0.0003
5.	C	0.0001
6.	C	0.0000
7.	C	0.0001
8.	H	0.0000
9.	C	0.0001
10.	H	0.0000
11.	C	0.0060
12.	C	0.0000
13.	C	0.0000
14.	H	0.0000
15.	H	0.0000
16.	H	0.0000
17.	C	0.0000
18.	H	0.0000
19.	C	0.0005
20.	B	0.0004
21.	C	0.0000
22.	H	0.0000
23.	H	0.0000
24.	H	0.0000
25.	C	0.0003
26.	H	0.0000
27.	H	0.0000
28.	H	0.0001
29.	C	0.0000
30.	H	0.0000
31.	C	0.0000
32.	H	0.0000
33.	C	0.0000
34.	H	0.0000
35.	C	0.0001
36.	H	0.0000
37.	H	0.0000
38.	H	0.0001
39.	C	0.0001
40.	H	0.0000
41.	H	0.0001
42.	H	0.0000
43.	C	0.9307
44.	H	0.0021
45.	H	0.0020
46.	H	0.0000

(Occupancy)	Bond orbital / Coefficients / Hybrids
	Lewis
1. (1.99972) CR (1) O 1	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
2. (1.99974) CR (1) O 2	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
3. (1.99947) CR (1) N 3	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
4. (1.99882) CR (1) C 4	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
5. (1.99891) CR (1) C 5	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
6. (1.99889) CR (1) C 6	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

7. (1.99915) CR (1) C 7	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
8. (1.99916) CR (1) C 9	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
9. (1.99900) CR (1) C 11	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
10. (1.99902) CR (1) C 12	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
11. (1.99933) CR (1) C 13	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
12. (1.99924) CR (1) C 17	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
13. (1.99898) CR (1) C 19	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
14. (1.99909) CR (1) B 20	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
15. (1.99939) CR (1) C 21	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
16. (1.99937) CR (1) C 25	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
17. (1.99918) CR (1) C 29	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
18. (1.99904) CR (1) C 31	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
19. (1.99926) CR (1) C 33	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
20. (1.99934) CR (1) C 35	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
21. (1.99937) CR (1) C 39	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
22. (1.99934) CR (1) C 43	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
23. (1.95075) LP (1) O 1	s(26.75%)p 2.73(73.16%)d 0.00(0.09%)	0.0000	0.5172	0.0041	-0.0028	0.0697
		0.0063	0.1220	0.0010	-0.8437	0.0017
		-0.0010	0.0046	0.0080	0.0007	-0.0294
24. (1.86132) LP (2) O 1	s(0.00%)p 1.00(99.89%)d 0.00(0.11%)	0.0000	0.0016	-0.0005	0.0003	-0.0342
		0.0009	0.9888	-0.0006	0.1412	-0.0002
		-0.0049	-0.0016	0.0320	0.0042	0.0081
25. (1.95124) LP (1) O 2	s(29.28%)p 2.41(70.63%)d 0.00(0.08%)	0.0000	0.5411	0.0026	-0.0032	0.1978
		0.0064	-0.0276	0.0003	0.8163	-0.0016
		-0.0005	-0.0120	0.0033	-0.0005	-0.0263
26. (1.87542) LP (2) O 2	s(0.18%)p99.99(99.72%)d 0.60(0.11%)					

				0.0000	0.0419	-0.0009	0.0002	-0.1577
				-0.0007	-0.9858	0.0007	-0.0230	-0.0001
				0.0097	0.0049	0.0303	0.0044	0.0012
27.	(1.70604)	LP (1) N 3	s(16.87%)p 4.93(83.13%)d 0.00(0.00%)	0.0000	0.4105	-0.0151	-0.0002	-0.5178
				0.0098	0.7496	-0.0343	0.0093	0.0007
				0.0020	0.0002	0.0005	-0.0033	-0.0006
28.	(0.99238)	LP (1) C 12	s(0.00%)p 1.00(100.00%)d 0.00(0.00%)	0.0000	0.0012	-0.0008	0.0000	0.0881
				0.0022	-0.0950	-0.0028	-0.9916	0.0000
				-0.0002	0.0017	0.0010	0.0003	-0.0001
29.	(1.97858)	BD (1) O 1- C 19	s(26.59%)p 2.76(73.27%)d 0.01(0.14%)	0.0000	0.5156	0.0035	0.0014	-0.8194
	(67.76%)	0.8232* O 1		-0.0080	-0.0633	-0.0005	0.2389	-0.0106
				0.0062	-0.0292	-0.0040	0.0231	0.0009
	(32.24%)	0.5678* C 19	s(18.50%)p 4.40(81.32%)d 0.01(0.19%)	0.0000	0.4299	0.0132	-0.0025	0.8393
				0.0089	0.0586	0.0079	-0.3213	-0.0435
				0.0057	-0.0231	-0.0015	0.0331	-0.0139
30.	(1.98758)	BD (1) O 1- B 20	s(46.62%)p 1.14(53.24%)d 0.00(0.15%)	0.0000	0.6827	-0.0048	0.0022	0.5661
	(81.31%)	0.9017* O 1		0.0033	-0.0469	0.0017	0.4578	-0.0087
				-0.0034	0.0289	-0.0051	0.0106	0.0219
	(18.69%)	0.4323* B 20	s(28.76%)p 2.46(70.87%)d 0.01(0.37%)	0.0000	0.5363	-0.0012	-0.0052	-0.5101
				0.0136	-0.0146	0.0056	-0.6675	-0.0501
				-0.0046	0.0531	0.0003	0.0153	0.0248
31.	(1.97756)	BD (1) O 2- C 11	s(26.74%)p 2.73(73.12%)d 0.01(0.14%)	0.0000	0.5171	0.0047	0.0019	-0.8292
	(67.63%)	0.8224* O 2		-0.0060	0.1577	0.0009	-0.1362	0.0110
				-0.0112	0.0248	-0.0057	0.0252	-0.0054
	(32.37%)	0.5689* C 11	s(18.27%)p 4.46(81.54%)d 0.01(0.18%)	0.0000	0.4273	0.0127	-0.0028	0.8570
				0.0144	-0.1942	-0.0068	0.2034	0.0412
				-0.0161	0.0144	-0.0031	0.0319	-0.0180
32.	(1.98564)	BD (1) O 2- B 20	s(43.75%)p 1.28(56.11%)d 0.00(0.14%)	0.0000	0.6615	-0.0044	0.0024	0.4965
	(81.11%)	0.9006* O 2		0.0045	-0.0383	-0.0018	-0.5594	0.0092
				-0.0016	-0.0221	-0.0010	0.0059	0.0293
	(18.89%)	0.4346* B 20	s(28.86%)p 2.45(70.79%)d 0.01(0.35%)	0.0000	0.5372	-0.0020	-0.0047	-0.4040
				0.0240	-0.0273	-0.0057	0.7355	0.0486
				-0.0020	-0.0462	-0.0012	0.0088	0.0360
33.	(1.97815)	BD (1) N 3- C 6	s(29.50%)p 2.39(70.43%)d 0.00(0.07%)	0.0000	0.5431	0.0011	-0.0002	0.7956
	(62.23%)	0.7889* N 3		0.0069	0.2510	-0.0013	0.0908	0.0038
				0.0050	0.0040	-0.0004	0.0236	-0.0105
	(37.77%)	0.6146* C 6	s(26.15%)p 2.82(73.74%)d 0.00(0.12%)	0.0000	0.5113	0.0058	-0.0026	-0.8098
				-0.0083	-0.2771	-0.0068	-0.0688	0.0005
				0.0148	0.0053	0.0012	0.0241	-0.0183
34.	(1.97649)	BD (1) N 3- C 13	s(24.81%)p 3.03(75.13%)d 0.00(0.05%)	0.0000	0.4981	0.0058	0.0006	-0.1378
	(63.31%)	0.7956* N 3		-0.0125	-0.3583	-0.0046	-0.7768	-0.0181
				0.0021	-0.0041	0.0189	-0.0059	0.0115
	(36.69%)	0.6058* C 13	s(20.73%)p 3.82(79.15%)d 0.01(0.12%)	0.0000	0.4553	0.0064	0.0018	0.0904
				-0.0057	0.3949	0.0024	0.7920	0.0071
				0.0030	0.0062	0.0225	-0.0050	0.0247
35.	(1.98228)	BD (1) N 3- C 21	s(28.80%)p 2.47(71.14%)d 0.00(0.06%)	0.0000	0.5366	0.0107	0.0002	-0.2806
	(63.02%)	0.7939* N 3		-0.0159	-0.4953	-0.0067	0.6219	0.0172
				0.0064	-0.0004	-0.0201	-0.0101	0.0047
	(36.98%)	0.6081* C 21	s(22.03%)p 3.53(77.84%)d 0.01(0.13%)	0.0000	0.4692	0.0110	0.0026	0.2424
				-0.0028	0.5531	0.0109	-0.6430	-0.0125
				0.0108	-0.0130	-0.0280	-0.0085	0.0119
36.	(1.96463)	BD (1) C 4- C 5	s(29.27%)p 2.41(70.67%)d 0.00(0.06%)	0.0000	0.5409	0.0091	0.0009	0.7206
	(48.29%)	0.6949* C 4						

					0.0228	-0.4242	0.0002	0.0827	0.0008
					-0.0154	0.0035	-0.0027	0.0112	-0.0163
	(51.71%)	0.7191*	C	5	s(33.93%)	p 1.95(66.03%)	d 0.00(0.04%)		
					0.0000	0.5824	-0.0041	-0.0006	-0.6623
					0.0110	0.4642	0.0007	-0.0777	0.0006
					-0.0132	0.0033	-0.0019	0.0076	-0.0126
37.	(1.97423)	BD (1)	C	4-	C	7			
	(50.76%)	0.7124*	C	4	s(35.21%)	p 1.84(64.74%)	d 0.00(0.05%)		
					0.0000	0.5928	0.0251	-0.0001	0.0346
					-0.0130	0.7990	0.0379	-0.0785	-0.0050
					0.0076	-0.0006	-0.0037	-0.0169	-0.0132
	(49.24%)	0.7017*	C	7	s(35.37%)	p 1.83(64.57%)	d 0.00(0.05%)		
					0.0000	0.5947	0.0005	0.0041	-0.0887
					-0.0225	-0.7936	0.0012	0.0871	-0.0026
					0.0029	0.0001	-0.0046	-0.0175	-0.0136
38.	(1.68986)	BD (2)	C	4-	C	7			
	(47.75%)	0.6910*	C	4	s(0.00%)	p 1.00(99.95%)	d 0.00(0.05%)		
					0.0000	0.0030	0.0001	0.0000	0.0518
					0.0004	-0.1019	-0.0053	-0.9930	-0.0174
					0.0000	-0.0136	-0.0167	0.0027	0.0024
	(52.25%)	0.7228*	C	7	s(0.00%)	p 1.00(99.97%)	d 0.00(0.03%)		
					0.0000	0.0037	0.0021	-0.0004	0.0662
					-0.0032	-0.1134	-0.0002	-0.9910	0.0204
					-0.0012	-0.0047	0.0163	-0.0016	-0.0038
39.	(1.95829)	BD (1)	C	4-	B	20			
	(70.19%)	0.8378*	C	4	s(35.23%)	p 1.84(64.74%)	d 0.00(0.02%)		
					0.0000	0.5932	-0.0205	-0.0004	-0.6890
					0.0371	-0.4109	0.0490	0.0079	-0.0023
					0.0115	-0.0007	-0.0011	0.0004	-0.0095
	(29.81%)	0.5460*	B	20	s(34.36%)	p 1.91(65.53%)	d 0.00(0.11%)		
					0.0000	0.5860	0.0073	0.0097	0.6623
					0.0012	0.4621	0.0321	-0.0461	-0.0011
					0.0268	-0.0038	-0.0015	0.0056	-0.0185
40.	(1.97060)	BD (1)	C	5-	C	6			
	(50.17%)	0.7083*	C	5	s(31.97%)	p 2.13(67.97%)	d 0.00(0.06%)		
					0.0000	0.5654	0.0046	-0.0001	-0.0824
					0.0009	-0.8190	0.0030	0.0472	-0.0007
					0.0047	0.0004	-0.0018	-0.0184	-0.0145
	(49.83%)	0.7059*	C	6	s(35.26%)	p 1.83(64.68%)	d 0.00(0.05%)		
					0.0000	0.5938	-0.0053	0.0013	0.1043
					0.0031	0.7970	-0.0073	-0.0268	0.0021
					0.0040	0.0003	-0.0022	-0.0183	-0.0126
41.	(1.96694)	BD (1)	C	5-	C	12			
	(50.78%)	0.7126*	C	5	s(34.05%)	p 1.94(65.90%)	d 0.00(0.05%)		
					0.0000	0.5835	0.0010	0.0013	0.7412
					-0.0061	0.3299	0.0008	0.0279	0.0003
					0.0112	0.0014	0.0000	0.0137	-0.0135
	(49.22%)	0.7016*	C	12	s(31.80%)	p 2.14(68.15%)	d 0.00(0.05%)		
					0.0000	0.5639	-0.0035	0.0015	-0.7535
					0.0050	-0.3355	0.0040	-0.0341	0.0007
					0.0125	0.0019	-0.0003	0.0115	-0.0142
42.	(1.97771)	BD (1)	C	6-	C	31			
	(50.70%)	0.7120*	C	6	s(38.51%)	p 1.60(61.45%)	d 0.00(0.05%)		
					0.0000	0.6205	0.0060	0.0007	0.5683
					-0.0010	-0.5343	-0.0147	0.0763	0.0022
					-0.0177	0.0024	-0.0023	0.0021	-0.0110
	(49.30%)	0.7022*	C	31	s(34.79%)	p 1.87(65.15%)	d 0.00(0.06%)		
					0.0000	0.5898	0.0000	0.0037	-0.6378
					-0.0168	0.4852	-0.0165	-0.0937	-0.0002
					-0.0185	0.0042	-0.0030	0.0050	-0.0153
43.	(1.76205)	BD (2)	C	6-	C	31			
	(49.62%)	0.7044*	C	6	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
					0.0000	0.0038	0.0020	0.0002	-0.0968
					-0.0018	0.0434	0.0016	0.9941	-0.0139
					0.0018	0.0170	-0.0086	-0.0016	0.0034
	(50.38%)	0.7098*	C	31	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
					0.0000	0.0034	0.0017	0.0000	-0.1088
					-0.0007	0.0445	0.0010	0.9927	-0.0191
					-0.0021	-0.0125	0.0154	0.0006	-0.0035
44.	(1.98327)	BD (1)	C	7-	H	8			
	(60.38%)	0.7770*	C	7	s(31.58%)	p 2.16(68.35%)	d 0.00(0.07%)		
					0.0000	0.5620	-0.0004	-0.0036	-0.6624
					-0.0092	0.4848	0.0094	-0.0977	-0.0032
					-0.0202	0.0044	-0.0033	0.0069	-0.0136
	(39.62%)	0.6295*	H	8	s(99.93%)	p 0.00(0.07%)			
					0.9996	-0.0016	0.0225	-0.0146	0.0035
45.	(1.97979)	BD (1)	C	7-	C	17			

	(49.80%)	0.7057* C 7	s(32.87%)p 2.04(67.08%)d 0.00(0.05%)	0.0000	0.5733	0.0021	0.0008	0.7403	-0.0087	0.3486	0.0314	0.0117	-0.0029	0.0130	0.0011	-0.0003	0.0116	-0.0131
	(50.20%)	0.7085* C 17	s(33.16%)p 2.01(66.79%)d 0.00(0.05%)	0.0000	0.5759	-0.0027	0.0017	-0.7394	-0.0163	-0.3462	0.0250	-0.0203	-0.0035	0.0131	0.0011	-0.0003	0.0104	-0.0134
46. (1.98166)	BD (1) C 9- H 10	0.7772* C 9	s(31.30%)p 2.19(68.64%)d 0.00(0.07%)	0.0000	0.5594	-0.0011	-0.0041	0.7366	0.0093	0.3785	0.0111	0.0179	-0.0003	0.0171	0.0011	0.0001	0.0124	-0.0143
	(60.40%)			0.0000	0.5594	-0.0011	-0.0041	0.7366	0.0093	0.3785	0.0111	0.0179	-0.0003	0.0171	0.0011	0.0001	0.0124	-0.0143
	(39.60%)	0.6293* H 10	s(99.93%)p 0.00(0.07%)	0.9996	-0.0011	-0.0236	-0.0127	-0.0005										
47. (1.97539)	BD (1) C 9- C 12	0.6966* C 9	s(33.24%)p 2.01(66.70%)d 0.00(0.05%)	0.0000	0.5766	-0.0045	0.0033	-0.0231	0.0228	-0.8116	0.0019	0.0848	0.0008	0.0017	0.0004	-0.0044	-0.0177	-0.0145
	(48.53%)			0.0000	0.5766	-0.0045	0.0033	-0.0231	0.0228	-0.8116	0.0019	0.0848	0.0008	0.0017	0.0004	-0.0044	-0.0177	-0.0145
	(51.47%)	0.7174* C 12	s(34.09%)p 1.93(65.87%)d 0.00(0.04%)	0.0000	0.5839	0.0024	-0.0003	0.0822	0.0223	0.8042	0.0001	-0.0690	0.0007	0.0008	0.0003	-0.0033	-0.0158	-0.0112
48. (1.97918)	BD (1) C 9- C 17	0.7097* C 9	s(35.29%)p 1.83(64.66%)d 0.00(0.05%)	0.0000	0.5940	0.0065	0.0021	-0.6710	0.0070	0.4312	0.0323	-0.0970	-0.0022	-0.0153	0.0040	-0.0025	0.0086	-0.0132
	(50.37%)			0.0000	0.5940	0.0065	0.0021	-0.6710	0.0070	0.4312	0.0323	-0.0970	-0.0022	-0.0153	0.0040	-0.0025	0.0086	-0.0132
	(49.63%)	0.7045* C 17	s(35.24%)p 1.84(64.70%)d 0.00(0.05%)	0.0000	0.5936	0.0040	0.0030	0.6660	0.0265	-0.4402	0.0187	0.0933	-0.0001	-0.0169	0.0039	-0.0030	0.0070	-0.0135
49. (1.74982)	BD (2) C 9- C 17	0.7141* C 9	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	-0.0013	0.0004	0.0000	-0.0770	-0.0002	0.1048	-0.0001	0.9911	-0.0224	-0.0022	-0.0178	0.0047	0.0009	-0.0033
	(50.99%)			0.0000	-0.0013	0.0004	0.0000	-0.0770	-0.0002	0.1048	-0.0001	0.9911	-0.0224	-0.0022	-0.0178	0.0047	0.0009	-0.0033
	(49.01%)	0.7001* C 17	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0027	-0.0006	0.0000	-0.0732	0.0000	0.1030	-0.0014	0.9915	-0.0246	0.0024	0.0133	-0.0132	0.0004	0.0041
50. (1.97796)	BD (1) C 11- C 19	0.7066* C 11	s(27.50%)p 2.63(72.44%)d 0.00(0.06%)	0.0000	0.5241	-0.0173	0.0003	-0.1123	-0.0174	-0.2019	0.0001	-0.8188	0.0150	0.0021	0.0036	0.0097	-0.0018	0.0231
	(49.92%)			0.0000	0.5241	-0.0173	0.0003	-0.1123	-0.0174	-0.2019	0.0001	-0.8188	0.0150	0.0021	0.0036	0.0097	-0.0018	0.0231
	(50.08%)	0.7077* C 19	s(27.45%)p 2.64(72.48%)d 0.00(0.06%)	0.0000	0.5236	-0.0182	0.0003	0.0347	-0.0202	0.2001	0.0020	0.8264	-0.0121	0.0001	0.0040	0.0095	-0.0019	0.0231
51. (1.98045)	BD (1) C 11- C 25	0.7063* C 11	s(26.30%)p 2.80(73.65%)d 0.00(0.05%)	0.0000	0.5128	-0.0017	0.0007	-0.0969	-0.0003	0.8420	-0.0009	0.1340	0.0145	-0.0049	-0.0026	0.0051	-0.0192	-0.0088
	(49.88%)			0.0000	0.5128	-0.0017	0.0007	-0.0969	-0.0003	0.8420	-0.0009	0.1340	0.0145	-0.0049	-0.0026	0.0051	-0.0192	-0.0088
	(50.12%)	0.7079* C 25	s(25.67%)p 2.89(74.29%)d 0.00(0.04%)	0.0000	0.5066	-0.0076	0.0010	0.1022	0.0056	-0.8423	0.0188	-0.1499	0.0131	-0.0032	-0.0006	0.0061	-0.0161	-0.0085
52. (1.98029)	BD (1) C 11- C 43	0.7059* C 11	s(27.85%)p 2.59(72.10%)d 0.00(0.05%)	0.0000	0.5275	0.0140	0.0007	-0.4906	0.0118	-0.4602	-0.0028	0.5180	0.0095	0.0128	-0.0144	-0.0114	-0.0004	0.0020
	(49.83%)			0.0000	0.5275	0.0140	0.0007	-0.4906	0.0118	-0.4602	-0.0028	0.5180	0.0095	0.0128	-0.0144	-0.0114	-0.0004	0.0020
	(50.17%)	0.7083* C 43	s(26.62%)p 2.75(73.34%)d 0.00(0.04%)	0.0000	0.5159	-0.0047	0.0017	0.4917	-0.0013	0.4454	-0.0081	-0.5412	0.0165	0.0102	-0.0125	-0.0114	0.0011	0.0026
53. (1.97669)	BD (1) C 12- C 29	0.7159* C 12	s(33.99%)p 1.94(65.97%)d 0.00(0.04%)	0.0000	0.5830	0.0025	-0.0005	0.6459	0.0131	-0.4808	0.0177	0.1041	0.0005	-0.0159	0.0036	-0.0033	0.0023	-0.0109
	(51.25%)			0.0000	0.5830	0.0025	-0.0005	0.6459	0.0131	-0.4808	0.0177	0.1041	0.0005	-0.0159	0.0036	-0.0033	0.0023	-0.0109
	(48.75%)	0.6982* C 29	s(33.37%)p 1.99(66.57%)d 0.00(0.05%)	0.0000	0.5777	-0.0050	0.0030	-0.6172	0.0171	0.5200	0.0173	-0.1178	0.0012					

					-0.0173	0.0049	-0.0037	0.0036	-0.0140
54.	(1.99377)	BD (1) C 13-	H 14		s(26.19%)	p 2.81(73.72%)	d 0.00(0.08%)		
	(60.37%)	0.7770*	C 13		0.0000	0.5118	-0.0018	-0.0008	0.4338
					-0.0052	-0.7403	-0.0038	0.0261	-0.0191
					-0.0214	-0.0003	-0.0018	-0.0123	-0.0151
	(39.63%)	0.6295*	H 14		s(99.95%)	p 0.00(0.05%)			
					0.9997	0.0013	-0.0108	0.0199	0.0023
55.	(1.99040)	BD (1) C 13-	H 15		s(26.65%)	p 2.75(73.27%)	d 0.00(0.08%)		
	(61.65%)	0.7852*	C 13		0.0000	0.5163	-0.0010	-0.0003	0.3219
					-0.0069	0.5247	-0.0120	-0.5945	-0.0120
					0.0109	-0.0132	-0.0210	-0.0043	0.0052
	(38.35%)	0.6193*	H 15		s(99.95%)	p 0.00(0.05%)			
					0.9997	0.0001	-0.0069	-0.0131	0.0174
56.	(1.99016)	BD (1) C 13-	H 16		s(26.37%)	p 2.79(73.55%)	d 0.00(0.08%)		
	(61.27%)	0.7827*	C 13		0.0000	0.5135	0.0010	0.0000	-0.8361
					0.0064	-0.1394	-0.0039	-0.1296	-0.0162
					0.0088	0.0066	-0.0003	0.0211	-0.0137
	(38.73%)	0.6224*	H 16		s(99.94%)	p 0.00(0.06%)			
					0.9997	0.0011	0.0235	0.0024	0.0062
57.	(1.98267)	BD (1) C 17-	H 18		s(31.43%)	p 2.18(68.50%)	d 0.00(0.07%)		
	(60.32%)	0.7766*	C 17		0.0000	0.5606	0.0000	-0.0037	0.0547
					-0.0001	0.8216	0.0111	-0.0829	-0.0013
					0.0036	-0.0001	-0.0045	-0.0206	-0.0141
	(39.68%)	0.6299*	H 18		s(99.92%)	p 0.00(0.08%)			
					0.9996	-0.0008	-0.0021	-0.0286	0.0027
58.	(1.98042)	BD (1) C 19-	C 35		s(27.97%)	p 2.57(71.98%)	d 0.00(0.05%)		
	(50.02%)	0.7072*	C 19		0.0000	0.5287	0.0135	0.0008	-0.4793
					0.0109	0.5401	0.0017	-0.4451	-0.0114
					-0.0140	0.0127	-0.0116	-0.0025	-0.0016
	(49.98%)	0.7070*	C 35		s(26.50%)	p 2.77(73.46%)	d 0.00(0.04%)		
					0.0000	0.5148	-0.0042	0.0017	0.4907
					-0.0014	-0.5293	0.0079	0.4618	-0.0164
					-0.0124	0.0107	-0.0117	-0.0011	-0.0009
59.	(1.98108)	BD (1) C 19-	C 39		s(26.00%)	p 2.84(73.95%)	d 0.00(0.05%)		
	(49.46%)	0.7032*	C 19		0.0000	0.5099	-0.0005	0.0005	-0.2486
					-0.0006	-0.8150	0.0010	-0.1154	-0.0140
					0.0115	0.0035	0.0038	-0.0160	-0.0097
	(50.54%)	0.7109*	C 39		s(25.36%)	p 2.94(74.61%)	d 0.00(0.04%)		
					0.0000	0.5035	-0.0084	0.0007	0.2730
					-0.0005	0.8099	-0.0202	0.1228	-0.0131
					0.0098	0.0017	0.0047	-0.0127	-0.0086
60.	(1.99241)	BD (1) C 21-	H 22		s(25.88%)	p 2.86(74.04%)	d 0.00(0.08%)		
	(60.27%)	0.7764*	C 21		0.0000	0.5087	-0.0036	-0.0011	0.4682
					-0.0114	-0.7181	-0.0066	-0.0712	0.0173
					-0.0229	-0.0021	0.0049	-0.0096	-0.0141
	(39.73%)	0.6303*	H 22		s(99.95%)	p 0.00(0.05%)			
					0.9998	0.0015	-0.0106	0.0194	-0.0009</

				0.0000	0.4927	0.0012	-0.0007	-0.7916
				-0.0066	0.2469	0.0203	-0.2614	0.0052
				-0.0111	0.0136	-0.0043	0.0193	-0.0096
	(39.43%)	0.6279* H 27	s(99.95%)p 0.00(0.05%)	0.9997	-0.0002	0.0202	-0.0074	0.0060
65. (1.98586)	BD (1) C 25- H 28							
	(61.15%)	0.7820* C 25	s(24.83%)p 3.02(75.09%)d 0.00(0.07%)	0.0000	0.4983	0.0025	-0.0002	0.5958
				0.0006	0.4504	0.0165	-0.4390	0.0100
				0.0164	-0.0163	-0.0131	0.0052	-0.0022
	(38.85%)	0.6233* H 28	s(99.96%)p 0.00(0.04%)	0.9998	0.0001	-0.0150	-0.0111	0.0096
66. (1.98239)	BD (1) C 29- H 30							
	(60.49%)	0.7777* C 29	s(31.76%)p 2.15(68.17%)d 0.00(0.06%)	0.0000	0.5636	0.0000	-0.0037	0.7664
				0.0142	0.2988	0.0014	0.0695	0.0022
				0.0144	0.0035	0.0010	0.0153	-0.0139
	(39.51%)	0.6286* H 30	s(99.92%)p 0.00(0.08%)	0.9996	-0.0011	-0.0262	-0.0093	-0.0024
67. (1.97989)	BD (1) C 29- C 33							
	(50.08%)	0.7077* C 29	s(34.69%)p 1.88(65.26%)d 0.00(0.05%)	0.0000	0.5890	0.0057	0.0019	-0.1284
				0.0285	-0.7951	-0.0155	0.0530	0.0036
				0.0069	0.0002	-0.0022	-0.0161	-0.0133
	(49.92%)	0.7066* C 33	s(34.89%)p 1.86(65.06%)d 0.00(0.05%)	0.0000	0.5907	0.0017	0.0026	0.1172
				0.0312	0.7967	0.0052	-0.0337	0.0028
				0.0044	0.0005	-0.0022	-0.0171	-0.0136
68. (1.75443)	BD (2) C 29- C 33							
	(49.64%)	0.7046* C 29	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0024	-0.0006	-0.0002	0.1205
				-0.0016	-0.0836	-0.0004	-0.9888	0.0221
				-0.0013	0.0080	0.0170	-0.0021	-0.0005
	(50.36%)	0.7097* C 33	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000	0.0053	-0.0009	0.0001	0.1212
				-0.0024	-0.0636	0.0009	-0.9900	0.0274
				0.0022	0.0013	-0.0175	0.0011	0.0025
69. (1.98090)	BD (1) C 31- H 32							
	(60.58%)	0.7784* C 31	s(31.74%)p 2.15(68.19%)d 0.00(0.06%)	0.0000	0.5634	-0.0012	-0.0037	-0.1050
				0.0104	-0.8185	-0.0158	0.0234	0.0012
				0.0070	0.0003	-0.0010	-0.0196	-0.0144
	(39.42%)	0.6278* H 32	s(99.92%)p 0.00(0.08%)	0.9996	-0.0011	0.0030	0.0274	-0.0008
70. (1.97223)	BD (1) C 31- C 33							
	(50.87%)	0.7133* C 31	s(33.29%)p 2.00(66.67%)d 0.00(0.04%)	0.0000	0.5769	0.0030	0.0010	0.7545
				0.0160	0.3031	-0.0267	0.0672	0.0029
				0.0125	0.0030	0.0008	0.0096	-0.0136
	(49.13%)	0.7009* C 33	s(33.07%)p 2.02(66.88%)d 0.00(0.05%)	0.0000	0.5751	-0.0001	0.0021	-0.7492
				0.0058	-0.3191	-0.0306	-0.0682	0.0026
				0.0122	0.0034	0.0006	0.0120	-0.0136
71. (1.98322)	BD (1) C 33- H 34							
	(60.47%)	0.7776* C 33	s(31.86%)p 2.14(68.07%)d 0.00(0.07%)	0.0000	0.5645	-0.0005	-0.0036	0.6398
				0.0101	-0.5082	-0.0071	0.1140	0.0023
				-0.0204	0.0049	-0.0038	0.0048	-0.0138
	(39.53%)	0.6287* H 34	s(99.93%)p 0.00(0.07%)	0.9996	-0.0007	-0.0217	0.0162	-0.0037
72. (1.98600)	BD (1) C 35- H 36							
	(61.36%)	0.7833* C 35	s(24.82%)p 3.03(75.11%)d 0.00(0.07%)	0.0000	0.4982	0.0036	-0.0001	-0.0307
				-0.0058	-0.2637	0.0156	-0.8248	-0.0051
				0.0010	0.0013	0.0147	-0.0018	0.0223
	(38.64%)	0.6216* H 36	s(99.95%)p 0.00(0.05%)	0.9998	0.0004	0.0002	0.0054	0.0211
73. (1.98563)	BD (1) C 35- H 37							
	(61.43%)	0.7838* C 35	s(24.69%)p 3.05(75.23%)d 0.00(0.07%)	0.0000	0.4969	0.0017	-0.0004	0.3188
				-0.0079	0.8058	0.0052	0.0307	-0.0161
				0.0160	0.0003	0.0032	-0.0162	-0.0135
	(38.57%)	0.6210* H 37	s(99.95%)p 0.00(0.05%)	0.9998	0.0002	-0.0084	-0.0202	0.0003
74. (1.98155)	BD (1) C 35- H 38							
	(60.74%)	0.7794* C 35	s(23.87%)p 3.19(76.06%)d 0.00(0.08%)	0.0000	0.4885	0.0000	-0.0009	-0.8097

				-0.0140	0.0066	0.0112	0.3232	-0.0122
				0.0016	-0.0177	0.0000	0.0200	-0.0071
	(39.26%)	0.6266*	H 38	s(99.95%)	p 0.00(0.05%)			
				0.9998	-0.0005	0.0212	-0.0011	-0.0069
75. (1.98815)	BD (1) C 39-	H 40						
	(61.22%)	0.7824*	C 39	s(25.02%)	p 2.99(74.90%)	d 0.00(0.07%)		
				0.0000	0.5002	0.0039	0.0000	-0.0630
				-0.0049	-0.1613	-0.0152	-0.8478	0.0006
				0.0001	0.0034	0.0090	0.0002	0.0253
	(38.78%)	0.6228*	H 40	s(99.95%)	p 0.00(0.05%)			
				0.9997	0.0000	0.0014	0.0043	0.0222
76. (1.98390)	BD (1) C 39-	H 41						
	(60.92%)	0.7805*	C 39	s(24.73%)	p 3.04(75.20%)	d 0.00(0.08%)		
				0.0000	0.4973	0.0020	-0.0004	-0.7766
				-0.0099	-0.1039	-0.0183	0.3709	-0.0049
				0.0042	-0.0184	-0.0029	0.0193	-0.0056
	(39.08%)	0.6252*	H 41	s(99.95%)	p 0.00(0.05%)			
				0.9997	-0.0001	0.0204	0.0036	-0.0089
77. (1.98640)	BD (1) C 39-	H 42						
	(60.43%)	0.7774*	C 39	s(24.75%)	p 3.04(75.17%)	d 0.00(0.08%)		
				0.0000	0.4975	0.0029	-0.0002	0.5634
				-0.0057	-0.5536	-0.0177	0.3571	-0.0050
				-0.0199	0.0124	-0.0130	0.0007	-0.0060
	(39.57%)	0.6290*	H 42	s(99.96%)	p 0.00(0.04%)			
				0.9998	-0.0001	-0.0131	0.0135	-0.0082
78. (1.98587)	BD (1) C 43-	H 44						
	(61.49%)	0.7841*	C 43	s(24.94%)	p 3.01(74.99%)	d 0.00(0.07%)		
				0.0000	0.4994	0.0034	0.0000	0.1358
				-0.0077	0.2611	-0.0134	0.8143	0.0059
				0.0017	0.0070	0.0142	-0.0014	0.0215
	(38.51%)	0.6206*	H 44	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0005	-0.0037	-0.0056	-0.0206
79. (1.98584)	BD (1) C 43-	H 45						
	(61.02%)	0.7812*	C 43	s(24.44%)	p 3.09(75.48%)	d 0.00(0.07%)		
				0.0000	0.4944	0.0018	-0.0005	0.1807
				-0.0065	-0.8474	-0.0048	-0.0617	0.0171
				-0.0096	-0.0003	0.0050	-0.0207	-0.0135
	(38.98%)	0.6243*	H 45	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0002	-0.0048	0.0214	0.0005
80. (1.98173)	BD (1) C 43-	H 46						
	(60.75%)	0.7794*	C 43	s(23.88%)	p 3.18(76.05%)	d 0.00(0.08%)		
				0.0000	0.4886	0.0005	-0.0008	-0.8403
				-0.0134	0.1205	-0.0078	-0.1982	0.0144
				-0.0077	0.0122	-0.0016	0.0208	-0.0111
	(39.25%)	0.6265*	H 46	s(99.95%)	p 0.00(0.05%)			
				0.9997	-0.0004	0.0222	-0.0024	0.0038
----- non-Lewis -----								
81. (0.99157)	LV (1) C 5			s(0.00%)	p 1.00(100.00%)	d 0.00(0.00%)		
				0.0000	0.0023	0.0011	0.0001	-0.0687
				-0.0042	0.0659	0.0021	0.9954	0.0106
				0.0005	-0.0019	-0.0042	-0.0003	-0.0005
82. (0.41567)	LV (1) B 20			s(7.89%)	p11.67(92.07%)	d 0.01(0.04%)		
				0.0000	0.2806	-0.0135	-0.0043	0.3657
				-0.0098	-0.8858	0.0304	-0.0355	-0.0028
				0.0006	-0.0025	0.0015	-0.0147	-0.0145
83. (0.04469)	BD*(1) O 1-	C 19						
	(32.24%)	0.5678*	O 1	s(26.59%)	p 2.76(73.27%)	d 0.01(0.14%)		
				0.0000	-0.5156	-0.0035	-0.0014	0.8194
				0.0080	0.0633	0.0005	-0.2389	0.0106
				-0.0062	0.0292	0.0040	-0.0231	-0.0009
	(67.76%)	-0.8232*	C 19	s(18.50%)	p 4.40(81.32%)	d 0.01(0.19%)		
				0.0000	-0.4299	-0.0132	0.0025	-0.8393
				-0.0089	-0.0586	-0.0079	0.3213	0.0435
				-0.0057	0.0231	0.0015	-0.0331	0.0139
84. (0.03356)	BD*(1) O 1-	B 20						
	(18.69%)	0.4323*	O 1	s(46.62%)	p 1.14(53.24%)	d 0.00(0.15%)		
				0.0000	-0.6827	0.0048	-0.0022	-0.5661
				-0.0033	0.0469	-0.0017	-0.4578	0.0087
				0.0034	-0.0289	0.0051	-0.0106	-0.0219
	(81.31%)	-0.9017*	B 20	s(28.76%)	p 2.46(70.87%)	d 0.01(0.37%)		
				0.0000	-0.5363	0.0012	0.0052	0.5101
				-0.0136	0.0146	-0.0056	0.6675	0.0501
				0.0046	-0.0531	-0.0003	-0.0153	-0.0248
85. (0.04274)	BD*(1) O 2-	C 11						
	(32.37%)	0.5689*	O 2	s(26.74%)	p 2.73(73.12%)	d 0.01(0.14%)		
				0.0000	-0.5171	-0.0047	-0.0019	0.8292
				0.0060	-0.1577	-0.0009	0.1362	-0.0110

					0.0112	-0.0248	0.0057	-0.0252	0.0054
	(67.63%)	-0.8224*	C 11	s(18.27%)p 4.46(81.54%)d 0.01(0.18%)	0.0000	-0.4273	-0.0127	0.0028	-0.8570
					-0.0144	0.1942	0.0068	-0.2034	-0.0412
					0.0161	-0.0144	0.0031	-0.0319	0.0180
86.	(0.03879)	BD*(1)	O 2- B 20						
	(18.89%)	0.4346*	O 2	s(43.75%)p 1.28(56.11%)d 0.00(0.14%)	0.0000	-0.6615	0.0044	-0.0024	-0.4965
					-0.0045	0.0383	0.0018	0.5594	-0.0092
					0.0016	0.0221	0.0010	-0.0059	-0.0293
	(81.11%)	-0.9006*	B 20	s(28.86%)p 2.45(70.79%)d 0.01(0.35%)	0.0000	-0.5372	0.0020	0.0047	0.4040
					-0.0240	0.0273	0.0057	-0.7355	-0.0486
					0.0020	0.0462	0.0012	-0.0088	-0.0360
87.	(0.03675)	BD*(1)	N 3- C 6						
	(37.77%)	0.6146*	N 3	s(29.50%)p 2.39(70.43%)d 0.00(0.07%)	0.0000	-0.5431	-0.0011	0.0002	-0.7956
					-0.0069	-0.2510	0.0013	-0.0908	-0.0038
					-0.0050	-0.0040	0.0004	-0.0236	0.0105
	(62.23%)	-0.7889*	C 6	s(26.15%)p 2.82(73.74%)d 0.00(0.12%)	0.0000	-0.5113	-0.0058	0.0026	0.8098
					0.0083	0.2771	0.0068	0.0688	-0.0005
					-0.0148	-0.0053	-0.0012	-0.0241	0.0183
88.	(0.01693)	BD*(1)	N 3- C 13						
	(36.69%)	0.6058*	N 3	s(24.81%)p 3.03(75.13%)d 0.00(0.05%)	0.0000	-0.4981	-0.0058	-0.0006	0.1378
					0.0125	0.3583	0.0046	0.7768	0.0181
					-0.0021	0.0041	-0.0189	0.0059	-0.0115
	(63.31%)	-0.7956*	C 13	s(20.73%)p 3.82(79.15%)d 0.01(0.12%)	0.0000	-0.4553	-0.0064	-0.0018	-0.0904
					0.0057	-0.3949	-0.0024	-0.7920	-0.0071
					-0.0030	-0.0062	-0.0225	0.0050	-0.0247
89.	(0.01491)	BD*(1)	N 3- C 21						
	(36.98%)	0.6081*	N 3	s(28.80%)p 2.47(71.14%)d 0.00(0.06%)	0.0000	-0.5366	-0.0107	-0.0002	0.2806
					0.0159	0.4953	0.0067	-0.6219	-0.0172
					-0.0064	0.0004	0.0201	0.0101	-0.0047
	(63.02%)	-0.7939*	C 21	s(22.03%)p 3.53(77.84%)d 0.01(0.13%)	0.0000	-0.4692	-0.0110	-0.0026	-0.2424
					0.0028	-0.5531	-0.0109	0.6430	0.0125
					-0.0108	0.0130	0.0280	0.0085	-0.0119
90.	(0.02819)	BD*(1)	C 4- C 5						
	(51.71%)	0.7191*	C 4	s(29.27%)p 2.41(70.67%)d 0.00(0.06%)	0.0000	-0.5409	-0.0091	-0.0009	-0.7206
					-0.0228	0.4242	-0.0002	-0.0827	-0.0008
					0.0154	-0.0035	0.0027	-0.0112	0.0163
	(48.29%)	-0.6949*	C 5	s(33.93%)p 1.95(66.03%)d 0.00(0.04%)	0.0000	-0.5824	0.0041	0.0006	0.6623
					-0.0110	-0.4642	-0.0007	0.0777	-0.0006
					0.0132	-0.0033	0.0019	-0.0076	0.0126
91.	(0.02147)	BD*(1)	C 4- C 7						
	(49.24%)	0.7017*	C 4	s(35.21%)p 1.84(64.74%)d 0.00(0.05%)	0.0000	-0.5928	-0.0251	0.0001	-0.0346
					0.0130	-0.7990	-0.0379	0.0785	0.0050
					-0.0076	0.0006	0.0037	0.0169	0.0132
	(50.76%)	-0.7124*	C 7	s(35.37%)p 1.83(64.57%)d 0.00(0.05%)	0.0000	-0.5947	-0.0005	-0.0041	0.0887
					0.0225	0.7936	-0.0012	-0.0871	0.0026
					-0.0029	-0.0001	0.0046	0.0175	0.0136
92.	(0.22854)	BD*(2)	C 4- C 7						
	(52.25%)	0.7228*	C 4	s(0.00%)p 1.00(99.95%)d 0.00(0.05%)	0.0000	-0.0030	-0.0001	0.0000	-0.0518
					-0.0004	0.1019	0.0053	0.9930	0.0174
					0.0000	0.0136	0.0167	-0.0027	-0.0024
	(47.75%)	-0.6910*	C 7	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000	-0.0037	-0.0021	0.0004	-0.0662
					0.0032	0.1134	0.0002	0.9910	-0.0204
					0.0012	0.0047	-0.0163	0.0016	0.0038
93.	(0.05313)	BD*(1)	C 4- B 20						
	(29.81%)	0.5460*	C 4	s(35.23%)p 1.84(64.74%)d 0.00(0.02%)	0.0000	-0.5932	0.0205	0.0004	0.6890
					-0.0371	0.4109	-0.0490	-0.0079	0.0023
					-0.0115	0.0007	0.0011	-0.0004	0.0095
	(70.19%)	-0.8378*	B 20	s(34.36%)p 1.91(65.53%)d 0.00(0.11%)	0.0000	-0.5860	-0.0073	-0.0097	-0.6623
					-0.0012	-0.4621	-0.0321	0.0461	0.0011
					-0.0268	0.0038	0.0015	-0.0056	0.0185

103. (0.25682) BD*(2) C 9- C 17
 (49.01%) 0.7001* C 9 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)
 0.0000 0.0013 -0.0004 0.0000 0.0770
 0.0002 -0.1048 0.0001 -0.9911 0.0224
 0.0022 0.0178 -0.0047 -0.0009 0.0033
 (50.99%) -0.7141* C 17 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)
 0.0000 -0.0027 0.0006 0.0000 0.0732
 0.0000 -0.1030 0.0014 -0.9915 0.0246
 -0.0024 -0.0133 0.0132 -0.0004 -0.0041

104. (0.05809) BD*(1) C 11- C 19
 (50.08%) 0.7077* C 11 s(27.50%)p 2.63(72.44%)d 0.00(0.06%)
 0.0000 0.5241 -0.0173 0.0003 -0.1123
 -0.0174 -0.2019 0.0001 -0.8188 0.0150
 0.0021 0.0036 0.0097 -0.0018 0.0231
 (49.92%) -0.7066* C 19 s(27.45%)p 2.64(72.48%)d 0.00(0.06%)
 0.0000 0.5236 -0.0182 0.0003 0.0347
 -0.0202 0.2001 0.0020 0.8264 -0.0121
 0.0001 0.0040 0.0095 -0.0019 0.0231

105. (0.03327) BD*(1) C 11- C 25
 (50.12%) 0.7079* C 11 s(26.30%)p 2.80(73.65%)d 0.00(0.05%)
 0.0000 0.5128 -0.0017 0.0007 -0.0969
 -0.0003 0.8420 -0.0009 0.1340 0.0145
 -0.0049 -0.0026 0.0051 -0.0192 -0.0088
 (49.88%) -0.7063* C 25 s(25.67%)p 2.89(74.29%)d 0.00(0.04%)
 0.0000 0.5066 -0.0076 0.0010 0.1022
 0.0056 -0.8423 0.0188 -0.1499 0.0131
 -0.0032 -0.0006 0.0061 -0.0161 -0.0085

106. (0.02713) BD*(1) C 11- C 43
 (50.17%) 0.7083* C 11 s(27.85%)p 2.59(72.10%)d 0.00(0.05%)
 0.0000 0.5275 0.0140 0.0007 -0.4906
 0.0118 -0.4602 -0.0028 0.5180 0.0095
 0.0128 -0.0144 -0.0114 -0.0004 0.0020
 (49.83%) -0.7059* C 43 s(26.62%)p 2.75(73.34%)d 0.00(0.04%)
 0.0000 0.5159 -0.0047 0.0017 0.4917
 -0.0013 0.4454 -0.0081 -0.5412 0.0165
 0.0102 -0.0125 -0.0114 0.0011 0.0026

107. (0.02260) BD*(1) C 12- C 29
 (48.75%) 0.6982* C 12 s(33.99%)p 1.94(65.97%)d 0.00(0.04%)
 0.0000 -0.5830 -0.0025 0.0005 -0.6459
 -0.0131 0.4808 -0.0177 -0.1041 -0.0005
 0.0159 -0.0036 0.0033 -0.0023 0.0109
 (51.25%) -0.7159* C 29 s(33.37%)p 1.99(66.57%)d 0.00(0.05%)
 0.0000 -0.5777 0.0050 -0.0030 0.6172
 -0.0171 -0.5200 -0.0173 0.1178 -0.0012
 0.0173 -0.0049 0.0037 -0.0036 0.0140

108. (0.00922) BD*(1) C 13- H 14
 (39.63%) 0.6295* C 13 s(26.19%)p 2.81(73.72%)d 0.00(0.08%)
 0.0000 -0.5118 0.0018 0.0008 -0.4338
 0.0052 0.7403 0.0038 -0.0261 0.0191
 0.0214 0.0003 0.0018 0.0123 0.0151
 (60.37%) -0.7770* H 14 s(99.95%)p 0.00(0.05%)
 -0.9997 -0.0013 0.0108 -0.0199 -0.0023

109. (0.00520) BD*(1) C 13- H 15
 (38.35%) 0.6193* C 13 s(26.65%)p 2.75(73.27%)d 0.00(0.08%)
 0.0000 -0.5163 0.0010 0.0003 -0.3219
 0.0069 -0.5247 0.0120 0.5945 0.0120
 -0.0109 0.0132 0.0210 0.0043 -0.0052
 (61.65%) -0.7852* H 15 s(99.95%)p 0.00(0.05%)
 -0.9997 -0.0001 0.0069 0.0131 -0.0174

110. (0.00848) BD*(1) C 13- H 16
 (38.73%) 0.6224* C 13 s(26.37%)p 2.79(73.55%)d 0.00(0.08%)
 0.0000 -0.5135 -0.0010 0.0000 0.8361
 -0.0064 0.1394 0.0039 0.1296 0.0162
 -0.0088 -0.0066 0.0003 -0.0211 0.0137
 (61.27%) -0.7827* H 16 s(99.94%)p 0.00(0.06%)
 -0.9997 -0.0011 -0.0235 -0.0024 -0.0062

111. (0.01070) BD*(1) C 17- H 18
 (39.68%) 0.6299* C 17 s(31.43%)p 2.18(68.50%)d 0.00(0.07%)
 0.0000 -0.5606 0.0000 0.0037 -0.0547
 0.0001 -0.8216 -0.0111 0.0829 0.0013
 -0.0036 0.0001 0.0045 0.0206 0.0141
 (60.32%) -0.7766* H 18 s(99.92%)p 0.00(0.08%)
 -0.9996 0.0008 0.0021 0.0286 -0.0027

112. (0.02658) BD*(1) C 19- C 35
 (49.98%) 0.7070* C 19 s(27.97%)p 2.57(71.98%)d 0.00(0.05%)
 0.0000 0.5287 0.0135 0.0008 -0.4793
 0.0109 0.5401 0.0017 -0.4451 -0.0114

				-0.0140	0.0127	-0.0116	-0.0025	-0.0016
(50.02%)	-0.7072*	C 35	s(26.50%)p 2.77(73.46%)d 0.00(0.04%)	0.0000	0.5148	-0.0042	0.0017	0.4907
				-0.0014	-0.5293	0.0079	0.4618	-0.0164
				-0.0124	0.0107	-0.0117	-0.0011	-0.0009
113.	(0.03513)	BD*(1) C 19-	C 39	s(26.00%)p 2.84(73.95%)d 0.00(0.05%)	0.0000	0.5099	-0.0005	0.0005
(50.54%)	0.7109*	C 19	s(26.00%)p 2.84(73.95%)d 0.00(0.05%)	-0.0006	-0.8150	0.0010	-0.1154	-0.0140
				0.0115	0.0035	0.0038	-0.0160	-0.0097
(49.46%)	-0.7032*	C 39	s(25.36%)p 2.94(74.61%)d 0.00(0.04%)	0.0000	0.5035	-0.0084	0.0007	0.2730
				-0.0005	0.8099	-0.0202	0.1228	-0.0131
				0.0098	0.0017	0.0047	-0.0127	-0.0086
114.	(0.01059)	BD*(1) C 21-	H 22	s(25.88%)p 2.86(74.04%)d 0.00(0.08%)	0.0000	-0.5087	0.0036	0.0011
(39.73%)	0.6303*	C 21	s(25.88%)p 2.86(74.04%)d 0.00(0.08%)	0.0114	0.7181	0.0066	0.0712	-0.0173
				0.0229	0.0021	-0.0049	0.0096	0.0141
(60.27%)	-0.7764*	H 22	s(99.95%)p 0.00(0.05%)	-0.9998	-0.0015	0.0106	-0.0194	0.0009
115.	(0.00888)	BD*(1) C 21-	H 23	s(25.89%)p 2.86(74.04%)d 0.00(0.08%)	0.0000	-0.5088	-0.0005	0.0003
(38.94%)	0.6240*	C 21	s(25.89%)p 2.86(74.04%)d 0.00(0.08%)	-0.0040	0.1754	0.0073	0.0961	-0.0169
				-0.0094	-0.0069	-0.0029	-0.0210	0.0130
(61.06%)	-0.7814*	H 23	s(99.94%)p 0.00(0.06%)	-0.9997	-0.0012	-0.0233	-0.0044	0.0006
116.	(0.00698)	BD*(1) C 21-	H 24	s(26.18%)p 2.82(73.74%)d 0.00(0.07%)	0.0000	-0.5117	0.0016	0.0003
(38.02%)	0.6166*	C 21	s(26.18%)p 2.82(73.74%)d 0.00(0.07%)	0.0106	-0.3818	0.0140	-0.7553	-0.0038
				-0.0036	-0.0083	-0.0192	0.0029	-0.0169
(61.98%)	-0.7873*	H 24	s(99.95%)p 0.00(0.05%)	-0.9997	-0.0009	0.0017	0.0098	0.0210
117.	(0.00659)	BD*(1) C 25-	H 26	s(25.08%)p 2.98(74.84%)d 0.00(0.07%)	0.0000	-0.5008	-0.0047	0.0000
(38.73%)	0.6223*	C 25	s(25.08%)p 2.98(74.84%)d 0.00(0.07%)	-0.0022	-0.1608	-0.0169	-0.8458	0.0015
				-0.0007	-0.0037	-0.0083	-0.0002	-0.0254
(61.27%)	-0.7827*	H 26	s(99.95%)p 0.00(0.05%)	-0.9997	0.0000	0.0029	0.0045	0.0217
118.	(0.00778)	BD*(1) C 25-	H 27	s(24.27%)p 3.12(75.65%)d 0.00(0.08%)	0.0000	-0.4927	-0.0012	0.0007
(39.43%)	0.6279*	C 25	s(24.27%)p 3.12(75.65%)d 0.00(0.08%)	0.0066	-0.2469	-0.0203	0.2614	-0.0052
				0.0111	-0.0136	0.0043	-0.0193	0.0096
(60.57%)	-0.7783*	H 27	s(99.95%)p 0.00(0.05%)	-0.9997	0.0002	-0.0202	0.0074	-0.0060
119.	(0.00671)	BD*(1) C 25-	H 28	s(24.83%)p 3.02(75.09%)d 0.00(0.07%)	0.0000	-0.4983	-0.0025	0.0002
(38.85%)	0.6233*	C 25	s(24.83%)p 3.02(75.09%)d 0.00(0.07%)	-0.0006	-0.4504	-0.0165	0.4390	-0.0100
				-0.0164	0.0163	0.0131	-0.0052	0.0022
(61.15%)	-0.7820*	H 28	s(99.96%)p 0.00(0.04%)	-0.9998	-0.0001	0.0150	0.0111	-0.0096
120.	(0.01130)	BD*(1) C 29-	H 30	s(31.76%)p 2.15(68.17%)d 0.00(0.06%)	0.0000	-0.5636	0.0000	0.0037
(39.51%)	0.6286*	C 29	s(31.76%)p 2.15(68.17%)d 0.00(0.06%)	-0.0142	-0.2988	-0.0014	-0.0695	-0.0022
				-0.0144	-0.0035	-0.0010	-0.0153	0.0139
(60.49%)	-0.7777*	H 30	s(99.92%)p 0.00(0.08%)	-0.9996	0.0011			

	(49.64%)	-0.7046*	C 33	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 -0.0053 0.0009 -0.0001 -0.1212	0.0024 0.0636 -0.0009 0.9900 -0.0274	-0.0022 -0.0013 0.0175 -0.0011 -0.0025
123. (0.01260)	BD*(1) C 31- H 32	(39.42%)	0.6278* C 31	s(31.74%)p 2.15(68.19%)d 0.00(0.06%)	0.0000 -0.5634 0.0012 0.0037 0.1050	-0.0104 0.8185 0.0158 -0.0234 -0.0012	-0.0070 -0.0003 0.0010 0.0196 0.0144
	(60.58%)	-0.7784* H 32	s(99.92%)p 0.00(0.08%)	-0.9996 0.0011 -0.0030 -0.0274 0.0008			
124. (0.01675)	BD*(1) C 31- C 33	(49.13%)	0.7009* C 31	s(33.29%)p 2.00(66.67%)d 0.00(0.04%)	0.0000 -0.5769 -0.0030 -0.0010 -0.7545	-0.0160 -0.3031 0.0267 -0.0672 -0.0029	-0.0125 -0.0030 -0.0008 -0.0096 0.0136
	(50.87%)	-0.7133* C 33	s(33.07%)p 2.02(66.88%)d 0.00(0.05%)	0.0000 -0.5751 0.0001 -0.0021 0.7492	-0.0058 0.3191 0.0306 0.0682 -0.0026	-0.0122 -0.0034 -0.0006 -0.0120 0.0136	
125. (0.01008)	BD*(1) C 33- H 34	(39.53%)	0.6287* C 33	s(31.86%)p 2.14(68.07%)d 0.00(0.07%)	0.0000 -0.5645 0.0005 0.0036 -0.6398	-0.0101 0.5082 0.0071 -0.1140 -0.0023	0.0204 -0.0049 0.0038 -0.0048 0.0138
	(60.47%)	-0.7776* H 34	s(99.93%)p 0.00(0.07%)	-0.9996 0.0007 0.0217 -0.0162 0.0037			
126. (0.00755)	BD*(1) C 35- H 36	(38.64%)	0.6216* C 35	s(24.82%)p 3.03(75.11%)d 0.00(0.07%)	0.0000 -0.4982 -0.0036 0.0001 0.0307	0.0058 0.2637 -0.0156 0.8248 0.0051	-0.0010 -0.0013 -0.0147 0.0018 -0.0223
	(61.36%)	-0.7833* H 36	s(99.95%)p 0.00(0.05%)	-0.9998 -0.0004 -0.0002 -0.0054 -0.0211			
127. (0.00759)	BD*(1) C 35- H 37	(38.57%)	0.6210* C 35	s(24.69%)p 3.05(75.23%)d 0.00(0.07%)	0.0000 -0.4969 -0.0017 0.0004 -0.3188	0.0079 -0.8058 -0.0052 -0.0307 0.0161	-0.0160 -0.0003 -0.0032 0.0162 0.0135
	(61.43%)	-0.7838* H 37	s(99.95%)p 0.00(0.05%)	-0.9998 -0.0002 0.0084 0.0202 -0.0003			
128. (0.00671)	BD*(1) C 35- H 38	(39.26%)	0.6266* C 35	s(23.87%)p 3.19(76.06%)d 0.00(0.08%)	0.0000 -0.4885 0.0000 0.0009 0.8097	0.0140 -0.0066 -0.0112 -0.3232 0.0122	-0.0016 0.0177 0.0000 -0.0200 0.0071
	(60.74%)	-0.7794* H 38	s(99.95%)p 0.00(0.05%)	-0.9998 0.0005 -0.0212 0.0011 0.0069			
129. (0.00665)	BD*(1) C 39- H 40	(38.78%)	0.6228* C 39	s(25.02%)p 2.99(74.90%)d 0.00(0.07%)	0.0000 -0.5002 -0.0039 0.0000 0.0630	0.0049 0.1613 0.0152 0.8478 -0.0006	-0.0001 -0.0034 -0.0090 -0.0002 -0.0253
	(61.22%)	-0.7824* H 40	s(99.95%)p 0.00(0.05%)	-0.9997 0.0000 -0.0014 -0.0043 -0.0222			
130. (0.00769)	BD*(1) C 39- H 41	(39.08%)	0.6252* C 39	s(24.73%)p 3.04(75.20%)d 0.00(0.08%)	0.0000 -0.4973 -0.0020 0.0004 0.7766	0.0099 0.1039 0.0183 -0.3709 0.0049	-0.0042 0.0184 0.0029 -0.0193 0.0056
	(60.92%)	-0.7805* H 41	s(99.95%)p 0.00(0.05%)	-0.9997 0.0001 -0.0204 -0.0036 0.0089			
131. (0.00748)	BD*(1) C 39- H 42	(39.57%)	0.6290* C 39	s(24.75%)p 3.04(75.17%)d 0.00(0.08%)	0.0000 -0.4975 -0.0029 0.0002 -0.5634	0.0057 0.5536 0.0177 -0.3571 0.0050	0.0199 -0.0124 0.0130 -0.0007 0.0060
	(60.43%)	-0.7774* H 42	s(99.96%)p 0.00(0.04%)	-0.9998 0.0001 0.0131 -0.0135 0.0082			
132. (0.00757)	BD*(1) C 43- H 44	(38.51%)	0.6206* C 43	s(24.94%)p 3.01(74.99%)d 0.00(0.07%)	0.0000 -0.4994 -0.0034 0.0000 -0.1358	0.0077 -0.2611 0.0134 -0.8143 -0.0059	-0.0017 -0.0070 -0.0142 0.0014 -0.0215
	(61.49%)	-0.7841* H 44	s(99.95%)p 0.00(0.05%)	-0.9998 -0.0005 0.0037 0.0056 0.0206			
133. (0.00786)	BD*(1) C 43- H 45						

	(38.98%)	0.6243* C 43	s(24.44%)p 3.09(75.48%)d 0.00(0.07%)	0.0000 -0.4944 -0.0018 0.0005 -0.1807	0.0065 0.8474 0.0048 0.0617 -0.0171	0.0096 0.0003 -0.0050 0.0207 0.0135
	(61.02%)	-0.7812* H 45	s(99.95%)p 0.00(0.05%)	-0.9998 -0.0002 0.0048 -0.0214 -0.0005		
134. (0.00716)	BD*(1) C 43- H 46					
	(39.25%)	0.6265* C 43	s(23.88%)p 3.18(76.05%)d 0.00(0.08%)	0.0000 -0.4886 -0.0005 0.0008 0.8403	0.0134 -0.1205 0.0078 0.1982 -0.0144	0.0077 -0.0122 0.0016 -0.0208 0.0111
	(60.75%)	-0.7794* H 46	s(99.95%)p 0.00(0.05%)	-0.9997 0.0004 -0.0222 0.0024 -0.0038		
135. (0.00168)	RY (1) O 1		s(6.29%)p14.14(88.85%)d 0.77(4.86%)	0.0000 -0.0104 0.2496 -0.0207 -0.0002	-0.0975 0.0001 0.6989 -0.0018 -0.6250	-0.1144 0.1285 0.0186 0.0996 -0.0936
136. (0.00157)	RY (2) O 1		s(9.36%)p 9.08(84.98%)d 0.60(5.66%)	0.0000 -0.0065 0.3044 0.0298 0.0031	-0.1866 0.0032 -0.6850 -0.0001 -0.5881	0.1234 0.1413 -0.0392 0.0109 -0.1404
137. (0.00059)	RY (3) O 1		s(6.23%)p14.73(91.83%)d 0.31(1.94%)	0.0000 0.0038 0.2467 0.0385 0.0043	-0.8962 0.0005 0.0562 -0.0021 0.3345	-0.1197 0.0669 0.0089 0.0108 0.0194
138. (0.00022)	RY (4) O 1		s(70.52%)p 0.26(18.43%)d 0.16(11.06%)	0.0000 0.0000 0.8194 0.1837 0.0027	0.3097 0.0002 0.0676 0.0020 0.2894	0.2949 -0.0050 -0.0023 0.0908 0.1239
139. (0.00013)	RY (5) O 1		s(24.55%)p 0.24(5.81%)d 2.84(69.64%)	0.0000 0.0071 -0.0402 0.4938 0.0013	-0.0779 -0.0036 0.0032 -0.0234 -0.2269	-0.0546 -0.2857 0.0729 -0.3986 0.6690
140. (0.00008)	RY (6) O 1		s(16.32%)p 0.29(4.77%)d 4.84(78.92%)			
141. (0.00004)	RY (7) O 1		s(10.68%)p 0.21(2.26%)d 8.15(87.05%)			
142. (0.00003)	RY (8) O 1		s(2.72%)p 0.32(0.86%)d35.43(96.42%)			
143. (0.00002)	RY (9) O 1		s(6.22%)p 0.20(1.22%)d14.89(92.57%)			
144. (0.00001)	RY (10) O 1		s(47.16%)p 0.03(1.44%)d 1.09(51.39%)			
145. (0.00201)	RY (1) O 2		s(1.82%)p52.59(95.81%)d 1.30(2.37%)	0.0000 -0.0044 0.1325 0.0252 -0.0007	0.2954 -0.0021 0.8659 -0.0016 0.3480	-0.1123 -0.0606 -0.0172 -0.0728 -0.0425
146. (0.00145)	RY (2) O 2		s(13.37%)p 5.91(79.01%)d 0.57(7.62%)	0.0000 -0.0113 0.3648 -0.0218 0.0013	-0.1867 -0.0010 -0.3217 0.0022 0.8073	0.0659 -0.2330 0.0186 0.0807 -0.1037
147. (0.00058)	RY (3) O 2		s(12.55%)p 6.73(84.43%)d 0.24(3.02%)	0.0000 0.0052 0.3514 0.0441 0.0049	-0.8374 -0.0022 0.2961 -0.0007 -0.2352	-0.1251 -0.0780 -0.0056 -0.0916 0.0082
148. (0.00016)	RY (4) O 2		s(67.39%)p 0.27(17.86%)d 0.22(14.75%)	0.0000 0.0009 0.7593 0.3119 0.0026	0.3217 -0.0005 -0.0669 0.0023 -0.2658	0.2769 0.1151 -0.1082 0.1341 0.1671
149. (0.00013)	RY (5) O 2		s(21.72%)p 0.53(11.43%)d 3.08(66.85%)	0.0000 0.0056 -0.2077 0.4171 0.0026	-0.1718 0.0049 0.0253 0.0253 0.2889	0.2039 0.4390 0.0541 -0.2872 0.5906
150. (0.00006)	RY (6) O 2		s(7.20%)p 1.07(7.71%)d11.81(85.09%)			
151. (0.00005)	RY (7) O 2		s(22.43%)p 0.05(1.02%)d 3.41(76.55%)			
152. (0.00003)	RY (8) O 2		s(0.95%)p 1.76(1.67%)d99.99(97.37%)			
153. (0.00002)	RY (9) O 2		s(0.95%)p 0.82(0.78%)d99.99(98.26%)			
154. (0.00001)	RY (10) O 2		s(51.66%)p 0.01(0.70%)d 0.92(47.63%)			
155. (0.00197)	RY (1) N 3		s(4.13%)p21.11(87.23%)d 2.09(8.64%)	0.0000 0.0157 0.2025 -0.0091 -0.0160	-0.1066 0.0276 0.9258 0.0026 -0.0527	0.2407 -0.0451 0.0019 -0.0124 0.1621
156. (0.00092)	RY (2) N 3		s(1.60%)p57.30(91.63%)d 4.24(6.77%)	0.0000 -0.0111 0.1228 -0.0281 0.0030	-0.7797 0.0154 -0.1127 -0.0169 0.5432	0.1675 0.1479 -0.0706 0.1031 -0.0470
157. (0.00090)	RY (3) N 3		s(0.26%)p99.99(83.43%)d61.68(16.31%)	0.0000 0.0043 0.0435 0.0270 -0.0028	0.4957 -0.0045 0.1048 -0.0232 0.7596	-0.2088 0.0766 -0.2181 0.0106 0.2568
158. (0.00058)	RY (4) N 3		s(0.16%)p 8.68(1.40%)d99.99(98.44%)	0.0000 -0.0017 0.0386 -0.0110 -0.0008		

					-0.0359	0.0014	-0.0246	-0.0076	0.1099
					0.0171	-0.9363	-0.2400	0.1462	-0.1685
159.	(0.00045)	RY	(5)	N	3	s(	6.51%)	p	1.32(8.58%)d13.05(84.92%)
						0.0000	0.0015	0.2441	-0.0740 -0.0066
						0.2521	-0.0045	0.0426	-0.0134 0.1419
						0.3247	0.1471	-0.0867	-0.2701 -0.8010
160.	(0.00033)	RY	(6)	N	3	s(	19.17%)	p	0.32(6.06%)d 3.90(74.77%)
						0.0000	-0.0062	0.4377	-0.0096 -0.0220
						0.1995	-0.0078	-0.1160	0.0015 -0.0824
						0.2133	0.1186	0.0725	0.8264 -0.0018
161.	(0.00026)	RY	(7)	N	3	s(	0.49%)	p	16.15(7.91%)d99.99(91.60%)
						0.0000	-0.0023	0.0384	0.0585 0.0031
						-0.0572	0.0044	-0.0367	-0.0188 -0.2722
						0.0181	0.1990	-0.9325	0.0108 0.0795
162.	(0.00018)	RY	(8)	N	3	s(	36.73%)	p	0.09(3.47%)d 1.63(59.80%)
						0.0000	0.0055	0.6009	-0.0785 -0.0020
						-0.1450	0.0141	0.0653	0.0031 -0.0958
						-0.7534	0.0086	0.0279	-0.0940 -0.1440
163.	(0.00010)	RY	(9)	N	3	s(	41.80%)	p	0.21(8.91%)d 1.18(49.30%)
						0.0000	-0.0096	0.5592	0.3243 0.0173
						0.0583	0.0120	-0.2895	0.0038 -0.0372
						0.3599	-0.1296	0.0702	-0.4300 0.3961
164.	(0.00003)	RY	(10)	N	3	s(	89.17%)	p	0.02(1.56%)d 0.10(9.27%)
165.	(0.00475)	RY	(1)	C	4	s(	0.78%)	p	99.99(94.32%)d 6.28(4.90%)
						0.0000	0.0418	0.0773	0.0081 -0.0250
						-0.9022	-0.0302	-0.3496	0.0049 -0.0736
						-0.2032	0.0055	-0.0294	-0.0818 0.0099
166.	(0.00354)	RY	(2)	C	4	s(	1.04%)	p	94.25(97.58%)d 1.34(1.39%)
						0.0000	0.0370	0.0947	-0.0032 -0.0272
						0.3599	0.0179	-0.9146	-0.0002 0.0931
						0.0297	-0.0020	0.0130	-0.1132 -0.0009
167.	(0.00155)	RY	(3)	C	4	s(	0.62%)	p	99.99(95.54%)d 6.20(3.84%)
						0.0000	0.0027	0.0786	-0.0034 -0.0021
						-0.0951	-0.0039	0.0646	-0.0173 0.9705
						0.0019	0.1572	-0.1089	0.0247 0.0349
168.	(0.00107)	RY	(4)	C	4	s(	97.46%)	p	0.02(1.98%)d 0.01(0.56%)
						0.0000	-0.0149	0.9871	-0.0051 -0.0164
						0.0384	-0.0247	0.1118	0.0025 -0.0705
						0.0353	-0.0546	0.0337	-0.0040 -0.0142
169.	(0.00050)	RY	(5)	C	4	s(	0.14%)	p	18.92(2.60%)d99.99(97.26%)
						0.0000	-0.0008	0.0361	-0.0083 -0.0008
						0.0284	0.0004	-0.0168	0.0147 -0.1572
						0.1055	0.2933	-0.9133	0.0438 0.1985
170.	(0.00017)	RY	(6)	C	4	s(	0.16%)	p	7.92(1.27%)d99.99(98.57%)
						0.0000	-0.0065	0.0210	0.0335 0.0033
						0.0030	-0.0083	0.0416	-0.0151 -0.1032
						0.0857	0.8749	0.2683	-0.3607 -0.1041
171.	(0.00016)	RY	(7)	C	4	s(	0.88%)	p	1.74(1.54%)d99.99(97.58%)
						0.0000	-0.0072	-0.0366	0.0863 0.0172
						-0.0525	-0.0205	0.0943	0.0060 0.0545
						0.3843	-0.3443	-0.1189	-0.8338 0.0100
172.	(0.00009)	RY	(8)	C	4	s(	15.09%)	p	0.26(3.95%)d 5.36(80.96%)
173.	(0.00004)	RY	(9)	C	4	s(	83.53%)	p	0.01(0.81%)d 0.19(15.66%)
174.	(0.00004)	RY	(10)	C	4	s(	0.59%)	p	0.53(0.31%)d99.99(99.10%)
175.	(0.00560)	RY	(1)	C	5	s(	0.15%)	p	99.99(93.92%)d38.35(5.92%)
						0.0000	-0.0021	0.0385	0.0075 0.0010
						-0.0152	0.0079	0.9612	-0.0014 -0.1230
						0.0276	-0.0243	-0.0175	-0.2398 -0.0072
176.	(0.00406)	RY	(2)	C	5	s(	0.75%)	p	99.99(93.99%)d 6.99(5.25%)
						0.0000	-0.0034	0.0849	-0.0174 0.0151
						0.9653	-0.0012	0.0095	0.0041 0.0886
						-0.2116	0.0190	-0.0313	-0.0787 -0.0157
177.	(0.00084)	RY	(3)	C	5	s(	0.43%)	p	99.99(46.97%)d99.99(52.61%)
						0.0000	0.0001	0.0647	0.0088 0.0007
						0.0523	0.0015	-0.0919	0.0089 -0.6771
						-0.1290	-0.4628	0.5305	-0.0168 -0.1165
178.	(0.00062)	RY	(4)	C	5	s(	96.54%)	p	0.01(0.88%)d 0.03(2.59%)
						0.0000	-0.0030	0.9825	-0.0020 -0.0050
						-0.0769	0.0056	-0.0351	-0.0022 0.0395
						0.0712	0.1082	0.0237	0.0003 -0.0923
179.	(0.00050)	RY	(5)	C	5	s(	0.77%)	p	6.56(5.05%)d99.99(94.18%)
						0.0000	-0.0007	0.0872	-0.0097 -0.0012
						-0.0190	-0.0012	0.0264	-0.0061 0.2222
						-0.0051	-0.8383	-0.4657	0.1275 -0.0767
180.	(0.00027)	RY	(6)	C	5	s(	0.15%)	p	99.99(47.13%)d99.99(52.71%)
						0.0000	0.0006	0.0296	0.0254 0.0006
						0.0455	0.0014	-0.1000	0.0050 -0.6777

181.	(0.00014)	RY	(7)	C	5	0.0473 0.1901 -0.6908 -0.0173 0.1063 s(10.33%)p 0.63(6.56%)d 8.04(83.11%) -0.0000 0.0048 0.0366 0.3193 0.0123 -0.1991 0.0105 -0.1353 -0.0017 0.0856 -0.6517 -0.0262 -0.0884 -0.6259 0.0779
182.	(0.00009)	RY	(8)	C	5	s(0.95%)p 4.84(4.58%)d99.72(94.47%)
183.	(0.00007)	RY	(9)	C	5	s(87.73%)p 0.01(0.96%)d 0.13(11.31%)
184.	(0.00002)	RY	(10)	C	5	s(2.25%)p 0.02(0.05%)d43.41(97.70%)
185.	(0.00567)	RY	(1)	C	6	s(0.30%)p99.99(91.87%)d26.49(7.84%) 0.0000 -0.0142 0.0523 -0.0040 -0.0059 -0.3104 -0.0009 -0.9067 0.0002 0.0115 0.0589 -0.0331 -0.0120 -0.2657 0.0555
186.	(0.00385)	RY	(2)	C	6	s(1.21%)p76.13(92.40%)d 5.26(6.38%) 0.0000 -0.0033 0.1087 0.0173 0.0003 0.9042 -0.0017 -0.3253 0.0013 -0.0258 0.2181 0.0357 0.0422 0.1147 -0.0065
187.	(0.00264)	RY	(3)	C	6	s(0.01%)p 1.00(89.42%)d 0.12(10.57%) 0.0000 0.0035 0.0076 -0.0021 0.0014 -0.0226 -0.0009 0.0088 -0.0184 -0.9451 -0.0257 0.3030 0.0385 -0.0710 0.0820
188.	(0.00143)	RY	(4)	C	6	s(97.38%)p 0.02(1.49%)d 0.01(1.14%) 0.0000 -0.0032 0.9868 0.0018 0.0046 -0.1049 0.0117 0.0606 -0.0021 0.0052 -0.0221 0.0052 0.0016 0.1040 -0.0039
189.	(0.00087)	RY	(5)	C	6	s(0.00%)p 1.00(0.44%)d99.99(99.56%) 0.0000 0.0000 0.0012 0.0037 0.0018 0.0062 -0.0016 0.0122 -0.0127 0.0633 0.1275 0.2938 -0.9352 0.0161 0.1350
190.	(0.00041)	RY	(6)	C	6	s(0.88%)p 5.90(5.20%)d99.99(93.92%) 0.0000 0.0036 0.0134 0.0929 0.0186 -0.1551 -0.0119 0.1649 0.0003 0.0157 0.9385 0.0533 0.1426 -0.1874 -0.0105
191.	(0.00019)	RY	(7)	C	6	s(2.37%)p 4.13(9.79%)d37.03(87.84%) 0.0000 0.0086 0.0988 0.1178 -0.0238 0.2102 -0.0190 0.1847 -0.0037 0.1366 -0.2033 0.1589 0.0450 -0.8839 0.1689
192.	(0.00015)	RY	(8)	C	6	s(0.13%)p72.66(9.25%)d99.99(90.62%) 0.0000 0.0030 0.0341 -0.0102 -0.0062 0.0740 -0.0075 0.0684 0.0078 -0.2867 0.0561 -0.8649 -0.3038 -0.2173 -0.1244
193.	(0.00009)	RY	(9)	C	6	s(92.45%)p 0.00(0.19%)d 0.08(7.36%)
194.	(0.00003)	RY	(10)	C	6	s(5.36%)p 0.02(0.13%)d17.64(94.52%)
195.	(0.00528)	RY	(1)	C	7	s(1.08%)p84.83(91.84%)d 6.53(7.08%) 0.0000 0.0310 0.0993 0.0032 0.0136 0.7707 -0.0031 -0.5611 0.0012 0.0967 -0.2560 0.0344 -0.0104 0.0617 -0.0119
196.	(0.00199)	RY	(2)	C	7	s(0.06%)p99.99(97.71%)d38.36(2.23%) 0.0000 0.0066 -0.0043 0.0228 0.0115 -0.5709 0.0164 -0.8052 0.0023 0.0496 0.0907 0.0122 0.0437 0.1097 0.0050
197.	(0.00070)	RY	(3)	C	7	s(0.25%)p99.99(79.69%)d81.33(20.06%) 0.0000 0.0012 0.0482 -0.0120 -0.0036 -0.0408 0.0015 0.0989 0.0193 0.8860 0.0480 0.3995 0.1907 -0.0439 0.0199
198.	(0.00046)	RY	(4)	C	7	s(8.35%)p 1.68(14.01%)d 9.30(77.64%) 0.0000 -0.0015 0.2889 -0.0065 -0.0008 0.0135 0.0018 -0.0112 0.0035 -0.3738 0.0216 0.4245 0.7432 -0.1876 -0.0903
199.	(0.00039)	RY	(5)	C	7	s(85.15%)p 0.01(0.76%)d 0.17(14.09%) 0.0000 -0.0022 0.9227 0.0040 -0.0043 -0.0498 0.0052 0.0161 -0.0006 0.0694 0.1486 -0.1880 -0.2521 -0.1396 0.0215
200.	(0.00008)	RY	(6)	C	7	s(27.22%)p 0.07(1.91%)d 2.60(70.88%)
201.	(0.00007)	RY	(7)	C	7	s(69.34%)p 0.01(0.84%)d 0.43(29.82%)
202.	(0.00002)	RY	(8)	C	7	s(0.89%)p 1.32(1.17%)d99.99(97.94%)
203.	(0.00001)	RY	(9)	C	7	s(7.83%)p 0.80(6.24%)d10.98(85.93%)
204.	(0.00001)	RY	(10)	C	7	s(0.01%)p99.99(5.86%)d99.99(94.13%)
205.	(0.00124)	RY	(1)	H	8	s(99.79%)p 0.00(0.21%) 0.0026 0.9989 -0.0273 0.0301 0.0210
206.	(0.00016)	RY	(2)	H	8	s(0.07%)p99.99(99.93%) -0.0002 0.0267 0.0859 -0.1175 -0.9890
207.	(0.00005)	RY	(3)	H	8	s(0.00%)p 1.00(100.00%)
208.	(0.00001)	RY	(4)	H	8	s(0.21%)p99.99(99.79%)
209.	(0.00430)	RY	(1)	C	9	s(0.13%)p99.99(92.83%)d52.87(7.03%) 0.0000 0.0294 -0.0189 0.0104 -0.0092 -0.8786 -0.0075 -0.3930 -0.0012 -0.0431 0.2069 -0.0101 0.0393 0.1603 -0.0137

210. (0.00209) RY (2) C 9	s(0.77%)p99.99(97.11%)d 2.74(2.11%) 0.0000 -0.0147 0.0813 0.0299 0.0127 -0.4023 -0.0174 0.8907 -0.0001 -0.1246 0.0648 -0.0187 -0.0044 -0.1286 -0.0066
211. (0.00081) RY (3) C 9	s(0.25%)p99.99(75.37%)d96.12(24.38%) 0.0000 -0.0004 0.0503 -0.0017 0.0021 0.0815 -0.0015 -0.0912 -0.0226 -0.8592 -0.0573 -0.0474 0.4755 -0.0557 -0.0955
212. (0.00049) RY (4) C 9	s(0.89%)p21.94(19.56%)d89.22(79.54%) 0.0000 0.0003 0.0944 0.0025 0.0013 -0.0357 -0.0012 0.0322 -0.0033 0.4397 -0.1318 -0.5180 0.6859 -0.0349 -0.1952
213. (0.00027) RY (5) C 9	s(94.94%)p 0.01(1.03%)d 0.04(4.03%) 0.0000 0.0001 0.9741 -0.0231 0.0060 -0.0175 -0.0025 -0.0993 0.0020 0.0101 -0.0879 0.0660 -0.1289 -0.0773 -0.0747
214. (0.00009) RY (6) C 9	s(39.45%)p 0.02(0.87%)d 1.51(59.68%)
215. (0.00006) RY (7) C 9	s(55.86%)p 0.03(1.69%)d 0.76(42.46%)
216. (0.00001) RY (8) C 9	s(4.97%)p 0.64(3.18%)d18.46(91.84%)
217. (0.00001) RY (9) C 9	s(0.11%)p46.16(4.95%)d99.99(94.95%)
218. (0.00001) RY (10) C 9	s(2.79%)p 1.23(3.43%)d33.58(93.77%)
219. (0.00118) RY (1) H 10	s(99.65%)p 0.00(0.35%) 0.0024 0.9983 0.0583 -0.0052 0.0064
220. (0.00017) RY (2) H 10	s(0.00%)p 1.00(100.00%) 0.0001 0.0006 0.0882 -0.1189 -0.9890
221. (0.00004) RY (3) H 10	s(0.12%)p99.99(99.88%)
222. (0.00001) RY (4) H 10	s(0.30%)p99.99(99.70%)
223. (0.00574) RY (1) C 11	s(5.32%)p17.52(93.16%)d 0.29(1.52%) 0.0000 -0.0260 0.2267 0.0332 -0.0211 0.6245 0.0068 -0.4813 -0.0231 0.5558 0.0709 -0.0747 0.0633 -0.0194 -0.0146
224. (0.00370) RY (2) C 11	s(0.24%)p99.99(95.77%)d16.32(3.98%) 0.0000 0.0008 0.0418 0.0263 -0.0023 0.5852 0.0010 0.7840 -0.0133 0.0204 -0.1536 -0.0825 -0.0894 -0.0294 0.0246
225. (0.00277) RY (3) C 11	s(1.15%)p82.53(95.10%)d 3.26(3.75%) 0.0000 -0.0276 0.1018 0.0200 -0.0185 -0.4832 -0.0003 0.3074 0.0107 0.7890 -0.1541 0.0373 0.0270 -0.0070 0.1077
226. (0.00127) RY (4) C 11	s(16.40%)p 0.24(3.92%)d 4.86(79.67%) 0.0000 0.0003 0.4050 -0.0054 0.0003 -0.0857 0.0177 0.1754 -0.0123 -0.0261 0.6486 -0.2532 0.0870 0.5498 -0.0448
227. (0.00118) RY (5) C 11	s(21.74%)p 0.17(3.66%)d 3.43(74.60%) 0.0000 0.0026 0.4661 -0.0098 -0.0069 -0.1281 -0.0054 -0.0710 -0.0226 -0.1206 -0.5096 -0.5172 -0.0417 -0.0152 -0.4657
228. (0.00067) RY (6) C 11	s(3.18%)p 0.44(1.41%)d30.01(95.41%) 0.0000 0.0038 0.1780 0.0091 0.0444 -0.0882 -0.0090 0.0380 0.0052 -0.0530 0.3483 -0.4281 -0.0430 -0.7333 0.3316
229. (0.00060) RY (7) C 11	s(41.15%)p 0.03(1.25%)d 1.40(57.60%) 0.0000 0.0036 0.6401 -0.0427 -0.0071 -0.0226 0.0028 0.0095 -0.0144 -0.1080 0.0325 0.6295 -0.3851 -0.1730 -0.0196
230. (0.00042) RY (8) C 11	s(9.43%)p 0.40(3.81%)d 9.20(86.76%) 0.0000 0.0034 0.3026 -0.0524 0.0016 0.0222 0.0083 -0.0757 0.0133 -0.1778 -0.3714 -0.0194 0.3508 0.2300 0.7439
231. (0.00032) RY (9) C 11	s(2.14%)p 0.86(1.83%)d44.96(96.03%) 0.0000 0.0029 0.1403 -0.0409 -0.0018 0.0108 -0.0149 0.1266 0.0046 -0.0441 0.0795 0.2696 0.8385 -0.2725 -0.3223
232. (0.00003) RY (10) C 11	s(99.33%)p 0.00(0.35%)d 0.00(0.33%)
233. (0.00541) RY (1) C 12	s(0.82%)p99.99(94.92%)d 5.21(4.26%) 0.0000 0.0249 0.0869 -0.0033 0.0061 -0.7656 -0.0011 -0.6017 0.0006 -0.0302 -0.1066 -0.0053 -0.0316 -0.1737 -0.0068
234. (0.00465) RY (2) C 12	s(0.00%)p 1.00(93.98%)d 0.06(6.02%) 0.0000 0.0043 0.0025 -0.0030 -0.0051 -0.5975 0.0163 0.7597 -0.0054 -0.0738 -0.1994 0.0367 -0.0041 0.1379 0.0053
235. (0.00068) RY (3) C 12	s(0.04%)p99.99(6.74%)d99.99(93.23%) 0.0000 -0.0001 0.0191 0.0000 0.0000 0.0165 -0.0002 -0.0136 0.0008 -0.2587 -0.1013 -0.1428 0.9265 -0.0653 -0.1971
236. (0.00056) RY (4) C 12	s(0.70%)p68.20(47.88%)d73.25(51.42%)

			0.0000	-0.0002	0.0835	0.0064	0.0002
			-0.0465	0.0007	0.0336	-0.0014	0.6895
			-0.0711	-0.6970	0.0554	0.0697	-0.1239
237.	(0.00036)	RY (5) C 12	s(97.16%)	p 0.01(1.10%)	d 0.02(1.74%)		
			0.0000	-0.0054	0.9849	0.0387	-0.0060
			0.0807	-0.0029	0.0614	-0.0010	-0.0259
238.	(0.00025)	RY (6) C 12	s(0.11%)	p99.99(45.25%)	d99.99(54.63%)		
			0.0000	-0.0004	0.0333	-0.0038	-0.0007
			0.0548	-0.0009	-0.0201	-0.0013	-0.6702
			-0.0581	-0.6650	-0.3039	0.0748	-0.0525
239.	(0.00013)	RY (7) C 12	s(44.75%)	p 0.04(1.97%)	d 1.19(53.28%)		
			0.0000	-0.0015	-0.0613	0.6661	-0.0150
			0.1295	-0.0064	0.0477	-0.0007	0.0203
			-0.5356	-0.0164	-0.0464	-0.4536	0.1942
240.	(0.00009)	RY (8) C 12	s(18.49%)	p 0.26(4.81%)	d 4.15(76.70%)		
241.	(0.00007)	RY (9) C 12	s(31.85%)	p 0.11(3.35%)	d 2.03(64.79%)		
242.	(0.00001)	RY (10) C 12	s(6.19%)	p 0.00(0.01%)	d15.15(93.80%)		
243.	(0.00260)	RY (1) C 13	s(2.61%)	p34.15(89.13%)	d 3.17(8.26%)		
			0.0000	0.0029	0.1614	0.0051	-0.0008
			0.1075	-0.0126	-0.8040	0.0045	0.4828
			0.0234	0.0188	-0.2244	0.0997	0.1464
244.	(0.00191)	RY (2) C 13	s(0.00%)	p 1.00(88.27%)	d 0.13(11.73%)		
			0.0000	-0.0001	0.0037	-0.0001	-0.0177
			-0.9114	-0.0074	0.0211	-0.0046	0.2264
			-0.1263	-0.2730	-0.0154	-0.0963	0.1316
245.	(0.00092)	RY (3) C 13	s(50.71%)	p 0.90(45.72%)	d 0.07(3.58%)		
			0.0000	0.0135	0.7118	0.0146	0.0066
			0.0745	-0.0087	0.4521	-0.0145	0.4969
			0.1366	0.0892	0.0122	0.0731	-0.0606
246.	(0.00024)	RY (4) C 13	s(23.06%)	p 0.49(11.23%)	d 2.85(65.71%)		
			0.0000	-0.0072	0.4428	-0.1857	-0.0135
			0.1058	0.0203	-0.2096	0.0048	-0.2379
			-0.5146	-0.3656	0.1426	-0.3562	-0.3338
247.	(0.00014)	RY (5) C 13	s(16.41%)	p 2.45(40.14%)	d 2.65(43.45%)		
			0.0000	-0.0158	0.4041	0.0238	0.0090
			-0.2900	0.0065	-0.1312	0.0203	-0.5473
			0.0854	0.3278	-0.4554	0.3142	-0.1166
248.	(0.00005)	RY (6) C 13	s(15.54%)	p 0.69(10.68%)	d 4.75(73.78%)		
249.	(0.00004)	RY (7) C 13	s(3.69%)	p 2.73(10.08%)	d23.35(86.23%)		
250.	(0.00002)	RY (8) C 13	s(24.61%)	p 0.13(3.20%)	d 2.93(72.19%)		
251.	(0.00001)	RY (9) C 13	s(8.51%)	p 0.07(0.57%)	d10.68(90.92%)		
252.	(0.00001)	RY (10) C 13	s(54.91%)	p 0.02(1.30%)	d 0.80(43.79%)		
253.	(0.00145)	RY (1) H 14	s(99.91%)	p 0.00(0.09%)			
			-0.0010	0.9996	-0.0001	-0.0159	0.0253
254.	(0.00007)	RY (2) H 14	s(0.03%)	p99.99(99.97%)			
255.	(0.00005)	RY (3) H 14	s(0.05%)	p99.99(99.95%)			
256.	(0.00001)	RY (4) H 14	s(0.07%)	p99.99(99.93%)			
257.	(0.00067)	RY (1) H 15	s(99.45%)	p 0.01(0.55%)			
			-0.0004	0.9973	0.0147	-0.0660	-0.0301
258.	(0.00007)	RY (2) H 15	s(0.22%)	p99.99(99.78%)			
259.	(0.00003)	RY (3) H 15	s(0.33%)	p99.99(99.67%)			
260.	(0.00000)	RY (4) H 15	s(0.05%)	p99.99(99.95%)			
261.	(0.00145)	RY (1) H 16	s(99.79%)	p 0.00(0.21%)			
			-0.0008	0.9989	-0.0110	-0.0431	0.0112
262.	(0.00008)	RY (2) H 16	s(0.14%)	p99.99(99.86%)			
263.	(0.00004)	RY (3) H 16	s(0.04%)	p99.99(99.96%)			
264.	(0.00001)	RY (4) H 16	s(0.09%)	p99.99(99.91%)			
265.	(0.00421)	RY (1) C 17	s(0.10%)	p99.99(93.19%)	d65.63(6.70%)		
			0.0000	0.0306	0.0078	-0.0046	-0.0023
			-0.1240	-0.0144	-0.9530	0.0022	0.0906
			0.0305	-0.0221	-0.0264	-0.2546	-0.0093
266.	(0.00234)	RY (2) C 17	s(0.14%)	p99.99(98.84%)	d 7.25(1.02%)		
			0.0000	-0.0022	0.0304	0.0219	-0.0282
			0.9829	0.0051	-0.1193	-0.0004	0.0848
			0.0972	-0.0228	0.0081	0.0112	-0.0074
267.	(0.00067)	RY (3) C 17	s(0.00%)	p 1.00(13.64%)	d 6.33(86.36%)		
			0.0000	0.0000	0.0054	0.0034	0.0013
			0.0387	-0.0023	-0.0405	-0.0207	-0.3645
			0.0992	0.9122	0.0731	-0.0758	0.1029
268.	(0.00053)	RY (4) C 17	s(1.18%)	p66.79(78.83%)	d16.94(19.99%)		
			0.0000	-0.0001	0.1086	0.0004	0.0001
			0.0570	-0.0009	-0.0951	-0.0132	-0.8808
			-0.0717	-0.3586	0.2385	0.0195	-0.0945
269.	(0.00033)	RY (5) C 17	s(95.87%)	p 0.01(1.18%)	d 0.03(2.95%)		
			0.0000	-0.0022	0.9788	-0.0247	-0.0040
			-0.0381	0.0037	-0.0120	0.0016	0.1007

270.	(0.00011)	RY	(6)	C 17	-0.0233 0.0613 -0.0304 0.1274 -0.0896 s(5.00%)p 0.18(0.91%)d18.82(94.09%) 0.0000 0.0009 0.0084 0.2235 -0.0235 0.0912 0.0037 -0.0018 -0.0021 0.0136 -0.9439 0.0832 -0.0757 -0.1533 0.1179
271.	(0.00006)	RY	(7)	C 17	s(82.11%)p 0.00(0.28%)d 0.21(17.61%)
272.	(0.00001)	RY	(8)	C 17	s(5.71%)p 1.10(6.30%)d15.41(87.99%)
273.	(0.00001)	RY	(9)	C 17	s(9.94%)p 0.03(0.34%)d 9.03(89.72%)
274.	(0.00000)	RY	(10)	C 17	s(0.10%)p62.71(6.52%)d99.99(93.37%)
275.	(0.00098)	RY	(1)	H 18	s(99.76%)p 0.00(0.24%) 0.0022 0.9988 -0.0048 0.0486 0.0052
276.	(0.00015)	RY	(2)	H 18	s(0.01%)p99.99(99.99%) -0.0002 0.0109 0.0919 -0.1083 -0.9898 s(0.01%)p 1.00(99.99%)
277.	(0.00005)	RY	(3)	H 18	s(0.30%)p99.99(99.70%)
278.	(0.00001)	RY	(4)	H 18	s(5.39%)p17.29(93.22%)d 0.26(1.39%) 0.0000 -0.0265 0.2283 0.0329 -0.0192 0.6017 -0.0024 0.4072 0.0279 -0.6351 -0.0243 0.0849 0.0550 -0.0301 -0.0463
279.	(0.00584)	RY	(1)	C 19	s(0.85%)p99.99(96.48%)d 3.15(2.67%) 0.0000 0.0099 0.0911 0.0101 0.0069 0.6177 -0.0013 -0.7514 0.0169 0.1354 0.0771 0.0723 -0.1127 0.0316 -0.0430
280.	(0.00385)	RY	(2)	C 19	s(1.22%)p77.67(94.85%)d 3.22(3.93%) 0.0000 -0.0259 0.1031 0.0300 -0.0190 -0.4548 0.0013 -0.4783 -0.0046 -0.7158 0.1342 0.0065 -0.0187 0.0619 0.1307
281.	(0.00263)	RY	(3)	C 19	s(11.33%)p 0.18(1.99%)d 7.65(86.68%) 0.0000 0.0000 0.3365 -0.0033 -0.0003 -0.0922 -0.0179 -0.1000 0.0107 0.0313 -0.8207 0.1934 0.1658 0.3475 -0.0873
282.	(0.00125)	RY	(4)	C 19	s(32.21%)p 0.18(5.67%)d 1.93(62.12%) 0.0000 0.0017 0.5672 -0.0177 -0.0043 -0.1719 0.0059 0.0858 0.0233 0.1385 0.4293 0.3062 -0.1394 0.1921 -0.5356
283.	(0.00121)	RY	(5)	C 19	s(2.86%)p 0.47(1.34%)d33.49(95.80%) 0.0000 0.0041 0.1690 0.0058 0.0440 -0.0861 0.0019 -0.0252 -0.0121 0.0567 -0.1241 0.5980 -0.0875 -0.7271 0.2206
284.	(0.00067)	RY	(6)	C 19	s(37.11%)p 0.02(0.89%)d 1.67(62.00%) 0.0000 0.0032 0.6073 -0.0478 -0.0046 -0.0284 -0.0014 0.0011 0.0128 0.0888 -0.0915 -0.6678 -0.2083 -0.3076 0.1664
285.	(0.00062)	RY	(7)	C 19	s(8.13%)p 0.48(3.88%)d10.83(87.99%) 0.0000 0.0028 0.2806 -0.0502 -0.0022 0.0499 -0.0100 0.0962 -0.0131 0.1636 0.2713 0.1950 0.1783 0.3925 0.7632
286.	(0.00040)	RY	(8)	C 19	s(1.80%)p 0.88(1.58%)d53.56(96.61%) 0.0000 0.0029 0.1214 -0.0573 0.0004 -0.0021 0.0140 -0.1160 -0.0079 0.0457 0.1398 -0.1146 0.9227 -0.2405 -0.1557
287.	(0.00032)	RY	(9)	C 19	s(99.19%)p 0.00(0.37%)d 0.00(0.44%)
288.	(0.00003)	RY	(10)	C 19	s(0.02%)p99.99(97.58%)d99.99(2.40%) 0.0000 -0.0040 0.0115 0.0048 -0.0006 -0.0759 0.0028 0.1164 0.0811 -0.9746 0.0143 0.1525 0.0003 0.0096 -0.0215
289.	(0.01744)	RY	(1)	B 20	s(4.47%)p19.81(88.53%)d 1.57(7.00%) 0.0000 0.0356 0.2036 -0.0445 0.0164 -0.5342 -0.0041 -0.7732 0.0045 -0.0416 -0.2385 0.0557 0.0533 -0.0217 -0.0821
290.	(0.00614)	RY	(2)	B 20	s(29.28%)p 2.19(64.12%)d 0.23(6.59%) 0.0000 -0.0016 0.5411 0.0054 -0.0408 -0.5956 0.0007 0.5223 0.0003 0.1096 0.1234 -0.0802 0.0152 0.0808 -0.1936
291.	(0.00483)	RY	(3)	B 20	s(48.56%)p 0.64(31.24%)d 0.42(20.21%) 0.0000 -0.0030 0.6963 -0.0272 0.0112 0.5272 -0.0192 -0.1758 -0.0029 -0.0558 -0.0546 -0.0373 -0.3760 0.1747 -0.1605
292.	(0.00196)	RY	(4)	B 20	s(12.13%)p 0.38(4.63%)d 6.86(83.24%) 0.0000 -0.0094 0.3404 0.0733 0.0170 0.1927 -0.0125 -0.0929 0.0074 0.0055 0.2557 0.1808 0.7984 0.0901 0.2980
293.	(0.00157)	RY	(5)	B 20	s(0.48%)p15.16(7.27%)d99.99(92.25%) 0.0000 -0.0090 0.0025 0.0686 0.0047 -0.1471 -0.0132 -0.2155 -0.0233 -0.0622 0.7277 -0.3062 -0.3288 0.0581 0.4332
294.	(0.00117)	RY	(6)	B 20	s(5.74%)p 0.43(2.46%)d16.01(91.81%)
295.	(0.00108)	RY	(7)	B 20	

		0.0000	-0.0047	0.2365	0.0374	0.0280
		-0.0463	0.0078	0.1465	-0.0031	0.0092
		-0.3954	0.0736	-0.1734	-0.4852	0.7006
296.	(0.00074) RY (8) B 20	s(0.04%)p72.06(3.07%)d99.99(96.88%)	0.0000	0.0026	0.0185	0.0088
			-0.0032	0.0629	0.0040	0.0037
			-0.0529	-0.1548	-0.2673	-0.9087
			0.2675	-0.0035	0.0069	s(96.21%)p 0.00(0.10%)d 0.04(3.69%)
297.	(0.00027) RY (9) B 20		0.0000	0.0017	-0.0234	0.9806
			-0.0057	-0.0244	-0.0088	-0.0149
			0.0021	0.0086	-0.1129	0.0227
			-0.0524	0.1427	-0.0229	s(3.20%)p 0.54(1.74%)d29.67(95.05%)
298.	(0.00019) RY (10) B 20		0.0000	0.0141	0.0887	0.1549
			-0.0328	0.0996	0.0060	-0.0779
			-0.0023	-0.0186	0.2974	-0.0517
			-0.8334	-0.3990	s(1.26%)p71.55(89.92%)d 7.02(8.82%)	0.0000
299.	(0.00317) RY (1) C 21		0.0034	0.1120	0.0012	0.0039
			0.3323	-0.0103	-0.7213	-0.0100
			-0.5179	0.0028	-0.0837	0.1457
			0.1614	0.1842	s(0.01%)p99.99(89.09%)d99.99(10.89%)	0.0000
300.	(0.00241) RY (2) C 21		0.0034	0.0108	-0.0001	0.0188
			0.8318	0.0100	0.0576	0.0052
			0.4419	0.1499	-0.1426	0.0347
			0.1102	-0.2298	s(44.96%)p 1.19(53.45%)d 0.04(1.59%)	0.0000
301.	(0.00088) RY (3) C 21		0.0112	0.6702	0.0178	-0.0012
			0.1720	-0.0210	0.5320	0.0189
			-0.4702	0.1152	-0.0046	0.0181
			0.0451	-0.0148	s(20.41%)p 0.34(6.99%)d 3.56(72.60%)	0.0000
302.	(0.00026) RY (4) C 21		-0.0036	0.3786	-0.2464	-0.0139
			0.0871	0.0206	-0.2102	-0.0027
			0.1323	-0.6073	0.2519	-0.0514
			-0.4761	-0.2538	s(26.32%)p 1.32(34.70%)d 1.48(38.98%)	0.0000
303.	(0.00014) RY (5) C 21		-0.0129	0.5012	-0.1090	0.0132
			-0.3561	0.0133	-0.2144	-0.0158
			0.4166	0.0816	-0.1614	0.4138
			0.4195	-0.0996	s(25.65%)p 0.16(4.03%)d 2.74(70.32%)	0.0000
304.	(0.00006) RY (6) C 21		0.0000	0.0000	0.0000	0.0000
305.	(0.00004) RY (7) C 21		0.0000	0.0000	0.0000	0.0000
306.	(0.00002) RY (8) C 21		0.0000	0.0000	0.0000	0.0000
307.	(0.00001) RY (9) C 21		0.0000	0.0000	0.0000	0.0000
308.	(0.00001) RY (10) C 21		0.0000	0.0000	0.0000	0.0000
309.	(0.00149) RY (1) H 22		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
310.	(0.00007) RY (2) H 22		0.0000	0.0000	0.0000	0.0000
311.	(0.00005) RY (3) H 22		0.0000	0.0000	0.0000	0.0000
312.	(0.00001) RY (4) H 22		0.0000	0.0000	0.0000	0.0000
313.	(0.00122) RY (1) H 23		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
314.	(0.00008) RY (2) H 23		0.0000	0.0000	0.0000	0.0000
315.	(0.00004) RY (3) H 23		0.0000	0.0000	0.0000	0.0000
316.	(0.00001) RY (4) H 23		0.0000	0.0000	0.0000	0.0000
317.	(0.00101) RY (1) H 24		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
318.	(0.00007) RY (2) H 24		0.0000	0.0000	0.0000	0.0000
319.	(0.00003) RY (3) H 24		0.0000	0.0000	0.0000	0.0000
320.	(0.00001) RY (4) H 24		0.0000	0.0000	0.0000	0.0000
321.	(0.00225) RY (1) C 25		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
322.	(0.00207) RY (2) C 25		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
323.	(0.00111) RY (3) C 25		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
324.	(0.00017) RY (4) C 25		0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000
325.	(0.00009) RY (5) C 25		0.0000	0.0000	0.0000	0.0000
326.	(0.00003) RY (6) C 25		0.0000	0.0000	0.0000	0.0000
327.	(0.00001) RY (7) C 25		0.0000	0.0000	0.0000	0.0000
328.	(0.00001) RY (8) C 25		0.0000	0.0000	0.0000	0.0000
329.	(0.00001) RY (9) C 25		0.0000	0.0000	0.0000	0.0000
330.	(0.00000) RY (10) C 25		0.0000	0.0000	0.0000	0.0000

331.	(0.00127)	RY	(1)	H	26	s(99.38%)p 0.01(0.62%)
						0.0000 0.9969 0.0242 -0.0736 0.0131
332.	(0.00007)	RY	(2)	H	26	s(0.52%)p99.99(99.48%)
333.	(0.00006)	RY	(3)	H	26	s(0.09%)p99.99(99.91%)
334.	(0.00001)	RY	(4)	H	26	s(0.05%)p99.99(99.95%)
335.	(0.00110)	RY	(1)	H	27	s(98.93%)p 0.01(1.07%)
						0.0010 0.9946 -0.0579 -0.0792 -0.0329
336.	(0.00008)	RY	(2)	H	27	s(0.87%)p99.99(99.13%)
337.	(0.00007)	RY	(3)	H	27	s(0.02%)p99.99(99.98%)
338.	(0.00001)	RY	(4)	H	27	s(0.23%)p99.99(99.77%)
339.	(0.00094)	RY	(1)	H	28	s(99.71%)p 0.00(0.29%)
						-0.0005 0.9986 0.0202 -0.0411 0.0281
340.	(0.00009)	RY	(2)	H	28	s(0.15%)p99.99(99.85%)
341.	(0.00007)	RY	(3)	H	28	s(0.09%)p99.99(99.91%)
342.	(0.00000)	RY	(4)	H	28	s(0.10%)p99.99(99.90%)
343.	(0.00399)	RY	(1)	C	29	s(0.10%)p99.99(92.62%)d71.37(7.28%)
						0.0000 0.0309 -0.0082 -0.0007 -0.0121
						-0.8861 -0.0023 -0.3730 -0.0004 -0.0405
						0.1829 0.0030 0.0436 0.1933 -0.0087
344.	(0.00210)	RY	(2)	C	29	s(0.12%)p99.99(97.90%)d16.31(1.98%)
						0.0000 -0.0120 0.0247 0.0215 -0.0048
						0.3725 0.0210 -0.9057 0.0002 0.1395
						-0.1021 0.0191 -0.0185 0.0930 0.0047
345.	(0.00073)	RY	(3)	C	29	s(0.94%)p66.42(62.25%)d39.28(36.81%)
						0.0000 -0.0008 0.0968 0.0033 -0.0022
						-0.0756 0.0015 0.0850 0.0226 0.7804
						-0.1101 -0.3393 0.4704 -0.0179 -0.1387
346.	(0.00052)	RY	(4)	C	29	s(0.74%)p44.61(33.22%)d88.69(66.04%)
						0.0000 0.0004 0.0859 0.0080 0.0000
						0.0603 0.0022 -0.0735 -0.0004 -0.5684
						-0.1085 -0.1414 0.7796 -0.0578 -0.1326
347.	(0.00022)	RY	(5)	C	29	s(94.12%)p 0.00(0.39%)d 0.06(5.49%)
						0.0000 -0.0013 0.9696 0.0311 0.0012
						-0.0521 0.0078 -0.0014 -0.0033 -0.0335
						-0.0579 0.0691 -0.1489 -0.1237 -0.0965
348.	(0.00008)	RY	(6)	C	29	s(30.87%)p 0.04(1.11%)d 2.20(68.02%)
349.	(0.00006)	RY	(7)	C	29	s(63.77%)p 0.02(1.17%)d 0.55(35.06%)
350.	(0.00001)	RY	(8)	C	29	s(4.58%)p 0.91(4.17%)d19.92(91.25%)
351.	(0.00001)	RY	(9)	C	29	s(0.29%)p15.30(4.37%)d99.99(95.34%)
352.	(0.00001)	RY	(10)	C	29	s(4.65%)p 0.61(2.85%)d19.90(92.50%)
353.	(0.00111)	RY	(1)	H	30	s(99.74%)p 0.00(0.26%)
						0.0022 0.9987 0.0317 0.0346 -0.0187
354.	(0.00016)	RY	(2)	H	30	s(0.04%)p99.99(99.96%)
						0.0000 0.0190 -0.1270 0.1015 0.9865
355.	(0.00004)	RY	(3)	H	30	s(0.07%)p99.99(99.93%)
356.	(0.00001)	RY	(4)	H	30	s(0.22%)p99.99(99.78%)
357.	(0.00360)	RY	(1)	C	31	s(0.62%)p99.99(92.29%)d11.41(7.09%)
						0.0000 -0.0306 0.0706 0.0171 -0.0040
						-0.1694 -0.0115 -0.9449 0.0017 0.0343
						-0.0858 0.0379 0.0008 0.2486 0.0166
358.	(0.00233)	RY	(2)	C	31	s(2.36%)p40.69(96.00%)d 0.70(1.65%)
						0.0000 0.0112 0.1522 0.0175 0.0198
						-0.9576 -0.0108 0.1775 -0.0008 -0.1047
						0.1198 -0.0202 0.0158 0.0378 -0.0018
359.	(0.00097)	RY	(3)	C	31	s(0.10%)p99.99(95.78%)d40.32(4.12%)
						0.0000 0.0000 0.0319 0.0024 -0.0011
						-0.0933 0.0001 0.0517 0.0152 0.9727
						-0.0320 0.0013 0.1986 -0.0213 -0.0158
360.	(0.00062)	RY	(4)	C	31	s(0.59%)p 0.23(0.14%)d99.99(99.27%)
						0.0000 -0.0003 0.0768 -0.0031 0.0011
						0.0305 -0.0013 -0.0024 -0.0144 -0.0146
						-0.0770 -0.9655 0.0678 0.1252 -0.1851
361.	(0.00033)	RY	(5)	C	31	s(93.99%)p 0.03(3.29%)d 0.03(2.72%)
						0.0000 -0.0007 0.9682 -0.0494 -0.0047
						0.1638 -0.0024 0.0761 -0.0008 -0.0149
						-0.0497 0.1070 -0.0266 0.1009 -0.0492
362.	(0.00008)	RY	(6)	C	31	s(78.90%)p 0.00(0.36%)d 0.26(20.74%)
363.	(0.00006)	RY	(7)	C	31	s(20.39%)p 0.09(1.84%)d 3.81(77.77%)
364.	(0.00002)	RY	(8)	C	31	s(1.95%)p 3.00(5.84%)d47.36(92.21%)
365.	(0.00001)	RY	(9)	C	31	s(1.05%)p 0.20(0.21%)d93.75(98.73%)
366.	(0.00001)	RY	(10)	C	31	s(0.23%)p19.05(4.29%)d99.99(95.48%)
367.	(0.00102)	RY	(1)	H	32	s(99.69%)p 0.00(0.31%)
						0.0025 0.9985 -0.0008 -0.0512 -0.0209
368.	(0.00018)	RY	(2)	H	32	s(0.05%)p99.99(99.95%)
						0.0003 0.0223 -0.1372 0.0337 0.9897
369.	(0.00005)	RY	(3)	H	32	s(0.00%)p 1.00(100.00%)
370.	(0.00001)	RY	(4)	H	32	s(0.33%)p99.99(99.67%)

371. (0.00420) RY (1) C 33	s(0.13%)p99.99(93.16%)d51.40(6.71%) 0.0000 0.0312 0.0181 -0.0019 -0.0126 -0.7300 0.0059 0.6225 -0.0023 -0.1047 -0.2488 0.0230 -0.0278 0.0620 -0.0075
372. (0.00231) RY (2) C 33	s(0.21%)p99.99(98.53%)d 5.85(1.26%) 0.0000 -0.0037 0.0461 0.0023 -0.0163 0.6356 -0.0233 0.7607 -0.0005 0.0432 0.0459 0.0218 0.0293 0.0951 -0.0088
373. (0.00098) RY (3) C 33	s(0.30%)p99.99(63.55%)d99.99(36.15%) 0.0000 -0.0004 0.0541 -0.0100 -0.0028 -0.0861 0.0022 0.0378 0.0270 0.7911 0.0333 -0.4845 -0.3402 0.0822 -0.0555
374. (0.00044) RY (4) C 33	s(0.00%)p 1.00(29.97%)d 2.34(70.03%) 0.0000 0.0003 0.0050 -0.0034 -0.0001 0.0747 -0.0012 -0.0077 -0.0021 -0.5422 0.0627 -0.3552 -0.7494 0.0904 0.0208
375. (0.00025) RY (5) C 33	s(95.27%)p 0.01(0.61%)d 0.04(4.12%) 0.0000 -0.0016 0.9755 -0.0332 0.0052 -0.0488 -0.0004 -0.0362 -0.0019 -0.0490 0.1615 0.0419 0.0359 0.0596 -0.0925
376. (0.00009) RY (6) C 33	s(7.92%)p 0.13(1.01%)d11.50(91.07%)
377. (0.00006) RY (7) C 33	s(75.44%)p 0.00(0.32%)d 0.32(24.23%)
378. (0.00001) RY (8) C 33	s(2.50%)p 2.53(6.32%)d36.51(91.19%)
379. (0.00001) RY (9) C 33	s(18.39%)p 0.01(0.24%)d 4.43(81.38%)
380. (0.00000) RY (10) C 33	s(0.01%)p 1.00(6.33%)d14.79(93.66%)
381. (0.00089) RY (1) H 34	s(99.72%)p 0.00(0.28%) 0.0019 0.9986 0.0239 -0.0441 -0.0180
382. (0.00016) RY (2) H 34	s(0.06%)p99.99(99.94%) 0.0000 0.0236 -0.1265 0.0610 0.9898
383. (0.00005) RY (3) H 34	s(0.05%)p99.99(99.95%)
384. (0.00001) RY (4) H 34	s(0.26%)p99.99(99.74%)
385. (0.00225) RY (1) C 35	s(3.59%)p25.25(90.53%)d 1.64(5.89%) 0.0000 0.0086 0.1891 0.0039 0.0003 -0.6437 -0.0099 -0.6763 -0.0024 0.1829 0.0550 -0.0770 -0.0595 -0.2076 -0.0572
386. (0.00188) RY (2) C 35	s(0.85%)p99.99(91.55%)d 8.93(7.60%) 0.0000 0.0085 0.0914 -0.0097 0.0068 -0.2374 0.0068 0.4257 0.0142 0.8232 0.0787 0.0814 -0.0015 0.0830 0.2373
387. (0.00070) RY (3) C 35	s(37.26%)p 1.61(59.96%)d 0.07(2.78%) 0.0000 0.0232 0.6084 0.0440 -0.0021 0.6147 -0.0010 -0.3474 0.0024 0.3178 0.0012 -0.0167 0.0903 0.0743 -0.1177
388. (0.00015) RY (4) C 35	s(13.18%)p 1.32(17.36%)d 5.27(69.46%) 0.0000 -0.0139 0.3326 -0.1450 0.0237 -0.3237 -0.0036 0.2172 -0.0074 -0.1448 -0.0803 -0.2828 0.3017 0.5819 -0.4226
389. (0.00005) RY (5) C 35	s(22.67%)p 0.74(16.77%)d 2.67(60.56%)
390. (0.00003) RY (6) C 35	s(19.36%)p 0.71(13.72%)d 3.46(66.92%)
391. (0.00002) RY (7) C 35	s(62.12%)p 0.00(0.07%)d 0.61(37.81%)
392. (0.00001) RY (8) C 35	s(26.07%)p 0.13(3.37%)d 2.71(70.57%)
393. (0.00001) RY (9) C 35	s(3.24%)p 0.89(2.89%)d29.00(93.87%)
394. (0.00000) RY (10) C 35	s(11.78%)p 0.33(3.94%)d 7.15(84.28%)
395. (0.00134) RY (1) H 36	s(99.31%)p 0.01(0.69%) -0.0004 0.9965 0.0591 -0.0566 0.0148
396. (0.00008) RY (2) H 36	s(0.53%)p99.99(99.47%)
397. (0.00006) RY (3) H 36	s(0.16%)p99.99(99.84%)
398. (0.00001) RY (4) H 36	s(0.05%)p99.99(99.95%)
399. (0.00136) RY (1) H 37	s(99.65%)p 0.00(0.35%) -0.0001 0.9982 0.0497 -0.0120 0.0300
400. (0.00008) RY (2) H 37	s(0.33%)p99.99(99.67%)
401. (0.00007) RY (3) H 37	s(0.02%)p99.99(99.98%)
402. (0.00001) RY (4) H 37	s(0.05%)p99.99(99.95%)
403. (0.00094) RY (1) H 38	s(99.22%)p 0.01(0.78%) 0.0011 0.9961 -0.0095 -0.0639 0.0600
404. (0.00009) RY (2) H 38	s(0.63%)p99.99(99.37%)
405. (0.00007) RY (3) H 38	s(0.03%)p99.99(99.97%)
406. (0.00001) RY (4) H 38	s(0.17%)p99.99(99.83%)
407. (0.00216) RY (1) C 39	s(4.24%)p21.58(91.52%)d 1.00(4.24%) 0.0000 0.0149 0.2053 -0.0080 0.0050 -0.1625 0.0093 0.1791 0.0109 0.9254 0.0024 0.0182 0.1768 0.0318 0.0990
408. (0.00200) RY (2) C 39	s(6.85%)p12.76(87.45%)d 0.83(5.70%) 0.0000 0.0117 0.2615 -0.0027 -0.0003 -0.6652 0.0076 0.6069 -0.0043 -0.2520 -0.1453 -0.0249 -0.1553 -0.0822 -0.0664
409. (0.00094) RY (3) C 39	s(28.01%)p 2.45(68.71%)d 0.12(3.28%)

			0.0000	0.0234	0.5276	0.0352	0.0004
			0.6729	0.0023	0.4795	0.0001	-0.0660
			0.0943	-0.0155	-0.1152	0.0817	-0.0609
410.	(0.00018)	RY (4) C 39	s(1.31%)p 3.07(4.01%)d72.39(94.68%)				
			0.0000	0.0049	-0.0135	0.1135	-0.0238
			0.1813	0.0003	0.0729	0.0105	-0.0355
			-0.5759	0.2807	0.3185	-0.6455	0.1351
411.	(0.00010)	RY (5) C 39	s(57.44%)p 0.64(36.71%)d 0.10(5.85%)				
412.	(0.00003)	RY (6) C 39	s(2.95%)p 1.17(3.46%)d31.71(93.59%)				
413.	(0.00002)	RY (7) C 39	s(5.48%)p 0.39(2.14%)d16.84(92.38%)				
414.	(0.00001)	RY (8) C 39	s(11.41%)p 0.07(0.76%)d 7.69(87.82%)				
415.	(0.00001)	RY (9) C 39	s(66.09%)p 0.01(0.81%)d 0.50(33.10%)				
416.	(0.00001)	RY (10) C 39	s(16.35%)p 0.28(4.54%)d 4.84(79.11%)				
417.	(0.00134)	RY (1) H 40	s(99.42%)p 0.01(0.58%)				
			0.0001	0.9971	0.0264	0.0687	-0.0195
418.	(0.00007)	RY (2) H 40	s(0.51%)p99.99(99.49%)				
419.	(0.00006)	RY (3) H 40	s(0.07%)p99.99(99.93%)				
420.	(0.00001)	RY (4) H 40	s(0.05%)p99.99(99.95%)				
421.	(0.00102)	RY (1) H 41	s(98.89%)p 0.01(1.11%)				
			0.0008	0.9944	-0.0325	0.0932	0.0374
422.	(0.00008)	RY (2) H 41	s(1.00%)p99.37(99.00%)				
423.	(0.00007)	RY (3) H 41	s(0.00%)p 1.00(100.00%)				
424.	(0.00001)	RY (4) H 41	s(0.17%)p99.99(99.83%)				
425.	(0.00092)	RY (1) H 42	s(99.72%)p 0.00(0.28%)				
			-0.0003	0.9986	0.0278	0.0422	-0.0169
426.	(0.00009)	RY (2) H 42	s(0.21%)p99.99(99.79%)				
427.	(0.00008)	RY (3) H 42	s(0.04%)p99.99(99.96%)				
428.	(0.00001)	RY (4) H 42	s(0.08%)p99.99(99.92%)				
429.	(0.00227)	RY (1) C 43	s(2.71%)p33.57(91.11%)d 2.27(6.17%)				
			0.0000	0.0070	0.1646	0.0008	0.0028
			-0.5464	0.0093	0.7803	0.0022	-0.0594
			0.0072	0.0821	-0.0735	-0.2050	-0.0866
430.	(0.00181)	RY (2) C 43	s(0.92%)p99.15(91.49%)d 8.22(7.59%)				
			0.0000	0.0086	0.0948	-0.0128	0.0025
			-0.4390	-0.0073	-0.3423	-0.0145	-0.7777
			-0.0994	-0.0222	0.0246	0.0410	0.2515
431.	(0.00072)	RY (3) C 43	s(37.33%)p 1.59(59.27%)d 0.09(3.40%)				
			0.0000	0.0237	0.6090	0.0432	-0.0008
			0.5908	0.0017	0.2653	-0.0022	-0.4161
			0.0023	-0.0060	0.0927	0.0707	-0.1429
432.	(0.00015)	RY (4) C 43	s(10.12%)p 1.64(16.57%)d 7.24(73.31%)				
			0.0000	-0.0133	0.2896	-0.1311	0.0249
			-0.3316	-0.0005	-0.1558	0.0046	0.1756
			-0.0413	0.1151	0.2703	0.6298	-0.4984
433.	(0.00006)	RY (5) C 43	s(25.31%)p 0.80(20.19%)d 2.15(54.51%)				
434.	(0.00003)	RY (6) C 43	s(20.01%)p 0.62(12.37%)d 3.38(67.62%)				
435.	(0.00002)	RY (7) C 43	s(78.25%)p 0.00(0.19%)d 0.28(21.55%)				
436.	(0.00001)	RY (8) C 43	s(13.61%)p 0.20(2.73%)d 6.15(83.66%)				
437.	(0.00001)	RY (9) C 43	s(3.23%)p 0.81(2.62%)d29.11(94.15%)				
438.	(0.00000)	RY (10) C 43	s(8.62%)p 0.42(3.60%)d10.18(87.78%)				
439.	(0.00136)	RY (1) H 44	s(99.37%)p 0.01(0.63%)				
			-0.0006	0.9968	0.0599	0.0449	-0.0271
440.	(0.00008)	RY (2) H 44	s(0.51%)p99.99(99.49%)				
441.	(0.00006)	RY (3) H 44	s(0.12%)p99.99(99.88%)				
442.	(0.00000)	RY (4) H 44	s(0.05%)p99.99(99.95%)				
443.	(0.00148)	RY (1) H 45	s(99.68%)p 0.00(0.32%)				
			-0.0001	0.9984	0.0427	0.0034	-0.0365
444.	(0.00009)	RY (2) H 45	s(0.29%)p99.99(99.71%)				
445.	(0.00007)	RY (3) H 45	s(0.02%)p99.99(99.98%)				
446.	(0.00001)	RY (4) H 45	s(0.05%)p99.99(99.95%)				
447.	(0.00102)	RY (1) H 46	s(99.13%)p 0.01(0.87%)				
			0.0009	0.9957	-0.0077	0.0658	-0.0654
448.	(0.00009)	RY (2) H 46	s(0.73%)p99.99(99.27%)				
449.	(0.00007)	RY (3) H 46	s(0.01%)p 1.00(99.99%)				
450.	(0.00001)	RY (4) H 46	s(0.18%)p99.99(99.82%)				

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
1. CR (1) O 1	279. RY (1) C 19	1.96	19.77	0.176
1. CR (1) O 1	289. RY (1) B 20	2.63	19.60	0.203
1. CR (1) O 1	291. RY (3) B 20	0.53	19.89	0.092

2. CR (1) O 2	223. RY (1) C 11	1.99	19.76	0.177
2. CR (1) O 2	289. RY (1) B 20	2.46	19.60	0.196
2. CR (1) O 2	291. RY (3) B 20	0.71	19.89	0.106
3. CR (1) N 3	82. LV (1) B 20	10.16	14.31	0.340
3. CR (1) N 3	96. BD* (1) C 6- C 31	0.66	14.84	0.088
3. CR (1) N 3	185. RY (1) C 6	0.51	15.48	0.080
3. CR (1) N 3	186. RY (2) C 6	0.90	15.54	0.106
3. CR (1) N 3	301. RY (3) C 21	0.72	15.23	0.093
4. CR (1) C 4	93. BD* (1) C 4- B 20	0.84	10.47	0.084
4. CR (1) C 4	94. BD* (1) C 5- C 6	0.71	10.56	0.077
4. CR (1) C 4	95. BD* (1) C 5- C 12	1.26	10.56	0.103
4. CR (1) C 4	98. BD* (1) C 7- H 8	0.70	10.75	0.077
4. CR (1) C 4	99. BD* (1) C 7- C 17	0.76	10.54	0.080
4. CR (1) C 4	175. RY (1) C 5	0.53	11.37	0.070
4. CR (1) C 4	176. RY (2) C 5	0.99	11.40	0.095
4. CR (1) C 4	196. RY (2) C 7	1.17	10.81	0.100
4. CR (1) C 4	290. RY (2) B 20	2.03	10.90	0.133
4. CR (1) C 4	292. RY (4) B 20	0.89	11.21	0.089
5. CR (1) C 5	91. BD* (1) C 4- C 7	0.60	10.65	0.071
5. CR (1) C 5	93. BD* (1) C 4- B 20	0.97	10.50	0.090
5. CR (1) C 5	94. BD* (1) C 5- C 6	0.51	10.59	0.065
5. CR (1) C 5	96. BD* (1) C 6- C 31	1.14	10.63	0.098
5. CR (1) C 5	101. BD* (1) C 9- C 12	0.63	10.58	0.073
5. CR (1) C 5	107. BD* (1) C 12- C 29	0.73	10.57	0.078
5. CR (1) C 5	165. RY (1) C 4	0.55	11.54	0.071
5. CR (1) C 5	166. RY (2) C 4	1.01	11.26	0.095
5. CR (1) C 5	185. RY (1) C 6	1.81	11.27	0.128
5. CR (1) C 5	233. RY (1) C 12	1.72	11.30	0.124
6. CR (1) C 6	90. BD* (1) C 4- C 5	0.73	10.66	0.079
6. CR (1) C 6	94. BD* (1) C 5- C 6	0.88	10.65	0.086
6. CR (1) C 6	95. BD* (1) C 5- C 12	0.95	10.64	0.090
6. CR (1) C 6	96. BD* (1) C 6- C 31	0.60	10.69	0.071
6. CR (1) C 6	123. BD* (1) C 31- H 32	0.83	10.79	0.085
6. CR (1) C 6	124. BD* (1) C 31- C 33	0.66	10.62	0.074
6. CR (1) C 6	175. RY (1) C 5	1.65	11.46	0.123
6. CR (1) C 6	358. RY (2) C 31	1.38	10.87	0.109
7. CR (1) C 7	90. BD* (1) C 4- C 5	0.69	10.59	0.076
7. CR (1) C 7	91. BD* (1) C 4- C 7	0.53	10.64	0.067
7. CR (1) C 7	93. BD* (1) C 4- B 20	1.58	10.49	0.115
7. CR (1) C 7	102. BD* (1) C 9- C 17	0.73	10.64	0.079
7. CR (1) C 7	111. BD* (1) C 17- H 18	0.52	10.76	0.067
7. CR (1) C 7	166. RY (2) C 4	1.57	11.25	0.118
7. CR (1) C 7	168. RY (4) C 4	0.72	11.34	0.081
7. CR (1) C 7	266. RY (2) C 17	1.04	10.76	0.094
8. CR (1) C 9	95. BD* (1) C 5- C 12	0.69	10.58	0.076
8. CR (1) C 9	99. BD* (1) C 7- C 17	0.89	10.56	0.087
8. CR (1) C 9	107. BD* (1) C 12- C 29	1.16	10.56	0.099
8. CR (1) C 9	111. BD* (1) C 17- H 18	0.63	10.76	0.074
8. CR (1) C 9	233. RY (1) C 12	0.80	11.29	0.085
8. CR (1) C 9	234. RY (2) C 12	0.87	11.42	0.089
8. CR (1) C 9	266. RY (2) C 17	1.58	10.77	0.116
9. CR (1) C 11	85. BD* (1) O 2- C 11	0.83	10.41	0.083
9. CR (1) C 11	86. BD* (1) O 2- B 20	1.85	10.53	0.125
9. CR (1) C 11	281. RY (3) C 19	1.05	11.05	0.096
9. CR (1) C 11	431. RY (3) C 43	0.58	11.09	0.071
10. CR (1) C 12	90. BD* (1) C 4- C 5	1.05	10.62	0.094
10. CR (1) C 12	94. BD* (1) C 5- C 6	0.93	10.62	0.089
10. CR (1) C 12	95. BD* (1) C 5- C 12	0.61	10.61	0.072
10. CR (1) C 12	100. BD* (1) C 9- H 10	0.60	10.78	0.072
10. CR (1) C 12	102. BD* (1) C 9- C 17	0.64	10.67	0.074
10. CR (1) C 12	120. BD* (1) C 29- H 30	0.58	10.78	0.070
10. CR (1) C 12	121. BD* (1) C 29- C 33	0.61	10.64	0.072
10. CR (1) C 12	176. RY (2) C 5	1.50	11.46	0.117
10. CR (1) C 12	210. RY (2) C 9	0.89	10.82	0.088
10. CR (1) C 12	344. RY (2) C 29	0.95	10.81	0.090
11. CR (1) C 13	88. BD* (1) N 3- C 13	0.60	10.32	0.070
11. CR (1) C 13	257. RY (1) H 15	0.51	10.70	0.066
11. CR (1) C 13	261. RY (1) H 16	0.56	10.79	0.069
12. CR (1) C 17	91. BD* (1) C 4- C 7	0.76	10.65	0.080
12. CR (1) C 17	98. BD* (1) C 7- H 8	0.55	10.78	0.069
12. CR (1) C 17	100. BD* (1) C 9- H 10	0.70	10.76	0.078
12. CR (1) C 17	101. BD* (1) C 9- C 12	0.97	10.58	0.090
12. CR (1) C 17	196. RY (2) C 7	1.11	10.84	0.098
12. CR (1) C 17	210. RY (2) C 9	1.41	10.80	0.110
13. CR (1) C 19	83. BD* (1) O 1- C 19	0.86	10.41	0.084
13. CR (1) C 19	84. BD* (1) O 1- B 20	1.93	10.56	0.128
13. CR (1) C 19	225. RY (3) C 11	0.88	11.09	0.088

13. CR (1) C 19	387. RY (3) C 35	0.58	11.08	0.071
14. CR (1) B 20	82. LV (1) B 20	2.03	6.77	0.105
14. CR (1) B 20	83. BD* (1) O 1- C 19	1.48	6.99	0.091
14. CR (1) B 20	85. BD* (1) O 2- C 11	1.26	6.99	0.084
14. CR (1) B 20	91. BD* (1) C 4- C 7	1.22	7.31	0.084
15. CR (1) C 21	317. RY (1) H 24	0.51	10.69	0.066
16. CR (1) C 25	224. RY (2) C 11	1.09	11.00	0.098
16. CR (1) C 25	225. RY (3) C 11	0.66	10.95	0.076
17. CR (1) C 29	95. BD* (1) C 5- C 12	0.73	10.59	0.078
17. CR (1) C 29	101. BD* (1) C 9- C 12	1.10	10.59	0.096
17. CR (1) C 29	124. BD* (1) C 31- C 33	0.84	10.57	0.084
17. CR (1) C 29	125. BD* (1) C 33- H 34	0.61	10.77	0.072
17. CR (1) C 29	234. RY (2) C 12	1.55	11.43	0.119
17. CR (1) C 29	372. RY (2) C 33	1.37	10.77	0.108
18. CR (1) C 31	87. BD* (1) N 3- C 6	1.45	10.36	0.109
18. CR (1) C 31	94. BD* (1) C 5- C 6	1.18	10.60	0.100
18. CR (1) C 31	96. BD* (1) C 6- C 31	0.69	10.64	0.076
18. CR (1) C 31	121. BD* (1) C 29- C 33	0.68	10.62	0.076
18. CR (1) C 31	125. BD* (1) C 33- H 34	0.51	10.76	0.066
18. CR (1) C 31	186. RY (2) C 6	2.45	11.34	0.149
18. CR (1) C 31	372. RY (2) C 33	1.13	10.77	0.099
19. CR (1) C 33	96. BD* (1) C 6- C 31	0.76	10.65	0.080
19. CR (1) C 33	107. BD* (1) C 12- C 29	0.87	10.58	0.086
19. CR (1) C 33	120. BD* (1) C 29- H 30	0.65	10.77	0.074
19. CR (1) C 33	123. BD* (1) C 31- H 32	0.66	10.75	0.075
19. CR (1) C 33	344. RY (2) C 29	1.30	10.80	0.106
19. CR (1) C 33	358. RY (2) C 31	0.81	10.83	0.084
20. CR (1) C 35	280. RY (2) C 19	1.57	11.03	0.117
21. CR (1) C 39	280. RY (2) C 19	0.55	11.04	0.070
21. CR (1) C 39	281. RY (3) C 19	1.14	10.94	0.100
22. CR (1) C 43	224. RY (2) C 11	1.12	11.01	0.099
22. CR (1) C 43	225. RY (3) C 11	0.93	10.96	0.090
23. LP (1) O 1	86. BD* (1) O 2- B 20	3.89	0.88	0.052
23. LP (1) O 1	93. BD* (1) C 4- B 20	1.35	0.92	0.032
23. LP (1) O 1	104. BD* (1) C 11- C 19	3.58	0.80	0.048
23. LP (1) O 1	112. BD* (1) C 19- C 35	1.30	0.86	0.030
23. LP (1) O 1	279. RY (1) C 19	2.56	1.35	0.053
23. LP (1) O 1	280. RY (2) C 19	0.68	1.50	0.028
23. LP (1) O 1	289. RY (1) B 20	5.33	1.19	0.071
23. LP (1) O 1	290. RY (2) B 20	0.74	1.36	0.028
23. LP (1) O 1	291. RY (3) B 20	1.48	1.48	0.042
24. LP (2) O 1	82. LV (1) B 20	42.64	0.35	0.109
24. LP (2) O 1	93. BD* (1) C 4- B 20	3.10	0.74	0.043
24. LP (2) O 1	104. BD* (1) C 11- C 19	1.06	0.62	0.023
24. LP (2) O 1	112. BD* (1) C 19- C 35	2.36	0.67	0.036
24. LP (2) O 1	113. BD* (1) C 19- C 39	7.72	0.63	0.062
24. LP (2) O 1	130. BD* (1) C 39- H 41	0.76	0.90	0.023
24. LP (2) O 1	282. RY (4) C 19	0.73	2.42	0.037
24. LP (2) O 1	293. RY (5) B 20	0.90	2.10	0.039
25. LP (1) O 2	84. BD* (1) O 1- B 20	3.54	0.91	0.051
25. LP (1) O 2	93. BD* (1) C 4- B 20	0.68	0.93	0.022
25. LP (1) O 2	104. BD* (1) C 11- C 19	4.06	0.81	0.051
25. LP (1) O 2	106. BD* (1) C 11- C 43	0.86	0.87	0.024
25. LP (1) O 2	223. RY (1) C 11	2.68	1.36	0.054
25. LP (1) O 2	224. RY (2) C 11	0.52	1.49	0.025
25. LP (1) O 2	227. RY (5) C 11	0.53	2.46	0.032
25. LP (1) O 2	289. RY (1) B 20	5.15	1.20	0.070
25. LP (1) O 2	291. RY (3) B 20	1.93	1.49	0.048
26. LP (2) O 2	82. LV (1) B 20	30.43	0.34	0.091
26. LP (2) O 2	93. BD* (1) C 4- B 20	5.24	0.73	0.055
26. LP (2) O 2	104. BD* (1) C 11- C 19	0.61	0.61	0.017
26. LP (2) O 2	105. BD* (1) C 11- C 25	7.00	0.64	0.060
26. LP (2) O 2	106. BD* (1) C 11- C 43	2.66	0.67	0.038
26. LP (2) O 2	118. BD* (1) C 25- H 27	0.91	0.90	0.026
26. LP (2) O 2	226. RY (4) C 11	0.76	2.37	0.038
27. LP (1) N 3	82. LV (1) B 20	164.20	0.44	0.239
27. LP (1) N 3	84. BD* (1) O 1- B 20	0.96	0.80	0.025
27. LP (1) N 3	86. BD* (1) O 2- B 20	2.19	0.78	0.037
27. LP (1) N 3	93. BD* (1) C 4- B 20	2.21	0.82	0.038
27. LP (1) N 3	94. BD* (1) C 5- C 6	2.68	0.92	0.044
27. LP (1) N 3	96. BD* (1) C 6- C 31	6.06	0.96	0.068
27. LP (1) N 3	108. BD* (1) C 13- H 14	2.73	0.97	0.046
27. LP (1) N 3	109. BD* (1) C 13- H 15	0.56	0.99	0.021
27. LP (1) N 3	110. BD* (1) C 13- H 16	0.91	0.99	0.027
27. LP (1) N 3	114. BD* (1) C 21- H 22	3.47	0.97	0.052
27. LP (1) N 3	115. BD* (1) C 21- H 23	1.12	0.98	0.030
27. LP (1) N 3	116. BD* (1) C 21- H 24	0.74	0.99	0.024

27. LP (1) N 3	185. RY (1) C 6	1.62	1.60	0.045
27. LP (1) N 3	243. RY (1) C 13	0.61	1.22	0.024
27. LP (1) N 3	290. RY (2) B 20	1.37	1.26	0.037
27. LP (1) N 3	294. RY (6) B 20	0.63	2.30	0.034
27. LP (1) N 3	297. RY (9) B 20	0.80	3.39	0.046
27. LP (1) N 3	299. RY (1) C 21	0.79	1.22	0.028
28. LP (1) C 12	92. BD*(2) C 4- C 7	1.12	0.17	0.012
28. LP (1) C 12	97. BD*(2) C 6- C 31	1.00	0.13	0.010
28. LP (1) C 12	103. BD*(2) C 9- C 17	87.73	0.15	0.101
28. LP (1) C 12	122. BD*(2) C 29- C 33	98.62	0.13	0.101
28. LP (1) C 12	177. RY (3) C 5	1.14	1.46	0.036
28. LP (1) C 12	179. RY (5) C 5	1.37	1.97	0.046
28. LP (1) C 12	180. RY (6) C 5	0.76	1.48	0.030
28. LP (1) C 12	211. RY (3) C 9	5.36	1.03	0.066
28. LP (1) C 12	236. RY (4) C 12	1.48	1.43	0.041
28. LP (1) C 12	238. RY (6) C 12	1.21	1.50	0.038
28. LP (1) C 12	345. RY (3) C 29	4.70	1.19	0.067
29. BD (1) O 1- C 19	82. LV (1) B 20	1.22	0.84	0.029
29. BD (1) O 1- C 19	84. BD*(1) O 1- B 20	1.49	1.21	0.038
29. BD (1) O 1- C 19	85. BD*(1) O 2- C 11	1.13	1.06	0.031
29. BD (1) O 1- C 19	86. BD*(1) O 2- B 20	1.64	1.18	0.039
29. BD (1) O 1- C 19	93. BD*(1) C 4- B 20	1.68	1.23	0.041
29. BD (1) O 1- C 19	106. BD*(1) C 11- C 43	1.20	1.17	0.033
29. BD (1) O 1- C 19	128. BD*(1) C 35- H 38	1.15	1.39	0.036
29. BD (1) O 1- C 19	130. BD*(1) C 39- H 41	0.93	1.39	0.032
29. BD (1) O 1- C 19	289. RY (1) B 20	2.92	1.50	0.059
30. BD (1) O 1- B 20	83. BD*(1) O 1- C 19	1.03	1.16	0.031
30. BD (1) O 1- B 20	112. BD*(1) C 19- C 35	1.18	1.26	0.034
30. BD (1) O 1- B 20	279. RY (1) C 19	3.62	1.76	0.071
30. BD (1) O 1- B 20	289. RY (1) B 20	0.87	1.59	0.033
31. BD (1) O 2- C 11	82. LV (1) B 20	2.04	0.83	0.037
31. BD (1) O 2- C 11	83. BD*(1) O 1- C 19	1.14	1.05	0.031
31. BD (1) O 2- C 11	84. BD*(1) O 1- B 20	1.40	1.20	0.037
31. BD (1) O 2- C 11	86. BD*(1) O 2- B 20	1.40	1.18	0.036
31. BD (1) O 2- C 11	93. BD*(1) C 4- B 20	1.36	1.22	0.036
31. BD (1) O 2- C 11	112. BD*(1) C 19- C 35	1.12	1.16	0.032
31. BD (1) O 2- C 11	118. BD*(1) C 25- H 27	1.08	1.39	0.035
31. BD (1) O 2- C 11	134. BD*(1) C 43- H 46	1.23	1.38	0.037
31. BD (1) O 2- C 11	289. RY (1) B 20	2.80	1.49	0.058
32. BD (1) O 2- B 20	85. BD*(1) O 2- C 11	0.84	1.12	0.027
32. BD (1) O 2- B 20	92. BD*(2) C 4- C 7	0.84	0.88	0.024
32. BD (1) O 2- B 20	106. BD*(1) C 11- C 43	1.39	1.23	0.037
32. BD (1) O 2- B 20	223. RY (1) C 11	3.46	1.71	0.069
32. BD (1) O 2- B 20	289. RY (1) B 20	0.88	1.55	0.033
33. BD (1) N 3- C 6	82. LV (1) B 20	14.27	0.83	0.097
33. BD (1) N 3- C 6	89. BD*(1) N 3- C 21	0.51	1.06	0.021
33. BD (1) N 3- C 6	93. BD*(1) C 4- B 20	0.50	1.22	0.022
33. BD (1) N 3- C 6	94. BD*(1) C 5- C 6	1.25	1.32	0.036
33. BD (1) N 3- C 6	95. BD*(1) C 5- C 12	2.62	1.31	0.052
33. BD (1) N 3- C 6	96. BD*(1) C 6- C 31	1.76	1.36	0.044
33. BD (1) N 3- C 6	110. BD*(1) C 13- H 16	0.99	1.39	0.033
33. BD (1) N 3- C 6	115. BD*(1) C 21- H 23	1.11	1.38	0.035
33. BD (1) N 3- C 6	124. BD*(1) C 31- C 33	1.35	1.28	0.037
33. BD (1) N 3- C 6	176. RY (2) C 5	0.90	2.16	0.039
33. BD (1) N 3- C 6	244. RY (2) C 13	0.69	1.66	0.030
33. BD (1) N 3- C 6	290. RY (2) B 20	0.63	1.66	0.029
33. BD (1) N 3- C 6	300. RY (2) C 21	0.79	1.64	0.032
34. BD (1) N 3- C 13	82. LV (1) B 20	12.78	0.77	0.089
34. BD (1) N 3- C 13	87. BD*(1) N 3- C 6	0.61	1.02	0.022
34. BD (1) N 3- C 13	94. BD*(1) C 5- C 6	0.79	1.26	0.028
34. BD (1) N 3- C 13	97. BD*(2) C 6- C 31	3.33	0.72	0.044
34. BD (1) N 3- C 13	116. BD*(1) C 21- H 24	1.44	1.33	0.039
34. BD (1) N 3- C 13	187. RY (3) C 6	0.84	1.57	0.032
34. BD (1) N 3- C 13	299. RY (1) C 21	0.77	1.56	0.031
35. BD (1) N 3- C 21	82. LV (1) B 20	12.60	0.82	0.091
35. BD (1) N 3- C 21	87. BD*(1) N 3- C 6	0.74	1.06	0.025
35. BD (1) N 3- C 21	94. BD*(1) C 5- C 6	1.15	1.30	0.035
35. BD (1) N 3- C 21	97. BD*(2) C 6- C 31	1.62	0.77	0.031
35. BD (1) N 3- C 21	109. BD*(1) C 13- H 15	0.90	1.37	0.031
35. BD (1) N 3- C 21	115. BD*(1) C 21- H 23	0.64	1.37	0.026
35. BD (1) N 3- C 21	116. BD*(1) C 21- H 24	0.53	1.37	0.024
35. BD (1) N 3- C 21	187. RY (3) C 6	0.78	1.62	0.032
35. BD (1) N 3- C 21	243. RY (1) C 13	0.72	1.60	0.030
36. BD (1) C 4- C 5	82. LV (1) B 20	0.63	0.74	0.019
36. BD (1) C 4- C 5	84. BD*(1) O 1- B 20	0.53	1.10	0.022
36. BD (1) C 4- C 5	91. BD*(1) C 4- C 7	2.81	1.28	0.054
36. BD (1) C 4- C 5	93. BD*(1) C 4- B 20	3.66	1.13	0.057

36. BD (1) C 4- C 5	94. BD* (1) C 5- C 6	3.49	1.22	0.058
36. BD (1) C 4- C 5	95. BD* (1) C 5- C 12	4.66	1.22	0.067
36. BD (1) C 4- C 5	96. BD* (1) C 6- C 31	3.16	1.26	0.056
36. BD (1) C 4- C 5	98. BD* (1) C 7- H 8	2.71	1.41	0.055
36. BD (1) C 4- C 5	107. BD* (1) C 12- C 29	2.12	1.20	0.045
36. BD (1) C 4- C 5	185. RY (1) C 6	0.58	1.90	0.030
36. BD (1) C 4- C 5	186. RY (2) C 6	0.71	1.96	0.033
36. BD (1) C 4- C 5	196. RY (2) C 7	0.73	1.47	0.029
36. BD (1) C 4- C 5	233. RY (1) C 12	0.54	1.93	0.029
36. BD (1) C 4- C 5	234. RY (2) C 12	0.83	2.06	0.037
36. BD (1) C 4- C 5	290. RY (2) B 20	0.66	1.56	0.029
37. BD (1) C 4- C 7	82. LV (1) B 20	0.90	0.77	0.023
37. BD (1) C 4- C 7	90. BD* (1) C 4- C 5	3.42	1.26	0.059
37. BD (1) C 4- C 7	93. BD* (1) C 4- B 20	5.71	1.16	0.073
37. BD (1) C 4- C 7	94. BD* (1) C 5- C 6	2.95	1.25	0.054
37. BD (1) C 4- C 7	98. BD* (1) C 7- H 8	3.49	1.44	0.063
37. BD (1) C 4- C 7	99. BD* (1) C 7- C 17	2.35	1.23	0.048
37. BD (1) C 4- C 7	111. BD* (1) C 17- H 18	1.50	1.43	0.041
37. BD (1) C 4- C 7	175. RY (1) C 5	0.89	2.07	0.038
37. BD (1) C 4- C 7	176. RY (2) C 5	0.59	2.10	0.032
37. BD (1) C 4- C 7	266. RY (2) C 17	1.24	1.44	0.038
38. BD (2) C 4- C 7	81. LV (1) C 5	72.05	0.14	0.089
38. BD (2) C 4- C 7	84. BD* (1) O 1- B 20	2.93	0.68	0.040
38. BD (2) C 4- C 7	86. BD* (1) O 2- B 20	4.19	0.66	0.047
38. BD (2) C 4- C 7	103. BD* (2) C 9- C 17	20.38	0.28	0.067
38. BD (2) C 4- C 7	180. RY (6) C 5	0.96	1.62	0.035
38. BD (2) C 4- C 7	267. RY (3) C 17	0.98	2.01	0.039
39. BD (1) C 4- B 20	83. BD* (1) O 1- C 19	1.98	0.80	0.036
39. BD (1) C 4- B 20	85. BD* (1) O 2- C 11	1.30	0.80	0.029
39. BD (1) C 4- B 20	90. BD* (1) C 4- C 5	2.93	1.07	0.050
39. BD (1) C 4- B 20	91. BD* (1) C 4- C 7	3.91	1.13	0.059
39. BD (1) C 4- B 20	95. BD* (1) C 5- C 12	6.83	1.06	0.076
39. BD (1) C 4- B 20	99. BD* (1) C 7- C 17	3.29	1.05	0.052
39. BD (1) C 4- B 20	175. RY (1) C 5	2.12	1.88	0.056
39. BD (1) C 4- B 20	195. RY (1) C 7	1.64	1.87	0.049
40. BD (1) C 5- C 6	88. BD* (1) N 3- C 13	0.71	0.95	0.023
40. BD (1) C 5- C 6	89. BD* (1) N 3- C 21	1.15	1.01	0.030
40. BD (1) C 5- C 6	90. BD* (1) C 4- C 5	3.79	1.27	0.062
40. BD (1) C 5- C 6	91. BD* (1) C 4- C 7	2.01	1.32	0.046
40. BD (1) C 5- C 6	95. BD* (1) C 5- C 12	3.78	1.25	0.061
40. BD (1) C 5- C 6	96. BD* (1) C 6- C 31	4.74	1.30	0.070
40. BD (1) C 5- C 6	101. BD* (1) C 9- C 12	2.08	1.25	0.045
40. BD (1) C 5- C 6	123. BD* (1) C 31- H 32	2.29	1.40	0.051
40. BD (1) C 5- C 6	165. RY (1) C 4	1.05	2.21	0.043
40. BD (1) C 5- C 6	234. RY (2) C 12	1.67	2.09	0.053
40. BD (1) C 5- C 6	358. RY (2) C 31	0.86	1.48	0.032
41. BD (1) C 5- C 12	87. BD* (1) N 3- C 6	2.91	1.00	0.048
41. BD (1) C 5- C 12	90. BD* (1) C 4- C 5	4.36	1.25	0.066
41. BD (1) C 5- C 12	93. BD* (1) C 4- B 20	1.71	1.15	0.040
41. BD (1) C 5- C 12	94. BD* (1) C 5- C 6	4.15	1.24	0.064
41. BD (1) C 5- C 12	100. BD* (1) C 9- H 10	1.97	1.41	0.047
41. BD (1) C 5- C 12	101. BD* (1) C 9- C 12	2.85	1.23	0.053
41. BD (1) C 5- C 12	107. BD* (1) C 12- C 29	2.82	1.22	0.052
41. BD (1) C 5- C 12	120. BD* (1) C 29- H 30	1.75	1.40	0.044
41. BD (1) C 5- C 12	166. RY (2) C 4	0.73	1.91	0.033
41. BD (1) C 5- C 12	186. RY (2) C 6	1.17	1.98	0.043
42. BD (1) C 6- C 31	87. BD* (1) N 3- C 6	1.01	1.06	0.029
42. BD (1) C 6- C 31	90. BD* (1) C 4- C 5	1.99	1.31	0.046
42. BD (1) C 6- C 31	94. BD* (1) C 5- C 6	5.20	1.30	0.074
42. BD (1) C 6- C 31	123. BD* (1) C 31- H 32	3.80	1.45	0.066
42. BD (1) C 6- C 31	124. BD* (1) C 31- C 33	2.82	1.27	0.053
42. BD (1) C 6- C 31	125. BD* (1) C 33- H 34	1.49	1.47	0.042
42. BD (1) C 6- C 31	155. RY (1) N 3	0.56	2.20	0.031
42. BD (1) C 6- C 31	176. RY (2) C 5	1.60	2.15	0.052
42. BD (1) C 6- C 31	371. RY (1) C 33	0.71	2.03	0.034
42. BD (1) C 6- C 31	372. RY (2) C 33	1.10	1.47	0.036
43. BD (2) C 6- C 31	81. LV (1) C 5	54.68	0.18	0.089
43. BD (2) C 6- C 31	88. BD* (1) N 3- C 13	1.57	0.54	0.026
43. BD (2) C 6- C 31	89. BD* (1) N 3- C 21	1.07	0.59	0.022
43. BD (2) C 6- C 31	110. BD* (1) C 13- H 16	0.73	0.92	0.023
43. BD (2) C 6- C 31	115. BD* (1) C 21- H 23	0.52	0.91	0.019
43. BD (2) C 6- C 31	122. BD* (2) C 29- C 33	17.07	0.31	0.065
43. BD (2) C 6- C 31	177. RY (3) C 5	1.05	1.64	0.037
43. BD (2) C 6- C 31	373. RY (3) C 33	1.72	1.36	0.043
44. BD (1) C 7- H 8	90. BD* (1) C 4- C 5	3.99	1.14	0.060
44. BD (1) C 7- H 8	91. BD* (1) C 4- C 7	2.13	1.19	0.045
44. BD (1) C 7- H 8	99. BD* (1) C 7- C 17	0.81	1.11	0.027

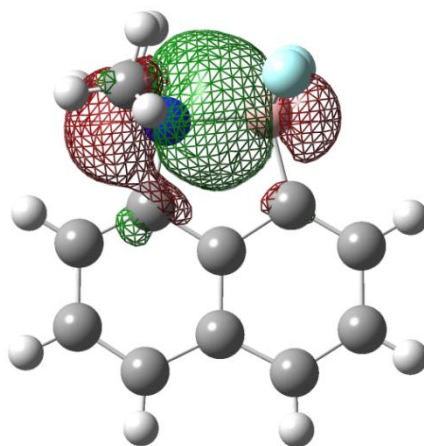
44. BD (1) C 7- H 8	102. BD* (1) C 9- C 17	3.21	1.19	0.055
44. BD (1) C 7- H 8	165. RY (1) C 4	0.93	2.08	0.039
44. BD (1) C 7- H 8	265. RY (1) C 17	0.73	1.88	0.033
45. BD (1) C 7- C 17	91. BD* (1) C 4- C 7	3.02	1.29	0.056
45. BD (1) C 7- C 17	93. BD* (1) C 4- B 20	3.42	1.13	0.055
45. BD (1) C 7- C 17	98. BD* (1) C 7- H 8	2.15	1.41	0.049
45. BD (1) C 7- C 17	100. BD* (1) C 9- H 10	2.42	1.39	0.052
45. BD (1) C 7- C 17	102. BD* (1) C 9- C 17	2.54	1.28	0.051
45. BD (1) C 7- C 17	111. BD* (1) C 17- H 18	2.21	1.40	0.050
45. BD (1) C 7- C 17	165. RY (1) C 4	1.51	2.18	0.051
45. BD (1) C 7- C 17	166. RY (2) C 4	1.01	1.89	0.039
45. BD (1) C 7- C 17	210. RY (2) C 9	1.38	1.43	0.040
46. BD (1) C 9- H 10	95. BD* (1) C 5- C 12	3.74	1.14	0.058
46. BD (1) C 9- H 10	99. BD* (1) C 7- C 17	4.25	1.12	0.062
46. BD (1) C 9- H 10	101. BD* (1) C 9- C 12	1.28	1.13	0.034
46. BD (1) C 9- H 10	102. BD* (1) C 9- C 17	1.75	1.20	0.041
46. BD (1) C 9- H 10	234. RY (2) C 12	1.07	1.97	0.041
46. BD (1) C 9- H 10	265. RY (1) C 17	0.91	1.89	0.037
47. BD (1) C 9- C 12	94. BD* (1) C 5- C 6	3.29	1.24	0.057
47. BD (1) C 9- C 12	95. BD* (1) C 5- C 12	3.49	1.24	0.059
47. BD (1) C 9- C 12	100. BD* (1) C 9- H 10	2.62	1.41	0.054
47. BD (1) C 9- C 12	102. BD* (1) C 9- C 17	2.83	1.30	0.054
47. BD (1) C 9- C 12	107. BD* (1) C 12- C 29	2.87	1.22	0.053
47. BD (1) C 9- C 12	111. BD* (1) C 17- H 18	2.03	1.42	0.048
47. BD (1) C 9- C 12	121. BD* (1) C 29- C 33	1.49	1.26	0.039
47. BD (1) C 9- C 12	175. RY (1) C 5	1.13	2.05	0.043
47. BD (1) C 9- C 12	265. RY (1) C 17	0.65	1.99	0.032
47. BD (1) C 9- C 12	266. RY (2) C 17	1.32	1.43	0.039
47. BD (1) C 9- C 12	343. RY (1) C 29	0.81	2.00	0.036
48. BD (1) C 9- C 17	98. BD* (1) C 7- H 8	1.61	1.45	0.043
48. BD (1) C 9- C 17	99. BD* (1) C 7- C 17	2.47	1.25	0.050
48. BD (1) C 9- C 17	100. BD* (1) C 9- H 10	3.29	1.43	0.061
48. BD (1) C 9- C 17	101. BD* (1) C 9- C 12	3.17	1.26	0.056
48. BD (1) C 9- C 17	107. BD* (1) C 12- C 29	3.73	1.24	0.061
48. BD (1) C 9- C 17	111. BD* (1) C 17- H 18	2.99	1.45	0.059
48. BD (1) C 9- C 17	195. RY (1) C 7	0.59	2.08	0.031
48. BD (1) C 9- C 17	196. RY (2) C 7	1.04	1.52	0.035
48. BD (1) C 9- C 17	233. RY (1) C 12	2.28	1.97	0.060
49. BD (2) C 9- C 17	92. BD* (2) C 4- C 7	14.32	0.32	0.061
49. BD (2) C 9- C 17	197. RY (3) C 7	1.68	1.14	0.039
50. BD (1) C 11- C 19	84. BD* (1) O 1- B 20	0.99	1.04	0.029
50. BD (1) C 11- C 19	86. BD* (1) O 2- B 20	0.95	1.02	0.028
50. BD (1) C 11- C 19	93. BD* (1) C 4- B 20	0.61	1.06	0.023
50. BD (1) C 11- C 19	105. BD* (1) C 11- C 25	0.51	0.97	0.020
50. BD (1) C 11- C 19	106. BD* (1) C 11- C 43	0.85	1.00	0.026
50. BD (1) C 11- C 19	112. BD* (1) C 19- C 35	0.84	1.00	0.026
50. BD (1) C 11- C 19	117. BD* (1) C 25- H 26	1.12	1.25	0.033
50. BD (1) C 11- C 19	126. BD* (1) C 35- H 36	1.25	1.24	0.035
50. BD (1) C 11- C 19	129. BD* (1) C 39- H 40	1.10	1.23	0.033
50. BD (1) C 11- C 19	132. BD* (1) C 43- H 44	1.23	1.24	0.035
50. BD (1) C 11- C 19	321. RY (1) C 25	0.78	1.50	0.030
50. BD (1) C 11- C 19	386. RY (2) C 35	0.71	1.49	0.029
50. BD (1) C 11- C 19	407. RY (1) C 39	0.76	1.51	0.030
50. BD (1) C 11- C 19	430. RY (2) C 43	0.67	1.49	0.028
51. BD (1) C 11- C 25	86. BD* (1) O 2- B 20	1.33	1.00	0.033
51. BD (1) C 11- C 25	104. BD* (1) C 11- C 19	0.65	0.93	0.022
51. BD (1) C 11- C 25	106. BD* (1) C 11- C 43	0.54	0.99	0.021
51. BD (1) C 11- C 25	113. BD* (1) C 19- C 39	1.76	0.94	0.036
51. BD (1) C 11- C 25	117. BD* (1) C 25- H 26	1.63	1.23	0.040
51. BD (1) C 11- C 25	118. BD* (1) C 25- H 27	1.55	1.22	0.039
51. BD (1) C 11- C 25	119. BD* (1) C 25- H 28	1.56	1.24	0.039
51. BD (1) C 11- C 25	133. BD* (1) C 43- H 45	1.79	1.22	0.042
51. BD (1) C 11- C 25	145. RY (1) O 2	0.59	1.89	0.030
51. BD (1) C 11- C 25	280. RY (2) C 19	0.65	1.63	0.029
51. BD (1) C 11- C 25	429. RY (1) C 43	0.78	1.40	0.029
52. BD (1) C 11- C 43	83. BD* (1) O 1- C 19	0.84	0.91	0.025
52. BD (1) C 11- C 43	86. BD* (1) O 2- B 20	1.95	1.03	0.040
52. BD (1) C 11- C 43	104. BD* (1) C 11- C 19	0.87	0.96	0.026
52. BD (1) C 11- C 43	105. BD* (1) C 11- C 25	0.58	0.99	0.021
52. BD (1) C 11- C 43	119. BD* (1) C 25- H 28	1.32	1.26	0.036
52. BD (1) C 11- C 43	132. BD* (1) C 43- H 44	1.86	1.25	0.043
52. BD (1) C 11- C 43	133. BD* (1) C 43- H 45	1.86	1.24	0.043
52. BD (1) C 11- C 43	134. BD* (1) C 43- H 46	1.57	1.23	0.039
52. BD (1) C 11- C 43	146. RY (2) O 2	0.81	1.91	0.035
52. BD (1) C 11- C 43	281. RY (3) C 19	0.81	1.55	0.032
52. BD (1) C 11- C 43	322. RY (2) C 25	0.86	1.44	0.031
53. BD (1) C 12- C 29	90. BD* (1) C 4- C 5	3.32	1.25	0.058

53. BD (1) C 12- C 29	95. BD* (1) C 5- C 12	3.30	1.24	0.057
53. BD (1) C 12- C 29	101. BD* (1) C 9- C 12	2.99	1.23	0.054
53. BD (1) C 12- C 29	102. BD* (1) C 9- C 17	1.45	1.30	0.039
53. BD (1) C 12- C 29	120. BD* (1) C 29- H 30	2.52	1.41	0.053
53. BD (1) C 12- C 29	121. BD* (1) C 29- C 33	2.41	1.27	0.049
53. BD (1) C 12- C 29	125. BD* (1) C 33- H 34	1.97	1.41	0.047
53. BD (1) C 12- C 29	175. RY (1) C 5	1.36	2.06	0.047
53. BD (1) C 12- C 29	209. RY (1) C 9	0.85	2.00	0.037
53. BD (1) C 12- C 29	372. RY (2) C 33	1.40	1.41	0.040
54. BD (1) C 13- H 14	109. BD* (1) C 13- H 15	1.12	1.22	0.033
54. BD (1) C 13- H 14	110. BD* (1) C 13- H 16	1.15	1.22	0.033
55. BD (1) C 13- H 15	82. LV (1) B 20	0.55	0.66	0.017
55. BD (1) C 13- H 15	89. BD* (1) N 3- C 21	2.29	0.89	0.040
55. BD (1) C 13- H 15	108. BD* (1) C 13- H 14	1.06	1.19	0.032
55. BD (1) C 13- H 15	110. BD* (1) C 13- H 16	1.43	1.21	0.037
56. BD (1) C 13- H 16	82. LV (1) B 20	0.52	0.66	0.017
56. BD (1) C 13- H 16	87. BD* (1) N 3- C 6	2.00	0.90	0.038
56. BD (1) C 13- H 16	108. BD* (1) C 13- H 14	1.06	1.19	0.032
56. BD (1) C 13- H 16	109. BD* (1) C 13- H 15	1.30	1.21	0.035
57. BD (1) C 17- H 18	91. BD* (1) C 4- C 7	3.34	1.20	0.057
57. BD (1) C 17- H 18	99. BD* (1) C 7- C 17	0.89	1.12	0.028
57. BD (1) C 17- H 18	101. BD* (1) C 9- C 12	4.58	1.13	0.064
57. BD (1) C 17- H 18	102. BD* (1) C 9- C 17	1.58	1.20	0.039
57. BD (1) C 17- H 18	195. RY (1) C 7	0.80	1.95	0.035
57. BD (1) C 17- H 18	209. RY (1) C 9	0.87	1.90	0.036
58. BD (1) C 19- C 35	84. BD* (1) O 1- B 20	1.93	1.05	0.040
58. BD (1) C 19- C 35	85. BD* (1) O 2- C 11	0.91	0.91	0.026
58. BD (1) C 19- C 35	104. BD* (1) C 11- C 19	0.92	0.96	0.026
58. BD (1) C 19- C 35	113. BD* (1) C 19- C 39	0.51	0.97	0.020
58. BD (1) C 19- C 35	126. BD* (1) C 35- H 36	1.81	1.25	0.042
58. BD (1) C 19- C 35	127. BD* (1) C 35- H 37	1.84	1.25	0.043
58. BD (1) C 19- C 35	128. BD* (1) C 35- H 38	1.49	1.23	0.038
58. BD (1) C 19- C 35	131. BD* (1) C 39- H 42	1.36	1.24	0.037
58. BD (1) C 19- C 35	135. RY (1) O 1	0.80	1.91	0.035
58. BD (1) C 19- C 35	225. RY (3) C 11	0.67	1.58	0.029
58. BD (1) C 19- C 35	408. RY (2) C 39	0.88	1.46	0.032
59. BD (1) C 19- C 39	84. BD* (1) O 1- B 20	1.42	1.03	0.034
59. BD (1) C 19- C 39	104. BD* (1) C 11- C 19	0.59	0.93	0.021
59. BD (1) C 19- C 39	105. BD* (1) C 11- C 25	1.66	0.96	0.036
59. BD (1) C 19- C 39	127. BD* (1) C 35- H 37	1.77	1.23	0.042
59. BD (1) C 19- C 39	129. BD* (1) C 39- H 40	1.61	1.22	0.040
59. BD (1) C 19- C 39	130. BD* (1) C 39- H 41	1.55	1.21	0.039
59. BD (1) C 19- C 39	131. BD* (1) C 39- H 42	1.61	1.22	0.040
59. BD (1) C 19- C 39	136. RY (2) O 1	0.56	1.87	0.029
59. BD (1) C 19- C 39	224. RY (2) C 11	0.50	1.60	0.025
59. BD (1) C 19- C 39	385. RY (1) C 35	0.75	1.40	0.029
60. BD (1) C 21- H 22	82. LV (1) B 20	0.50	0.66	0.016
60. BD (1) C 21- H 22	115. BD* (1) C 21- H 23	1.15	1.21	0.033
60. BD (1) C 21- H 22	116. BD* (1) C 21- H 24	1.13	1.22	0.033
61. BD (1) C 21- H 23	87. BD* (1) N 3- C 6	2.93	0.90	0.046
61. BD (1) C 21- H 23	114. BD* (1) C 21- H 22	1.04	1.19	0.031
61. BD (1) C 21- H 23	116. BD* (1) C 21- H 24	1.32	1.21	0.036
62. BD (1) C 21- H 24	88. BD* (1) N 3- C 13	3.12	0.83	0.045
62. BD (1) C 21- H 24	114. BD* (1) C 21- H 22	1.07	1.18	0.032
62. BD (1) C 21- H 24	115. BD* (1) C 21- H 23	1.45	1.20	0.037
63. BD (1) C 25- H 26	104. BD* (1) C 11- C 19	3.20	0.88	0.047
63. BD (1) C 25- H 26	105. BD* (1) C 11- C 25	0.92	0.91	0.026
63. BD (1) C 25- H 26	118. BD* (1) C 25- H 27	1.15	1.17	0.033
63. BD (1) C 25- H 26	119. BD* (1) C 25- H 28	1.37	1.19	0.036
64. BD (1) C 25- H 27	85. BD* (1) O 2- C 11	3.83	0.84	0.051
64. BD (1) C 25- H 27	105. BD* (1) C 11- C 25	0.54	0.92	0.020
64. BD (1) C 25- H 27	117. BD* (1) C 25- H 26	1.11	1.19	0.032
64. BD (1) C 25- H 27	119. BD* (1) C 25- H 28	1.03	1.19	0.031
64. BD (1) C 25- H 27	224. RY (2) C 11	0.74	1.56	0.030
65. BD (1) C 25- H 28	85. BD* (1) O 2- C 11	0.75	0.83	0.022
65. BD (1) C 25- H 28	105. BD* (1) C 11- C 25	0.85	0.91	0.025
65. BD (1) C 25- H 28	106. BD* (1) C 11- C 43	2.69	0.94	0.045
65. BD (1) C 25- H 28	117. BD* (1) C 25- H 26	1.23	1.18	0.034
65. BD (1) C 25- H 28	118. BD* (1) C 25- H 27	1.09	1.17	0.032
65. BD (1) C 25- H 28	225. RY (3) C 11	0.83	1.51	0.032
66. BD (1) C 29- H 30	95. BD* (1) C 5- C 12	3.80	1.14	0.059
66. BD (1) C 29- H 30	107. BD* (1) C 12- C 29	1.25	1.12	0.033
66. BD (1) C 29- H 30	121. BD* (1) C 29- C 33	1.50	1.17	0.037
66. BD (1) C 29- H 30	124. BD* (1) C 31- C 33	4.02	1.12	0.060
66. BD (1) C 29- H 30	233. RY (1) C 12	0.90	1.86	0.036
66. BD (1) C 29- H 30	234. RY (2) C 12	0.53	1.98	0.029
66. BD (1) C 29- H 30	371. RY (1) C 33	0.85	1.88	0.036

67. BD (1) C 29- C 33	101. BD* (1) C 9- C 12	3.60	1.25	0.060
67. BD (1) C 29- C 33	107. BD* (1) C 12- C 29	2.77	1.24	0.052
67. BD (1) C 29- C 33	120. BD* (1) C 29- H 30	2.97	1.43	0.058
67. BD (1) C 29- C 33	123. BD* (1) C 31- H 32	1.94	1.41	0.047
67. BD (1) C 29- C 33	124. BD* (1) C 31- C 33	2.26	1.23	0.047
67. BD (1) C 29- C 33	125. BD* (1) C 33- H 34	2.89	1.43	0.057
67. BD (1) C 29- C 33	233. RY (1) C 12	2.82	1.97	0.067
67. BD (1) C 29- C 33	358. RY (2) C 31	1.01	1.49	0.035
68. BD (2) C 29- C 33	97. BD* (2) C 6- C 31	16.84	0.29	0.063
68. BD (2) C 29- C 33	235. RY (3) C 12	0.54	2.12	0.030
68. BD (2) C 29- C 33	359. RY (3) C 31	1.36	0.92	0.032
69. BD (1) C 31- H 32	94. BD* (1) C 5- C 6	4.83	1.16	0.067
69. BD (1) C 31- H 32	96. BD* (1) C 6- C 31	2.16	1.20	0.046
69. BD (1) C 31- H 32	121. BD* (1) C 29- C 33	2.93	1.18	0.053
69. BD (1) C 31- H 32	124. BD* (1) C 31- C 33	1.15	1.13	0.032
69. BD (1) C 31- H 32	186. RY (2) C 6	1.20	1.90	0.043
69. BD (1) C 31- H 32	371. RY (1) C 33	0.85	1.89	0.036
70. BD (1) C 31- C 33	87. BD* (1) N 3- C 6	7.14	1.00	0.076
70. BD (1) C 31- C 33	96. BD* (1) C 6- C 31	3.87	1.28	0.063
70. BD (1) C 31- C 33	120. BD* (1) C 29- H 30	2.08	1.40	0.048
70. BD (1) C 31- C 33	121. BD* (1) C 29- C 33	2.31	1.26	0.048
70. BD (1) C 31- C 33	123. BD* (1) C 31- H 32	2.60	1.39	0.054
70. BD (1) C 31- C 33	125. BD* (1) C 33- H 34	2.13	1.41	0.049
70. BD (1) C 31- C 33	185. RY (1) C 6	2.84	1.92	0.066
70. BD (1) C 31- C 33	344. RY (2) C 29	1.29	1.43	0.038
71. BD (1) C 33- H 34	96. BD* (1) C 6- C 31	3.28	1.19	0.056
71. BD (1) C 33- H 34	107. BD* (1) C 12- C 29	4.09	1.13	0.061
71. BD (1) C 33- H 34	121. BD* (1) C 29- C 33	1.48	1.17	0.037
71. BD (1) C 33- H 34	124. BD* (1) C 31- C 33	0.90	1.12	0.028
71. BD (1) C 33- H 34	343. RY (1) C 29	0.84	1.91	0.036
71. BD (1) C 33- H 34	357. RY (1) C 31	0.69	1.89	0.032
72. BD (1) C 35- H 36	104. BD* (1) C 11- C 19	3.86	0.89	0.052
72. BD (1) C 35- H 36	112. BD* (1) C 19- C 35	1.01	0.94	0.028
72. BD (1) C 35- H 36	127. BD* (1) C 35- H 37	1.30	1.18	0.035
72. BD (1) C 35- H 36	128. BD* (1) C 35- H 38	1.11	1.16	0.032
72. BD (1) C 35- H 36	280. RY (2) C 19	0.58	1.59	0.027
73. BD (1) C 35- H 37	83. BD* (1) O 1- C 19	0.66	0.84	0.021
73. BD (1) C 35- H 37	112. BD* (1) C 19- C 35	0.94	0.94	0.027
73. BD (1) C 35- H 37	113. BD* (1) C 19- C 39	3.10	0.90	0.047
73. BD (1) C 35- H 37	126. BD* (1) C 35- H 36	1.21	1.18	0.034
73. BD (1) C 35- H 37	128. BD* (1) C 35- H 38	1.09	1.16	0.032
73. BD (1) C 35- H 37	281. RY (3) C 19	0.62	1.48	0.027
74. BD (1) C 35- H 38	83. BD* (1) O 1- C 19	4.77	0.84	0.057
74. BD (1) C 35- H 38	112. BD* (1) C 19- C 35	0.64	0.95	0.022
74. BD (1) C 35- H 38	126. BD* (1) C 35- H 36	1.07	1.18	0.032
74. BD (1) C 35- H 38	127. BD* (1) C 35- H 37	1.02	1.19	0.031
74. BD (1) C 35- H 38	279. RY (1) C 19	0.76	1.44	0.030
75. BD (1) C 39- H 40	104. BD* (1) C 11- C 19	2.94	0.90	0.046
75. BD (1) C 39- H 40	113. BD* (1) C 19- C 39	0.87	0.91	0.025
75. BD (1) C 39- H 40	130. BD* (1) C 39- H 41	1.22	1.18	0.034
75. BD (1) C 39- H 40	131. BD* (1) C 39- H 42	1.32	1.18	0.035
76. BD (1) C 39- H 41	83. BD* (1) O 1- C 19	3.97	0.85	0.052
76. BD (1) C 39- H 41	113. BD* (1) C 19- C 39	0.59	0.91	0.021
76. BD (1) C 39- H 41	129. BD* (1) C 39- H 40	1.21	1.19	0.034
76. BD (1) C 39- H 41	131. BD* (1) C 39- H 42	1.18	1.19	0.033
76. BD (1) C 39- H 41	280. RY (2) C 19	0.57	1.60	0.027
77. BD (1) C 39- H 42	83. BD* (1) O 1- C 19	0.59	0.85	0.020
77. BD (1) C 39- H 42	112. BD* (1) C 19- C 35	2.44	0.95	0.043
77. BD (1) C 39- H 42	113. BD* (1) C 19- C 39	0.81	0.91	0.024
77. BD (1) C 39- H 42	129. BD* (1) C 39- H 40	1.16	1.19	0.033
77. BD (1) C 39- H 42	130. BD* (1) C 39- H 41	1.14	1.18	0.033
77. BD (1) C 39- H 42	281. RY (3) C 19	0.86	1.49	0.032
78. BD (1) C 43- H 44	104. BD* (1) C 11- C 19	3.99	0.89	0.053
78. BD (1) C 43- H 44	106. BD* (1) C 11- C 43	1.10	0.95	0.029
78. BD (1) C 43- H 44	133. BD* (1) C 43- H 45	1.29	1.18	0.035
78. BD (1) C 43- H 44	134. BD* (1) C 43- H 46	1.13	1.17	0.032
78. BD (1) C 43- H 44	224. RY (2) C 11	0.70	1.56	0.029
79. BD (1) C 43- H 45	85. BD* (1) O 2- C 11	0.67	0.84	0.021
79. BD (1) C 43- H 45	105. BD* (1) C 11- C 25	3.09	0.92	0.048
79. BD (1) C 43- H 45	106. BD* (1) C 11- C 43	0.94	0.95	0.027
79. BD (1) C 43- H 45	132. BD* (1) C 43- H 44	1.17	1.18	0.033
79. BD (1) C 43- H 45	134. BD* (1) C 43- H 46	1.07	1.17	0.032
79. BD (1) C 43- H 45	225. RY (3) C 11	0.87	1.51	0.032
80. BD (1) C 43- H 46	85. BD* (1) O 2- C 11	4.68	0.84	0.056
80. BD (1) C 43- H 46	106. BD* (1) C 11- C 43	0.68	0.95	0.023
80. BD (1) C 43- H 46	132. BD* (1) C 43- H 44	1.08	1.19	0.032
80. BD (1) C 43- H 46	133. BD* (1) C 43- H 45	1.01	1.18	0.031

80. BD (1) C 43- H 46	223. RY (1) C 11	0.76	1.44	0.030

5



Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	1.5227	0.0167	0.1036	0.0087	0.0018	0.0357	0.0130	1.2518
2. C	1.5227	0.0000	1.2917	0.0102	0.0011	0.0316	0.0002	0.0377	0.0155
3. C	0.0167	1.2917	0.0000	1.5533	0.0367	0.0003	0.0331	0.0010	0.0588
4. C	0.1036	0.0102	1.5533	0.0000	0.0101	0.0355	0.0005	0.0095	0.0106
5. C	0.0087	0.0011	0.0367	0.0101	0.0000	1.5448	0.0105	0.1094	0.0105
6. C	0.0018	0.0316	0.0003	0.0355	1.5448	0.0000	1.3097	0.0130	0.0552
7. C	0.0357	0.0002	0.0331	0.0005	0.0105	1.3097	0.0000	1.5114	0.0118
8. C	0.0130	0.0377	0.0010	0.0095	0.1094	0.0130	1.5114	0.0000	1.2487
9. C	1.2518	0.0155	0.0588	0.0106	0.0105	0.0552	0.0118	1.2487	0.0000
10. C	0.0114	0.0632	0.0112	1.2691	1.2679	0.0116	0.0652	0.0162	1.2317
11. C	0.0089	0.0057	0.0004	0.0026	0.0001	0.0003	0.0004	0.0018	0.0081
12. C	0.0088	0.0052	0.0004	0.0023	0.0001	0.0002	0.0003	0.0019	0.0079
13. N	0.9299	0.0118	0.0103	0.0007	0.0003	0.0002	0.0032	0.0066	0.0093
14. B	0.0059	0.0059	0.0002	0.0002	0.0034	0.0081	0.0147	0.7893	0.0147
15. F	0.0016	0.0010	0.0002	0.0001	0.0025	0.0004	0.0064	0.0184	0.0051
16. F	0.0017	0.0010	0.0001	0.0001	0.0025	0.0004	0.0065	0.0182	0.0050
17. H	0.0052	0.9209	0.0049	0.0065	0.0003	0.0000	0.0003	0.0002	0.0087
18. H	0.0060	0.0036	0.9260	0.0054	0.0002	0.0002	0.0000	0.0002	0.0003
19. H	0.0003	0.0087	0.0054	0.9238	0.0011	0.0001	0.0000	0.0003	0.0076
20. H	0.0001	0.0000	0.0001	0.0010	0.9259	0.0058	0.0089	0.0004	0.0075
21. H	0.0003	0.0000	0.0002	0.0001	0.0054	0.9311	0.0044	0.0063	0.0003
22. H	0.0001	0.0002	0.0000	0.0003	0.0065	0.0034	0.9250	0.0072	0.0091
23. H	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
24. H	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0001
25. H	0.0064	0.0014	0.0001	0.0006	0.0000	0.0000	0.0001	0.0006	0.0004
26. H	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
27. H	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002
28. H	0.0068	0.0012	0.0001	0.0006	0.0000	0.0000	0.0001	0.0006	0.0004

Atom	10	11	12	13	14	15	16	17	18
1. C	0.0114	0.0089	0.0088	0.9299	0.0059	0.0016	0.0017	0.0052	0.0060
2. C	0.0632	0.0057	0.0052	0.0118	0.0059	0.0010	0.0010	0.9209	0.0036
3. C	0.0112	0.0004	0.0004	0.0103	0.0002	0.0002	0.0001	0.0049	0.9260
4. C	1.2691	0.0026	0.0023	0.0007	0.0002	0.0001	0.0001	0.0065	0.0054
5. C	1.2679	0.0001	0.0001	0.0003	0.0034	0.0025	0.0025	0.0003	0.0002
6. C	0.0116	0.0003	0.0002	0.0002	0.0081	0.0004	0.0004	0.0000	0.0002
7. C	0.0652	0.0004	0.0003	0.0032	0.0147	0.0064	0.0065	0.0003	0.0000
8. C	0.0162	0.0018	0.0019	0.0066	0.7893	0.0184	0.0182	0.0002	0.0002
9. C	1.2317	0.0081	0.0079	0.0093	0.0147	0.0051	0.0050	0.0087	0.0003
10. C	0.0000	0.0003	0.0003	0.0072	0.0079	0.0004	0.0004	0.0003	0.0082
11. C	0.0003	0.0000	0.0098	0.9163	0.0048	0.0018	0.0064	0.0002	0.0000
12. C	0.0003	0.0098	0.0000	0.9200	0.0048	0.0062	0.0016	0.0002	0.0000

13.	N	0.0072	0.9163	0.9200	0.0000	0.4475	0.0187	0.0184	0.0023	0.0004
14.	B	0.0079	0.0048	0.0048	0.4475	0.0000	0.7348	0.7297	0.0001	0.0001
15.	F	0.0004	0.0018	0.0062	0.0187	0.7348	0.0000	0.0320	0.0000	0.0000
16.	F	0.0004	0.0064	0.0016	0.0184	0.7297	0.0320	0.0000	0.0000	0.0000
17.	H	0.0003	0.0002	0.0002	0.0023	0.0001	0.0000	0.0000	0.0000	0.0014
18.	H	0.0082	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000	0.0014	0.0000
19.	H	0.0045	0.0000	0.0000	0.0004	0.0003	0.0000	0.0000	0.0001	0.0018
20.	H	0.0041	0.0000	0.0000	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
21.	H	0.0082	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
22.	H	0.0002	0.0000	0.0000	0.0003	0.0009	0.0003	0.0003	0.0000	0.0000
23.	H	0.0000	0.9280	0.0075	0.0016	0.0003	0.0002	0.0013	0.0000	0.0000
24.	H	0.0000	0.9426	0.0004	0.0036	0.0056	0.0007	0.0021	0.0001	0.0000
25.	H	0.0002	0.9306	0.0003	0.0026	0.0003	0.0002	0.0021	0.0000	0.0000
26.	H	0.0000	0.0078	0.9286	0.0019	0.0004	0.0015	0.0002	0.0000	0.0000
27.	H	0.0000	0.0004	0.9425	0.0036	0.0059	0.0020	0.0007	0.0002	0.0000
28.	H	0.0002	0.0004	0.9313	0.0025	0.0002	0.0014	0.0002	0.0000	0.0000

Atom	19	20	21	22	23	24	25	26	27
1. C	0.0003	0.0001	0.0003	0.0001	0.0005	0.0004	0.0064	0.0004	0.0005
2. C	0.0087	0.0000	0.0000	0.0002	0.0001	0.0002	0.0014	0.0001	0.0002
3. C	0.0054	0.0001	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
4. C	0.9238	0.0010	0.0001	0.0003	0.0000	0.0000	0.0006	0.0000	0.0000
5. C	0.0011	0.9259	0.0054	0.0065	0.0000	0.0000	0.0000	0.0000	0.0000
6. C	0.0001	0.0058	0.9311	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000
7. C	0.0000	0.0089	0.0044	0.9250	0.0000	0.0001	0.0001	0.0000	0.0002
8. C	0.0003	0.0004	0.0063	0.0072	0.0001	0.0002	0.0006	0.0001	0.0002
9. C	0.0076	0.0075	0.0003	0.0091	0.0001	0.0001	0.0004	0.0001	0.0002
10. C	0.0045	0.0041	0.0082	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000
11. C	0.0000	0.0000	0.0000	0.0000	0.9280	0.9426	0.9306	0.0078	0.0004
12. C	0.0000	0.0000	0.0000	0.0000	0.0075	0.0004	0.0003	0.9286	0.9425
13. N	0.0004	0.0003	0.0001	0.0003	0.0016	0.0036	0.0026	0.0019	0.0036
14. B	0.0003	0.0004	0.0001	0.0009	0.0003	0.0056	0.0003	0.0004	0.0059
15. F	0.0000	0.0000	0.0000	0.0003	0.0002	0.0007	0.0002	0.0015	0.0020
16. F	0.0000	0.0000	0.0000	0.0003	0.0013	0.0021	0.0021	0.0002	0.0007
17. H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
18. H	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19. H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20. H	0.0002	0.0000	0.0018	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
21. H	0.0000	0.0018	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000
22. H	0.0000	0.0002	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0022	0.0005	0.0001
24. H	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000	0.0016	0.0001	0.0003
25. H	0.0000	0.0000	0.0000	0.0000	0.0022	0.0016	0.0000	0.0001	0.0001
26. H	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.0001	0.0000	0.0018
27. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0003	0.0001	0.0018	0.0000
28. H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0024	0.0016

Atom		28
1.	C	0.0068
2.	C	0.0012
3.	C	0.0001
4.	C	0.0006
5.	C	0.0000
6.	C	0.0000
7.	C	0.0001
8.	C	0.0006
9.	C	0.0004
10.	C	0.0002
11.	C	0.0004
12.	C	0.9313
13.	N	0.0025
14.	B	0.0002
15.	F	0.0014
16.	F	0.0002
17.	H	0.0000
18.	H	0.0000
19.	H	0.0000
20.	H	0.0000
21.	H	0.0000
22.	H	0.0000
23.	H	0.0001
24.	H	0.0001
25.	H	0.0001
26.	H	0.0024
27.	H	0.0016

28. H 0.0000

(Occupancy)		Bond orbital / Coefficients / Hybrids			
-----		Lewis -----			
1.	(1.99887) CR (1) C 1	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
2.	(1.99902) CR (1) C 2	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
3.	(1.99924) CR (1) C 3	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
4.	(1.99914) CR (1) C 4	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
5.	(1.99916) CR (1) C 5	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
6.	(1.99922) CR (1) C 6	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
7.	(1.99917) CR (1) C 7	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
8.	(1.99889) CR (1) C 8	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
9.	(1.99891) CR (1) C 9	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
10.	(1.99901) CR (1) C 10	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
11.	(1.99938) CR (1) C 11	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
12.	(1.99938) CR (1) C 12	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
13.	(1.99947) CR (1) N 13	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
14.	(1.99902) CR (1) B 14	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
15.	(1.99995) CR (1) F 15	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
16.	(1.99995) CR (1) F 16	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
17.	(0.99140) LP (1) C 10	s(0.00%)p 1.00(100.00%)d 0.00(0.00%)			
		0.0000	0.0005	-0.0001	0.0000
		-0.0002	-0.0005	-0.0002	1.0000
		0.0002	-0.0019	0.0004	-0.0001
18.	(1.98459) LP (1) F 15	s(50.20%)p 0.99(49.76%)d 0.00(0.04%)			
		0.0000	0.7085	-0.0005	-0.0034
		0.0003	-0.2076	0.0004	-0.6028
		-0.0052	-0.0128	-0.0096	-0.0015
19.	(1.93443) LP (2) F 15	s(0.22%)p99.99(99.70%)d 0.34(0.08%)			

				0.0000	0.0468	0.0012	-0.0007	-0.8814
				0.0005	0.1439	0.0011	0.4467	0.0004
				-0.0080	-0.0123	0.0088	-0.0130	0.0171
20.	(1.92188)	LP (3) F 15		s(0.09%)p99.99(99.83%)d 0.92(0.08%)				
				0.0000	0.0297	-0.0020	-0.0009	0.0238
				0.0006	-0.9371	-0.0013	0.3457	0.0002
				-0.0129	0.0064	-0.0169	0.0104	0.0149
21.	(1.98485)	LP (1) F 16		s(51.23%)p 0.95(48.74%)d 0.00(0.04%)				
				0.0000	0.7157	-0.0006	-0.0033	-0.2981
				0.0003	-0.2139	0.0005	0.5940	-0.0015
				-0.0051	0.0121	0.0095	-0.0013	-0.0094
22.	(1.93551)	LP (2) F 16		s(0.26%)p99.99(99.67%)d 0.28(0.07%)				
				0.0000	0.0510	0.0011	-0.0008	-0.8788
				0.0007	0.1315	0.0011	-0.4552	-0.0003
				-0.0082	0.0115	-0.0086	-0.0127	0.0169
23.	(1.92362)	LP (3) F 16		s(0.08%)p99.99(99.84%)d 0.96(0.08%)				
				0.0000	0.0285	-0.0021	-0.0009	0.0428
				0.0006	-0.9351	-0.0012	-0.3495	-0.0002
				-0.0124	-0.0067	0.0160	0.0106	0.0145
24.	(1.97852)	BD (1) C 1- C 2		(50.92%) 0.7136* C 1 s(38.52%)p 1.59(61.43%)d 0.00(0.04%)				
				0.0000	0.6207	0.0045	0.0005	0.2131
				-0.0101	0.7541	0.0120	-0.0002	-0.0003
				0.0097	0.0000	0.0000	-0.0148	-0.0111
				(49.08%) 0.7006* C 2 s(35.05%)p 1.85(64.88%)d 0.00(0.07%)				
				0.0000	0.5920	0.0022	0.0036	-0.3165
				-0.0241	-0.7402	0.0052	0.0112	-0.0006
				0.0138	0.0001	-0.0003	-0.0144	-0.0161
25.	(1.76704)	BD (2) C 1- C 2		(50.16%) 0.7082* C 1 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)				
				0.0000	0.0048	0.0008	0.0001	0.0054
				-0.0001	-0.0058	0.0007	-0.9997	0.0152
				0.0001	-0.0102	-0.0159	0.0004	0.0001
				(49.84%) 0.7060* C 2 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)				
				0.0000	-0.0021	0.0005	0.0001	0.0094
				-0.0006	-0.0208	0.0007	-0.9994	0.0158
				-0.0001	0.0027	0.0208	-0.0002	-0.0002
26.	(1.96976)	BD (1) C 1- C 9		(49.87%) 0.7062* C 1 s(35.37%)p 1.83(64.58%)d 0.00(0.05%)				
				0.0000	0.5947	-0.0051	0.0015	0.4983
				-0.0019	-0.6304	0.0064	0.0091	-0.0004
				-0.0176	0.0002	-0.0004	-0.0056	-0.0131
				(50.13%) 0.7081* C 9 s(32.14%)p 2.11(67.80%)d 0.00(0.06%)				
				0.0000	0.5669	0.0038	0.0000	-0.4888
				0.0010	0.6626	-0.0047	-0.0001	0.0000
				-0.0182	0.0001	-0.0001	-0.0045	-0.0148
27.	(1.98043)	BD (1) C 1- N 13		(37.33%) 0.6110* C 1 s(26.02%)p 2.84(73.86%)d 0.00(0.12%)				
				0.0000	0.5100	0.0076	-0.0023	-0.8396
				-0.0143	-0.1828	0.0034	-0.0010	-0.0002
				0.0146	-0.0002	-0.0001	0.0247	-0.0188
				(62.67%) 0.7916* N 13 s(26.35%)p 2.79(73.58%)d 0.00(0.07%)				
				0.0000	0.5133	0.0033	-0.0004	0.8125
				0.0079	0.2750	0.0024	-0.0070	-0.0006
				0.0176	-0.0003	-0.0003	0.0154	-0.0113
28.	(1.97131)	BD (1) C 2- C 3		(50.93%) 0.7136* C 2 s(33.53%)p 1.98(66.42%)d 0.00(0.05%)				
				0.0000	0.5791	0.0045	0.0008	0.8056
				0.0023	0.1190	0.0323	0.0038	-0.0005
				0.0014	0.0000	-0.0001	0.0160	-0.0145
				(49.07%) 0.7005* C 3 s(32.88%)p 2.04(67.07%)d 0.00(0.05%)				
				0.0000	0.5734	0.0011	0.0018	-0.8113
				-0.0115	-0.1067	0.0303	0.0045	-0.0005
				0.0051	0.0001	-0.0001	0.0166	-0.0146
29.	(1.98138)	BD (1) C 2- H 17		(61.23%) 0.7825* C 2 s(31.25%)p 2.20(68.68%)d 0.00(0.07%)				
				0.0000	0.5590	-0.0044	-0.0034	-0.5000
				0.0040	0.6605	0.0141	-0.0197	-0.0003
				-0.0208	0.0011	-0.0013	-0.0045	-0.0149
				(38.77%) 0.6226* H 17 s(99.94%)p 0.00(0.06%)				
				0.9997	0.0011	0.0136	-0.0196	0.0007
30.	(1.97943)	BD (1) C 3- C 4		(49.93%) 0.7066* C 3 s(35.87%)p 1.79(64.07%)d 0.00(0.05%)				
				0.0000	0.5989	0.0037	0.0024	0.5049
				0.0318	-0.6201	0.0114	0.0141	-0.0003
				-0.0177	0.0002	-0.0004	-0.0051	-0.0141
				(50.07%) 0.7076* C 4 s(34.95%)p 1.86(65.00%)d 0.00(0.05%)				

				0.0000	0.5911	0.0076	0.0018	-0.5117
				0.0167	0.6220	0.0295	-0.0009	-0.0005
				-0.0179	0.0002	-0.0003	-0.0017	-0.0140
31.	(1.75235)	BD (2) C	3- C 4					
	(50.55%)		0.7110* C	3 s(0.00%)	p 1.00(99.97%)	d 0.00(0.03%)		
				0.0000	0.0013	-0.0007	0.0001	0.0030
				-0.0006	0.0264	-0.0005	0.9992	-0.0249
				0.0000	0.0074	-0.0171	0.0005	0.0003
	(49.45%)		0.7032* C	4 s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	0.0006	-0.0005	-0.0001	0.0142
				-0.0006	0.0127	-0.0005	0.9994	-0.0193
				-0.0002	-0.0169	0.0110	-0.0004	-0.0003
32.	(1.98240)	BD (1) C	3- H 18					
	(60.96%)		0.7808* C	3 s(31.09%)	p 2.21(68.84%)	d 0.00(0.07%)		
				0.0000	0.5576	-0.0033	-0.0032	0.2920
				0.0047	0.7763	0.0066	-0.0222	-0.0003
				0.0134	-0.0006	-0.0015	-0.0164	-0.0147
	(39.04%)		0.6248* H	18 s(99.93%)	p 0.00(0.07%)			
				0.9997	-0.0008	-0.0092	-0.0247	0.0008
33.	(1.97597)	BD (1) C	4- C 10					
	(48.81%)		0.6986* C	4 s(33.80%)	p 1.96(66.14%)	d 0.00(0.06%)		
				0.0000	0.5814	-0.0048	0.0034	-0.2629
				0.0241	-0.7691	-0.0053	0.0131	-0.0002
				0.0122	-0.0002	-0.0003	-0.0136	-0.0149
	(51.19%)		0.7155* C	10 s(34.01%)	p 1.94(65.95%)	d 0.00(0.04%)		
				0.0000	0.5832	0.0025	-0.0003	0.3120
				0.0205	0.7495	-0.0062	0.0008	0.0002
				0.0098	-0.0001	-0.0002	-0.0133	-0.0117
34.	(1.98133)	BD (1) C	4- H 19					
	(60.92%)		0.7805* C	4 s(31.08%)	p 2.22(68.86%)	d 0.00(0.06%)		
				0.0000	0.5575	-0.0018	-0.0040	0.8174
				0.0093	0.1421	0.0058	-0.0138	-0.0003
				0.0073	-0.0011	-0.0003	0.0195	-0.0143
	(39.08%)		0.6252* H	19 s(99.93%)	p 0.00(0.07%)			
				0.9996	-0.0012	-0.0263	-0.0052	0.0006
35.	(1.97895)	BD (1) C	5- C 6					
	(50.35%)		0.7096* C	5 s(35.54%)	p 1.81(64.41%)	d 0.00(0.05%)		
				0.0000	0.5961	0.0071	0.0020	-0.3538
				0.0231	-0.7195	-0.0259	-0.0076	-0.0001
				0.0153	0.0002	0.0003	-0.0092	-0.0136
	(49.65%)		0.7046* C	6 s(34.77%)	p 1.87(65.17%)	d 0.00(0.06%)		
				0.0000	0.5897	0.0030	0.0030	0.3463
				0.0316	0.7285	-0.0038	0.0075	0.0003
				0.0145	0.0003	0.0005	-0.0118	-0.0144
36.	(1.74262)	BD (2) C	5- C 6					
	(50.96%)		0.7139* C	5 s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	0.0032	-0.0004	0.0000	0.0176
				-0.0004	0.0045	0.0002	-0.9994	0.0211
				-0.0003	0.0137	0.0135	-0.0002	0.0003
	(49.04%)		0.7003* C	6 s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	0.0036	-0.0004	-0.0001	0.0186
				-0.0006	-0.0014	0.0004	-0.9993	0.0248
				0.0003	-0.0046	-0.0189	0.0000	-0.0004
37.	(1.97534)	BD (1) C	5- C 10					
	(48.41%)		0.6958* C	5 s(33.19%)	p 2.01(66.75%)	d 0.00(0.06%)		
				0.0000	0.5761	-0.0034	0.0034	-0.4347
				0.0212	0.6913	0.0123	-0.0027	0.0007
				-0.0168	0.0001	0.0001	-0.0071	-0.0150
	(51.59%)		0.7183* C	10 s(34.10%)	p 1.93(65.86%)	d 0.00(0.04%)		
				0.0000	0.5839	0.0024	-0.0005	0.4795
				0.0168	-0.6545	0.0117	0.0005	0.0002
				-0.0142	-0.0001	0.0001	-0.0071	-0.0115
38.	(1.98192)	BD (1) C	5- H 20					
	(60.74%)		0.7794* C	5 s(31.10%)	p 2.21(68.83%)	d 0.00(0.06%)		
				0.0000	0.5577	-0.0024	-0.0041	0.8276
				0.0102	0.0554	-0.0054	0.0167	0.0003
				0.0032	0.0011	0.0001	0.0206	-0.0142
	(39.26%)		0.6266* H	20 s(99.93%)	p 0.00(0.07%)			
				0.9996	0.0012	-0.0267	-0.0012	-0.0006
39.	(1.97945)	BD (1) C	6- C 7					
	(50.25%)		0.7088* C	6 s(33.54%)	p 1.98(66.41%)	d 0.00(0.05%)		
				0.0000	0.5792	-0.0029	0.0017	-0.8099
				-0.0002	-0.0839	-0.0298	-0.0129	0.0000
				0.0029	0.0004	0.0000	0.0166	-0.0135
	(49.75%)		0.7054* C	7 s(33.20%)	p 2.01(66.76%)	d 0.00(0.05%)		
				0.0000	0.5762	0.0009	0.0012	0.8127
				0.0096	0.0767	-0.0327	0.0047	-0.0002

						0.0043	0.0005	0.0001	0.0171	-0.0135
40.	(1.98204)	BD (1) C	6-	H 21		s(31.51%)	p 2.17(68.42%)	d 0.00(0.07%)		
	(60.26%)		0.7763*	C 6		0.0000	0.5613	0.0008	-0.0036	0.4720
						0.0063	-0.6791	-0.0114	0.0118	0.0004
						-0.0206	0.0007	-0.0008	-0.0059	-0.0148
	(39.74%)		0.6304*	H 21		s(99.92%)	p 0.00(0.08%)			
						0.9996	-0.0008	-0.0163	0.0224	-0.0005
41.	(1.97580)	BD (1) C	7-	C 8		s(35.27%)	p 1.83(64.67%)	d 0.00(0.05%)		
	(49.27%)		0.7020*	C 7		0.0000	0.5939	0.0046	0.0030	-0.4820
						-0.0256	0.6431	-0.0127	0.0020	0.0000
						-0.0170	-0.0001	0.0003	-0.0065	-0.0140
	(50.73%)		0.7122*	C 8		s(36.34%)	p 1.75(63.60%)	d 0.00(0.05%)		
						0.0000	0.6023	0.0259	-0.0005	0.4257
						-0.0009	-0.6734	-0.0357	-0.0077	-0.0005
						-0.0188	-0.0002	0.0003	-0.0014	-0.0132
42.	(1.98317)	BD (1) C	7-	H 22		s(31.36%)	p 2.19(68.57%)	d 0.00(0.07%)		
	(60.91%)		0.7805*	C 7		0.0000	0.5600	-0.0026	-0.0032	-0.3254
						-0.0033	-0.7614	-0.0086	-0.0067	-0.0002
						0.0156	0.0001	0.0001	-0.0145	-0.0141
	(39.09%)		0.6252*	H 22		s(99.93%)	p 0.00(0.07%)			
						0.9996	-0.0014	0.0117	0.0242	0.0001
43.	(1.96422)	BD (1) C	8-	C 9		s(29.60%)	p 2.38(70.33%)	d 0.00(0.07%)		
	(48.12%)		0.6937*	C 8		0.0000	0.5440	0.0111	0.0010	0.3981
						0.0197	0.7377	0.0133	0.0092	0.0003
						0.0166	0.0002	0.0004	-0.0092	-0.0174
	(51.88%)		0.7203*	C 9		s(33.87%)	p 1.95(66.09%)	d 0.00(0.04%)		
						0.0000	0.5820	-0.0022	-0.0006	-0.3313
						0.0047	-0.7423	0.0044	-0.0024	0.0001
						0.0132	0.0002	0.0003	-0.0083	-0.0132
44.	(1.96654)	BD (1) C	8-	B 14		s(33.85%)	p 1.95(66.12%)	d 0.00(0.03%)		
	(70.92%)		0.8421*	C 8		0.0000	0.5814	-0.0230	-0.0003	-0.8109
						0.0496	0.0086	-0.0341	-0.0022	-0.0001
						-0.0065	0.0001	0.0000	0.0106	-0.0098
	(29.08%)		0.5392*	B 14		s(34.20%)	p 1.92(65.66%)	d 0.00(0.13%)		
						0.0000	0.5845	-0.0095	0.0171	0.7869
						0.0530	-0.1852	-0.0142	0.0017	0.0002
						-0.0094	0.0001	0.0001	0.0297	-0.0194
45.	(1.96601)	BD (1) C	9-	C 10		s(33.93%)	p 1.95(66.02%)	d 0.00(0.05%)		
	(50.79%)		0.7127*	C 9		0.0000	0.5825	-0.0004	0.0013	0.8067
						-0.0047	0.0967	-0.0035	0.0058	0.0004
						0.0064	0.0002	0.0000	0.0162	-0.0136
	(49.21%)		0.7015*	C 10		s(31.78%)	p 2.14(68.17%)	d 0.00(0.05%)		
						0.0000	0.5637	-0.0034	0.0015	-0.8198
						0.0075	-0.0975	-0.0019	-0.0023	0.0003
						0.0038	0.0003	0.0000	0.0165	-0.0144
46.	(1.98088)	BD (1) C	11-	N 13		s(20.35%)	p 3.91(79.52%)	d 0.01(0.13%)		
	(36.08%)		0.6007*	C 11		0.0000	0.4510	0.0101	0.0022	0.3960
						-0.0003	-0.2981	-0.0068	-0.7412	-0.0115
						-0.0087	-0.0230	0.0162	0.0030	0.0196
	(63.92%)		0.7995*	N 13		s(23.65%)	p 3.23(76.31%)	d 0.00(0.05%)		
						0.0000	0.4862	0.0090	0.0001	-0.4010
						-0.0131	0.2966	-0.0067	0.7168	0.0165
						-0.0078	-0.0094	0.0159	0.0003	0.0090
47.	(1.98997)	BD (1) C	11-	H 23		s(25.77%)	p 2.88(74.15%)	d 0.00(0.08%)		
	(62.03%)		0.7876*	C 11		0.0000	0.5077	-0.0033	-0.0009	0.4661
						-0.0172	-0.2770	0.0077	0.6686	0.0063
						-0.0083	0.0210	-0.0131	0.0048	0.0088
	(37.97%)		0.6162*	H 23		s(99.95%)	p 0.00(0.05%)			
						0.9998	0.0007	-0.0095	0.0078	-0.0180
48.	(1.99361)	BD (1) C	11-	H 24		s(27.32%)	p 2.66(72.59%)	d 0.00(0.08%)		
	(60.45%)		0.7775*	C 11		0.0000	0.5227	-0.0012	-0.0003	-0.0158
						-0.0102	0.8509	0.0025	-0.0335	0.0188
						-0.0005	0.0008	-0.0038	-0.0245	-0.0144
	(39.55%)		0.6289*	H 24		s(99.94%)	p 0.00(0.06%)			
						0.9997	0.0011	0.0015	-0.0249	-0.0020
49.	(1.98985)	BD (1) C	11-	H 25		s(26.51%)	p 2.77(73.41%)	d 0.00(0.08%)		
	(61.59%)		0.7848*	C 11		0.0000	0.5149	0.0007	0.0000	-0.7901

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0.0005 -0.3302 0.0062 0.0231 0.0162
0.0172 0.0013 -0.0012 0.0166 -0.0146
( 38.41%) 0.6198* H 25 s( 99.94%)p 0.00( 0.06%)
0.9997 0.0015 0.0217 0.0105 -0.0036
50. (1.98197) BD ( 1) C 12- N 13
( 36.22%) 0.6018* C 12 s( 20.76%)p 3.81( 79.12%)d 0.01( 0.12%)
0.0000 0.4555 0.0103 0.0023 0.4233
0.0004 -0.3188 -0.0071 0.7143 0.0119
-0.0094 0.0239 -0.0166 0.0035 0.0173
( 63.78%) 0.7986* N 13 s( 24.12%)p 3.14( 75.83%)d 0.00( 0.05%)
0.0000 0.4910 0.0099 0.0000 -0.4207
-0.0139 0.3099 -0.0060 -0.6963 -0.0170
-0.0083 0.0100 -0.0160 0.0004 0.0082
51. (1.98977) BD ( 1) C 12- H 26
( 61.89%) 0.7867* C 12 s( 25.92%)p 2.85( 74.00%)d 0.00( 0.08%)
0.0000 0.5091 -0.0020 -0.0006 0.4063
-0.0164 -0.2973 0.0077 -0.6973 -0.0063
-0.0070 -0.0196 0.0139 0.0028 0.0117
( 38.11%) 0.6173* H 26 s( 99.95%)p 0.00( 0.05%)
0.9997 0.0008 -0.0082 0.0081 0.0194
52. (1.99316) BD ( 1) C 12- H 27
( 60.39%) 0.7771* C 12 s( 26.83%)p 2.72( 73.08%)d 0.00( 0.08%)
0.0000 0.5180 -0.0021 -0.0005 0.0315
-0.0106 0.8534 0.0018 0.0329 -0.0189
0.0031 -0.0008 0.0033 -0.0245 -0.0141
( 39.61%) 0.6294* H 27 s( 99.94%)p 0.00( 0.06%)
0.9997 0.0010 0.0000 -0.0246 0.0022
53. (1.98949) BD ( 1) C 12- H 28
( 61.49%) 0.7842* C 12 s( 26.45%)p 2.78( 73.47%)d 0.00( 0.08%)
0.0000 0.5143 0.0001 -0.0001 -0.8083
0.0008 -0.2835 0.0063 0.0254 -0.0166
0.0155 -0.0036 0.0004 0.0181 -0.0140
( 38.51%) 0.6206* H 28 s( 99.94%)p 0.00( 0.06%)
0.9997 0.0012 0.0223 0.0089 0.0025
54. (1.96438) BD ( 1) N 13- B 14
( 84.92%) 0.9215* N 13 s( 25.88%)p 2.86( 74.11%)d 0.00( 0.00%)
0.0000 0.5086 -0.0148 0.0006 -0.0302
-0.0138 -0.8596 0.0336 -0.0059 -0.0001
-0.0034 0.0000 0.0002 -0.0044 -0.0042
( 15.08%) 0.3883* B 14 s( 17.94%)p 4.55( 81.71%)d 0.02( 0.35%)
0.0000 0.4234 -0.0090 -0.0081 -0.1011
-0.0054 0.8975 0.0351 0.0070 -0.0002
-0.0024 0.0001 0.0007 -0.0503 -0.0315
55. (1.99422) BD ( 1) B 14- F 15
( 15.81%) 0.3976* B 14 s( 24.02%)p 3.15( 75.61%)d 0.02( 0.37%)
0.0000 0.4898 0.0125 -0.0117 -0.4239
-0.0207 -0.2712 -0.0166 -0.7080 -0.0296
0.0094 0.0444 0.0218 0.0065 0.0336
( 84.19%) 0.9176* F 15 s( 49.47%)p 1.02( 50.36%)d 0.00( 0.17%)
0.0000 0.7033 -0.0002 0.0042 0.3613
0.0016 0.2389 0.0020 0.5621 -0.0022
0.0119 0.0287 0.0194 0.0038 0.0185
56. (1.99404) BD ( 1) B 14- F 16
( 15.85%) 0.3981* B 14 s( 23.91%)p 3.17( 75.72%)d 0.02( 0.36%)
0.0000 0.4887 0.0122 -0.0119 -0.4288
-0.0214 -0.2822 -0.0176 0.7015 0.0294
0.0101 -0.0440 -0.0224 0.0065 0.0322
( 84.15%) 0.9173* F 16 s( 48.41%)p 1.06( 51.42%)d 0.00( 0.16%)
0.0000 0.6958 -0.0001 0.0042 0.3689
0.0017 0.2483 0.0020 -0.5626 0.0019
0.0122 -0.0280 -0.0194 0.0036 0.0173
57. (1.88415) 3C ( 1) C 7- C 8- C 9
( 33.00%) 0.5745* C 7 s( 0.00%)p 1.00( 99.95%)d 0.00( 0.05%)
0.0000 0.0002 0.0000 0.0000 0.0050
-0.0001 0.0067 0.0005 -0.9996 0.0131
0.0000 0.0079 -0.0213 -0.0002 -0.0005
( 47.75%) 0.6910* C 8 s( 0.00%)p 1.00( 99.97%)d 0.00( 0.03%)
0.0000 -0.0009 -0.0002 0.0000 0.0021
0.0001 0.0119 0.0007 -0.9995 -0.0208
0.0002 -0.0186 -0.0012 0.0001 0.0000
( 19.25%) 0.4388* C 9 s( 0.00%)p 1.00( 99.91%)d 0.00( 0.09%)
0.0000 0.0019 0.0001 0.0001 0.0055
-0.0001 0.0023 0.0005 -0.9995 -0.0067
-0.0001 0.0165 0.0247 0.0003 0.0005
----- non-Lewis -----
58. (0.02499) BD*( 1) C 1- C 2
( 49.08%) 0.7006* C 1 s( 38.52%)p 1.59( 61.43%)d 0.00( 0.04%)

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				0.0000	0.6207	0.0045	0.0005	0.2131
				-0.0101	0.7541	0.0120	-0.0002	-0.0003
				0.0097	0.0000	0.0000	-0.0148	-0.0111
	(50.92%)	-0.7136*	C 2	s(35.05%)	p 1.85	(64.88%)	d 0.00	(0.07%)
				0.0000	0.5920	0.0022	0.0036	-0.3165
				-0.0241	-0.7402	0.0052	0.0112	-0.0006
				0.0138	0.0001	-0.0003	-0.0144	-0.0161
59.	(0.30037)	BD*(2)	C 1- C 2					
	(49.84%)	0.7060*	C 1	s(0.00%)	p 1.00	(99.96%)	d 0.00	(0.04%)
				0.0000	0.0048	0.0008	0.0001	0.0054
				-0.0001	-0.0058	0.0007	-0.9997	0.0152
				0.0001	-0.0102	-0.0159	0.0004	0.0001
	(50.16%)	-0.7082*	C 2	s(0.00%)	p 1.00	(99.96%)	d 0.00	(0.04%)
				0.0000	-0.0021	0.0005	0.0001	0.0094
				-0.0006	-0.0208	0.0007	-0.9994	0.0158
				-0.0001	0.0027	0.0208	-0.0002	-0.0002
60.	(0.03199)	BD*(1)	C 1- C 9					
	(50.13%)	0.7081*	C 1	s(35.37%)	p 1.83	(64.58%)	d 0.00	(0.05%)
				0.0000	0.5947	-0.0051	0.0015	0.4983
				-0.0019	-0.6304	0.0064	0.0091	-0.0004
				-0.0176	0.0002	-0.0004	-0.0056	-0.0131
	(49.87%)	-0.7062*	C 9	s(32.14%)	p 2.11	(67.80%)	d 0.00	(0.06%)
				0.0000	0.5669	0.0038	0.0000	-0.4888
				0.0010	0.6626	-0.0047	-0.0001	0.0000
				-0.0182	0.0001	-0.0001	-0.0045	-0.0148
61.	(0.03895)	BD*(1)	C 1- N 13					
	(62.67%)	0.7916*	C 1	s(26.02%)	p 2.84	(73.86%)	d 0.00	(0.12%)
				0.0000	0.5100	0.0076	-0.0023	-0.8396
				-0.0143	-0.1828	0.0034	-0.0010	-0.0002
				0.0146	-0.0002	-0.0001	0.0247	-0.0188
	(37.33%)	-0.6110*	N 13	s(26.35%)	p 2.79	(73.58%)	d 0.00	(0.07%)
				0.0000	0.5133	0.0033	-0.0004	0.8125
				0.0079	0.2750	0.0024	-0.0070	-0.0006
				0.0176	-0.0003	-0.0003	0.0154	-0.0113
62.	(0.01664)	BD*(1)	C 2- C 3					
	(49.07%)	0.7005*	C 2	s(33.53%)	p 1.98	(66.42%)	d 0.00	(0.05%)
				0.0000	-0.5791	-0.0045	-0.0008	-0.8056
				-0.0023	-0.1190	-0.0323	-0.0038	0.0005
				-0.0014	0.0000	0.0001	-0.0160	0.0145
	(50.93%)	-0.7136*	C 3	s(32.88%)	p 2.04	(67.07%)	d 0.00	(0.05%)
				0.0000	-0.5734	-0.0011	-0.0018	0.8113
				0.0115	0.1067	-0.0303	-0.0045	0.0005
				-0.0051	-0.0001	0.0001	-0.0166	0.0146
63.	(0.01261)	BD*(1)	C 2- H 17					
	(38.77%)	0.6226*	C 2	s(31.25%)	p 2.20	(68.68%)	d 0.00	(0.07%)
				0.0000	-0.5590	0.0044	0.0034	0.5000
				-0.0040	-0.6605	-0.0141	0.0197	0.0003
				0.0208	-0.0011	0.0013	0.0045	0.0149
	(61.23%)	-0.7825*	H 17	s(99.94%)	p 0.00	(0.06%)		
				-0.9997	-0.0011	-0.0136	0.0196	-0.0007
64.	(0.01406)	BD*(1)	C 3- C 4					
	(50.07%)	0.7076*	C 3	s(35.87%)	p 1.79	(64.07%)	d 0.00	(0.05%)
				0.0000	0.5989	0.0037	0.0024	0.5049
				0.0318	-0.6201	0.0114	0.0141	-0.0003
				-0.0177	0.0002	-0.0004	-0.0051	-0.0141
	(49.93%)	-0.7066*	C 4	s(34.95%)	p 1.86	(65.00%)	d 0.00	(0.05%)
				0.0000	0.5911	0.0076	0.0018	-0.5117
				0.0167	0.6220	0.0295	-0.0009	-0.0005
				-0.0179	0.0002	-0.0003	-0.0017	-0.0140
65.	(0.25445)	BD*(2)	C 3- C 4					
	(49.45%)	0.7032*	C 3	s(0.00%)	p 1.00	(99.97%)	d 0.00	(0.03%)
				0.0000	0.0013	-0.0007	0.0001	0.0030
				-0.0006	0.0264	-0.0005	0.9992	-0.0249
				0.0000	0.0074	-0.0171	0.0005	0.0003
	(50.55%)	-0.7110*	C 4	s(0.00%)	p 1.00	(99.96%)	d 0.00	(0.04%)
				0.0000	0.0006	-0.0005	-0.0001	0.0142
				-0.0006	0.0127	-0.0005	0.9994	-0.0193
				-0.0002	-0.0169	0.0110	-0.0004	-0.0003
66.	(0.01066)	BD*(1)	C 3- H 18					
	(39.04%)	0.6248*	C 3	s(31.09%)	p 2.21	(68.84%)	d 0.00	(0.07%)
				0.0000	-0.5576	0.0033	0.0032	-0.2920
				-0.0047	-0.7763	-0.0066	0.0222	0.0003
				-0.0134	0.0006	0.0015	0.0164	0.0147
	(60.96%)	-0.7808*	H 18	s(99.93%)	p 0.00	(0.07%)		
				-0.9997	0.0008	0.0092	0.0247	-0.0008
67.	(0.02331)	BD*(1)	C 4- C 10					
	(51.19%)	0.7155*	C 4	s(33.80%)	p 1.96	(66.14%)	d 0.00	(0.06%)

				0.0000	0.5814	-0.0048	0.0034	-0.2629
				0.0241	-0.7691	-0.0053	0.0131	-0.0002
				0.0122	-0.0002	-0.0003	-0.0136	-0.0149
	(48.81%)	-0.6986*	C 10	s(34.01%)	p 1.94(65.95%)	d 0.00(0.04%)		
				0.0000	0.5832	0.0025	-0.0003	0.3120
				0.0205	0.7495	-0.0062	0.0008	0.0002
				0.0098	-0.0001	-0.0002	-0.0133	-0.0117
68.	(0.01225)	BD*(1)	C 4- H 19					
	(39.08%)	0.6252*	C 4	s(31.08%)	p 2.22(68.86%)	d 0.00(0.06%)		
				0.0000	-0.5575	0.0018	0.0040	-0.8174
				-0.0093	-0.1421	-0.0058	0.0138	0.0003
				-0.0073	0.0011	0.0003	-0.0195	0.0143
	(60.92%)	-0.7805*	H 19	s(99.93%)	p 0.00(0.07%)			
				-0.9996	0.0012	0.0263	0.0052	-0.0006
69.	(0.01478)	BD*(1)	C 5- C 6					
	(49.65%)	0.7046*	C 5	s(35.54%)	p 1.81(64.41%)	d 0.00(0.05%)		
				0.0000	0.5961	0.0071	0.0020	-0.3538
				0.0231	-0.7195	-0.0259	-0.0076	-0.0001
				0.0153	0.0002	0.0003	-0.0092	-0.0136
	(50.35%)	-0.7096*	C 6	s(34.77%)	p 1.87(65.17%)	d 0.00(0.06%)		
				0.0000	0.5897	0.0030	0.0030	0.3463
				0.0316	0.7285	-0.0038	0.0075	0.0003
				0.0145	0.0003	0.0005	-0.0118	-0.0144
70.	(0.25450)	BD*(2)	C 5- C 6					
	(49.04%)	0.7003*	C 5	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	-0.0032	0.0004	0.0000	-0.0176
				0.0004	-0.0045	-0.0002	0.9994	-0.0211
				0.0003	-0.0137	-0.0135	0.0002	-0.0003
	(50.96%)	-0.7139*	C 6	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	-0.0036	0.0004	0.0001	-0.0186
				0.0006	0.0014	-0.0004	0.9993	-0.0248
				-0.0003	0.0046	0.0189	0.0000	0.0004
71.	(0.02381)	BD*(1)	C 5- C 10					
	(51.59%)	0.7183*	C 5	s(33.19%)	p 2.01(66.75%)	d 0.00(0.06%)		
				0.0000	0.5761	-0.0034	0.0034	-0.4347
				0.0212	0.6913	0.0123	-0.0027	0.0007
				-0.0168	0.0001	0.0001	-0.0071	-0.0150
	(48.41%)	-0.6958*	C 10	s(34.10%)	p 1.93(65.86%)	d 0.00(0.04%)		
				0.0000	0.5839	0.0024	-0.0005	0.4795
				0.0168	-0.6545	0.0117	0.0005	0.0002
				-0.0142	-0.0001	0.0001	-0.0071	-0.0115
72.	(0.01223)	BD*(1)	C 5- H 20					
	(39.26%)	0.6266*	C 5	s(31.10%)	p 2.21(68.83%)	d 0.00(0.06%)		
				0.0000	-0.5577	0.0024	0.0041	-0.8276
				-0.0102	-0.0554	0.0054	-0.0167	-0.0003
				-0.0032	-0.0011	-0.0001	-0.0206	0.0142
	(60.74%)	-0.7794*	H 20	s(99.93%)	p 0.00(0.07%)			
				-0.9996	-0.0012	0.0267	0.0012	0.0006
73.	(0.01880)	BD*(1)	C 6- C 7					
	(49.75%)	0.7054*	C 6	s(33.54%)	p 1.98(66.41%)	d 0.00(0.05%)		
				0.0000	0.5792	-0.0029	0.0017	-0.8099
				-0.0002	-0.0839	-0.0298	-0.0129	0.0000
				0.0029	0.0004	0.0000	0.0166	-0.0135
	(50.25%)	-0.7088*	C 7	s(33.20%)	p 2.01(66.76%)	d 0.00(0.05%)		
				0.0000	0.5762	0.0009	0.0012	0.8127
				0.0096	0.0767	-0.0327	0.0047	-0.0002
				0.0043	0.0005	0.0001	0.0171	-0.0135
74.	(0.01092)	BD*(1)	C 6- H 21					
	(39.74%)	0.6304*	C 6	s(31.51%)	p 2.17(68.42%)	d 0.00(0.07%)		
				0.0000	-0.5613	-0.0008	0.0036	-0.4720
				-0.0063	0.6791	0.0114	-0.0118	-0.0004
				0.0206	-0.0007	0.0008	0.0059	0.0148
	(60.26%)	-0.7763*	H 21	s(99.92%)	p 0.00(0.08%)			
				-0.9996	0.0008	0.0163	-0.0224	0.0005
75.	(0.02062)	BD*(1)	C 7- C 8					
	(50.73%)	0.7122*	C 7	s(35.27%)	p 1.83(64.67%)	d 0.00(0.05%)		
				0.0000	0.5939	0.0046	0.0030	-0.4820
				-0.0256	0.6431	-0.0127	0.0020	0.0000
				-0.0170	-0.0001	0.0003	-0.0065	-0.0140
	(49.27%)	-0.7020*	C 8	s(36.34%)	p 1.75(63.60%)	d 0.00(0.05%)		
				0.0000	0.6023	0.0259	-0.0005	0.4257
				-0.0009	-0.6734	-0.0357	-0.0077	-0.0005
				-0.0188	-0.0002	0.0003	-0.0014	-0.0132
76.	(0.01285)	BD*(1)	C 7- H 22					
	(39.09%)	0.6252*	C 7	s(31.36%)	p 2.19(68.57%)	d 0.00(0.07%)		
				0.0000	-0.5600	0.0026	0.0032	0.3254
				0.0033	0.7614	0.0086	0.0067	0.0002

	(60.91%)	-0.7805*	H 22	s(99.93%)p 0.00(0.07%)	-0.0156 -0.0001 -0.0001 0.0145 0.0141 -0.9996 0.0014 -0.0117 -0.0242 -0.0001
77. (0.02714)	BD*(1) C 8-	C 9	(51.88%)	0.7203* C 8	s(29.60%)p 2.38(70.33%)d 0.00(0.07%) 0.0000 -0.5440 -0.0111 -0.0010 -0.3981 -0.0197 -0.7377 -0.0133 -0.0092 -0.0003 -0.0166 -0.0002 -0.0004 0.0092 0.0174 s(33.87%)p 1.95(66.09%)d 0.00(0.04%) 0.0000 -0.5820 0.0022 0.0006 0.3313 -0.0047 0.7423 -0.0044 0.0024 -0.0001 -0.0132 -0.0002 -0.0003 0.0083 0.0132
78. (0.06011)	BD*(1) C 8-	B 14	(29.08%)	0.5392* C 8	s(33.85%)p 1.95(66.12%)d 0.00(0.03%) 0.0000 -0.5814 0.0230 0.0003 0.8109 -0.0496 -0.0086 0.0341 0.0022 0.0001 0.0065 -0.0001 0.0000 -0.0106 0.0098 s(34.20%)p 1.92(65.66%)d 0.00(0.13%) 0.0000 -0.5845 0.0095 -0.0171 -0.7869 -0.0530 0.1852 0.0142 -0.0017 -0.0002 0.0094 -0.0001 -0.0001 -0.0297 0.0194
79. (0.03604)	BD*(1) C 9-	C 10	(49.21%)	0.7015* C 9	s(33.93%)p 1.95(66.02%)d 0.00(0.05%) 0.0000 0.5825 -0.0004 0.0013 0.8067 -0.0047 0.0967 -0.0035 0.0058 0.0004 0.0064 0.0002 0.0000 0.0162 -0.0136 s(31.78%)p 2.14(68.17%)d 0.00(0.05%) 0.0000 0.5637 -0.0034 0.0015 -0.8198 0.0075 -0.0975 -0.0019 -0.0023 0.0003 0.0038 0.0003 0.0000 0.0165 -0.0144
80. (0.01693)	BD*(1) C 11-	N 13	(63.92%)	0.7995* C 11	s(20.35%)p 3.91(79.52%)d 0.01(0.13%) 0.0000 0.4510 0.0101 0.0022 0.3960 -0.0003 -0.2981 -0.0068 -0.7412 -0.0115 -0.0087 -0.0230 0.0162 0.0030 0.0196 s(23.65%)p 3.23(76.31%)d 0.00(0.05%) 0.0000 0.4862 0.0090 0.0001 -0.4010 -0.0131 0.2966 -0.0067 0.7168 0.0165 -0.0078 -0.0094 0.0159 0.0003 0.0090
81. (0.00573)	BD*(1) C 11-	H 23	(37.97%)	0.6162* C 11	s(25.77%)p 2.88(74.15%)d 0.00(0.08%) 0.0000 -0.5077 0.0033 0.0009 -0.4661 0.0172 0.2770 -0.0077 -0.6686 -0.0063 0.0083 -0.0210 0.0131 -0.0048 -0.0088 s(99.95%)p 0.00(0.05%) -0.9998 -0.0007 0.0095 -0.0078 0.0180
82. (0.00877)	BD*(1) C 11-	H 24	(39.55%)	0.6289* C 11	s(27.32%)p 2.66(72.59%)d 0.00(0.08%) 0.0000 -0.5227 0.0012 0.0003 0.0158 0.0102 -0.8509 -0.0025 0.0335 -0.0188 0.0005 -0.0008 0.0038 0.0245 0.0144 s(99.94%)p 0.00(0.06%) -0.9997 -0.0011 -0.0015 0.0249 0.0020
83. (0.00722)	BD*(1) C 11-	H 25	(38.41%)	0.6198* C 11	s(26.51%)p 2.77(73.41%)d 0.00(0.08%) 0.0000 -0.5149 -0.0007 0.0000 0.7901 -0.0005 0.3302 -0.0062 -0.0231 -0.0162 -0.0172 -0.0013 0.0012 -0.0166 0.0146 s(99.94%)p 0.00(0.06%) -0.9997 -0.0015 -0.0217 -0.0105 0.0036
84. (0.01687)	BD*(1) C 12-	N 13	(63.78%)	0.7986* C 12	s(20.76%)p 3.81(79.12%)d 0.01(0.12%) 0.0000 0.4555 0.0103 0.0023 0.4233 0.0004 -0.3188 -0.0071 0.7143 0.0119 -0.0094 0.0239 -0.0166 0.0035 0.0173 s(24.12%)p 3.14(75.83%)d 0.00(0.05%) 0.0000 0.4910 0.0099 0.0000 -0.4207 -0.0139 0.3099 -0.0060 -0.6963 -0.0170 -0.0083 0.0100 -0.0160 0.0004 0.0082
85. (0.00627)	BD*(1) C 12-	H 26	(38.11%)	0.6173* C 12	s(25.92%)p 2.85(74.00%)d 0.00(0.08%) 0.0000 -0.5091 0.0020 0.0006 -0.4063 0.0164 0.2973 -0.0077 0.6973 0.0063 0.0070 0.0196 -0.0139 -0.0028 -0.0117 s(99.95%)p 0.00(0.05%) -0.9997 -0.0008 0.0082 -0.0081 -0.0194
86. (0.00894)	BD*(1) C 12-	H 27			

(39.61%) 0.6294* C 12 s(26.83%)p 2.72(73.08%)d 0.00(0.08%)
0.0000 -0.5180 0.0021 0.0005 -0.0315
0.0106 -0.8534 -0.0018 -0.0329 0.0189
-0.0031 0.0008 -0.0033 0.0245 0.0141
(60.39%) -0.7771* H 27 s(99.94%)p 0.00(0.06%)
-0.9997 -0.0010 0.0000 0.0246 -0.0022

87. (0.00705) BD*(1) C 12- H 28
(38.51%) 0.6206* C 12 s(26.45%)p 2.78(73.47%)d 0.00(0.08%)
0.0000 -0.5143 -0.0001 0.0001 0.8083
-0.0008 0.2835 -0.0063 -0.0254 0.0166
-0.0155 0.0036 -0.0004 -0.0181 0.0140
(61.49%) -0.7842* H 28 s(99.94%)p 0.00(0.06%)
-0.9997 -0.0012 -0.0223 -0.0089 -0.0025

88. (0.12171) BD*(1) N 13- B 14
(15.08%) 0.3883* N 13 s(25.88%)p 2.86(74.11%)d 0.00(0.00%)
0.0000 -0.5086 0.0148 -0.0006 0.0302
0.0138 0.8596 -0.0336 0.0059 0.0001
0.0034 0.0000 -0.0002 0.0044 0.0042
(84.92%) -0.9215* B 14 s(17.94%)p 4.55(81.71%)d 0.02(0.35%)
0.0000 -0.4234 0.0090 0.0081 0.1011
0.0054 -0.8975 -0.0351 -0.0070 0.0002
0.0024 -0.0001 -0.0007 0.0503 0.0315

89. (0.05779) BD*(1) B 14- F 15
(84.19%) 0.9176* B 14 s(24.02%)p 3.15(75.61%)d 0.02(0.37%)
0.0000 0.4898 0.0125 -0.0117 -0.4239
-0.0207 -0.2712 -0.0166 -0.7080 -0.0296
0.0094 0.0444 0.0218 0.0065 0.0336
(15.81%) -0.3976* F 15 s(49.47%)p 1.02(50.36%)d 0.00(0.17%)
0.0000 0.7033 -0.0002 0.0042 0.3613
0.0016 0.2389 0.0020 0.5621 -0.0022
0.0119 0.0287 0.0194 0.0038 0.0185

90. (0.05943) BD*(1) B 14- F 16
(84.15%) 0.9173* B 14 s(23.91%)p 3.17(75.72%)d 0.02(0.36%)
0.0000 0.4887 0.0122 -0.0119 -0.4288
-0.0214 -0.2822 -0.0176 0.7015 0.0294
0.0101 -0.0440 -0.0224 0.0065 0.0322
(15.85%) -0.3981* F 16 s(48.41%)p 1.06(51.42%)d 0.00(0.16%)
0.0000 0.6958 -0.0001 0.0042 0.3689
0.0017 0.2483 0.0020 -0.5626 0.0019
0.0122 -0.0280 -0.0194 0.0036 0.0173

91. (0.95632) 3Cn(1) C 7- C 8- C 9
(35.35%) 0.5945* C 7 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
0.0000 -0.0002 0.0000 0.0000 -0.0050
0.0001 -0.0067 -0.0005 0.9996 -0.0131
0.0000 -0.0079 0.0213 0.0002 0.0005
(0.03%) 0.0162* C 8 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0009 0.0002 0.0000 -0.0021
-0.0001 -0.0119 -0.0007 0.9995 0.0208
-0.0002 0.0186 0.0012 -0.0001 0.0000
(64.63%) 0.8039* C 9 s(0.00%)p 1.00(99.91%)d 0.00(0.09%)
0.0000 0.0019 0.0001 0.0001 0.0055
-0.0001 0.0023 0.0005 -0.9995 -0.0067
-0.0001 0.0165 0.0247 0.0003 0.0005

92. (0.07643) 3C*(1) C 7- C 8- C 9
(31.65%) 0.5626* C 7 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
0.0000 0.0002 0.0000 0.0000 0.0050
-0.0001 0.0067 0.0005 -0.9996 0.0131
0.0000 0.0079 -0.0213 -0.0002 -0.0005
(52.23%) -0.7227* C 8 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 -0.0009 -0.0002 0.0000 0.0021
0.0001 0.0119 0.0007 -0.9995 -0.0208
0.0002 -0.0186 -0.0012 0.0001 0.0000
(16.12%) 0.4015* C 9 s(0.00%)p 1.00(99.91%)d 0.00(0.09%)
0.0000 0.0019 0.0001 0.0001 0.0055
-0.0001 0.0023 0.0005 -0.9995 -0.0067
-0.0001 0.0165 0.0247 0.0003 0.0005

93. (0.00586) RY (1) C 1
s(0.27%)p99.99(92.32%)d27.36(7.41%)
0.0000 -0.0168 0.0492 -0.0030 -0.0017
-0.7355 -0.0026 0.6180 0.0002 -0.0183
-0.2595 0.0022 -0.0038 -0.0577 0.0586

94. (0.00365) RY (2) C 1
s(3.61%)p24.60(88.84%)d 2.09(7.55%)
0.0000 -0.0020 0.1886 0.0227 0.0017
0.5920 0.0012 0.7263 0.0027 0.1020
0.0148 -0.0266 -0.0153 0.2718 -0.0221

95. (0.00277) RY (3) C 1
s(0.08%)p99.99(90.79%)d99.99(9.13%)
0.0000 -0.0004 0.0291 -0.0012 0.0004
0.0743 0.0001 0.0655 -0.0191 -0.9475

96.	(0.00125)	RY	(4)	C	1	0.0094 0.2736 0.1237 0.0313 -0.0084 s(94.74%)p 0.04(3.35%)d 0.02(1.91%) 0.0000 -0.0033 0.9733 -0.0007 0.0099 -0.1014 -0.0075 -0.1518 0.0011 0.0067 0.1240 -0.0093 -0.0098 -0.0597 0.0029
97.	(0.00089)	RY	(5)	C	1	s(0.01%)p 1.00(0.41%)d99.99(99.58%) 0.0000 0.0001 0.0096 0.0011 -0.0002 0.0016 -0.0002 0.0027 -0.0122 0.0630 -0.0173 -0.2231 0.9724 -0.0081 -0.0100
98.	(0.00037)	RY	(6)	C	1	s(1.05%)p 6.70(7.04%)d87.41(91.91%) 0.0000 0.0015 0.0573 0.0850 0.0172 -0.1174 0.0175 -0.2367 0.0003 -0.0014 -0.4203 -0.0060 -0.0017 0.8610 -0.0330
99.	(0.00018)	RY	(7)	C	1	s(2.17%)p 3.92(8.51%)d41.17(89.32%) 0.0000 0.0114 0.0977 0.1096 -0.0296 0.2781 0.0086 -0.0814 0.0000 -0.0156 -0.8376 -0.0292 -0.0236 -0.4044 0.1632
100.	(0.00015)	RY	(8)	C	1	s(0.04%)p99.99(8.72%)d99.99(91.25%) 0.0000 0.0004 0.0120 0.0149 -0.0011 0.0038 0.0003 -0.0048 -0.0082 0.2950 -0.0324 0.9346 0.1944 -0.0114 0.0027
101.	(0.00009)	RY	(9)	C	1	s(92.82%)p 0.00(0.13%)d 0.08(7.04%)
102.	(0.00003)	RY	(10)	C	1	s(5.29%)p 0.01(0.05%)d17.88(94.65%)
103.	(0.00362)	RY	(1)	C	2	s(0.39%)p99.99(92.27%)d19.05(7.35%) 0.0000 -0.0275 0.0534 0.0159 -0.0115 -0.6075 0.0119 0.7438 0.0005 -0.0137 0.2670 -0.0017 0.0036 0.0438 0.0166
104.	(0.00230)	RY	(2)	C	2	s(1.53%)p63.35(96.89%)d 1.03(1.58%) 0.0000 0.0107 0.1231 0.0057 0.0136 -0.7576 0.0205 -0.6277 0.0001 0.0210 -0.0187 0.0074 0.0041 0.1238 0.0030
105.	(0.00096)	RY	(3)	C	2	s(0.01%)p99.99(95.54%)d99.99(4.44%) 0.0000 0.0000 0.0109 -0.0008 0.0004 -0.0051 0.0006 -0.0246 -0.0115 -0.9771 0.0027 -0.0719 0.1981 -0.0029 -0.0054
106.	(0.00062)	RY	(4)	C	2	s(0.06%)p 5.10(0.30%)d99.99(99.64%) 0.0000 -0.0001 0.0240 -0.0040 -0.0001 -0.0048 -0.0003 -0.0020 -0.0147 -0.0526 -0.0125 -0.8255 -0.5609 0.0116 0.0036
107.	(0.00034)	RY	(5)	C	2	s(94.98%)p 0.02(2.24%)d 0.03(2.79%) 0.0000 -0.0009 0.9681 -0.1122 -0.0067 0.1488 0.0041 0.0016 0.0007 0.0115 0.1540 0.0177 0.0096 -0.0171 -0.0589
108.	(0.00008)	RY	(6)	C	2	s(40.38%)p 0.03(1.28%)d 1.44(58.34%)
109.	(0.00007)	RY	(7)	C	2	s(59.67%)p 0.02(1.05%)d 0.66(39.28%)
110.	(0.00002)	RY	(8)	C	2	s(1.90%)p 3.26(6.19%)d48.48(91.92%)
111.	(0.00002)	RY	(9)	C	2	s(1.21%)p 0.19(0.23%)d81.40(98.56%)
112.	(0.00001)	RY	(10)	C	2	s(0.04%)p93.39(4.07%)d99.99(95.88%)
113.	(0.00440)	RY	(1)	C	3	s(0.12%)p99.99(93.43%)d55.59(6.45%) 0.0000 0.0292 0.0160 -0.0073 -0.0104 -0.2827 -0.0146 -0.9239 0.0004 0.0217 0.1717 -0.0035 -0.0028 -0.1864 -0.0160
114.	(0.00242)	RY	(2)	C	3	s(0.53%)p99.99(98.31%)d 2.21(1.16%) 0.0000 -0.0058 0.0722 -0.0032 -0.0279 0.9451 0.0130 -0.2982 0.0006 0.0074 0.0468 -0.0141 0.0063 0.0956 -0.0060
115.	(0.00096)	RY	(3)	C	3	s(0.01%)p 1.00(64.34%)d 0.55(35.65%) 0.0000 0.0000 0.0070 -0.0052 -0.0003 0.0070 -0.0005 -0.0220 -0.0251 -0.8014 0.0104 0.5955 -0.0423 0.0046 0.0010
116.	(0.00045)	RY	(4)	C	3	s(0.00%)p 1.00(29.31%)d 2.41(70.69%) 0.0000 -0.0001 0.0049 0.0040 0.0000 0.0101 0.0000 0.0088 0.0003 0.5412 0.0143 0.6947 -0.4731 0.0103 0.0145
117.	(0.00025)	RY	(5)	C	3	s(94.58%)p 0.01(0.83%)d 0.05(4.59%) 0.0000 -0.0021 0.9645 -0.1244 0.0060 -0.0901 0.0053 0.0072 0.0007 0.0043 -0.0176 -0.0059 0.0034 0.1815 -0.1124
118.	(0.00011)	RY	(6)	C	3	s(6.63%)p 0.13(0.84%)d13.95(92.53%) 0.0000 -0.0015 0.1605 0.2014 -0.0229 0.0876 0.0090 -0.0112 0.0001 0.0003 -0.6658 0.0154 -0.0050 -0.6904 0.0707
119.	(0.00006)	RY	(7)	C	3	s(80.18%)p 0.00(0.24%)d 0.24(19.58%)
120.	(0.00001)	RY	(8)	C	3	s(1.00%)p 5.53(5.54%)d93.28(93.46%)
121.	(0.00001)	RY	(9)	C	3	s(17.08%)p 0.05(0.81%)d 4.81(82.10%)
122.	(0.00000)	RY	(10)	C	3	s(0.03%)p99.99(6.39%)d99.99(93.58%)
123.	(0.00429)	RY	(1)	C	4	s(0.09%)p99.99(92.91%)d79.06(7.00%)

					0.0000	0.0289	-0.0068	-0.0026	-0.0140
					-0.9594	-0.0057	-0.0913	-0.0002	0.0072
					0.0851	-0.0011	0.0027	0.2504	-0.0091
124.	(0.00222)	RY	(2)	C 4	s(0.17%)p99.99(97.89%)d11.15(1.94%)				
					0.0000	-0.0144	0.0305	0.0246	0.0082
					-0.0997	-0.0206	0.9839	0.0003	-0.0182
					0.1245	0.0010	-0.0059	-0.0620	0.0021
125.	(0.00073)	RY	(3)	C 4	s(0.01%)p99.99(58.37%)d99.99(41.61%)				
					0.0000	0.0000	0.0097	-0.0046	-0.0002
					-0.0057	-0.0001	-0.0119	-0.0212	-0.7636
					0.0007	0.0419	0.6435	-0.0116	-0.0124
126.	(0.00052)	RY	(4)	C 4	s(0.01%)p99.99(37.32%)d99.99(62.66%)				
					0.0000	0.0000	0.0080	-0.0068	-0.0001
					-0.0024	0.0000	-0.0158	0.0010	-0.6107
					0.0010	0.2738	-0.7426	0.0119	0.0100
127.	(0.00022)	RY	(5)	C 4	s(95.55%)p 0.00(0.25%)d 0.04(4.20%)				
					0.0000	-0.0020	0.9772	-0.0261	0.0068
					-0.0403	-0.0088	-0.0244	0.0006	0.0128
					-0.1215	-0.0048	-0.0044	-0.1004	-0.1307
128.	(0.00009)	RY	(6)	C 4	s(29.73%)p 0.04(1.10%)d 2.33(69.17%)				
129.	(0.00006)	RY	(7)	C 4	s(66.04%)p 0.02(1.30%)d 0.49(32.66%)				
130.	(0.00001)	RY	(8)	C 4	s(4.05%)p 0.94(3.81%)d22.77(92.15%)				
131.	(0.00001)	RY	(9)	C 4	s(0.26%)p16.64(4.26%)d99.99(95.48%)				
132.	(0.00001)	RY	(10)	C 4	s(4.26%)p 0.67(2.84%)d21.82(92.91%)				
133.	(0.00422)	RY	(1)	C 5	s(0.25%)p99.99(92.61%)d29.05(7.14%)				
					0.0000	-0.0275	0.0401	-0.0095	0.0150
					0.9486	-0.0029	0.1612	0.0000	0.0082
					-0.0414	-0.0031	0.0011	-0.2639	0.0081
134.	(0.00224)	RY	(2)	C 5	s(0.47%)p99.99(97.51%)d 4.30(2.02%)				
					0.0000	-0.0159	0.0613	0.0261	0.0021
					0.1529	0.0238	-0.9751	0.0003	0.0187
					-0.1413	-0.0034	0.0009	-0.0135	-0.0029
135.	(0.00080)	RY	(3)	C 5	s(0.00%)p 1.00(73.97%)d 0.35(26.03%)				
					0.0000	-0.0001	0.0040	-0.0002	0.0002
					0.0118	0.0011	-0.0165	-0.0218	-0.8595
					0.0068	0.1970	-0.4705	0.0011	0.0001
136.	(0.00047)	RY	(4)	C 5	s(0.05%)p99.99(20.99%)d99.99(78.95%)				
					0.0000	0.0000	0.0229	-0.0017	0.0001
					-0.0056	-0.0003	0.0081	-0.0037	0.4581
					0.0056	-0.1078	-0.8819	-0.0011	-0.0135
137.	(0.00031)	RY	(5)	C 5	s(96.66%)p 0.01(0.98%)d 0.02(2.36%)				
					0.0000	0.0003	0.9818	-0.0519	0.0049
					-0.0840	0.0059	0.0510	-0.0001	-0.0101
					-0.0132	0.0008	0.0228	-0.1205	-0.0913
138.	(0.00009)	RY	(6)	C 5	s(30.03%)p 0.04(1.14%)d 2.29(68.83%)				
139.	(0.00006)	RY	(7)	C 5	s(65.52%)p 0.02(1.41%)d 0.50(33.07%)				
140.	(0.00001)	RY	(8)	C 5	s(4.55%)p 0.56(2.55%)d20.41(92.90%)				
141.	(0.00001)	RY	(9)	C 5	s(0.08%)p66.61(5.06%)d99.99(94.86%)				
142.	(0.00001)	RY	(10)	C 5	s(2.56%)p 1.49(3.82%)d36.62(93.62%)				
143.	(0.00424)	RY	(1)	C 6	s(0.13%)p99.99(93.14%)d50.50(6.73%)				
					0.0000	0.0322	0.0162	-0.0059	-0.0080
					-0.6182	0.0114	0.7409	0.0005	-0.0034
					-0.2410	-0.0031	-0.0035	-0.0948	-0.0134
144.	(0.00218)	RY	(2)	C 6	s(0.22%)p99.99(98.70%)d 4.99(1.08%)				
					0.0000	-0.0006	0.0397	0.0242	-0.0204
					0.7641	-0.0176	0.6342	-0.0002	0.0167
					-0.0452	0.0054	0.0028	0.0932	-0.0047
145.	(0.00067)	RY	(3)	C 6	s(0.00%)p 1.00(13.23%)d 6.56(86.77%)				
					0.0000	-0.0001	0.0064	0.0009	-0.0002
					-0.0015	0.0000	-0.0003	0.0207	0.3631
					0.0118	-0.8324	-0.4173	0.0111	-0.0201
146.	(0.00050)	RY	(4)	C 6	s(0.02%)p99.99(79.83%)d99.99(20.15%)				
					0.0000	0.0002	0.0117	0.0051	-0.0001
					0.0162	-0.0004	0.0077	-0.0136	-0.8932
					0.0064	-0.1847	-0.4090	-0.0063	-0.0064
147.	(0.00030)	RY	(5)	C 6	s(96.34%)p 0.00(0.19%)d 0.04(3.47%)				
					0.0000	-0.0027	0.9815	-0.0051	-0.0012
					-0.0418	-0.0038	-0.0099	-0.0004	0.0066
					0.1305	0.0109	0.0102	0.0466	-0.1236
148.	(0.00011)	RY	(6)	C 6	s(4.13%)p 0.23(0.97%)d22.96(94.90%)				
					0.0000	0.0017	0.0124	0.2029	-0.0177
					0.0740	-0.0166	0.0596	-0.0004	0.0066
					0.3420	-0.0148	0.0173	-0.9083	0.0804
149.	(0.00006)	RY	(7)	C 6	s(87.28%)p 0.00(0.25%)d 0.14(12.48%)				
150.	(0.00001)	RY	(8)	C 6	s(1.94%)p 3.47(6.73%)d47.13(91.34%)				
151.	(0.00001)	RY	(9)	C 6	s(10.10%)p 0.00(0.03%)d 8.89(89.86%)				
152.	(0.00000)	RY	(10)	C 6	s(0.01%)p 1.00(6.97%)d13.35(93.02%)				

153.	(0.00517)	RY	(1)	C	7	s(1.19%)p76.29(91.13%)d 6.43(7.68%) 0.0000 0.0306 0.1043 -0.0115 0.0113 0.3611 0.0138 0.8835 0.0006 0.0024 0.1864 0.0019 0.0030 -0.2046 -0.0140
154.	(0.00216)	RY	(2)	C	7	s(0.06%)p99.99(98.10%)d29.74(1.84%) 0.0000 0.0020 0.0101 0.0226 0.0232 -0.9102 -0.0105 0.3896 0.0002 -0.0086 0.0503 -0.0021 0.0000 0.1258 0.0065
155.	(0.00075)	RY	(3)	C	7	s(0.03%)p99.99(93.22%)d99.99(6.75%) 0.0000 0.0001 0.0174 -0.0008 0.0004 -0.0097 -0.0006 -0.0005 0.0070 0.9654 -0.0068 -0.0254 0.2585 -0.0020 0.0042
156.	(0.00058)	RY	(4)	C	7	s(0.09%)p15.95(1.47%)d99.99(98.43%) 0.0000 -0.0002 0.0302 -0.0038 0.0000 -0.0070 -0.0003 -0.0038 0.0165 0.1200 -0.0065 0.9243 -0.3603 -0.0145 0.0048
157.	(0.00040)	RY	(5)	C	7	s(93.02%)p 0.01(0.67%)d 0.07(6.31%) 0.0000 -0.0045 0.9632 -0.0500 0.0037 -0.0428 -0.0101 -0.0662 -0.0005 -0.0201 -0.2345 -0.0331 -0.0017 -0.0821 -0.0149
158.	(0.00008)	RY	(6)	C	7	s(58.70%)p 0.02(0.95%)d 0.69(40.35%)
159.	(0.00008)	RY	(7)	C	7	s(36.25%)p 0.05(1.89%)d 1.71(61.86%)
160.	(0.00002)	RY	(8)	C	7	s(4.29%)p 1.44(6.17%)d20.89(89.54%)
161.	(0.00001)	RY	(9)	C	7	s(6.52%)p 0.18(1.15%)d14.16(92.33%)
162.	(0.00001)	RY	(10)	C	7	s(0.01%)p 1.00(5.31%)d17.85(94.69%)
163.	(0.00502)	RY	(1)	C	8	s(0.21%)p99.99(94.59%)d24.45(5.20%) 0.0000 0.0325 0.0313 0.0095 -0.0330 -0.9603 0.0187 -0.1493 0.0000 -0.0063 0.0112 -0.0007 0.0032 -0.2276 0.0056
164.	(0.00207)	RY	(2)	C	8	s(0.20%)p99.99(97.78%)d10.11(2.02%) 0.0000 0.0385 -0.0187 -0.0130 -0.0216 -0.1417 -0.0278 0.9780 0.0004 -0.0042 -0.1340 -0.0057 -0.0010 -0.0469 0.0003
165.	(0.00181)	RY	(3)	C	8	s(0.00%)p 1.00(94.33%)d 0.06(5.67%) 0.0000 0.0005 0.0013 0.0001 -0.0003 -0.0065 -0.0003 0.0039 -0.0241 0.9709 -0.0042 0.2033 0.1239 -0.0009 0.0023
166.	(0.00056)	RY	(4)	C	8	s(93.68%)p 0.00(0.44%)d 0.06(5.89%) 0.0000 -0.0122 0.9677 0.0129 -0.0321 0.0560 0.0119 -0.0020 -0.0008 0.0062 -0.1734 0.0348 -0.1183 -0.1091 -0.0409
167.	(0.00049)	RY	(5)	C	8	s(1.47%)p 0.19(0.28%)d66.86(98.25%) 0.0000 -0.0017 0.1212 0.0036 -0.0041 0.0095 0.0015 -0.0009 0.0060 -0.0513 -0.0225 -0.3256 0.9359 -0.0074 0.0080
168.	(0.00019)	RY	(6)	C	8	s(0.01%)p 1.00(5.43%)d17.42(94.57%) 0.0000 -0.0007 -0.0046 0.0060 0.0005 0.0025 0.0014 -0.0027 -0.0126 -0.2326 -0.0552 0.9211 0.3069 -0.0038 0.0012
169.	(0.00015)	RY	(7)	C	8	s(4.19%)p 0.44(1.83%)d22.42(93.98%) 0.0000 0.0094 0.1648 -0.1211 -0.0121 0.0187 -0.0273 0.1302 -0.0008 -0.0096 0.9618 0.0507 0.0181 -0.0970 0.0490
170.	(0.00007)	RY	(8)	C	8	s(39.15%)p 0.07(2.75%)d 1.48(58.10%)
171.	(0.00004)	RY	(9)	C	8	s(60.77%)p 0.03(1.77%)d 0.62(37.47%)
172.	(0.00003)	RY	(10)	C	8	s(0.53%)p 1.49(0.79%)d99.99(98.68%)
173.	(0.00509)	RY	(1)	C	9	s(0.01%)p 1.00(94.23%)d 0.06(5.76%) 0.0000 -0.0019 0.0078 0.0054 0.0028 0.2522 -0.0103 -0.9373 -0.0005 -0.0013 -0.2348 -0.0018 -0.0018 -0.0497 -0.0021
174.	(0.00394)	RY	(2)	C	9	s(1.48%)p62.78(93.19%)d 3.59(5.33%) 0.0000 -0.0001 0.1204 -0.0188 0.0104 0.9276 0.0051 0.2667 -0.0001 -0.0087 -0.0163 -0.0051 -0.0051 -0.2289 -0.0241
175.	(0.00162)	RY	(3)	C	9	s(0.00%)p 1.00(12.26%)d 7.16(87.74%) 0.0000 0.0001 0.0056 0.0001 0.0001 -0.0105 -0.0001 -0.0015 -0.0250 -0.3491 0.0066 -0.3690 -0.8609 -0.0001 -0.0089
176.	(0.00059)	RY	(4)	C	9	s(0.00%)p 1.00(42.22%)d 1.37(57.78%) 0.0000 -0.0003 0.0036 0.0010 -0.0002 0.0031 0.0000 0.0008 -0.0154 0.6496 0.0008 -0.7575 0.0618 0.0074 -0.0129
177.	(0.00050)	RY	(5)	C	9	s(93.24%)p 0.01(0.53%)d 0.07(6.24%) 0.0000 -0.0041 0.9656 0.0039 -0.0030 -0.0679 -0.0053 -0.0239 0.0003 0.0055 0.0103 0.0133 0.0005 0.2160 -0.1244
178.	(0.00036)	RY	(6)	C	9	s(0.02%)p99.99(45.59%)d99.99(54.39%)

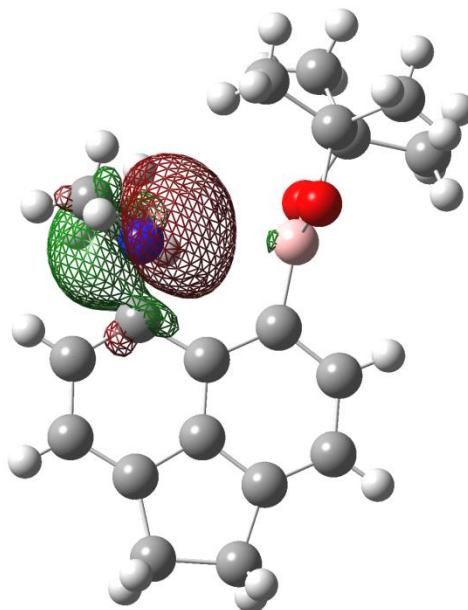
		0.0000	0.0002	0.0121	0.0045	0.0003
		-0.0104	0.0000	-0.0012	0.0081	-0.6751
		0.0004	-0.5380	0.5044	-0.0107	-0.0040
179.	(0.00018) RY (7) C 9	s(10.67%)p 0.62(6.61%)d 7.76(82.72%)				
		0.0000	0.0030	0.1831	0.2704	0.0169
		-0.2506	-0.0032	0.0529	-0.0002	0.0151
		-0.2851	0.0034	-0.0058	-0.8629	0.0356
180.	(0.00009) RY (8) C 9	s(0.84%)p 5.61(4.71%)d99.99(94.46%)				
181.	(0.00006) RY (9) C 9	s(91.18%)p 0.01(0.82%)d 0.09(8.00%)				
182.	(0.00002) RY (10) C 9	s(2.62%)p 0.01(0.03%)d37.16(97.35%)				
183.	(0.00519) RY (1) C 10	s(0.92%)p99.99(94.65%)d 4.80(4.43%)				
		0.0000	0.0245	0.0927	-0.0047	0.0036
		-0.9660	0.0015	-0.1155	-0.0002	-0.0050
		-0.0505	-0.0006	0.0024	-0.2040	-0.0100
184.	(0.00489) RY (2) C 10	s(0.02%)p99.99(94.17%)d99.99(5.81%)				
		0.0000	0.0008	0.0154	0.0031	-0.0045
		-0.1138	0.0163	0.9635	0.0002	0.0104
		-0.2338	-0.0001	-0.0019	0.0582	-0.0044
185.	(0.00070) RY (3) C 10	s(0.15%)p91.53(13.60%)d99.99(86.25%)				
		0.0000	-0.0001	0.0385	0.0024	-0.0007
		0.0073	-0.0003	0.0031	0.0014	-0.3687
		-0.0030	0.3911	-0.8421	-0.0206	0.0054
186.	(0.00056) RY (4) C 10	s(0.10%)p99.99(43.48%)d99.99(56.42%)				
		0.0000	-0.0003	0.0310	0.0044	-0.0003
		0.0007	-0.0002	-0.0096	-0.0014	0.6593
		-0.0045	-0.5293	-0.5330	-0.0031	-0.0016
187.	(0.00037) RY (5) C 10	s(97.56%)p 0.01(1.19%)d 0.01(1.25%)				
		0.0000	-0.0056	0.9869	0.0404	-0.0066
		0.1087	-0.0012	-0.0037	0.0000	-0.0025
		-0.0157	0.0051	0.0505	-0.0572	-0.0803
188.	(0.00025) RY (6) C 10	s(0.00%)p 1.00(42.92%)d 1.33(57.07%)				
		0.0000	0.0003	0.0060	-0.0023	-0.0002
		0.0021	0.0002	0.0060	-0.0008	-0.6551
		-0.0026	-0.7528	-0.0627	0.0077	0.0026
189.	(0.00014) RY (7) C 10	s(42.44%)p 0.05(2.12%)d 1.31(55.45%)				
		0.0000	-0.0021	-0.0724	0.6474	-0.0164
		0.1429	-0.0026	0.0215	0.0000	-0.0002
		-0.1567	-0.0091	0.0147	-0.7067	0.1736
190.	(0.00008) RY (8) C 10	s(18.60%)p 0.25(4.58%)d 4.13(76.82%)				
191.	(0.00006) RY (9) C 10	s(33.97%)p 0.10(3.31%)d 1.85(62.71%)				
192.	(0.00001) RY (10) C 10	s(6.34%)p 0.00(0.01%)d14.77(93.66%)				
193.	(0.00339) RY (1) C 11	s(0.26%)p99.99(94.88%)d18.49(4.85%)				
		0.0000	-0.0010	0.0505	-0.0088	-0.0022
		-0.1022	0.0058	0.9019	-0.0096	-0.3532
		0.0925	0.0350	-0.1725	0.0303	0.0899
194.	(0.00223) RY (2) C 11	s(1.10%)p81.00(89.50%)d 8.50(9.40%)				
		0.0000	-0.0012	0.1050	0.0056	-0.0213
		-0.7561	0.0035	-0.2956	-0.0005	-0.4852
		-0.0116	0.1785	0.0498	-0.1117	0.2168
195.	(0.00100) RY (3) C 11	s(44.37%)p 1.10(48.61%)d 0.16(7.01%)				
		0.0000	0.0135	0.6653	0.0302	-0.0024
		0.4376	0.0167	-0.2076	0.0186	-0.5009
		0.0314	-0.0446	-0.0847	0.2443	-0.0173
196.	(0.00028) RY (4) C 11	s(28.55%)p 0.19(5.35%)d 2.32(66.11%)				
		0.0000	-0.0061	0.4979	-0.1938	0.0007
		-0.0395	-0.0250	0.1384	-0.0022	0.1792
		-0.1293	0.1795	0.2094	-0.6757	-0.3342
197.	(0.00011) RY (5) C 11	s(20.26%)p 1.94(39.29%)d 2.00(40.45%)				
		0.0000	-0.0155	0.4280	-0.1385	0.0155
		-0.3773	0.0018	0.0156	-0.0184	0.4997
		0.2649	0.0307	-0.4175	0.3876	-0.0940
198.	(0.00005) RY (6) C 11	s(6.15%)p 1.34(8.21%)d13.93(85.65%)				
199.	(0.00004) RY (7) C 11	s(20.01%)p 0.24(4.74%)d 3.76(75.25%)				
200.	(0.00002) RY (8) C 11	s(4.53%)p 0.65(2.96%)d20.43(92.51%)				
201.	(0.00001) RY (9) C 11	s(3.26%)p 0.17(0.54%)d29.48(96.20%)				
202.	(0.00000) RY (10) C 11	s(71.54%)p 0.09(6.25%)d 0.31(22.21%)				
203.	(0.00347) RY (1) C 12	s(0.19%)p99.99(94.68%)d26.74(5.12%)				
		0.0000	0.0002	0.0429	-0.0088	-0.0010
		-0.0541	0.0069	0.9017	0.0093	0.3616
		0.0984	-0.0181	0.1737	0.0442	0.0954
204.	(0.00234) RY (2) C 12	s(1.03%)p87.23(89.48%)d 9.25(9.49%)				
		0.0000	-0.0004	0.1011	0.0061	-0.0214
		-0.7415	0.0047	-0.2711	0.0017	0.5207
		-0.0030	-0.1593	-0.0461	-0.1154	0.2325
205.	(0.00099) RY (3) C 12	s(43.71%)p 1.13(49.44%)d 0.16(6.85%)				
		0.0000	0.0132	0.6602	0.0317	-0.0036
		0.4564	0.0178	-0.2253	-0.0186	0.4844

206.	(0.00028)	RY	(4)	C 12	0.0205 0.0408 0.0807 0.2443 -0.0149 s(27.74%)p 0.16(4.55%)d 2.44(67.71%) 0.0000 -0.0050 0.4835 -0.2089 -0.0016 -0.0380 -0.0245 0.1467 0.0027 -0.1482 -0.1171 -0.1863 -0.1871 -0.6945 -0.3336
207.	(0.00011)	RY	(5)	C 12	s(22.01%)p 1.79(39.31%)d 1.76(38.68%) 0.0000 -0.0154 0.4480 -0.1383 0.0158 -0.3953 0.0005 0.0310 0.0177 -0.4851 0.2493 -0.0448 0.4091 0.3851 -0.0832
208.	(0.00005)	RY	(6)	C 12	s(11.44%)p 0.60(6.84%)d 7.14(81.71%)
209.	(0.00004)	RY	(7)	C 12	s(18.31%)p 0.32(5.81%)d 4.14(75.87%)
210.	(0.00002)	RY	(8)	C 12	s(4.66%)p 0.55(2.56%)d19.92(92.78%)
211.	(0.00001)	RY	(9)	C 12	s(3.60%)p 0.15(0.55%)d26.62(95.85%)
212.	(0.00000)	RY	(10)	C 12	s(67.35%)p 0.11(7.08%)d 0.38(25.57%)
213.	(0.00171)	RY	(1)	N 13	s(5.30%)p15.22(80.58%)d 2.67(14.12%) 0.0000 0.0116 0.2296 -0.0109 0.0042 0.2345 -0.0366 -0.8636 -0.0026 0.0599 -0.1392 0.0074 0.0219 0.3001 0.1769
214.	(0.00124)	RY	(2)	N 13	s(0.03%)p99.99(84.29%)d99.99(15.68%) 0.0000 0.0001 0.0180 -0.0029 0.0005 0.0130 -0.0030 -0.0549 0.0292 -0.9159 -0.0121 -0.0834 -0.3862 0.0150 0.0176
215.	(0.00063)	RY	(3)	N 13	s(0.00%)p 1.00(4.73%)d20.12(95.26%) 0.0000 -0.0019 0.0022 0.0037 0.0024 -0.1029 -0.0006 -0.0180 0.0118 -0.1905 0.0241 0.9426 0.2496 0.0154 0.0327
216.	(0.00062)	RY	(4)	N 13	s(0.30%)p99.99(59.20%)d99.99(40.50%) 0.0000 0.0127 0.0094 0.0526 -0.0071 0.7573 -0.0005 0.1357 0.0002 -0.0085 0.2247 0.0646 0.0120 -0.3739 0.4586
217.	(0.00053)	RY	(5)	N 13	s(0.53%)p58.98(31.47%)d99.99(68.00%) 0.0000 -0.0072 -0.0347 0.0639 0.0124 -0.5493 -0.0044 -0.1116 -0.0020 0.0173 0.4536 -0.0900 -0.0117 -0.0545 0.6805
218.	(0.00036)	RY	(6)	N 13	s(20.11%)p 0.34(6.80%)d 3.64(73.10%) 0.0000 -0.0044 0.4484 -0.0032 -0.0250 0.1541 -0.0081 0.2080 0.0015 0.0159 0.6304 0.0187 -0.0526 0.5413 -0.1936
219.	(0.00025)	RY	(7)	N 13	s(0.01%)p99.99(12.11%)d99.99(87.88%) 0.0000 0.0001 -0.0029 0.0117 0.0023 -0.0261 -0.0001 -0.0122 0.0159 0.3464 -0.0352 0.3024 -0.8853 -0.0469 0.0114
220.	(0.00011)	RY	(8)	N 13	s(73.27%)p 0.08(6.04%)d 0.28(20.69%) 0.0000 -0.0067 0.7980 0.3097 0.0181 -0.1454 -0.0064 0.1972 -0.0003 -0.0030 -0.3788 -0.0150 0.0241 -0.1908 0.1619
221.	(0.00010)	RY	(9)	N 13	s(4.30%)p 3.29(14.16%)d18.96(81.54%)
222.	(0.00003)	RY	(10)	N 13	s(96.15%)p 0.01(0.78%)d 0.03(3.07%)
223.	(0.01856)	RY	(1)	B 14	s(6.90%)p12.56(86.66%)d 0.93(6.44%) 0.0000 0.0015 0.2479 0.0869 0.0640 -0.8479 0.0235 -0.3398 0.0091 -0.1656 -0.0367 0.0270 0.0101 -0.0489 0.2447
224.	(0.01738)	RY	(2)	B 14	s(0.15%)p99.99(96.21%)d23.54(3.64%) 0.0000 0.0004 0.0365 0.0145 0.0107 -0.1446 0.0049 -0.0629 -0.0535 0.9666 -0.0059 -0.1694 -0.0764 -0.0082 0.0418
225.	(0.01061)	RY	(3)	B 14	s(0.49%)p99.99(86.12%)d27.30(13.39%) 0.0000 -0.0128 0.0516 0.0455 -0.0283 0.3754 0.0609 -0.8460 0.0002 -0.0045 -0.1188 -0.0011 -0.0039 0.3300 0.1042
226.	(0.00358)	RY	(4)	B 14	s(73.04%)p 0.01(0.78%)d 0.36(26.19%) 0.0000 -0.0001 0.8519 -0.0680 -0.0064 0.0857 -0.0072 0.0165 -0.0001 0.0065 0.1739 0.0051 0.0078 0.0361 -0.4798
227.	(0.00154)	RY	(5)	B 14	s(0.00%)p 1.00(1.88%)d52.07(98.11%) 0.0000 -0.0001 -0.0026 0.0032 -0.0004 -0.0035 0.0001 0.0028 0.0396 0.1314 -0.0114 0.9120 -0.3862 0.0084 -0.0039
228.	(0.00126)	RY	(6)	B 14	s(0.01%)p 1.00(2.15%)d45.60(97.85%) 0.0000 0.0003 0.0082 0.0021 0.0001 0.0013 0.0011 0.0090 -0.0460 -0.1388 0.0052 -0.3670 -0.9185 0.0089 -0.0035
229.	(0.00061)	RY	(7)	B 14	s(5.59%)p 2.52(14.09%)d14.36(80.32%) 0.0000 -0.0017 0.2054 0.1173 0.0015 0.0041 0.0488 0.3721 0.0012 0.0037 0.0659 -0.0010 0.0119 0.7760 0.4433
230.	(0.00033)	RY	(8)	B 14	s(34.98%)p 0.25(8.88%)d 1.61(56.15%)

				0.0000	-0.0038	0.2808	0.5205	0.0100
				0.2970	0.0033	0.0208	0.0010	0.0028
				0.2281	0.0073	-0.0044	-0.4838	0.5247
231.	(0.00030)	RY	(9)	B	14	s(69.84%)	p 0.02(1.27%)	d 0.41(28.89%)
						0.0000	0.0094	-0.1226
						0.8266	-0.0422	-0.0948
						-0.0122	0.0422	-0.0007
						-0.0011	-0.2706	-0.0078
						0.0060	0.1604	-0.4357
232.	(0.00020)	RY	(10)	B	14	s(8.91%)	p 0.37(3.28%)	d 9.85(87.81%)
						0.0000	0.0011	0.2687
						-0.1301	-0.0020	0.1047
						-0.0087	0.1474	0.0001
						0.0011	-0.9079	-0.0084
						-0.0004	-0.1474	0.1792
233.	(0.00047)	RY	(1)	F	15	s(74.66%)	p 0.25(18.73%)	d 0.09(6.61%)
						0.0000	-0.0011	0.8624
						-0.0527	-0.0019	0.3805
						-0.0064	0.2039	0.0005
						0.0305	0.0086	0.1336
						0.0904	-0.1074	-0.1687
234.	(0.00025)	RY	(2)	F	15	s(3.29%)	p28.91(95.03%)	d 0.51(1.68%)
						0.0000	0.0000	0.1354
						0.1206	-0.0010	-0.6724
						0.0005	0.6280	0.0009
						0.3222	-0.0057	0.0790
						-0.0983	-0.0188	-0.0230
235.	(0.00010)	RY	(3)	F	15	s(19.24%)	p 3.32(63.88%)	d 0.88(16.87%)
236.	(0.00005)	RY	(4)	F	15	s(1.22%)	p15.17(18.53%)	d65.68(80.25%)
237.	(0.00005)	RY	(5)	F	15	s(6.40%)	p 8.76(56.07%)	d 5.86(37.53%)
238.	(0.00002)	RY	(6)	F	15	s(59.37%)	p 0.26(15.16%)	d 0.43(25.47%)
239.	(0.00002)	RY	(7)	F	15	s(15.12%)	p 1.05(15.82%)	d 4.57(69.06%)
240.	(0.00001)	RY	(8)	F	15	s(12.92%)	p 0.93(12.05%)	d 5.81(75.04%)
241.	(0.00000)	RY	(9)	F	15	s(6.45%)	p 0.34(2.19%)	d14.16(91.36%)
242.	(0.00000)	RY	(10)	F	15	s(1.34%)	p 2.15(2.89%)	d71.41(95.77%)
243.	(0.00047)	RY	(1)	F	16	s(73.84%)	p 0.27(19.58%)	d 0.09(6.59%)
						0.0000	-0.0013	0.8575
						-0.0555	-0.0021	0.3883
						-0.0064	0.2083	-0.0003
						-0.0388	0.0152	-0.1359
						-0.0864	-0.1017	-0.1713
244.	(0.00024)	RY	(2)	F	16	s(3.52%)	p26.98(94.93%)	d 0.44(1.55%)
						0.0000	0.0000	0.1387
						0.1263	-0.0010	-0.6739
						0.0005	0.6300	-0.0009
						-0.3134	-0.0064	-0.0731
						0.0973	-0.0161	-0.0193
245.	(0.00009)	RY	(3)	F	16	s(19.71%)	p 3.22(63.52%)	d 0.85(16.77%)
246.	(0.00005)	RY	(4)	F	16	s(2.60%)	p 5.32(13.87%)	d32.07(83.53%)
247.	(0.00004)	RY	(5)	F	16	s(4.69%)	p13.40(62.81%)	d 6.94(32.51%)
248.	(0.00002)	RY	(6)	F	16	s(63.39%)	p 0.24(15.47%)	d 0.33(21.13%)
249.	(0.00002)	RY	(7)	F	16	s(11.55%)	p 1.38(15.98%)	d 6.27(72.47%)
250.	(0.00001)	RY	(8)	F	16	s(13.69%)	p 0.70(9.64%)	d 5.60(76.67%)
251.	(0.00000)	RY	(9)	F	16	s(0.46%)	p 3.56(1.63%)	d99.99(97.92%)
252.	(0.00000)	RY	(10)	F	16	s(6.57%)	p 0.44(2.92%)	d13.79(90.52%)
253.	(0.00096)	RY	(1)	H	17	s(99.66%)	p 0.00(0.34%)	-0.0023
						0.9983	0.0471	-0.0287
						-0.0177	s(0.04%)	p99.99(99.96%)
254.	(0.00017)	RY	(2)	H	17	-0.0002	0.0188	-0.0055
						0.0267	0.9995	s(0.05%)
255.	(0.00005)	RY	(3)	H	17	p99.99(99.95%)	s(0.31%)	p99.99(99.69%)
256.	(0.00001)	RY	(4)	H	17	s(99.84%)	p 0.00(0.16%)	0.0018
257.	(0.00089)	RY	(1)	H	18	0.9992	0.0130	0.0366
						0.0117	s(0.02%)	p99.99(99.98%)
258.	(0.00015)	RY	(2)	H	18	0.0000	0.0129	-0.0028
						-0.0311	-0.9994	s(0.00%)
259.	(0.00005)	RY	(3)	H	18	p 1.00(100.00%)	s(0.22%)	p99.99(99.78%)
260.	(0.00001)	RY	(4)	H	18	s(99.72%)	p 0.00(0.28%)	0.0023
261.	(0.00111)	RY	(1)	H	19	0.9986	0.0465	-0.0234
						0.0107	s(0.01%)	p99.99(99.99%)
262.	(0.00015)	RY	(2)	H	19	0.0001	0.0112	-0.0164
						-0.0128	-0.9997	s(0.12%)
263.	(0.00004)	RY	(3)	H	19	p99.99(99.88%)	s(0.22%)	p99.99(99.78%)
264.	(0.00001)	RY	(4)	H	19	s(99.70%)	p 0.00(0.30%)	-0.0024
265.	(0.00118)	RY	(1)	H	20	0.9985	-0.0451	-0.0307
						0.0059	s(0.00%)	p 1.00(100.00%)
266.	(0.00016)	RY	(2)	H	20	-0.0001	0.0070	0.0202
						0.0062	-0.9998	s(0.10%)
267.	(0.00004)	RY	(3)	H	20	p99.99(99.90%)	s(0.27%)	p99.99(99.73%)
268.	(0.00001)	RY	(4)	H	20	s(99.60%)	p 0.00(0.40%)	0.0023
269.	(0.00095)	RY	(1)	H	21	0.9980	0.0078	-0.0620
						-0.0105	s(0.01%)	p99.99(99.99%)
270.	(0.00015)	RY	(2)	H	21	0.0001	0.0110	-0.0205
						0.0050	0.9997	s(0.10%)
271.	(0.00005)	RY	(3)	H	21	p99.99(99.90%)	s(0.37%)	p99.99(99.63%)
272.	(0.00001)	RY	(4)	H	21	s(99.83%)	p 0.00(0.17%)	0.0024
273.	(0.00106)	RY	(1)	H	22	0.9992	0.0029	-0.0404
						-0.0032	s(0.00%)	p 1.00(100.00%)
274.	(0.00015)	RY	(2)	H	22	0.0000	0.0031	-0.0054
						-0.0042	1.0000	

275.	(0.00005)	RY	(3)	H	22	s(0.03%)p99.99(99.97%)
276.	(0.00001)	RY	(4)	H	22	s(0.20%)p99.99(99.80%)
277.	(0.00103)	RY	(1)	H	23	s(99.47%)p 0.01(0.53%)
						-0.0009 0.9973 -0.0099 0.0678 0.0247
278.	(0.00007)	RY	(2)	H	23	s(0.35%)p99.99(99.65%)
279.	(0.00004)	RY	(3)	H	23	s(0.18%)p99.99(99.82%)
280.	(0.00000)	RY	(4)	H	23	s(0.05%)p99.99(99.95%)
281.	(0.00120)	RY	(1)	H	24	s(99.86%)p 0.00(0.14%)
						-0.0003 0.9993 -0.0072 0.0314 -0.0187
282.	(0.00005)	RY	(2)	H	24	s(0.02%)p99.99(99.98%)
283.	(0.00004)	RY	(3)	H	24	s(0.02%)p99.99(99.98%)
284.	(0.00001)	RY	(4)	H	24	s(0.17%)p99.99(99.83%)
285.	(0.00165)	RY	(1)	H	25	s(99.59%)p 0.00(0.41%)
						-0.0015 0.9980 -0.0265 0.0580 -0.0007
286.	(0.00007)	RY	(2)	H	25	s(0.38%)p99.99(99.62%)
287.	(0.00004)	RY	(3)	H	25	s(0.01%)p99.99(99.99%)
288.	(0.00001)	RY	(4)	H	25	s(0.07%)p99.99(99.93%)
289.	(0.00117)	RY	(1)	H	26	s(99.17%)p 0.01(0.83%)
						-0.0010 0.9958 -0.0100 0.0858 -0.0289
290.	(0.00007)	RY	(2)	H	26	s(0.59%)p99.99(99.41%)
291.	(0.00004)	RY	(3)	H	26	s(0.24%)p99.99(99.76%)
292.	(0.00000)	RY	(4)	H	26	s(0.05%)p99.99(99.95%)
293.	(0.00121)	RY	(1)	H	27	s(99.90%)p 0.00(0.10%)
						-0.0004 0.9995 0.0136 0.0270 0.0115
294.	(0.00006)	RY	(2)	H	27	s(0.00%)p 1.00(100.00%)
295.	(0.00004)	RY	(3)	H	27	s(0.03%)p99.99(99.97%)
296.	(0.00001)	RY	(4)	H	27	s(0.13%)p99.99(99.87%)
297.	(0.00147)	RY	(1)	H	28	s(99.80%)p 0.00(0.20%)
						-0.0011 0.9990 -0.0225 0.0387 0.0036
298.	(0.00007)	RY	(2)	H	28	s(0.17%)p99.99(99.83%)
299.	(0.00004)	RY	(3)	H	28	s(0.01%)p99.99(99.99%)
300.	(0.00001)	RY	(4)	H	28	s(0.07%)p99.99(99.93%)

2



Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.9983	0.0065	0.0003	0.0003	0.0014	0.0106	0.0105	0.0060
2. C	0.9983	0.0000	0.0108	0.0105	0.0015	0.0004	0.0004	0.0065	1.0068
3. C	0.0065	0.0108	0.0000	1.2968	0.0135	0.0012	0.0306	0.0007	1.5186
4. C	0.0003	0.0105	1.2968	0.0000	1.5108	0.0336	0.0003	0.0299	0.0121
5. C	0.0003	0.0015	0.0135	1.5108	0.0000	0.0114	0.0323	0.0005	0.1017
6. C	0.0014	0.0004	0.0012	0.0336	0.0114	0.0000	1.5109	0.0119	0.0090
7. C	0.0106	0.0004	0.0306	0.0003	0.0323	1.5109	0.0000	1.3096	0.0012
8. C	0.0105	0.0065	0.0007	0.0299	0.0005	0.0119	1.3096	0.0000	0.0340
9. C	0.0060	1.0068	1.5186	0.0121	0.1017	0.0090	0.0012	0.0340	0.0000
10. C	0.0082	0.0083	0.0616	0.0104	1.2298	1.2496	0.0113	0.0628	0.0112
11. C	1.0059	0.0057	0.0351	0.0009	0.0086	0.1072	0.0123	1.5116	0.0148
12. C	0.0085	0.0088	0.0114	0.0555	0.0110	0.0117	0.0590	0.0116	1.2429
13. C	0.0000	0.0000	0.0004	0.0044	0.0082	0.0003	0.0003	0.0001	0.0015
14. C	0.0000	0.0000	0.0004	0.0107	0.0097	0.0003	0.0009	0.0001	0.0037
15. C	0.0000	0.0000	0.0000	0.0001	0.0002	0.0111	0.0008	0.0002	0.0000
16. C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0114	0.0011	0.0002	0.0000
17. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000
18. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000
19. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0003	0.0000	0.0000
20. C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0001	0.0000	0.0000
21. O	0.0000	0.0000	0.0001	0.0007	0.0004	0.0075	0.0069	0.0004	0.0002
22. O	0.0000	0.0000	0.0001	0.0007	0.0004	0.0076	0.0076	0.0006	0.0002
23. B	0.0005	0.0003	0.0002	0.0028	0.0018	0.8473	0.0195	0.0093	0.0004
24. N	0.0003	0.0004	0.0089	0.0295	0.9980	0.0038	0.0023	0.0004	0.0050
25. H	0.9147	0.0023	0.0010	0.0002	0.0001	0.0034	0.0001	0.0069	0.0023
26. H	0.9201	0.0025	0.0008	0.0002	0.0001	0.0030	0.0001	0.0063	0.0025
27. H	0.0024	0.9181	0.0064	0.0002	0.0029	0.0001	0.0003	0.0008	0.0034
28. H	0.0024	0.9150	0.0073	0.0002	0.0032	0.0002	0.0003	0.0010	0.0035
29. H	0.0001	0.0017	0.9304	0.0045	0.0058	0.0003	0.0001	0.0002	0.0062
30. H	0.0002	0.0003	0.0048	0.9290	0.0054	0.0001	0.0002	0.0000	0.0059
31. H	0.0003	0.0002	0.0000	0.0003	0.0001	0.0062	0.9294	0.0036	0.0003
32. H	0.0017	0.0001	0.0002	0.0001	0.0004	0.0064	0.0042	0.9262	0.0002
33. H	0.0000	0.0000	0.0001	0.0014	0.0069	0.0001	0.0001	0.0000	0.0005
34. H	0.0000	0.0000	0.0001	0.0011	0.0005	0.0001	0.0001	0.0000	0.0003

35.	H	0.0000	0.0000	0.0000	0.0004	0.0006	0.0000	0.0000	0.0000	0.0001
36.	H	0.0000	0.0000	0.0002	0.0011	0.0072	0.0001	0.0001	0.0000	0.0005
37.	H	0.0000	0.0000	0.0001	0.0012	0.0005	0.0001	0.0001	0.0000	0.0002
38.	H	0.0000	0.0000	0.0000	0.0005	0.0006	0.0002	0.0000	0.0000	0.0001
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1.	C	0.0082	1.0059	0.0085	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0083	0.0057	0.0088	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0616	0.0351	0.0114	0.0004	0.0004	0.0000	0.0000	0.0000
4.	C	0.0104	0.0009	0.0555	0.0044	0.0107	0.0001	0.0001	0.0000
5.	C	1.2298	0.0086	0.0110	0.0082	0.0097	0.0002	0.0001	0.0000
6.	C	1.2496	0.1072	0.0117	0.0003	0.0003	0.0111	0.0114	0.0002
7.	C	0.0113	0.0123	0.0590	0.0003	0.0009	0.0008	0.0011	0.0002
8.	C	0.0628	1.5116	0.0116	0.0001	0.0001	0.0002	0.0002	0.0000
9.	C	0.0112	0.0148	1.2429	0.0015	0.0037	0.0000	0.0000	0.0000
10.	C	0.0000	0.0115	1.2482	0.0089	0.0057	0.0006	0.0006	0.0002
11.	C	0.0115	0.0000	1.2491	0.0002	0.0002	0.0003	0.0005	0.0001
12.	C	1.2482	1.2491	0.0000	0.0003	0.0003	0.0002	0.0002	0.0000
13.	C	0.0089	0.0002	0.0003	0.0000	0.0092	0.0000	0.0001	0.0000
14.	C	0.0057	0.0002	0.0003	0.0092	0.0000	0.0001	0.0001	0.0002
15.	C	0.0006	0.0003	0.0002	0.0000	0.0001	0.0000	0.9564	0.9988
16.	C	0.0006	0.0005	0.0002	0.0001	0.0001	0.9564	0.0000	0.0069
17.	C	0.0002	0.0001	0.0000	0.0000	0.0002	0.9988	0.0069	0.0000
18.	C	0.0001	0.0000	0.0000	0.0000	0.0001	0.9975	0.0063	0.0071
19.	C	0.0001	0.0001	0.0000	0.0001	0.0000	0.0070	0.9985	0.0013
20.	C	0.0001	0.0000	0.0000	0.0007	0.0002	0.0063	0.9983	0.0030
21.	O	0.0044	0.0015	0.0002	0.0002	0.0017	0.8572	0.0182	0.0159
22.	O	0.0047	0.0016	0.0002	0.0002	0.0004	0.0177	0.8601	0.0060
23.	B	0.0130	0.0032	0.0074	0.0006	0.0012	0.0096	0.0090	0.0084
24.	N	0.0187	0.0004	0.0075	0.9677	0.9547	0.0004	0.0003	0.0002
25.	H	0.0001	0.0032	0.0066	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0001	0.0037	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0001	0.0025	0.0063	0.0000	0.0001	0.0000	0.0000	0.0000
28.	H	0.0001	0.0023	0.0063	0.0000	0.0001	0.0000	0.0000	0.0000
29.	H	0.0002	0.0002	0.0089	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0076	0.0002	0.0004	0.0006	0.0001	0.0000	0.0000	0.0000
31.	H	0.0082	0.0060	0.0004	0.0000	0.0000	0.0001	0.0001	0.0000
32.	H	0.0002	0.0055	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0003	0.0000	0.0001	0.9384	0.0005	0.0000	0.0001	0.0000
34.	H	0.0003	0.0000	0.0000	0.9384	0.0003	0.0000	0.0000	0.0000
35.	H	0.0003	0.0000	0.0000	0.9346	0.0085	0.0000	0.0000	0.0000
36.	H	0.0005	0.0000	0.0001	0.0005	0.9399	0.0000	0.0000	0.0001
37.	H	0.0002	0.0000	0.0001	0.0003	0.9379	0.0000	0.0000	0.0000
38.	H	0.0002	0.0000	0.0000	0.0079	0.9330	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0039	0.0081	0.9310
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0061	0.0006	0.9300
41.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0037	0.0007	0.9279
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0038	0.0085	0.0009
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0060	0.0004	0.0005
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034	0.0008	0.0084
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0083	0.0038	0.0001
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0063	0.0001
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0035	0.0001
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0085	0.0041	0.0004
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0058	0.0002
50.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0009	0.0036	0.0002

Atom	19	20	21	22	23	24	25	26	27
1.	C	0.0000	0.0000	0.0000	0.0000	0.0005	0.0003	0.9147	0.9201
2.	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0004	0.0023	0.0025
3.	C	0.0000	0.0000	0.0001	0.0001	0.0002	0.0089	0.0010	0.0008
4.	C	0.0000	0.0001	0.0007	0.0007	0.0028	0.0295	0.0002	0.0002
5.	C	0.0000	0.0000	0.0004	0.0004	0.0018	0.9980	0.0001	0.0001

6.	C	0.0002	0.0003	0.0075	0.0076	0.8473	0.0038	0.0034	0.0030	0.0001
7.	C	0.0003	0.0001	0.0069	0.0076	0.0195	0.0023	0.0001	0.0001	0.0003
8.	C	0.0000	0.0000	0.0004	0.0006	0.0093	0.0004	0.0069	0.0063	0.0008
9.	C	0.0000	0.0000	0.0002	0.0002	0.0004	0.0050	0.0023	0.0025	0.0034
10.	C	0.0001	0.0001	0.0044	0.0047	0.0130	0.0187	0.0001	0.0001	0.0001
11.	C	0.0001	0.0000	0.0015	0.0016	0.0032	0.0004	0.0032	0.0037	0.0025
12.	C	0.0000	0.0000	0.0002	0.0002	0.0074	0.0075	0.0066	0.0061	0.0063
13.	C	0.0001	0.0007	0.0002	0.0002	0.0006	0.9677	0.0000	0.0000	0.0000
14.	C	0.0000	0.0002	0.0017	0.0004	0.0012	0.9547	0.0000	0.0000	0.0001
15.	C	0.0070	0.0063	0.8572	0.0177	0.0096	0.0004	0.0000	0.0000	0.0000
16.	C	0.9985	0.9983	0.0182	0.8601	0.0090	0.0003	0.0000	0.0000	0.0000
17.	C	0.0013	0.0030	0.0159	0.0060	0.0084	0.0002	0.0000	0.0000	0.0000
18.	C	0.0031	0.0079	0.0194	0.0018	0.0065	0.0002	0.0000	0.0000	0.0000
19.	C	0.0000	0.0070	0.0060	0.0157	0.0082	0.0001	0.0000	0.0000	0.0000
20.	C	0.0070	0.0000	0.0016	0.0191	0.0061	0.0009	0.0000	0.0000	0.0000
21.	O	0.0060	0.0016	0.0000	0.0490	0.8890	0.0064	0.0001	0.0000	0.0000
22.	O	0.0157	0.0191	0.0490	0.0000	0.9012	0.0059	0.0001	0.0000	0.0000
23.	B	0.0082	0.0061	0.8890	0.9012	0.0000	0.0608	0.0001	0.0001	0.0000
24.	N	0.0001	0.0009	0.0064	0.0059	0.0000	0.0000	0.0000	0.0000	0.0001
25.	H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0022	0.0016
26.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0022	0.0000	0.0014
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0016	0.0014	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0020	0.0016	0.0020
29.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0006	0.0000	0.0000	0.0001
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0002	0.0002	0.0015	0.0003	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0001	0.0001	0.0002	0.0001	0.0001	0.0001	0.0000
33.	H	0.0000	0.0002	0.0001	0.0001	0.0002	0.0058	0.0000	0.0000	0.0000
34.	H	0.0000	0.0001	0.0003	0.0001	0.0019	0.0218	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0032	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0005	0.0000	0.0002	0.0056	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0005	0.0005	0.0021	0.0221	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0008	0.0002	0.0002	0.0031	0.0000	0.0000	0.0000
39.	H	0.0001	0.0003	0.0010	0.0008	0.0001	0.0000	0.0000	0.0000	0.0000
40.	H	0.0001	0.0001	0.0098	0.0007	0.0003	0.0000	0.0000	0.0000	0.0000
41.	H	0.0001	0.0004	0.0020	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
42.	H	0.0004	0.0003	0.0023	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
43.	H	0.0003	0.0000	0.0109	0.0002	0.0008	0.0001	0.0000	0.0000	0.0000
44.	H	0.0002	0.0004	0.0014	0.0007	0.0011	0.0000	0.0000	0.0000	0.0000
45.	H	0.9293	0.0016	0.0008	0.0010	0.0001	0.0000	0.0000	0.0000	0.0000
46.	H	0.9320	0.0003	0.0006	0.0095	0.0003	0.0000	0.0000	0.0000	0.0000
47.	H	0.9274	0.0085	0.0001	0.0019	0.0002	0.0000	0.0000	0.0000	0.0000
48.	H	0.0009	0.9264	0.0003	0.0025	0.0002	0.0000	0.0000	0.0000	0.0000
49.	H	0.0006	0.9298	0.0002	0.0110	0.0008	0.0001	0.0000	0.0000	0.0000
50.	H	0.0084	0.9285	0.0005	0.0013	0.0009	0.0007	0.0000	0.0000	0.0000

	Atom	28	29	30	31	32	33	34	35	36
1.	C	0.0024	0.0001	0.0002	0.0003	0.0017	0.0000	0.0000	0.0000	0.0000
2.	C	0.9150	0.0017	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
3.	C	0.0073	0.9304	0.0048	0.0000	0.0002	0.0001	0.0001	0.0000	0.0002
4.	C	0.0002	0.0045	0.9290	0.0003	0.0001	0.0014	0.0011	0.0004	0.0011
5.	C	0.0032	0.0058	0.0054	0.0001	0.0004	0.0069	0.0005	0.0006	0.0072
6.	C	0.0002	0.0003	0.0001	0.0062	0.0064	0.0001	0.0001	0.0000	0.0001
7.	C	0.0003	0.0001	0.0002	0.9294	0.0042	0.0001	0.0001	0.0000	0.0001
8.	C	0.0010	0.0002	0.0000	0.0036	0.9262	0.0000	0.0000	0.0000	0.0000
9.	C	0.0035	0.0062	0.0059	0.0003	0.0002	0.0005	0.0003	0.0001	0.0005
10.	C	0.0001	0.0002	0.0076	0.0082	0.0002	0.0003	0.0003	0.0003	0.0005
11.	C	0.0023	0.0002	0.0002	0.0060	0.0055	0.0000	0.0000	0.0000	0.0000
12.	C	0.0063	0.0089	0.0004	0.0004	0.0092	0.0001	0.0000	0.0000	0.0001
13.	C	0.0000	0.0000	0.0006	0.0000	0.0000	0.9384	0.9384	0.9346	0.0005
14.	C	0.0001	0.0000	0.0001	0.0000	0.0000	0.0005	0.0003	0.0085	0.9399
15.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000
21.	O	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0003	0.0000	0.0005
22.	O	0.0000	0.0000	0.0000	0.0002	0.0001	0.0001	0.0001	0.0001	0.0000
23.	B	0.0000	0.0001	0.0000	0.0015	0.0002	0.0002	0.0019	0.0001	0.0002
24.	N	0.0002	0.0006	0.0034	0.0003	0.0001	0.0058	0.0218	0.0032	0.0056
25.	H	0.0020	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
26.	H	0.0016	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27.	H	0.0020	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0001	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

30.	H	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001
31.	H	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013	0.0023	0.0003
34.	H	0.0000	0.0000	0.0005	0.0000	0.0000	0.0013	0.0000	0.0011	0.0003
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023	0.0011	0.0000	0.0002
36.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0003	0.0003	0.0002	0.0000
37.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0003	0.0015	0.0000	0.0011
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0026
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0001

	Atom	37	38	39	40	41	42	43	44	45
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0012	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0005	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	0.0001	0.0002	0.0000	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000
7.	C	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0003	0.0079	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.9379	0.9330	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0039	0.0061	0.0037	0.0038	0.0060	0.0034	0.0083
16.	C	0.0000	0.0000	0.0081	0.0006	0.0007	0.0085	0.0004	0.0008	0.0038
17.	C	0.0000	0.0000	0.9310	0.9300	0.9279	0.0009	0.0005	0.0084	0.0001
18.	C	0.0000	0.0000	0.0016	0.0003	0.0089	0.9271	0.9301	0.9299	0.0003
19.	C	0.0000	0.0000	0.0001	0.0001	0.0001	0.0004	0.0003	0.0002	0.9293
20.	C	0.0000	0.0000	0.0003	0.0001	0.0004	0.0003	0.0000	0.0004	0.0016
21.	O	0.0005	0.0008	0.0010	0.0098	0.0020	0.0023	0.0109	0.0014	0.0008
22.	O	0.0005	0.0002	0.0008	0.0007	0.0001	0.0003	0.0002	0.0007	0.0010
23.	B	0.0021	0.0002	0.0001	0.0003	0.0002	0.0002	0.0008	0.0011	0.0001
24.	N	0.0221	0.0031	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0011	0.0026	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0023	0.0021	0.0001	0.0000	0.0002	0.0001
40.	H	0.0000	0.0000	0.0023	0.0000	0.0021	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0021	0.0021	0.0000	0.0000	0.0002	0.0006	0.0000
42.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0021	0.0019	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0021	0.0000	0.0020	0.0000
44.	H	0.0000	0.0000	0.0002	0.0000	0.0006	0.0019	0.0020	0.0000	0.0000
45.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0025
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0020
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0001
49.	H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0002

Atom	46	47	48	49	50
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1.	C	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0001
6.	C	0.0003	0.0000	0.0000	0.0003	0.0001
7.	C	0.0001	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0000	0.0003
14.	C	0.0000	0.0000	0.0000	0.0000	0.0001
15.	C	0.0006	0.0006	0.0085	0.0004	0.0009
16.	C	0.0063	0.0035	0.0041	0.0058	0.0036
17.	C	0.0001	0.0001	0.0004	0.0002	0.0002
18.	C	0.0001	0.0003	0.0003	0.0000	0.0004
19.	C	0.9320	0.9274	0.0009	0.0006	0.0084
20.	C	0.0003	0.0085	0.9264	0.9298	0.9285
21.	O	0.0006	0.0001	0.0003	0.0002	0.0005
22.	O	0.0095	0.0019	0.0025	0.0110	0.0013
23.	B	0.0003	0.0002	0.0002	0.0008	0.0009
24.	N	0.0000	0.0000	0.0000	0.0001	0.0007
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0004
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0001
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0001	0.0000
40.	H	0.0001	0.0000	0.0000	0.0001	0.0000
41.	H	0.0000	0.0000	0.0000	0.0001	0.0003
42.	H	0.0000	0.0001	0.0003	0.0000	0.0000
43.	H	0.0001	0.0001	0.0000	0.0000	0.0000
44.	H	0.0000	0.0002	0.0000	0.0000	0.0000
45.	H	0.0025	0.0020	0.0001	0.0000	0.0002
46.	H	0.0000	0.0021	0.0000	0.0000	0.0000
47.	H	0.0021	0.0000	0.0000	0.0002	0.0006
48.	H	0.0000	0.0000	0.0000	0.0024	0.0023
49.	H	0.0000	0.0002	0.0024	0.0000	0.0021
50.	H	0.0000	0.0006	0.0023	0.0021	0.0000

(Occupancy)		Bond orbital / Coefficients / Hybrids				
		Lewis				
1.	(1.99926) CR (1) C 1	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
2.	(1.99927) CR (1) C 2	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
3.	(1.99908) CR (1) C 3	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
4.	(1.99908) CR (1) C 4	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
5.	(1.99896) CR (1) C 5	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
6.	(1.99883) CR (1) C 6	s(100.00%)				
		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000

7. (1.99918) CR (1) C 7	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
8. (1.99908) CR (1) C 8	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
9. (1.99902) CR (1) C 9	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
10. (1.99888) CR (1) C 10	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
11. (1.99901) CR (1) C 11	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
12. (1.99890) CR (1) C 12	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
13. (1.99941) CR (1) C 13	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
14. (1.99936) CR (1) C 14	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
15. (1.99898) CR (1) C 15	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
16. (1.99897) CR (1) C 16	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
17. (1.99934) CR (1) C 17	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
18. (1.99937) CR (1) C 18	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
19. (1.99933) CR (1) C 19	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
20. (1.99935) CR (1) C 20	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
21. (1.99974) CR (1) O 21	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
22. (1.99974) CR (1) O 22	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
23. (1.99916) CR (1) B 23	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
24. (1.99947) CR (1) N 24	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
25. (0.99734) LP (1) C 12	s(0.00%)p 1.00(100.00%)d 0.00(0.00%)	0.0000	0.0005	-0.0004	-0.0002	-0.0656
		-0.0034	0.0259	0.0009	-0.9974	-0.0104
		-0.0001	0.0035	0.0016	0.0006	-0.0003
26. (1.95449) LP (1) O 21	s(29.06%)p 2.44(70.84%)d 0.00(0.11%)					

					0.0000	0.5390	0.0005	-0.0032	-0.1128
					-0.0052	0.0604	-0.0008	-0.8318	0.0007
					0.0001	-0.0075	0.0062	0.0005	-0.0311
27.	(1.80783)	LP (2) O 21			s(0.06%)p99.99(99.79%)d 2.25(0.15%)				
					0.0000	0.0254	-0.0001	-0.0005	0.0781
					0.0009	0.9928	-0.0017	0.0780	-0.0007
					0.0031	0.0031	0.0369	0.0059	0.0060
28.	(1.95596)	LP (1) O 22			s(29.86%)p 2.35(70.03%)d 0.00(0.11%)				
					0.0000	0.5465	0.0006	-0.0032	-0.1858
					-0.0057	-0.1131	-0.0005	0.8081	-0.0018
					-0.0015	0.0122	0.0087	0.0000	-0.0289
29.	(1.80038)	LP (2) O 22			s(0.09%)p99.99(99.76%)d 1.61(0.15%)				
					0.0000	0.0302	0.0007	0.0004	0.1583
					-0.0002	-0.9787	0.0001	-0.1211	0.0001
					-0.0061	-0.0067	0.0358	0.0071	0.0078
30.	(1.86329)	LP (1) N 24			s(15.88%)p 5.29(84.06%)d 0.00(0.05%)				
					0.0000	0.3985	-0.0027	-0.0015	0.5845
					-0.0128	-0.6519	0.0212	0.2709	-0.0049
					0.0174	-0.0092	0.0081	0.0005	0.0087
31.	(1.98144)	BD (1) C 1- C 2			s(23.66%)p 3.23(76.31%)d 0.00(0.04%)				
	(49.90%)	0.7064* C 1			0.0000	0.4864	-0.0012	0.0005	-0.3392
					-0.0140	0.8028	-0.0178	0.0551	0.0010
					-0.0096	-0.0011	0.0024	-0.0130	-0.0092
	(50.10%)	0.7078* C 2			s(24.92%)p 3.01(75.04%)d 0.00(0.03%)				
					0.0000	0.4992	-0.0003	0.0011	0.2772
					-0.0217	-0.8185	0.0031	-0.0562	0.0008
					-0.0124	-0.0011	0.0023	-0.0098	-0.0095
32.	(1.97832)	BD (1) C 1- C 11			s(25.58%)p 2.91(74.37%)d 0.00(0.05%)				
	(49.51%)	0.7036* C 1			0.0000	0.5057	-0.0063	0.0005	0.8578
					-0.0144	0.0597	-0.0182	-0.0609	0.0012
					0.0029	-0.0018	-0.0004	0.0187	-0.0095
	(50.49%)	0.7106* C 11			s(30.89%)p 2.24(69.07%)d 0.00(0.04%)				
					0.0000	0.5558	-0.0026	-0.0023	-0.8096
					0.0112	-0.1816	-0.0237	0.0391	-0.0009
					0.0014	-0.0022	0.0000	0.0155	-0.0114
33.	(1.97724)	BD (1) C 1- H 25			s(24.71%)p 3.04(75.22%)d 0.00(0.07%)				
	(61.68%)	0.7854* C 1			0.0000	0.4971	0.0011	-0.0011	-0.3166
					-0.0091	-0.3866	-0.0108	-0.7087	0.0040
					0.0087	0.0122	0.0169	-0.0026	0.0133
	(38.32%)	0.6190* H 25			s(99.95%)p 0.00(0.05%)				
					0.9997	0.0010	0.0084	0.0108	0.0189
34.	(1.97777)	BD (1) C 1- H 26			s(25.89%)p 2.86(74.04%)d 0.00(0.07%)				
	(61.25%)	0.7826* C 1			0.0000	0.5088	0.0052	0.0005	-0.2192
					-0.0116	-0.4492	-0.0151	0.7001	0.0033
					0.0068	-0.0079	-0.0195	-0.0054	0.0135
	(38.75%)	0.6225* H 26			s(99.93%)p 0.00(0.07%)				
					0.9996	-0.0006	0.0068	0.0141	-0.0215
35.	(1.97819)	BD (1) C 2- C 9			s(24.84%)p 3.02(75.11%)d 0.00(0.05%)				
	(49.48%)	0.7034* C 2			0.0000	0.4984	-0.0044	0.0008	0.6780
					-0.0204	0.5373	0.0055	-0.0478	0.0014
					0.0185	-0.0014	-0.0011	0.0042	-0.0101
	(50.52%)	0.7108* C 9			s(31.22%)p 2.20(68.74%)d 0.00(0.04%)				
					0.0000	0.5587	-0.0022	-0.0022	-0.7197
					-0.0045	-0.4087	0.0286	0.0389	0.0015
					0.0153	-0.0013	-0.0008	0.0028	-0.0112
36.	(1.97842)	BD (1) C 2- H 27			s(25.35%)p 2.94(74.58%)d 0.00(0.07%)				
	(61.49%)	0.7841* C 2			0.0000	0.5035	0.0032	-0.0004	-0.5476
					-0.0155	0.1663	0.0005	-0.6466	0.0017
					-0.0080	0.0206	-0.0086	0.0091	0.0084
	(38.51%)	0.6206* H 27			s(99.94%)p 0.00(0.06%)				
					0.9997	0.0008	0.0161	-0.0056	0.0177
37.	(1.97653)	BD (1) C 2- H 28			s(24.75%)p 3.04(75.18%)d 0.00(0.07%)				
	(61.62%)	0.7850* C 2			0.0000	0.4975	0.0011	-0.0009	-0.4034
					-0.0153	0.1150	0.0008	0.7587	-0.0008
					-0.0049	-0.0178	0.0083	0.0056	0.0167
	(38.38%)	0.6195* H 28			s(99.94%)p 0.00(0.06%)				
					0.9997	0.0009	0.0117	-0.0044	-0.0208
38.	(1.97149)	BD (1) C 3- C 4			s(33.04%)p 2.02(66.91%)d 0.00(0.04%)				
	(49.74%)	0.7053* C 3			0.0000	0.5748	0.0016	0.0007	0.7517

					-0.0087	0.3194	0.0291	-0.0333	0.0011
					0.0106	-0.0018	-0.0003	0.0125	-0.0132
	(50.26%)	0.7089*	C	4	s(34.20%)	p 1.92(65.76%)	d 0.00(0.04%)		
					0.0000	0.5848	0.0027	0.0021	-0.7464
					-0.0161	-0.3117	0.0273	0.0482	0.0011
					0.0118	-0.0018	-0.0005	0.0112	-0.0133
39.	(1.97806)	BD (1) C	3- C 9						
	(49.15%)	0.7011*	C	3	s(34.89%)	p 1.86(65.06%)	d 0.00(0.06%)		
					0.0000	0.5906	0.0001	0.0043	-0.1134
					-0.0258	-0.7981	0.0022	-0.0089	0.0012
					0.0051	-0.0002	0.0008	-0.0178	-0.0148
	(50.85%)	0.7131*	C	9	s(37.18%)	p 1.69(62.78%)	d 0.00(0.04%)		
					0.0000	0.6097	0.0094	0.0012	0.0261
					-0.0260	0.7910	0.0154	0.0204	0.0021
					0.0053	-0.0001	0.0008	-0.0166	-0.0117
40.	(1.73755)	BD (2) C	3- C 9						
	(51.86%)	0.7202*	C	3	s(0.00%)	p 1.00(99.97%)	d 0.00(0.03%)		
					0.0000	0.0001	0.0000	0.0001	-0.0523
					0.0002	0.0187	0.0010	-0.9981	0.0207
					0.0015	-0.0029	0.0182	0.0003	0.0012
	(48.14%)	0.6938*	C	9	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
					0.0000	0.0018	-0.0001	-0.0001	-0.0675
					-0.0005	0.0265	0.0010	-0.9971	0.0084
					-0.0005	-0.0109	-0.0176	-0.0010	0.0005
41.	(1.98277)	BD (1) C	3- H 29						
	(60.26%)	0.7763*	C	3	s(31.88%)	p 2.14(68.06%)	d 0.00(0.06%)		
					0.0000	0.5646	-0.0005	-0.0040	-0.6470
					-0.0105	0.5096	0.0141	0.0435	0.0008
					-0.0202	-0.0016	0.0010	0.0063	-0.0139
	(39.74%)	0.6304*	H 29		s(99.92%)	p 0.00(0.08%)			
					0.9996	-0.0011	0.0222	-0.0161	-0.0012
42.	(1.97852)	BD (1) C	4- C 5						
	(49.73%)	0.7052*	C	4	s(34.52%)	p 1.90(65.42%)	d 0.00(0.06%)		
					0.0000	0.5875	-0.0033	0.0027	0.6546
					0.0138	-0.4720	0.0159	-0.0508	-0.0002
					-0.0173	-0.0023	0.0015	0.0071	-0.0152
	(50.27%)	0.7090*	C	5	s(37.03%)	p 1.70(62.92%)	d 0.00(0.05%)		
					0.0000	0.6085	0.0020	0.0001	-0.6313
					0.0009	0.4766	0.0180	0.0566	-0.0003
					-0.0168	-0.0016	0.0016	0.0070	-0.0108
43.	(1.75229)	BD (2) C	4- C 5						
	(50.63%)	0.7116*	C	4	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
					0.0000	0.0065	0.0006	-0.0001	0.0702
					0.0005	-0.0019	-0.0028	0.9971	-0.0214
					-0.0009	0.0135	-0.0129	0.0011	-0.0022
	(49.37%)	0.7026*	C	5	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
					0.0000	0.0025	0.0024	0.0007	0.0768
					0.0068	-0.0195	-0.0040	0.9964	-0.0188
					0.0010	-0.0191	0.0067	-0.0021	0.0023
44.	(1.98011)	BD (1) C	4- H 30						
	(60.25%)	0.7762*	C	4	s(31.09%)	p 2.21(68.85%)	d 0.00(0.07%)		
					0.0000	0.5575	0.0023	-0.0037	0.0931
					-0.0105	0.8242	0.0179	-0.0086	-0.0005
					0.0070	-0.0005	-0.0010	-0.0200	-0.0148
	(39.75%)	0.6305*	H 30		s(99.92%)	p 0.00(0.08%)			
					0.9996	-0.0011	-0.0039	-0.0287	0.0007
45.	(1.97153)	BD (1) C	5- C 10						
	(48.88%)	0.6991*	C	5	s(34.29%)	p 1.91(65.65%)	d 0.00(0.05%)		
					0.0000	0.5856	-0.0069	0.0012	-0.0471
					0.0117	-0.8086	0.0094	-0.0137	0.0029
					0.0022	-0.0010	0.0016	-0.0194	-0.0119
	(51.12%)	0.7150*	C 10		s(33.35%)	p 2.00(66.60%)	d 0.00(0.05%)		
					0.0000	0.5775	0.0019	-0.0003	0.1164
					0.0115	0.8076	-0.0051	0.0051	-0.0005
					0.0023	-0.0006	0.0001	-0.0173	-0.0121
46.	(1.98268)	BD (1) C	5- N 24						
	(40.01%)	0.6326*	C	5	s(28.57%)	p 2.50(71.33%)	d 0.00(0.10%)		
					0.0000	0.5344	0.0108	-0.0013	0.7694
					0.0228	0.3432	-0.0014	-0.0540	0.0060
					0.0180	-0.0043	-0.0009	0.0193	-0.0168
	(59.99%)	0.7745*	N 24		s(30.72%)	p 2.25(69.18%)	d 0.00(0.10%)		
					0.0000	0.5543	-0.0024	0.0000	-0.7656
					-0.0017	-0.3157	-0.0052	0.0767	0.0083
					0.0106	-0.0008	0.0046	0.0267	-0.0108
47.	(1.96933)	BD (1) C	6- C 7						
	(50.88%)	0.7133*	C	6	s(33.24%)	p 2.01(66.71%)	d 0.00(0.05%)		
					0.0000	0.5763	0.0139	-0.0001	-0.1930

					-0.0027	-0.7928	-0.0296	-0.0208	-0.0024
					0.0100	0.0006	0.0009	-0.0135	-0.0147
	(49.12%)	0.7008*	C 7	s(35.77%)p 1.79(64.18%)d 0.00(0.05%)	0.0000	0.5981	-0.0008	0.0029	0.1796
					0.0199	0.7797	-0.0032	0.0346	-0.0017
					0.0070	0.0001	0.0014	-0.0163	-0.0139
48.	(1.72389)	BD (2) C	6- C 7						
	(50.10%)	0.7078*	C 6	s(0.01%)p 1.00(99.95%)d 0.00(0.04%)	0.0000	0.0090	0.0002	-0.0001	0.0100
					0.0002	0.0304	-0.0004	-0.9992	-0.0095
					0.0003	0.0098	0.0169	0.0008	0.0010
	(49.90%)	0.7064*	C 7	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000	-0.0031	0.0007	-0.0001	-0.0152
					0.0015	0.0502	-0.0011	-0.9983	0.0191
					0.0001	-0.0006	-0.0172	-0.0003	-0.0010
49.	(1.96766)	BD (1) C	6- C 10						
	(49.19%)	0.7013*	C 6	s(33.26%)p 2.01(66.69%)d 0.00(0.05%)	0.0000	0.5767	0.0051	0.0018	-0.5916
					-0.0077	0.5626	0.0104	0.0164	-0.0011
					-0.0174	-0.0005	0.0007	0.0035	-0.0147
	(50.81%)	0.7128*	C 10	s(34.21%)p 1.92(65.75%)d 0.00(0.04%)	0.0000	0.5849	0.0009	-0.0002	0.6303
					0.0005	-0.5090	0.0106	-0.0321	0.0001
					-0.0156	-0.0011	0.0005	0.0009	-0.0115
50.	(1.96069)	BD (1) C	6- B 23						
	(68.74%)	0.8291*	C 6	s(33.38%)p 2.00(66.60%)d 0.00(0.03%)	0.0000	0.5776	-0.0132	-0.0009	0.7819
					-0.0398	0.2292	-0.0076	0.0200	-0.0003
					0.0055	0.0012	0.0003	0.0119	-0.0104
	(31.26%)	0.5591*	B 23	s(38.52%)p 1.59(61.40%)d 0.00(0.08%)	0.0000	0.6206	-0.0020	0.0092	-0.7739
					-0.0024	-0.1132	-0.0117	-0.0461	0.0020
					0.0099	0.0036	0.0014	0.0163	-0.0204
51.	(1.97481)	BD (1) C	7- C 8						
	(49.75%)	0.7053*	C 7	s(33.30%)p 2.00(66.65%)d 0.00(0.05%)	0.0000	0.5771	0.0022	0.0021	-0.7714
					0.0066	-0.2652	-0.0318	-0.0033	-0.0008
					0.0113	-0.0001	0.0003	0.0132	-0.0139
	(50.25%)	0.7089*	C 8	s(33.29%)p 2.00(66.66%)d 0.00(0.05%)	0.0000	0.5770	0.0022	0.0003	0.7690
					0.0161	0.2716	-0.0285	-0.0196	-0.0014
					0.0122	-0.0006	0.0003	0.0113	-0.0135
52.	(1.98168)	BD (1) C	7- H 31						
	(60.43%)	0.7774*	C 7	s(30.76%)p 2.25(69.17%)d 0.00(0.07%)	0.0000	0.5546	-0.0003	-0.0037	0.6096
					0.0052	-0.5643	-0.0129	-0.0394	-0.0015
					-0.0222	-0.0022	0.0021	0.0012	-0.0150
	(39.57%)	0.6290*	H 31	s(99.93%)p 0.00(0.07%)	0.9996	-0.0012	-0.0193	0.0182	0.0016
53.	(1.97836)	BD (1) C	8- C 11						
	(49.01%)	0.7001*	C 8	s(35.09%)p 1.85(64.85%)d 0.00(0.06%)	0.0000	0.5923	0.0030	0.0036	-0.6224
					-0.0231	0.5072	-0.0196	0.0540	-0.0004
					-0.0189	-0.0022	0.0022	0.0032	-0.0147
	(50.99%)	0.7140*	C 11	s(37.34%)p 1.68(62.62%)d 0.00(0.04%)	0.0000	0.6110	0.0096	0.0011	0.5452
					-0.0115	-0.5700	-0.0247	-0.0579	-0

				0.0015	-0.4535	0.0029	-0.0577	-0.0001
				-0.0162	-0.0027	0.0015	0.0075	-0.0150
	(51.12%)	0.7150*	C 12	s(32.68%)	p 2.06(67.27%)	d 0.00(0.05%)		
				0.0000	0.5716	0.0009	-0.0005	-0.6423
				0.0043	0.5071	-0.0018	0.0557	0.0000
				-0.0161	-0.0024	0.0018	0.0065	-0.0139
57.	(1.96441)	BD (1)	C 10- C 12					
	(49.64%)	0.7046*	C 10	s(32.38%)	p 2.09(67.57%)	d 0.00(0.05%)		
				0.0000	0.5690	0.0005	0.0013	-0.7664
				0.0054	-0.2965	0.0010	0.0216	-0.0009
				0.0106	-0.0014	-0.0002	0.0135	-0.0142
	(50.36%)	0.7096*	C 12	s(34.84%)	p 1.87(65.11%)	d 0.00(0.05%)		
				0.0000	0.5903	-0.0014	0.0015	0.7515
				-0.0067	0.2909	-0.0039	-0.0415	0.0001
				0.0118	-0.0019	-0.0004	0.0132	-0.0134
58.	(1.96798)	BD (1)	C 11- C 12					
	(48.95%)	0.6997*	C 11	s(31.65%)	p 2.16(68.30%)	d 0.00(0.06%)		
				0.0000	0.5625	-0.0058	0.0015	0.2081
				0.0070	0.7994	-0.0031	0.0238	-0.0010
				0.0090	-0.0003	0.0011	-0.0157	-0.0152
	(51.05%)	0.7145*	C 12	s(32.42%)	p 2.08(67.53%)	d 0.00(0.05%)		
				0.0000	0.5694	0.0018	-0.0005	-0.1342
				0.0003	-0.8106	0.0047	-0.0120	-0.0003
				0.0078	-0.0003	0.0006	-0.0158	-0.0141
59.	(1.98400)	BD (1)	C 13- N 24					
	(39.34%)	0.6272*	C 13	s(22.12%)	p 3.52(77.78%)	d 0.00(0.11%)		
				0.0000	0.4702	0.0093	0.0023	-0.1660
				0.0161	-0.6904	-0.0175	-0.5225	0.0016
				0.0081	0.0046	0.0265	-0.0162	0.0009
	(60.66%)	0.7788*	N 24	s(27.34%)	p 2.65(72.58%)	d 0.00(0.08%)		
				0.0000	0.5229	0.0050	0.0007	0.1538
				0.0226	0.6673	-0.0042	0.5058	0.0200
				0.0017	-0.0081	0.0186	-0.0186	-0.0062
60.	(1.98874)	BD (1)	C 13- H 33					
	(60.39%)	0.7771*	C 13	s(26.00%)	p 2.84(73.92%)	d 0.00(0.08%)		
				0.0000	0.5099	0.0039	0.0000	0.8428
				-0.0028	0.1666	0.0055	-0.0299	0.0117
				0.0088	-0.0033	-0.0025	0.0226	-0.0133
	(39.61%)	0.6293*	H 33	s(99.94%)	p 0.00(0.06%)			
				0.9997	-0.0009	-0.0245	-0.0048	-0.0005
61.	(1.99460)	BD (1)	C 13- H 34					
	(59.86%)	0.7737*	C 13	s(26.09%)	p 2.83(73.83%)	d 0.00(0.08%)		
				0.0000	0.5107	-0.0068	-0.0011	-0.4520
				0.0085	0.6722	0.0134	-0.2859	0.0140
				-0.0195	0.0066	-0.0144	-0.0091	-0.0100
	(40.14%)	0.6336*	H 34	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0048	0.0102	-0.0182	0.0058
62.	(1.99003)	BD (1)	C 13- H 35					
	(61.18%)	0.7822*	C 13	s(25.75%)	p 2.88(74.17%)	d 0.00(0.08%)		
				0.0000	0.5075	-0.0012	-0.0005	-0.2380
				0.0114	-0.2046	0.0103	0.8019	-0.0008
				0.0029	-0.0119	-0.0123	0.0018	0.0213
	(38.82%)	0.6230*	H 35	s(99.95%)	p 0.00(0.05%)			
				0.9997	0.0007	0.0054	0.0054	-0.0211
63.	(1.97526)	BD (1)	C 14- N 24					
	(39.03%)	0.6247*	C 14	s(22.06%)	p 3.53(77.83%)	d 0.00(0.11%)		
				0.0000	0.4697	0.0076	0.0021	-0.2310
				0.0122	-0.1655	-0.0103	0.8350	0.0106
				0.0037	-0.0126	-0.0103	0.0009	0.0283
	(60.97%)	0.7808*	N 24	s(25.98%)	p 2.85(73.94%)	d 0.00(0.08%)		
				0.0000	0.5097	0.0019	0.0012	0.2174
				0.0209	0.1680	-0.0049	-0.8143	-0.0188
				0.0068	0.0025	-0.0152	-0.0036	0.0220
64.	(1.98884)	BD (1)	C 14- H 36					
	(60.23%)	0.7761*	C 14	s(25.76%)	p 2.88(74.16%)	d 0.00(0.08%)		
				0.0000	0.5076	0.0032	0.0000	0.8362
				0.0007	0.2049	-0.0035	-0.0130	-0.0136
				0.0109	0.0007	0.0013	0.0209	-0.0155
	(39.77%)	0.6306*	H 36	s(99.94%)	p 0.00(0.06%)			
				0.9997	-0.0011	-0.0247	-0.0039	0.0018
65.	(1.99521)	BD (1)	C 14- H 37					
	(59.94%)	0.7742*	C 14	s(25.76%)	p 2.88(74.15%)	d 0.00(0.08%)		
				0.0000	0.5075	-0.0067	-0.0014	-0.4741
				0.0086	0.6595	-0.0037	-0.2854	-0.0174
				-0.0193	0.0105	-0.0132	-0.0082	-0.0102
	(40.06%)	0.6329*	H 37	s(99.96%)	p 0.00(0.04%)			
				0.9998	0.0051	0.0108	-0.0151	0.0086

66.	(1.98906)	BD (1) C 14- H 38	(61.25%)	0.7826*	C 14	s(26.37%)p 2.79(73.55%)d 0.00(0.08%)	0.0000	0.5135	0.0004	-0.0001	-0.1465
						0.0090	-0.7032	0.0094	-0.4682	-0.0083	
						0.0062	0.0047	0.0219	-0.0150	-0.0036	
						0.9997	0.0006	0.0020	0.0190	0.0130	
						(38.75%)	0.6225*	H 38	s(99.95%)p 0.00(0.05%)		
67.	(1.97801)	BD (1) C 15- C 16	(50.04%)	0.7074*	C 15	s(27.57%)p 2.62(72.36%)d 0.00(0.07%)	0.0000	0.5248	-0.0167	0.0004	-0.0124
						0.0203	0.1715	0.0010	0.8328	-0.0120	
						0.0002	-0.0037	0.0089	-0.0016	0.0237	
						0.0000	0.5230	-0.0166	0.0004	0.0823	
						(49.96%)	0.7068*	C 16	s(27.38%)p 2.65(72.55%)d 0.00(0.07%)	0.0193	-0.1706
68.	(1.98017)	BD (1) C 15- C 17	(50.28%)	0.7091*	C 15	s(27.63%)p 2.62(72.32%)d 0.00(0.05%)	0.0000	0.5255	0.0126	0.0006	0.5019
						-0.0107	0.5326	0.0007	-0.4329	-0.0103	
						0.0144	-0.0122	-0.0108	-0.0022	-0.0023	
						0.0000	0.5104	-0.0045	0.0016	-0.5177	
						(49.72%)	0.7051*	C 17	s(26.05%)p 2.84(73.91%)d 0.00(0.04%)	0.0034	-0.5215
69.	(1.98069)	BD (1) C 15- C 18	(50.16%)	0.7082*	C 15	s(27.24%)p 2.67(72.71%)d 0.00(0.05%)	0.0000	0.5219	0.0005	0.0009	0.1844
						0.0038	-0.8173	0.0002	-0.1580	-0.0150	
						-0.0070	-0.0033	0.0060	-0.0179	-0.0090	
						0.0000	0.5035	-0.0068	0.0010	-0.1942	
						(49.84%)	0.7060*	C 18	s(25.35%)p 2.94(74.61%)d 0.00(0.04%)	-0.0019	0.8218
70.	(1.97763)	BD (1) C 15- O 21	(31.67%)	0.5628*	C 15	s(17.47%)p 4.71(82.34%)d 0.01(0.19%)	0.0000	0.4178	0.0104	-0.0030	-0.8433
						-0.0075	0.1353	0.0090	-0.3034	-0.0427	
						-0.0106	0.0211	-0.0029	0.0332	-0.0152	
						0.0000	0.5110	0.0020	0.0014	0.8266	
						(68.33%)	0.8266*	O 21	s(26.12%)p 2.82(73.73%)d 0.01(0.16%)	0.0042	-0.0947
71.	(1.98012)	BD (1) C 16- C 19	(50.38%)	0.7098*	C 16	s(27.52%)p 2.63(72.44%)d 0.00(0.05%)	0.0000	0.5244	0.0124	0.0005	0.4879
						-0.0127	-0.5039	-0.0007	0.4818	0.0090	
						-0.0136	0.0129	-0.0113	-0.0019	-0.0002	
						0.0000	0.5129	-0.0041	0.0016	-0.5125	
						(49.62%)	0.7044*	C 19	s(26.31%)p 2.80(73.65%)d 0.00(0.04%)	0.0028	0.4702
72.	(1.98081)	BD (1) C 16- C 20	(50.13%)	0.7080*	C 16	s(27.65%)p 2.61(72.30%)d 0.00(0.05%)	0.0000	0.5258	0.0011	0.0009	0.1147
						0.0019	0.8243	0.0008	0.1734	0.0163	
						0.0046	0.0027	0.0065	-0.0189	-0.0086	
						0.0000	0.5130	-0.0065	0.0013	-0.1137	
						(49.87%)	0.7062*	C 20	s(26.32%)p 2.80(73.63%)d 0.00(0.04%)	-0.0049	-0.8282
73.	(1.97803)	BD (1) C 16- O 22	(31.94%)	0.5652*	C 16	s(17.35%)p 4.75(82.47%)d 0.01(0.18%)	0.0000	0.4164	0.0095	-0.0030	-0.8597
						-0.0085	-0.1918	-0.0104	0.2163	0.0434	
						0.0157	-0.0138	-0.0025	0.0327	-0.0182	
						0.0000	0.5044	0.0018	0.0012	0.8370	
						(68.06%)	0.8250*	O 22	s(25.44%)p 2.92(74.40%)d 0.01(0.16%)	0.0021	0.1663
74.	(1.98661)	BD (1) C 17- H 39	(61.24%)	0.7826*	C 17	s(25.34%)p 2.94(74.59%)d 0.00(0.07%)	0.0000	0.5033	0.0050	0.0005	0.0453

75.	(1.98141)	BD (1) C 17- H 40	(60.87%)	0.7802*	C 17	s(24.36%)p 3.10(75.56%)d 0.00(0.07%)	0.0000	0.4936	0.0005	-0.0007	0.7960
							0.0143	-0.0090	0.0106	0.3485	-0.0120
							-0.0025	0.0182	-0.0006	0.0193	-0.0062
		(39.13%)	0.6255*	H 40	s(99.95%)p 0.00(0.05%)		0.9998	-0.0006	-0.0211	-0.0007	-0.0074
76.	(1.98548)	BD (1) C 17- H 41	(61.44%)	0.7838*	C 17	s(24.12%)p 3.14(75.81%)d 0.00(0.07%)	0.0000	0.4911	-0.0001	-0.0011	-0.3088
							0.0101	0.8133	0.0036	0.0302	-0.0157
							-0.0158	0.0002	0.0022	-0.0165	-0.0133
		(38.56%)	0.6210*	H 41	s(99.96%)p 0.00(0.04%)		0.9998	0.0001	0.0075	-0.0195	0.0007
77.	(1.98540)	BD (1) C 18- H 42	(61.60%)	0.7848*	C 18	s(25.41%)p 2.93(74.52%)d 0.00(0.07%)	0.0000	0.5041	0.0037	0.0000	-0.1039
							0.0002	-0.1481	-0.0168	-0.8439	0.0017
							0.0005	0.0054	0.0052	0.0005	0.0258
		(38.40%)	0.6197*	H 42	s(99.95%)p 0.00(0.05%)		0.9998	0.0003	0.0035	0.0037	0.0216
78.	(1.98191)	BD (1) C 18- H 43	(60.83%)	0.7799*	C 18	s(24.18%)p 3.13(75.74%)d 0.00(0.08%)	0.0000	0.4917	0.0015	-0.0005	0.8279
							0.0072	-0.1538	-0.0196	0.2189	-0.0054
							-0.0048	0.0135	-0.0026	0.0219	-0.0102
		(39.17%)	0.6259*	H 43	s(99.95%)p 0.00(0.05%)		0.9997	-0.0003	-0.0215	0.0051	-0.0054
79.	(1.98569)	BD (1) C 18- H 44	(61.23%)	0.7825*	C 18	s(24.92%)p 3.01(75.00%)d 0.00(0.08%)	0.0000	0.4992	0.0019	-0.0003	-0.5148
							0.0035	-0.5275	-0.0175	0.4543	-0.0098
							0.0159	-0.0154	-0.0164	0.0008	-0.0004
		(38.77%)	0.6226*	H 44	s(99.96%)p 0.00(0.04%)		0.9998	0.0004	0.0120	0.0133	-0.0106
80.	(1.98616)	BD (1) C 19- H 45	(61.40%)	0.7836*	C 19	s(24.46%)p 3.08(75.46%)d 0.00(0.07%)	0.0000	0.4946	0.0033	-0.0001	-0.0560
							0.0074	0.2771	-0.0143	0.8212	0.0067
							-0.0001	-0.0023	0.0158	-0.0023	0.0217
		(38.60%)	0.6213*	H 45	s(99.95%)p 0.00(0.05%)		0.9997	0.0001	0.0015	-0.0058	-0.0217
81.	(1.98136)	BD (1) C 19- H 46	(60.66%)	0.7789*	C 19	s(24.44%)p 3.09(75.48%)d 0.00(0.08%)	0.0000	0.4944	0.0017	-0.0002	0.8234
							0.0173	0.0732	-0.0098	-0.2664	0.0120
							0.0064	-0.0144	-0.0015	0.0206	-0.0096
		(39.34%)	0.6272*	H 46	s(99.94%)p 0.00(0.06%)		0.9997	-0.0008	-0.0237	-0.0012	0.0053
82.	(1.98655)	BD (1) C 19- H 47	(61.62%)	0.7850*	C 19	s(24.66%)p 3.05(75.27%)d 0.00(0.07%)	0.0000	0.4966	0.0001	-0.0011	-0.2351
							0.0086	-0.8342	-0.0007	-0.0336	0.0165
							0.0109	-0.0005	0.0019	-0.0195	-0.0133
		(38.38%)	0.6195*	H 47	s(99.96%)p 0.00(0.04%)		0.9998	0.0001	0.0055	0.0199	-0.0011
83.	(1.98461)	BD (1) C 20- H 48	(61.55%)	0.7846*	C 20	s(24.68%)p 3.05(75.24%)d 0.00(0.07%)	0.0000	0.4968	0.0043	0.0001	-0.2240
							0.0000	0.1464	0.0164	0.8250	-0.0004
							-0.0015	-0.0106	0.0069	0.0016	0.0237
		(38.45%)	0.6200*	H 48	s(99.95%)p 0.00(0.05%)		0.9997	0.0001	0.0065	-0.0043	-0.0212
84.	(1.98193)	BD (1) C 20- H 49	(60.82%)	0.7799*	C 20	s(24.22%)p 3.12(75.70%)d 0.00(0.08%)	0.0000	0.4922	0.0015	-0.0007	0.8357
							0.0053	0.2155	0.0199	-0.1079	0.0068
							0.0100	-0.0059	-0.0016	0.0216	-0.0128
		(39.18%)	0.6259*	H 49	s(99.95%)p 0.00(0.05%)		0.9997	-0.0003	-0.0216	-0.0072	0.0017
85.	(1.98503)	BD (1) C 20- H 50	(61.23%)	0.7825*	C 20	s(24.64%)p 3.06(75.29%)d 0.00(0.07%)	0.0000	0.4964	0.0012	-0.0005	-0.4873
							0.0016	0.4955	0.0149	-0.5192	0.0110
							-0.0146	0.0157	-0.0165	0.0004	0.0016
		(38.77%)	0.6227*	H 50	s(99.96%)p 0.00(0.04%)		0.9998	0.0005	0.0122	-0.0120	0.0112

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86. (1.98771) BD ( 1) O 21- B 23
    ( 81.39%) 0.9022* O 21 s( 44.71%)p 1.23( 55.11%)d 0.00( 0.18%)
                        0.0000 0.6686 -0.0004 0.0026 -0.5437
                        -0.0066 -0.0139 0.0033 0.5052 -0.0059
                        0.0024 -0.0306 -0.0063 0.0093 0.0277
    ( 18.61%) 0.4314* B 23 s( 30.71%)p 2.24( 68.91%)d 0.01( 0.38%)
                        0.0000 0.5541 0.0025 -0.0093 0.4674
                        -0.0208 0.1092 0.0073 -0.6737 -0.0663
                        0.0027 -0.0550 -0.0071 0.0077 0.0259

87. (1.98725) BD ( 1) O 22- B 23
    ( 81.38%) 0.9021* O 22 s( 44.55%)p 1.24( 55.26%)d 0.00( 0.19%)
                        0.0000 0.6674 -0.0004 0.0028 -0.4875
                        -0.0068 0.0111 -0.0028 -0.5611 0.0061
                        -0.0013 0.0261 -0.0061 0.0063 0.0331
    ( 18.62%) 0.4315* B 23 s( 30.56%)p 2.26( 69.06%)d 0.01( 0.38%)
                        0.0000 0.5527 0.0036 -0.0072 0.4040
                        -0.0291 -0.0289 -0.0085 0.7221 0.0645
                        -0.0054 0.0508 -0.0043 0.0044 0.0346

----- non-Lewis -----
88. (0.99131) LV ( 1) C 10 s( 0.00%)p 1.00(100.00%)d 0.00( 0.00%)
                        0.0000 0.0035 0.0010 0.0002 0.0363
                        0.0050 -0.0141 0.0013 0.9992 0.0088
                        0.0003 -0.0029 -0.0003 -0.0010 0.0002

89. (0.38143) LV ( 1) B 23 s( 0.07%)p99.99( 99.83%)d 1.53( 0.10%)
                        0.0000 0.0256 -0.0034 -0.0029 -0.1283
                        0.0007 0.9861 -0.0346 0.0907 0.0084
                        0.0318 0.0008 0.0023 -0.0042 -0.0003

90. (0.00847) BD*( 1) C 1- C 2
    ( 50.10%) 0.7078* C 1 s( 23.66%)p 3.23( 76.31%)d 0.00( 0.04%)
                        0.0000 -0.4864 0.0012 -0.0005 0.3392
                        0.0140 -0.8028 0.0178 -0.0551 -0.0010
                        0.0096 0.0011 -0.0024 0.0130 0.0092
    ( 49.90%) -0.7064* C 2 s( 24.92%)p 3.01( 75.04%)d 0.00( 0.03%)
                        0.0000 -0.4992 0.0003 -0.0011 -0.2772
                        0.0217 0.8185 -0.0031 0.0562 -0.0008
                        0.0124 0.0011 -0.0023 0.0098 0.0095

91. (0.02300) BD*( 1) C 1- C 11
    ( 50.49%) 0.7106* C 1 s( 25.58%)p 2.91( 74.37%)d 0.00( 0.05%)
                        0.0000 -0.5057 0.0063 -0.0005 -0.8578
                        0.0144 -0.0597 0.0182 0.0609 -0.0012
                        -0.0029 0.0018 0.0004 -0.0187 0.0095
    ( 49.51%) -0.7036* C 11 s( 30.89%)p 2.24( 69.07%)d 0.00( 0.04%)
                        0.0000 -0.5558 0.0026 0.0023 0.8096
                        -0.0112 0.1816 0.0237 -0.0391 0.0009
                        -0.0014 0.0022 0.0000 -0.0155 0.0114

92. (0.01109) BD*( 1) C 1- H 25
    ( 38.32%) 0.6190* C 1 s( 24.71%)p 3.04( 75.22%)d 0.00( 0.07%)
                        0.0000 -0.4971 -0.0011 0.0011 0.3166
                        0.0091 0.3866 0.0108 0.7087 -0.0040
                        -0.0087 -0.0122 -0.0169 0.0026 -0.0133
    ( 61.68%) -0.7854* H 25 s( 99.95%)p 0.00( 0.05%)
                        -0.9997 -0.0010 -0.0084 -0.0108 -0.0189

93. (0.01008) BD*( 1) C 1- H 26
    ( 38.75%) 0.6225* C 1 s( 25.89%)p 2.86( 74.04%)d 0.00( 0.07%)
                        0.0000 -0.5088 -0.0052 -0.0005 0.2192
                        0.0116 0.4492 0.0151 -0.7001 -0.0033
                        -0.0068 0.0079 0.0195 0.0054 -0.0135
    ( 61.25%) -0.7826* H 26 s( 99.93%)p 0.00( 0.07%)
                        -0.9996 0.0006 -0.0068 -0.0141 0.0215

94. (0.02252) BD*( 1) C 2- C 9
    ( 50.52%) 0.7108* C 2 s( 24.84%)p 3.02( 75.11%)d 0.00( 0.05%)
                        0.0000 -0.4984 0.0044 -0.0008 -0.6780
                        0.0204 -0.5373 -0.0055 0.0478 -0.0014
                        -0.0185 0.0014 0.0011 -0.0042 0.0101
    ( 49.48%) -0.7034* C 9 s( 31.22%)p 2.20( 68.74%)d 0.00( 0.04%)
                        0.0000 -0.5587 0.0022 0.0022 0.7197
                        0.0045 0.4087 -0.0286 -0.0389 -0.0015
                        -0.0153 0.0013 0.0008 -0.0028 0.0112

95. (0.01058) BD*( 1) C 2- H 27
    ( 38.51%) 0.6206* C 2 s( 25.35%)p 2.94( 74.58%)d 0.00( 0.07%)
                        0.0000 -0.5035 -0.0032 0.0004 0.5476
                        0.0155 -0.1663 -0.0005 0.6466 -0.0017
                        0.0080 -0.0206 0.0086 -0.0091 -0.0084
    ( 61.49%) -0.7841* H 27 s( 99.94%)p 0.00( 0.06%)
                        -0.9997 -0.0008 -0.0161 0.0056 -0.0177

96. (0.01078) BD*( 1) C 2- H 28
    ( 38.38%) 0.6195* C 2 s( 24.75%)p 3.04( 75.18%)d 0.00( 0.07%)

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					0.0000	-0.4975	-0.0011	0.0009	0.4034
					0.0153	-0.1150	-0.0008	-0.7587	0.0008
					0.0049	0.0178	-0.0083	-0.0056	-0.0167
	(61.62%)	-0.7850*	H 28	s(99.94%)p 0.00(0.06%)	-0.9997	-0.0009	-0.0117	0.0044	0.0208
97.	(0.01646)	BD*(1) C	3- C 4						
	(50.26%)	0.7089*	C 3	s(33.04%)p 2.02(66.91%)d 0.00(0.04%)	0.0000	-0.5748	-0.0016	-0.0007	-0.7517
					0.0087	-0.3194	-0.0291	0.0333	-0.0011
					-0.0106	0.0018	0.0003	-0.0125	0.0132
	(49.74%)	-0.7053*	C 4	s(34.20%)p 1.92(65.76%)d 0.00(0.04%)	0.0000	-0.5848	-0.0027	-0.0021	0.7464
					0.0161	0.3117	-0.0273	-0.0482	-0.0011
					-0.0118	0.0018	0.0005	-0.0112	0.0133
98.	(0.02212)	BD*(1) C	3- C 9						
	(50.85%)	0.7131*	C 3	s(34.89%)p 1.86(65.06%)d 0.00(0.06%)	0.0000	-0.5906	-0.0001	-0.0043	0.1134
					0.0258	0.7981	-0.0022	0.0089	-0.0012
					-0.0051	0.0002	-0.0008	0.0178	0.0148
	(49.15%)	-0.7011*	C 9	s(37.18%)p 1.69(62.78%)d 0.00(0.04%)	0.0000	-0.6097	-0.0094	-0.0012	-0.0261
					0.0260	-0.7910	-0.0154	-0.0204	-0.0021
					-0.0053	0.0001	-0.0008	0.0166	0.0117
99.	(0.27382)	BD*(2) C	3- C 9						
	(48.14%)	0.6938*	C 3	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000	-0.0001	0.0000	-0.0001	0.0523
					-0.0002	-0.0187	-0.0010	0.9981	-0.0207
					-0.0015	0.0029	-0.0182	-0.0003	-0.0012
	(51.86%)	-0.7202*	C 9	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	-0.0018	0.0001	0.0001	0.0675
					0.0005	-0.0265	-0.0010	0.9971	-0.0084
					0.0005	0.0109	0.0176	0.0010	-0.0005
100.	(0.01243)	BD*(1) C	3- H 29						
	(39.74%)	0.6304*	C 3	s(31.88%)p 2.14(68.06%)d 0.00(0.06%)	0.0000	-0.5646	0.0005	0.0040	0.6470
					0.0105	-0.5096	-0.0141	-0.0435	-0.0008
					0.0202	0.0016	-0.0010	-0.0063	0.0139
	(60.26%)	-0.7763*	H 29	s(99.92%)p 0.00(0.08%)	-0.9996	0.0011	-0.0222	0.0161	0.0012
101.	(0.02855)	BD*(1) C	4- C 5						
	(50.27%)	0.7090*	C 4	s(34.52%)p 1.90(65.42%)d 0.00(0.06%)	0.0000	-0.5875	0.0033	-0.0027	-0.6546
					-0.0138	0.4720	-0.0159	0.0508	0.0002
					0.0173	0.0023	-0.0015	-0.0071	0.0152
	(49.73%)	-0.7052*	C 5	s(37.03%)p 1.70(62.92%)d 0.00(0.05%)	0.0000	-0.6085	-0.0020	-0.0001	0.6313
					-0.0009	-0.4766	-0.0180	-0.0566	0.0003
					0.0168	0.0016	-0.0016	-0.0070	0.0108
102.	(0.29041)	BD*(2) C	4- C 5						
	(49.37%)	0.7026*	C 4	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0065	0.0006	-0.0001	0.0702
					0.0005	-0.0019	-0.0028	0.9971	-0.0214
					-0.0009	0.0135	-0.0129	0.0011	-0.0022
	(50.63%)	-0.7116*	C 5	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0025	0.0024	0.0007	0.0768
					0.0068	-0.0195	-0.0040	0.9964	-0.0188
					0.0010	-0.0191	0.0067	-0.0021	0.0023
103.	(0.01136)	BD*(1) C	4- H 30						
	(39.75%)	0.6305*	C 4	s(31.09%)p 2.21(68.85%)d 0.00(0.07%)	0.0000	-0.5575	-0.0023	0.0037	-0.0931
					0.0105	-0.8242	-0.0179	0.0086	0.0005
					-0.0070	0.0005	0.0010	0.0200	0.0148
	(60.25%)	-0.7762*	H 30	s(99.92%)p 0.00(0.08%)	-0.9996	0.0011	0.0039	0.0287	-0.0007
104.	(0.03578)	BD*(1) C	5- C 10						
	(51.12%)	0.7150*	C 5	s(34.29%)p 1.91(65.65%)d 0.00(0.05%)	0.0000	0.5856	-0.0069	0.0012	-0.0471
					0.0117	-0.8086	0.0094	-0.0137	0.0029
					0.0022	-0.0010	0.0016	-0.0194	-0.0119
	(48.88%)	-0.6991*	C 10	s(33.35%)p 2.00(66.60%)d 0.00(0.05%)	0.0000	0.5775	0.0019	-0.0003	0.1164
					0.0115	0.8076	-0.0051	0.0051	-0.0005
					0.0023	-0.0006	0.0001	-0.0173	-0.0121
105.	(0.02936)	BD*(1) C	5- N 24						
	(59.99%)	0.7745*	C 5	s(28.57%)p 2.50(71.33%)d 0.00(0.10%)	0.0000	0.5344	0.0108	-0.0013	0.7694
					0.0228	0.3432	-0.0014	-0.0540	0.0060

									0.0180	-0.0043	-0.0009	0.0193	-0.0168
	(40.01%)	-0.6326*	N 24	s(30.72%)p 2.25(69.18%)d 0.00(0.10%)					0.0000	0.5543	-0.0024	0.0000	-0.7656
									-0.0017	-0.3157	-0.0052	0.0767	0.0083
									0.0106	-0.0008	0.0046	0.0267	-0.0108
106.	(0.01882)	BD*(1) C	6- C 7	s(33.24%)p 2.01(66.71%)d 0.00(0.05%)					0.0000	-0.5763	-0.0139	0.0001	0.1930
	(49.12%)	0.7008*	C 6						0.0027	0.7928	0.0296	0.0208	0.0024
									-0.0100	-0.0006	-0.0009	0.0135	0.0147
	(50.88%)	-0.7133*	C 7	s(35.77%)p 1.79(64.18%)d 0.00(0.05%)					0.0000	-0.5981	0.0008	-0.0029	-0.1796
									-0.0199	-0.7797	0.0032	-0.0346	0.0017
									-0.0070	-0.0001	-0.0014	0.0163	0.0139
107.	(0.26395)	BD*(2) C	6- C 7	s(0.01%)p 1.00(99.95%)d 0.00(0.04%)					0.0000	0.0090	0.0002	-0.0001	0.0100
	(49.90%)	0.7064*	C 6						0.0002	0.0304	-0.0004	-0.9992	-0.0095
									0.0003	0.0098	0.0169	0.0008	0.0010
	(50.10%)	-0.7078*	C 7	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)					0.0000	-0.0031	0.0007	-0.0001	-0.0152
									0.0015	0.0502	-0.0011	-0.9983	0.0191
									0.0001	-0.0006	-0.0172	-0.0003	-0.0010
108.	(0.02982)	BD*(1) C	6- C 10	s(33.26%)p 2.01(66.69%)d 0.00(0.05%)					0.0000	0.5767	0.0051	0.0018	-0.5916
	(50.81%)	0.7128*	C 6						-0.0077	0.5626	0.0104	0.0164	-0.0011
									-0.0174	-0.0005	0.0007	0.0035	-0.0147
	(49.19%)	-0.7013*	C 10	s(34.21%)p 1.92(65.75%)d 0.00(0.04%)					0.0000	0.5849	0.0009	-0.0002	0.6303
									0.0005	-0.5090	0.0106	-0.0321	0.0001
									-0.0156	-0.0011	0.0005	0.0009	-0.0115
109.	(0.03014)	BD*(1) C	6- B 23	s(33.38%)p 2.00(66.60%)d 0.00(0.03%)					0.0000	-0.5776	0.0132	0.0009	-0.7819
	(31.26%)	0.5591*	C 6						0.0398	-0.2292	0.0076	-0.0200	0.0003
									-0.0055	-0.0012	-0.0003	-0.0119	0.0104
	(68.74%)	-0.8291*	B 23	s(38.52%)p 1.59(61.40%)d 0.00(0.08%)					0.0000	-0.6206	0.0020	-0.0092	0.7739
									0.0024	0.1132	0.0117	0.0461	-0.0020
									-0.0099	-0.0036	-0.0014	-0.0163	0.0204
110.	(0.01917)	BD*(1) C	7- C 8	s(33.30%)p 2.00(66.65%)d 0.00(0.05%)					0.0000	0.5771	0.0022	0.0021	-0.7714
	(50.25%)	0.7089*	C 7						0.0066	-0.2652	-0.0318	-0.0033	-0.0008
									0.0113	-0.0001	0.0003	0.0132	-0.0139
	(49.75%)	-0.7053*	C 8	s(33.29%)p 2.00(66.66%)d 0.00(0.05%)					0.0000	0.5770	0.0022	0.0003	0.7690
									0.0161	0.2716	-0.0285	-0.0196	-0.0014
									0.0122	-0.0006	0.0003	0.0113	-0.0135
111.	(0.01090)	BD*(1) C	7- H 31	s(30.76%)p 2.25(69.17%)d 0.00(0.07%)					0.0000	-0.5546	0.0003	0.0037</	

				0.0000	-0.5608	0.0031	0.0032	0.1344
				-0.0025	0.8154	0.0107	0.0437	0.0015
				-0.0076	-0.0003	-0.0027	0.0196	0.0139
	(60.80%)	-0.7797*	H 32	s(99.93%)	p 0.00(0.07%)			
				-0.9997	-0.0012	-0.0046	-0.0259	-0.0016
115.	(0.02839)	BD*(1) C 9-	C 12					
	(51.12%)	0.7150*	C 9	s(31.46%)	p 2.18(68.49%)	d 0.00(0.06%)		
				0.0000	0.5608	-0.0060	0.0015	0.6898
				0.0015	-0.4535	0.0029	-0.0577	-0.0001
				-0.0162	-0.0027	0.0015	0.0075	-0.0150
	(48.88%)	-0.6991*	C 12	s(32.68%)	p 2.06(67.27%)	d 0.00(0.05%)		
				0.0000	0.5716	0.0009	-0.0005	-0.6423
				0.0043	0.5071	-0.0018	0.0557	0.0000
				-0.0161	-0.0024	0.0018	0.0065	-0.0139
116.	(0.03339)	BD*(1) C 10-	C 12					
	(50.36%)	0.7096*	C 10	s(32.38%)	p 2.09(67.57%)	d 0.00(0.05%)		
				0.0000	-0.5690	-0.0005	-0.0013	0.7664
				-0.0054	0.2965	-0.0010	-0.0216	0.0009
				-0.0106	0.0014	0.0002	-0.0135	0.0142
	(49.64%)	-0.7046*	C 12	s(34.84%)	p 1.87(65.11%)	d 0.00(0.05%)		
				0.0000	-0.5903	0.0014	-0.0015	-0.7515
				0.0067	-0.2909	0.0039	0.0415	-0.0001
				-0.0118	0.0019	0.0004	-0.0132	0.0134
117.	(0.02892)	BD*(1) C 11-	C 12					
	(51.05%)	0.7145*	C 11	s(31.65%)	p 2.16(68.30%)	d 0.00(0.06%)		
				0.0000	0.5625	-0.0058	0.0015	0.2081
				0.0070	0.7994	-0.0031	0.0238	-0.0010
				0.0090	-0.0003	0.0011	-0.0157	-0.0152
	(48.95%)	-0.6997*	C 12	s(32.42%)	p 2.08(67.53%)	d 0.00(0.05%)		
				0.0000	0.5694	0.0018	-0.0005	-0.1342
				0.0003	-0.8106	0.0047	-0.0120	-0.0003
				0.0078	-0.0003	0.0006	-0.0158	-0.0141
118.	(0.01352)	BD*(1) C 13-	N 24					
	(60.66%)	0.7788*	C 13	s(22.12%)	p 3.52(77.78%)	d 0.00(0.11%)		
				0.0000	0.4702	0.0093	0.0023	-0.1660
				0.0161	-0.6904	-0.0175	-0.5225	0.0016
				0.0081	0.0046	0.0265	-0.0162	0.0009
	(39.34%)	-0.6272*	N 24	s(27.34%)	p 2.65(72.58%)	d 0.00(0.08%)		
				0.0000	0.5229	0.0050	0.0007	0.1538
				0.0226	0.6673	-0.0042	0.5058	0.0200
				0.0017	-0.0081	0.0186	-0.0186	-0.0062
119.	(0.00889)	BD*(1) C 13-	H 33					
	(39.61%)	0.6293*	C 13	s(26.00%)	p 2.84(73.92%)	d 0.00(0.08%)		
				0.0000	-0.5099	-0.0039	0.0000	-0.8428
				0.0028	-0.1666	-0.0055	0.0299	-0.0117
				-0.0088	0.0033	0.0025	-0.0226	0.0133
	(60.39%)	-0.7771*	H 33	s(99.94%)	p 0.00(0.06%)			
				-0.9997	0.0009	0.0245	0.0048	0.0005
120.	(0.01937)	BD*(1) C 13-	H 34					
	(40.14%)	0.6336*	C 13	s(26.09%)	p 2.83(73.83%)	d 0.00(0.08%)		
				0.0000	-0.5107	0.0068	0.0011	0.4520
				-0.0085	-0.6722	-0.0134	0.2859	-0.0140
				0.0195	-0.0066	0.0144	0.0091	0.0100
	(59.86%)	-0.7737*	H 34	s(99.95%)	p 0.00(0.05%)			
				-0.9998	-0.0048	-0.0102	0.0182	-0.0058
121.	(0.00690)	BD*(1) C 13-	H 35					
	(38.82%)	0.6230*	C 13	s(25.75%)	p 2.88(74.17%)	d 0.00(0.08%)		
				0.0000	-0.5075	0.0012	0.0005	0.2380
				-0.0114	0.2046	-0.0103	-0.8019	0.0008
				-0.0029	0.0119	0.0123	-0.0018	-0.0213
	(61.18%)	-0.7822*	H 35	s(99.95%)	p 0.00(0.05%)			
				-0.9997	-0.0007	-0.0054	-0.0054	0.0211
122.	(0.01480)	BD*(1) C 14-	N 24					
	(60.97%)	0.7808*	C 14	s(22.06%)	p 3.53(77.83%)	d 0.00(0.11%)		
				0.0000	0.4697	0.0076	0.0021	-0.2310
				0.0122	-0.1655	-0.0103	0.8350	0.0106
				0.0037	-0.0126	-0.0103	0.0009	0.0283
	(39.03%)	-0.6247*	N 24	s(25.98%)	p 2.85(73.94%)	d 0.00(0.08%)		
				0.0000	0.5097	0.0019	0.0012	0.2174
				0.0209	0.1680	-0.0049	-0.8143	-0.0188
				0.0068	0.0025	-0.0152	-0.0036	0.0220
123.	(0.00882)	BD*(1) C 14-	H 36					
	(39.77%)	0.6306*	C 14	s(25.76%)	p 2.88(74.16%)	d 0.00(0.08%)		
				0.0000	-0.5076	-0.0032	0.0000	-0.8362
				-0.0007	-0.2049	0.0035	0.0130	0.0136
				-0.0109	-0.0007	-0.0013	-0.0209	0.0155
	(60.23%)	-0.7761*	H 36	s(99.94%)	p 0.00(0.06%)			

				-0.9997	0.0011	0.0247	0.0039	-0.0018
124.	(0.01974)	BD*(1) C 14- H 37	s(25.76%)p 2.88(74.15%)d 0.00(0.08%)					
	(40.06%)	0.6329* C 14	0.0000 -0.5075 0.0067 0.0014 0.4741					
			-0.0086 -0.6595 0.0037 0.2854 0.0174					
			0.0193 -0.0105 0.0132 0.0082 0.0102					
	(59.94%)	-0.7742* H 37	s(99.96%)p 0.00(0.04%)					
			-0.9998 -0.0051 -0.0108 0.0151 -0.0086					
125.	(0.00714)	BD*(1) C 14- H 38	s(26.37%)p 2.79(73.55%)d 0.00(0.08%)					
	(38.75%)	0.6225* C 14	0.0000 -0.5135 -0.0004 0.0001 0.1465					
			-0.0090 0.7032 -0.0094 0.4682 0.0083					
			-0.0062 -0.0047 -0.0219 0.0150 0.0036					
	(61.25%)	-0.7826* H 38	s(99.95%)p 0.00(0.05%)					
			-0.9997 -0.0006 -0.0020 -0.0190 -0.0130					
126.	(0.05459)	BD*(1) C 15- C 16	s(27.57%)p 2.62(72.36%)d 0.00(0.07%)					
	(49.96%)	0.7068* C 15	0.0000 0.5248 -0.0167 0.0004 -0.0124					
			0.0203 0.1715 0.0010 0.8328 -0.0120					
			0.0002 -0.0037 0.0089 -0.0016 0.0237					
	(50.04%)	-0.7074* C 16	s(27.38%)p 2.65(72.55%)d 0.00(0.07%)					
			0.0000 0.5230 -0.0166 0.0004 0.0823					
			0.0193 -0.1706 -0.0008 -0.8301 0.0139					
			-0.0012 -0.0013 0.0087 -0.0017 0.0242					
127.	(0.02705)	BD*(1) C 15- C 17	s(27.63%)p 2.62(72.32%)d 0.00(0.05%)					
	(49.72%)	0.7051* C 15	0.0000 0.5255 0.0126 0.0006 0.5019					
			-0.0107 0.5326 0.0007 -0.4329 -0.0103					
			0.0144 -0.0122 -0.0108 -0.0022 -0.0023					
	(50.28%)	-0.7091* C 17	s(26.05%)p 2.84(73.91%)d 0.00(0.04%)					
			0.0000 0.5104 -0.0045 0.0016 -0.5177					
			0.0034 -0.5215 0.0075 0.4459 -0.0175					
			0.0132 -0.0102 -0.0108 -0.0002 -0.0019					
128.	(0.02849)	BD*(1) C 15- C 18	s(27.24%)p 2.67(72.71%)d 0.00(0.05%)					
	(49.84%)	0.7060* C 15	0.0000 0.5219 0.0005 0.0009 0.1844					
			0.0038 -0.8173 0.0002 -0.1580 -0.0150					
			-0.0070 -0.0033 0.0060 -0.0179 -0.0090					
	(50.16%)	-0.7082* C 18	s(25.35%)p 2.94(74.61%)d 0.00(0.04%)					
			0.0000 0.5035 -0.0068 0.0010 -0.1942					
			-0.0019 0.8218 -0.0164 0.1805 -0.0126					
			-0.0070 -0.0014 0.0074 -0.0156 -0.0083					
129.	(0.04979)	BD*(1) C 15- O 21	s(17.47%)p 4.71(82.34%)d 0.01(0.19%)					
	(68.33%)	0.8266* C 15	0.0000 0.4178 0.0104 -0.0030 -0.8433					
			-0.0075 0.1353 0.0090 -0.3034 -0.0427					
			-0.0106 0.0211 -0.0029 0.0332 -0.0152					
	(31.67%)	-0.5628* O 21	s(26.12%)p 2.82(73.73%)d 0.01(0.16%)					
			0.0000 0.5110 0.0020 0.0014 0.8266					
			0.0042 -0.0947 0.0005 0.2118 -0.0127					
			-0.0079 0.0306 -0.0062 0.0233 0.0011					
130.	(0.02662)	BD*(1) C 16- C 19	s(27.52%)p 2.63(72.44%)d 0.00(0.05%)					
	(49.62%)	0.7044* C 16	0.0000 0.5244 0.0124 0.0005 0.4879					
			-0.0127 -0.5039 -0.0007 0.4818 0.0090					
			-0.0136 0.0129 -0.0113 -0.0019 -0.0002					
	(50.38%)	-0.7098* C 19	s(26.31%)p 2.80(73.65%)d 0.00(0.04%)					
			0.0000 0.5129 -0.0041 0.0016 -0.5125					
			0.0028 0.4702 -0.0067 -0.5025 0.0170					
			-0.0121 0.0105 -0.0118 -0.0002 0.0003					
131.	(0.02842)	BD*(1) C 16- C 20	s(27.65%)p 2.61(72.30%)d 0.00(0.05%)					
	(49.87%)	0.7062* C 16	0.0000 0.5258 0.0011 0.0009 0.1147					
			0.0019 0.8243 0.0008 0.1734 0.0163					
			0.0046 0.0027 0.0065 -0.0189 -0.0086					
	(50.13%)	-0.7080* C 20	s(26.32%)p 2.80(73.63%)d 0.00(0.04%)					
			0.0000 0.5130 -0.0065 0.0013 -0.1137					
			-0.0049 -0.8282 0.0153 -0.1928 0.0119					
			0.0045 0.0009 0.0075 -0.0162 -0.0083					
132.	(0.04952)	BD*(1) C 16- O 22	s(17.35%)p 4.75(82.47%)d 0.01(0.18%)					
	(68.06%)	0.8250* C 16	0.0000 0.4164 0.0095 -0.0030 -0.8597					
			-0.0085 -0.1918 -0.0104 0.2163 0.0434					
			0.0157 -0.0138 -0.0025 0.0327 -0.0182					
	(31.94%)	-0.5652* O 22	s(25.44%)p 2.92(74.40%)d 0.01(0.16%)					
			0.0000 0.5044 0.0018 0.0012 0.8370					
			0.0021 0.1663 -0.0005 -0.1250 0.0129					

				0.0134	-0.0272	-0.0080	0.0245	-0.0043
133.	(0.00704)	BD*(1) C 17- H 39						
	(38.76%)	0.6225* C 17	s(25.34%)p 2.94(74.59%)d 0.00(0.07%)					
			0.0000 -0.5033 -0.0050 -0.0005 -0.0453					
			-0.0076 0.2562 -0.0134 0.8233 0.0079					
			0.0012 0.0014 -0.0141 0.0019 -0.0227					
	(61.24%)	-0.7826* H 39	s(99.94%)p 0.00(0.06%)					
			-0.9997 0.0001 0.0008 -0.0055 -0.0231					
134.	(0.00640)	BD*(1) C 17- H 40						
	(39.13%)	0.6255* C 17	s(24.36%)p 3.10(75.56%)d 0.00(0.07%)					
			0.0000 -0.4936 -0.0005 0.0007 -0.7960					
			-0.0143 0.0090 -0.0106 -0.3485 0.0120					
			0.0025 -0.0182 0.0006 -0.0193 0.0062					
	(60.87%)	-0.7802* H 40	s(99.95%)p 0.00(0.05%)					
			-0.9998 0.0006 0.0211 0.0007 0.0074					
135.	(0.00737)	BD*(1) C 17- H 41						
	(38.56%)	0.6210* C 17	s(24.12%)p 3.14(75.81%)d 0.00(0.07%)					
			0.0000 -0.4911 0.0001 0.0011 0.3088					
			-0.0101 -0.8133 -0.0036 -0.0302 0.0157					
			0.0158 -0.0002 -0.0022 0.0165 0.0133					
	(61.44%)	-0.7838* H 41	s(99.96%)p 0.00(0.04%)					
			-0.9998 -0.0001 -0.0075 0.0195 -0.0007					
136.	(0.00662)	BD*(1) C 18- H 42						
	(38.40%)	0.6197* C 18	s(25.41%)p 2.93(74.52%)d 0.00(0.07%)					
			0.0000 -0.5041 -0.0037 0.0000 0.1039					
			-0.0002 0.1481 0.0168 0.8439 -0.0017					
			-0.0005 -0.0054 -0.0052 -0.0005 -0.0258					
	(61.60%)	-0.7848* H 42	s(99.95%)p 0.00(0.05%)					
			-0.9998 -0.0003 -0.0035 -0.0037 -0.0216					
137.	(0.00729)	BD*(1) C 18- H 43						
	(39.17%)	0.6259* C 18	s(24.18%)p 3.13(75.74%)d 0.00(0.08%)					
			0.0000 -0.4917 -0.0015 0.0005 -0.8279					
			-0.0072 0.1538 0.0196 -0.2189 0.0054					
			0.0048 -0.0135 0.0026 -0.0219 0.0102					
	(60.83%)	-0.7799* H 43	s(99.95%)p 0.00(0.05%)					
			-0.9997 0.0003 0.0215 -0.0051 0.0054					
138.	(0.00723)	BD*(1) C 18- H 44						
	(38.77%)	0.6226* C 18	s(24.92%)p 3.01(75.00%)d 0.00(0.08%)					
			0.0000 -0.4992 -0.0019 0.0003 0.5148					
			-0.0035 0.5275 0.0175 -0.4543 0.0098					
			-0.0159 0.0154 0.0164 -0.0008 0.0004					
	(61.23%)	-0.7825* H 44	s(99.96%)p 0.00(0.04%)					
			-0.9998 -0.0004 -0.0120 -0.0133 0.0106					
139.	(0.00700)	BD*(1) C 19- H 45						
	(38.60%)	0.6213* C 19	s(24.46%)p 3.08(75.46%)d 0.00(0.07%)					
			0.0000 -0.4946 -0.0033 0.0001 0.0560					
			-0.0074 -0.2771 0.0143 -0.8212 -0.0067					
			0.0001 0.0023 -0.0158 0.0023 -0.0217					
	(61.40%)	-0.7836* H 45	s(99.95%)p 0.00(0.05%)					
			-0.9997 -0.0001 -0.0015 0.0058 0.0217					
140.	(0.00623)	BD*(1) C 19- H 46						
	(39.34%)	0.6272* C 19	s(24.44%)p 3.09(75.48%)d 0.00(0.08%)					
			0.0000 -0.4944 -0.0017 0.0002 -0.8234					
			-0.0173 -0.0732 0.0098 0.2664 -0.0120					
			-0.0064 0.0144 0.0015 -0.0206 0.0096					
	(60.66%)	-0.7789* H 46	s(99.94%)p 0.00(0.06%)					
			-0.9997 0.0008 0.0237 0.0012 -0.0053					
141.	(0.00719)	BD*(1) C 19- H 47						
	(38.38%)	0.6195* C 19	s(24.66%)p 3.05(75.27%)d 0.00(0.07%)					
			0.0000 -0.4966 -0.0001 0.0011 0.2351					
			-0.0086 0.8342 0.0007 0.0336 -0.0165					
			-0.0109 0.0005 -0.0019 0.0195 0.0133					
	(61.62%)	-0.7850* H 47	s(99.96%)p 0.00(0.04%)					
			-0.9998 -0.0001 -0.0055 -0.0199 0.0011					
142.	(0.00708)	BD*(1) C 20- H 48						
	(38.45%)	0.6200* C 20	s(24.68%)p 3.05(75.24%)d 0.00(0.07%)					
			0.0000 -0.4968 -0.0043 -0.0001 0.2240					
			0.0000 -0.1464 -0.0164 -0.8250 0.0004					
			0.0015 0.0106 -0.0069 -0.0016 -0.0237					
	(61.55%)	-0.7846* H 48	s(99.95%)p 0.00(0.05%)					
			-0.9997 -0.0001 -0.0065 0.0043 0.0212					
143.	(0.00764)	BD*(1) C 20- H 49						
	(39.18%)	0.6259* C 20	s(24.22%)p 3.12(75.70%)d 0.00(0.08%)					
			0.0000 -0.4922 -0.0015 0.0007 -0.8357					
			-0.0053 -0.2155 -0.0199 0.1079 -0.0068					
			-0.0100 0.0059 0.0016 -0.0216 0.0128					
	(60.82%)	-0.7799* H 49	s(99.95%)p 0.00(0.05%)					

					-0.9997	0.0003	0.0216	0.0072	-0.0017
144.	(0.00810)	BD*(1) C 20- H 50							
	(38.77%)	0.6227* C 20	s(24.64%)p 3.06(75.29%)d 0.00(0.07%)						
			0.0000 -0.4964 -0.0012 0.0005 0.4873						
			-0.0016 -0.4955 -0.0149 0.5192 -0.0110						
			0.0146 -0.0157 0.0165 -0.0004 -0.0016						
	(61.23%)	-0.7825* H 50	s(99.96%)p 0.00(0.04%)						
			-0.9998 -0.0005 -0.0122 0.0120 -0.0112						
145.	(0.03461)	BD*(1) O 21- B 23							
	(18.61%)	0.4314* O 21	s(44.71%)p 1.23(55.11%)d 0.00(0.18%)						
			0.0000 -0.6686 0.0004 -0.0026 0.5437						
			0.0066 0.0139 -0.0033 -0.5052 0.0059						
			-0.0024 0.0306 0.0063 -0.0093 -0.0277						
	(81.39%)	-0.9022* B 23	s(30.71%)p 2.24(68.91%)d 0.01(0.38%)						
			0.0000 -0.5541 -0.0025 0.0093 -0.4674						
			0.0208 -0.1092 -0.0073 0.6737 0.0663						
			-0.0027 0.0550 0.0071 -0.0077 -0.0259						
146.	(0.03443)	BD*(1) O 22- B 23							
	(18.62%)	0.4315* O 22	s(44.55%)p 1.24(55.26%)d 0.00(0.19%)						
			0.0000 -0.6674 0.0004 -0.0028 0.4875						
			0.0068 -0.0111 0.0028 0.5611 -0.0061						
			0.0013 -0.0261 0.0061 -0.0063 -0.0331						
	(81.38%)	-0.9021* B 23	s(30.56%)p 2.26(69.06%)d 0.01(0.38%)						
			0.0000 -0.5527 -0.0036 0.0072 -0.4040						
			0.0291 0.0289 0.0085 -0.7221 -0.0645						
			0.0054 -0.0508 0.0043 -0.0044 -0.0346						
147.	(0.00202)	RY (1) C 1	s(0.02%)p99.99(90.54%)d99.99(9.44%)						
			0.0000 -0.0011 0.0140 0.0001 0.0028						
			0.1179 0.0026 0.0224 0.0095 0.9439						
			0.0462 0.0880 0.2901 0.0006 0.0189						
148.	(0.00192)	RY (2) C 1	s(0.82%)p99.99(83.95%)d18.52(15.23%)						
			0.0000 0.0327 0.0815 0.0227 0.0068						
			0.3033 0.0088 0.8619 0.0021 -0.0667						
			0.3458 0.0314 -0.0402 -0.1729 -0.0128						
149.	(0.00088)	RY (3) C 1	s(2.88%)p32.75(94.45%)d 0.92(2.66%)						
			0.0000 0.0115 0.1694 0.0040 0.0053						
			0.8959 0.0002 -0.3622 -0.0009 -0.1034						
			-0.0265 0.0131 -0.0061 -0.1589 -0.0217						
150.	(0.00036)	RY (4) C 1	s(0.59%)p 0.86(0.51%)d99.99(98.90%)						
			0.0000 0.0002 0.0770 0.0019 0.0001						
			-0.0250 -0.0004 0.0034 0.0122 -0.0658						
			-0.0733 0.9781 -0.0574 0.0887 -0.1251						
151.	(0.00016)	RY (5) C 1	s(87.10%)p 0.02(1.90%)d 0.13(11.00%)						
			0.0000 0.0013 0.9331 -0.0197 -0.0005						
			-0.1198 -0.0008 0.0660 -0.0038 0.0164						
			-0.1686 -0.1257 0.0205 0.1971 -0.1629						
152.	(0.00004)	RY (6) C 1	s(2.86%)p 1.95(5.57%)d32.06(91.58%)						
153.	(0.00003)	RY (7) C 1	s(53.75%)p 0.11(6.09%)d 0.75(40.16%)						
154.	(0.00002)	RY (8) C 1	s(0.70%)p12.76(8.92%)d99.99(90.38%)						
155.	(0.00002)	RY (9) C 1	s(48.26%)p 0.15(7.46%)d 0.92(44.27%)						
156.	(0.00000)	RY (10) C 1	s(3.17%)p 0.21(0.67%)d30.37(96.16%)						
157.	(0.00193)	RY (1) C 2	s(0.11%)p99.99(88.91%)d99.99(10.98%)						
			0.0000 0.0086 0.0312 0.0067 0.0037						
			0.2709 -0.0011 -0.1343 0.0109 0.8930						
			-0.0741 0.2499 -0.1719 0.0911 -0.0635						
158.	(0.00174)	RY (2) C 2	s(0.52%)p99.99(82.54%)d32.45(16.94%)						
			0.0000 0.0283 0.0635 0.0197 0.0112						
			0.7759 -0.0016 -0.3617 -0.0037 -0.3042						
			-0.2096 -0.1024 0.0543 0.3345 0.0091						
159.	(0.00090)	RY (3) C 2	s(2.28%)p41.89(95.31%)d 1.06(2.41%)						
			0.0000 0.0097 0.1500 0.0131 0.0008						
			0.3907 0.0021 0.8947 0.0003 0.0047						
			-0.1414 0.0147 0.0291 -0.0532 -0.0154						
160.	(0.00037)	RY (4) C 2	s(0.17%)p 2.65(0.44%)d99.99(99.40%)						
			0.0000 -0.0012 0.0401 0.0061 0.0015						
			-0.0214 -0.0004 -0.0197 0.0101 -0.0585						
			0.0488 0.6782 0.7209 0.0903 -0.0617						
161.	(0.00018)	RY (5) C 2	s(89.13%)p 0.02(1.73%)d 0.10(9.14%)						
			0.0000 0.0022 0.9439 0.0181 -0.0019						
			-0.0158 0.0005 -0.1293 0.0008 -0.0165						
			0.2092 -0.0377 -0.0262 -0.1711 -0.1276						
162.	(0.00004)	RY (6) C 2	s(3.41%)p 1.81(6.17%)d26.48(90.42%)						
163.	(0.00003)	RY (7) C 2	s(60.14%)p 0.08(4.82%)d 0.58(35.04%)						
164.	(0.00002)	RY (8) C 2	s(33.33%)p 0.26(8.58%)d 1.74(58.09%)						
165.	(0.00002)	RY (9) C 2	s(8.06%)p 1.32(10.65%)d10.08(81.29%)						
166.	(0.00000)	RY (10) C 2	s(2.99%)p 0.31(0.93%)d32.14(96.08%)						
167.	(0.00423)	RY (1) C 3	s(0.13%)p99.99(92.35%)d58.77(7.52%)						

				0.0000	0.0344	0.0089	-0.0042	0.0099
				0.7589	-0.0052	-0.5864	-0.0024	-0.0596
				-0.2658	-0.0155	0.0099	0.0644	-0.0100
168.	(0.00208)	RY	(2)	C	3	s(0.08%)p99.99(97.97%)d24.03(1.95%)		
						0.0000	-0.0052	0.0270
						-0.0076	-0.0095	
						0.5932	-0.0173	0.7904
						0.0002	-0.0516	
						-0.0669	0.0151	0.0240
						-0.1190	-0.0062	
169.	(0.00087)	RY	(3)	C	3	s(0.09%)p99.99(86.67%)d99.99(13.24%)		
						0.0000	0.0003	0.0287
						-0.0090	0.0006	
						0.0753	-0.0010	-0.0041
						0.0201	0.9277	
						0.0062	0.3466	0.1049
						0.0170	-0.0299	
170.	(0.00053)	RY	(4)	C	3	s(0.02%)p99.99(8.27%)d99.99(91.70%)		
						0.0000	0.0006	-0.0078
						0.0132	0.0001	
						-0.0232	0.0010	-0.0231
						0.0072	-0.2857	
						0.0599	0.5230	0.7983
						0.0469	-0.0213	
171.	(0.00025)	RY	(5)	C	3	s(97.29%)p 0.00(0.28%)d 0.02(2.43%)		
						0.0000	-0.0005	0.9864
						-0.0012	-0.0021	
						-0.0043	0.0041	-0.0422
						-0.0006	-0.0311	
						0.0937	0.0042	-0.0069
						-0.1162	-0.0441	
172.	(0.00007)	RY	(6)	C	3	s(90.91%)p 0.00(0.25%)d 0.10(8.84%)		
173.	(0.00007)	RY	(7)	C	3	s(2.35%)p 0.74(1.74%)d40.79(95.91%)		
174.	(0.00002)	RY	(8)	C	3	s(5.04%)p 1.47(7.41%)d17.38(87.55%)		
175.	(0.00001)	RY	(9)	C	3	s(4.26%)p 0.01(0.04%)d22.45(95.70%)		
176.	(0.00000)	RY	(10)	C	3	s(0.01%)p99.99(5.02%)d99.99(94.97%)		
177.	(0.00365)	RY	(1)	C	4	s(0.30%)p99.99(93.60%)d20.16(6.09%)		
						0.0000	-0.0332	0.0376
						0.0225	0.0071	
						0.0517	0.0080	0.9659
						0.0021	-0.0186	
						-0.0809	-0.0227	0.0036
						0.2313	0.0195	
178.	(0.00232)	RY	(2)	C	4	s(2.10%)p45.80(95.98%)d 0.92(1.92%)		
						0.0000	0.0090	0.1420
						0.0267	-0.0170	
						0.9755	0.0096	-0.0624
						-0.0011	-0.0626	
						0.1256	0.0075	-0.0051
						0.0582	-0.0023	
179.	(0.00097)	RY	(3)	C	4	s(4.72%)p15.91(75.05%)d 4.29(20.24%)		
						0.0000	-0.0002	0.2166
						-0.0156	0.0017	
						-0.1030	-0.0010	-0.0266
						-0.0229	-0.8594	
						0.0527	0.4152	0.1242
						0.0933	-0.0556	
180.	(0.00062)	RY	(4)	C	4	s(2.62%)p 5.34(13.96%)d31.89(83.42%)		
						0.0000	0.0002	0.1610
						-0.0154	0.0029	
						-0.0501	-0.0011	-0.0230
						0.0058	-0.3695	
						0.0828	-0.8961	0.1269
						-0.0155	0.0897	
181.	(0.00043)	RY	(5)	C	4	s(86.89%)p 0.11(9.71%)d 0.04(3.40%)		
						0.0000	-0.0025	0.9314
						0.0373	0.0089	
						-0.1382	-0.0028	-0.0344
						0.0025	0.2769	
						0.0878	0.0451	-0.1092
						0.0841	-0.0726	
182.	(0.00007)	RY	(6)	C	4	s(13.84%)p 0.12(1.62%)d 6.11(84.54%)		
183.	(0.00006)	RY	(7)	C	4	s(84.45%)p 0.00(0.41%)d 0.18(15.14%)		
184.	(0.00003)	RY	(8)	C	4	s(1.59%)p 2.58(4.09%)d59.44(94.32%)		
185.	(0.00002)	RY	(9)	C	4	s(2.98%)p 0.12(0.36%)d32.49(96.67%)		
186.	(0.00001)	RY	(10)	C	4	s(0.71%)p 7.38(5.24%)d99.99(94.05%)		
187.	(0.00482)	RY	(1)	C	5	s(2.12%)p45.05(95.41%)d 1.17(2.47%)		
						0.0000	-0.0068	0.1447
						-0.0142	0.0169	
						-0.3745	0.0011	0.8993
						0.0065	0.0688	
						0.0696	0.0576	0.0245
						-0.1261	0.0054	
188.	(0.00461)	RY	(2)	C	5	s(0.09%)p99.99(90.48%)d99.99(9.43%)		
						0.0000	0.0206	0.0188
						0.0086	0.0046	
						-0.8870	-0.0083	-0.3422
						0.0057	0.0295	
						0.0947	0.0218	-0.0140
						0.2870	-0.0478	
189.	(0.00306)	RY	(3)	C	5	s(1.77%)p48.58(85.95%)d 6.94(12.28%)		
						0.0000	0.0058	0.1327
						0.0073	0.0032	
						-0.0695	-0.0005	0.0353
						-0.0235	-0.9235	
						0.0052	-0.3273	-0.0674
						-0.0512	0.0922	
190.	(0.00122)	RY	(4)	C	5	s(41.78%)p 0.16(6.85%)d 1.23(51.38%)		
						0.0000	0.0007	0.6418
						0.0762	-0.0189	
						0.0292	0.0051	-0.1862
						-0.0017	0.1805	
						0.5776	-0.1753	-0.1036
						-0.3707	0.0348	
191.	(0.00072)	RY	(5)	C	5	s(39.10%)p 0.05(2.01%)d 1.51(58.89%)		
						0.0000	-0.0052	0.6211
						-0.0720	-0.0026	
						0.1243	-0.0188	0.0283
						0.0078	-0.0589	
						-0.3294	0.3772	-0.3793
						0.4350	-0.0709	
192.	(0.00062)	RY	(6)	C	5	s(12.58%)p 0.03(0.41%)d 6.92(87.01%)		
						0.0000	-0.0041	0.3534
						-0.0307	-0.0033	
						0.0622	-0.0095	-0.0071
						-0.0083	-0.0006	
						-0.1026	-0.0873	0.8886
						0.2487	0.0194	
193.	(0.00016)	RY	(7)	C	5	s(0.54%)p19.73(10.70%)d99.99(88.75%)		
						0.0000	-0.0043	0.0488
						0.0550	-0.0021	
						0.0373	-0.0109	0.1060
						-0.0077	0.3070	
						-0.1972	-0.8092	-0.2221
						0.3471	0.1553	

194.	(0.00014)	RY	(8)	C	5	s(3.89%)p 2.05(7.97%)d22.65(88.14%) 0.0000 0.0103 0.1877 0.0598 0.0243 -0.2130 0.0113 -0.1555 -0.0016 0.0972 -0.6989 -0.0566 0.0245 -0.6139 0.1110
195.	(0.00009)	RY	(9)	C	5	s(93.45%)p 0.00(0.22%)d 0.07(6.33%)
196.	(0.00003)	RY	(10)	C	5	s(4.79%)p 0.03(0.12%)d19.85(95.09%)
197.	(0.00573)	RY	(1)	C	6	s(1.65%)p56.99(93.84%)d 2.74(4.51%) 0.0000 0.0318 0.1242 0.0052 0.0305 0.8594 -0.0006 0.4445 0.0008 -0.0380 -0.1266 -0.0031 0.0057 -0.1695 0.0173
198.	(0.00260)	RY	(2)	C	6	s(0.06%)p99.99(98.44%)d26.28(1.50%) 0.0000 -0.0015 -0.0022 0.0238 0.0072 0.4355 0.0272 -0.8824 0.0021 -0.1236 -0.1203 -0.0045 -0.0210 0.0105 -0.0025
199.	(0.00131)	RY	(3)	C	6	s(3.10%)p30.09(93.13%)d 1.22(3.78%) 0.0000 0.0023 0.1759 -0.0028 0.0035 0.0643 0.0039 -0.1017 -0.0071 0.9574 -0.0309 -0.1059 0.1578 0.0077 0.0259
200.	(0.00113)	RY	(4)	C	6	s(94.85%)p 0.04(3.99%)d 0.01(1.16%) 0.0000 -0.0076 0.9737 -0.0201 0.0112 -0.1038 0.0111 -0.0385 0.0018 -0.1654 0.0696 0.0228 -0.0366 0.0681 -0.0168
201.	(0.00051)	RY	(5)	C	6	s(0.01%)p 1.00(3.60%)d26.76(96.39%) 0.0000 -0.0003 0.0051 -0.0051 -0.0003 -0.0039 0.0001 -0.0016 0.0143 -0.1892 0.0436 -0.3272 0.9228 0.0317 0.0498
202.	(0.00018)	RY	(6)	C	6	s(1.37%)p 1.10(1.51%)d70.64(97.11%) 0.0000 0.0031 -0.0177 0.1159 -0.0051 0.0810 0.0242 -0.0842 0.0021 0.0298 0.8574 0.1323 0.0277 -0.4656 0.0305
203.	(0.00011)	RY	(7)	C	6	s(0.00%)p 1.00(0.22%)d99.99(99.78%) 0.0000 0.0003 0.0021 -0.0016 0.0010 -0.0132 0.0033 -0.0015 -0.0144 -0.0423 0.0901 -0.9276 -0.3357 -0.1247 -0.0317
204.	(0.00008)	RY	(8)	C	6	s(9.71%)p 0.45(4.39%)d 8.84(85.89%)
205.	(0.00004)	RY	(9)	C	6	s(51.39%)p 0.01(0.62%)d 0.93(47.99%)
206.	(0.00004)	RY	(10)	C	6	s(37.99%)p 0.01(0.31%)d 1.62(61.71%)
207.	(0.00476)	RY	(1)	C	7	s(0.30%)p99.99(93.01%)d22.22(6.69%) 0.0000 -0.0308 0.0452 -0.0042 0.0152 0.6923 -0.0026 -0.6709 0.0012 -0.0215 0.2583 0.0107 -0.0056 -0.0060 0.0046
208.	(0.00207)	RY	(2)	C	7	s(3.04%)p31.18(94.80%)d 0.71(2.16%) 0.0000 0.0076 0.1740 0.0094 -0.0090 0.6567 -0.0154 0.7110 0.0019 0.1043 0.0697 -0.0260 -0.0131 0.1260 -0.0057
209.	(0.00081)	RY	(3)	C	7	s(0.16%)p99.99(45.80%)d99.99(54.04%) 0.0000 0.0005 0.0383 -0.0130 0.0019 -0.0586 0.0011 -0.0805 0.0202 0.6691 0.0129 -0.6132 -0.4047 -0.0220 -0.0036
210.	(0.00053)	RY	(4)	C	7	s(0.21%)p99.99(47.63%)d99.99(52.16%) 0.0000 0.0000 0.0428 -0.0165 0.0014 -0.0339 0.0026 -0.0646 0.0022 0.6863 -0.0273 0.3447 0.6301 0.0680 0.0183
211.	(0.00044)	RY	(5)	C	7	s(91.62%)p 0.05(4.87%)d 0.04(3.51%) 0.0000 -0.0006 0.9572 -0.0057 0.0077 -0.1906 0.0042 -0.0807 -0.0006 -0.0757 0.1299 0.0146 -0.0146 0.1183 -0.0619
212.	(0.00011)	RY	(6)	C	7	s(3.38%)p 0.33(1.12%)d28.28(95.50%) 0.0000 0.0003 0.1578 0.0942 -0.0140 0.0743 -0.0173 0.0679 -0.0011 0.0240 -0.0683 0.0006 0.0761 -0.9696 0.0672
213.	(0.00006)	RY	(7)	C	7	s(94.31%)p 0.00(0.13%)d 0.06(5.57%)
214.	(0.00002)	RY	(8)	C	7	s(2.44%)p 2.51(6.13%)d37.43(91.42%)
215.	(0.00002)	RY	(9)	C	7	s(4.69%)p 0.03(0.15%)d20.27(95.15%)
216.	(0.00001)	RY	(10)	C	7	s(0.01%)p 1.00(6.40%)d14.63(93.59%)
217.	(0.00401)	RY	(1)	C	8	s(0.39%)p99.99(91.56%)d20.47(8.05%) 0.0000 -0.0316 0.0540 -0.0037 -0.0028 -0.2060 -0.0173 -0.9342 -0.0002 -0.0075 -0.0983 -0.0163 -0.0104 0.2651 0.0120
218.	(0.00231)	RY	(2)	C	8	s(0.05%)p99.99(98.38%)d32.09(1.57%) 0.0000 0.0049 -0.0096 0.0193 0.0247 -0.9652 -0.0073 0.2180 0.0002 0.0630 0.1080 0.0071 -0.0070 0.0628 0.0017
219.	(0.00077)	RY	(3)	C	8	s(0.05%)p99.99(93.89%)d99.99(6.06%) 0.0000 -0.0010 0.0230 -0.0013 0.0007 -0.0586 0.0005 0.0286 -0.0161 -0.9666 -0.0184 -0.1444 -0.1984 -0.0001 -0.0073

220.	(0.00053)	RY	(4)	C	8	s(0.59%)p 1.79(1.06%)d99.99(98.34%) 0.0000 0.0001 0.0755 -0.0156 0.0005 -0.0029 -0.0011 0.0088 0.0102 -0.1022 -0.0723 0.9669 -0.1859 0.0394 -0.0844
221.	(0.00029)	RY	(5)	C	8	s(95.66%)p 0.01(0.88%)d 0.04(3.47%) 0.0000 0.0005 0.9748 -0.0793 0.0033 -0.0045 -0.0064 0.0858 0.0004 0.0362 -0.1510 -0.0857 0.0286 0.0416 -0.0441
222.	(0.00008)	RY	(6)	C	8	s(21.66%)p 0.05(1.15%)d 3.56(77.19%)
223.	(0.00007)	RY	(7)	C	8	s(75.16%)p 0.01(0.53%)d 0.32(24.31%)
224.	(0.00002)	RY	(8)	C	8	s(3.51%)p 2.16(7.58%)d25.31(88.90%)
225.	(0.00001)	RY	(9)	C	8	s(3.07%)p 0.02(0.07%)d31.52(96.85%)
226.	(0.00000)	RY	(10)	C	8	s(0.02%)p99.99(4.92%)d99.99(95.06%)
227.	(0.00398)	RY	(1)	C	9	s(1.41%)p64.91(91.62%)d 4.94(6.97%) 0.0000 0.0138 0.1174 0.0122 0.0038 0.9534 0.0171 0.0823 0.0001 -0.0119 0.2546 -0.0024 -0.0339 0.0604 -0.0106
228.	(0.00357)	RY	(2)	C	9	s(0.55%)p99.99(93.48%)d10.77(5.96%) 0.0000 0.0259 0.0698 0.0017 -0.0169 0.0855 -0.0041 -0.9624 -0.0002 -0.0310 0.0131 0.0186 0.0031 -0.2414 -0.0288
229.	(0.00174)	RY	(3)	C	9	s(0.00%)p 1.00(84.07%)d 0.19(15.93%) 0.0000 0.0006 0.0021 -0.0012 -0.0012 -0.0132 0.0010 0.0282 -0.0158 -0.9162 0.0382 0.1862 0.3496 0.0244 -0.0193
230.	(0.00066)	RY	(4)	C	9	s(28.25%)p 0.15(4.28%)d 2.39(67.47%) 0.0000 -0.0064 0.5314 -0.0057 0.0045 -0.0802 -0.0107 0.0936 0.0054 -0.1657 -0.0270 0.4226 -0.6643 -0.1885 -0.1367
231.	(0.00060)	RY	(5)	C	9	s(52.17%)p 0.07(3.84%)d 0.84(43.99%) 0.0000 -0.0090 0.7221 -0.0100 0.0058 -0.0817 -0.0155 0.1228 -0.0048 0.1279 0.0823 -0.2896 0.4853 -0.3367 -0.0192
232.	(0.00016)	RY	(6)	C	9	s(0.26%)p43.14(11.40%)d99.99(88.34%) 0.0000 0.0015 0.0425 -0.0288 -0.0015 -0.0011 0.0018 -0.0133 0.0140 -0.3371 -0.0933 -0.8270 -0.4289 0.0247 0.0787
233.	(0.00014)	RY	(7)	C	9	s(15.50%)p 0.19(2.99%)d 5.26(81.50%) 0.0000 0.0077 0.3437 -0.1918 -0.0169 0.0903 0.0131 -0.1409 -0.0011 0.0384 -0.5888 0.0338 0.1078 0.6701 -0.0805
234.	(0.00008)	RY	(8)	C	9	s(34.58%)p 0.14(4.90%)d 1.75(60.52%)
235.	(0.00007)	RY	(9)	C	9	s(61.55%)p 0.06(3.40%)d 0.57(35.05%)
236.	(0.00001)	RY	(10)	C	9	s(5.87%)p 0.01(0.05%)d16.02(94.08%)
237.	(0.00680)	RY	(1)	C	10	s(0.92%)p99.99(95.19%)d 4.23(3.89%) 0.0000 0.0096 0.0953 0.0055 -0.0029 -0.8364 -0.0015 -0.5022 0.0045 0.0142 -0.0861 0.0075 0.0117 -0.1768 -0.0052
238.	(0.00507)	RY	(2)	C	10	s(0.11%)p99.99(94.67%)d47.45(5.22%) 0.0000 0.0017 0.0282 -0.0173 -0.0069 -0.5061 0.0158 0.8258 0.0013 0.0910 -0.1689 -0.0092 0.0086 0.1533 -0.0057
239.	(0.00074)	RY	(3)	C	10	s(1.72%)p21.46(36.88%)d35.74(61.41%) 0.0000 -0.0008 0.1299 0.0175 -0.0010 -0.0179 0.0000 0.0545 0.0066 -0.6045 -0.0687 0.5181 -0.5815 -0.0299 -0.0436
240.	(0.00059)	RY	(4)	C	10	s(95.20%)p 0.02(1.99%)d 0.03(2.81%) 0.0000 -0.0030 0.9757 -0.0075 0.0023 0.0849 0.0006 -0.0091 -0.0024 0.1123 0.0551 -0.0166 0.0715 0.1368 -0.0312
241.	(0.00052)	RY	(5)	C	10	s(0.07%)p99.99(39.44%)d99.99(60.49%) 0.0000 0.0001 0.0197 0.0190 0.0004 -0.0291 0.0004 0.0489 0.0061 -0.6254 0.0254 0.1244 0.7672 0.0029 0.0156
242.	(0.00035)	RY	(6)	C	10	s(0.91%)p22.67(20.73%)d85.72(78.36%) 0.0000 -0.0010 0.0823 0.0487 -0.0026 -0.0031 -0.0014 0.0519 0.0013 -0.4523 -0.0698 -0.8352 -0.2385 -0.1421 0.0636
243.	(0.00011)	RY	(7)	C	10	s(90.45%)p 0.01(0.88%)d 0.10(8.67%) 0.0000 0.0022 0.0312 0.9505 -0.0043 0.0423 -0.0014 0.0333 -0.0010 0.0768 -0.1677 0.0641 0.0302 -0.1601 0.1672
244.	(0.00009)	RY	(8)	C	10	s(5.02%)p 1.22(6.13%)d17.68(88.85%)
245.	(0.00009)	RY	(9)	C	10	s(2.47%)p 1.69(4.16%)d37.80(93.37%)
246.	(0.00002)	RY	(10)	C	10	s(3.18%)p 0.00(0.01%)d30.44(96.81%)
247.	(0.00444)	RY	(1)	C	11	s(0.94%)p97.93(92.41%)d 7.04(6.65%) 0.0000 0.0091 0.0960 0.0118 0.0135

		0.8710	-0.0115	0.4061	-0.0027	0.0124
		0.0801	-0.0178	-0.0196	0.2435	-0.0078
248.	(0.00318) RY (2) C 11	s(1.61%)p	57.16(92.09%)d	3.91(6.30%)		
		0.0000	0.0254	0.1243	0.0042	-0.0123
		-0.4091	-0.0037	0.8653	0.0027	0.0676
		-0.2436	-0.0127	0.0226	0.0473	-0.0275
249.	(0.00182) RY (3) C 11	s(0.01%)p	1.00(85.37%)d	0.17(14.63%)		
		0.0000	0.0006	0.0078	0.0022	-0.0013
		-0.0168	-0.0004	0.0638	-0.0150	-0.9215
		-0.0188	0.3567	-0.1277	0.0178	-0.0455
250.	(0.00065) RY (4) C 11	s(4.17%)p	1.03(4.30%)d	21.93(91.52%)		
		0.0000	-0.0023	0.2042	-0.0047	-0.0024
		0.0125	0.0043	-0.0571	-0.0069	0.1989
		-0.1590	0.1725	-0.9217	-0.0512	-0.0902
251.	(0.00060) RY (5) C 11	s(75.43%)p	0.07(5.00%)d	0.26(19.57%)		
		0.0000	-0.0112	0.8684	-0.0130	-0.0067
		0.0368	0.0174	-0.2126	0.0023	-0.0554
		-0.3537	-0.0606	0.2496	0.0157	-0.0661
252.	(0.00015) RY (6) C 11	s(15.15%)p	0.20(2.97%)d	5.41(81.89%)		
		0.0000	0.0080	0.3391	-0.1908	-0.0046
		-0.0211	-0.0208	0.1696	-0.0002	0.0058
		0.7040	0.0315	-0.0125	-0.5651	-0.0532
253.	(0.00014) RY (7) C 11	s(0.06%)p	99.99(10.39%)d	99.99(89.55%)		
		0.0000	-0.0004	0.0015	0.0244	0.0007
		-0.0155	-0.0003	0.0175	0.0141	-0.3212
		0.0084	-0.9100	-0.2463	-0.0460	0.0679
254.	(0.00008) RY (8) C 11	s(35.87%)p	0.12(4.32%)d	1.67(59.82%)		
255.	(0.00007) RY (9) C 11	s(62.54%)p	0.05(3.13%)d	0.55(34.33%)		
256.	(0.00001) RY (10) C 11	s(4.35%)p	0.02(0.09%)d	21.97(95.57%)		
257.	(0.00489) RY (1) C 12	s(0.08%)p	99.99(94.49%)d	69.58(5.43%)		
		0.0000	0.0001	0.0272	0.0065	-0.0020
		-0.3392	0.0104	0.9108	0.0022	0.0130
		0.1650	0.0205	-0.0079	-0.1630	-0.0053
258.	(0.00330) RY (2) C 12	s(0.57%)p	99.99(91.30%)d	14.33(8.14%)		
		0.0000	0.0020	0.0740	-0.0140	0.0131
		0.8951	0.0040	0.3313	-0.0031	-0.0422
		-0.1978	0.0155	0.0305	-0.2021	-0.0142
259.	(0.00060) RY (3) C 12	s(51.73%)p	0.04(2.09%)d	0.89(46.18%)		
		0.0000	-0.0039	0.7191	0.0137	-0.0023
		0.0107	-0.0006	-0.0217	0.0008	0.1426
		0.1336	0.5916	0.1631	0.1957	-0.1705
260.	(0.00054) RY (4) C 12	s(2.32%)p	0.16(0.37%)d	41.90(97.31%)		
		0.0000	-0.0010	0.1523	-0.0040	-0.0007
		0.0030	-0.0004	0.0020	-0.0009	0.0607
		0.1090	-0.4572	0.8634	0.0439	0.0683
261.	(0.00053) RY (5) C 12	s(34.05%)p	0.01(0.19%)d	1.93(65.76%)		
		0.0000	-0.0040	0.5835	-0.0060	-0.0022
		0.0208	-0.0003	-0.0050	-0.0027	-0.0382
		0.1140	-0.6503	-0.4569	0.0810	-0.0804
262.	(0.00033) RY (6) C 12	s(1.09%)p	89.32(97.14%)d	1.63(1.77%)		
		0.0000	-0.0006	0.1036	0.0116	0.0006
		-0.0557	0.0008	-0.0185	0.0109	-0.9838
		0.0149	0.0833	0.0966	-0.0263	-0.0228
263.	(0.00014) RY (7) C 12	s(9.18%)p	0.94(8.61%)d	8.96(82.21%)		
		0.0000	0.0032	0.2760	0.1249	0.0145
		-0.2633	0.0059	-0.1132	-0.0010	0.0607
		-0.6188	0.0000	0.0576	-0.6592	0.0357
264.	(0.00008) RY (8) C 12	s(12.03%)p	0.42(5.02%)d	6.90(82.96%)		
265.	(0.00006) RY (9) C 12	s(85.95%)p	0.01(0.83%)d	0.15(13.21%)		
266.	(0.00002) RY (10) C 12	s(3.06%)p	0.02(0.05%)d	31.65(96.89%)		
267.	(0.00245) RY (1) C 13	s(4.71%)p	17.12(80.60%)d	3.12(14.69%)		
		0.0000	0.0025	0.2169	-0.0047	0.0078
		0.3631	0.0121	0.2676	-0.0141	-0.7760
		-0.0784	-0.0442	0.0626	0.1208	0.3468
268.	(0.00172) RY (2) C 13	s(11.83%)p	5.46(64.55%)d	2.00(23.61%)		
		0.0000	0.0152	0.3436	0.0072	-0.0196
		-0.7749	0.0035	-0.0035	-0.0055	-0.2114
		0.3150	0.1959	-0.0099	0.2884	0.1237
269.	(0.00060) RY (3) C 13	s(6.45%)p	4.33(27.91%)d	10.18(65.64%)		
		0.0000	-0.0058	-0.1345	0.2153	-0.0089
		0.3815	0.0141	-0.2979	-0.0037	0.2112
		0.4305	0.3323	0.0236	0.4824	0.3569
270.	(0.00058) RY (4) C 13	s(20.23%)p	3.56(72.00%)d	0.38(7.77%)		
		0.0000	0.0046	0.4497	-0.0012	0.0015
		0.1313	0.0231	-0.8141	0.0162	-0.1978
		-0.0056	-0.0988	-0.0028	-0.1869	-0.1817
271.	(0.00006) RY (5) C 13	s(34.60%)p	0.65(22.33%)d	1.24(43.07%)		

272.	(0.00003)	RY	(6)	C 13	s(20.76%)p 0.55(11.35%)d 3.27(67.89%)
273.	(0.00002)	RY	(7)	C 13	s(35.22%)p 0.07(2.54%)d 1.77(62.24%)
274.	(0.00001)	RY	(8)	C 13	s(39.27%)p 0.04(1.63%)d 1.50(59.10%)
275.	(0.00000)	RY	(9)	C 13	s(19.39%)p 0.67(12.96%)d 3.49(67.65%)
276.	(0.00000)	RY	(10)	C 13	s(7.58%)p 0.58(4.43%)d11.61(87.99%)
277.	(0.00229)	RY	(1)	C 14	s(9.23%)p 8.22(75.87%)d 1.61(14.89%) 0.0000 0.0079 0.3037 -0.0063 0.0003 0.0714 0.0210 0.7414 0.0007 0.4511 -0.0393 -0.0284 0.3719 0.0211 0.0884
278.	(0.00175)	RY	(2)	C 14	s(4.37%)p15.95(69.66%)d 5.95(25.97%) 0.0000 0.0104 0.2087 0.0038 -0.0190 -0.8217 0.0007 0.0153 0.0033 -0.1444 0.1132 -0.3782 0.1503 0.2048 -0.1984
279.	(0.00079)	RY	(3)	C 14	s(14.71%)p 4.28(63.01%)d 1.52(22.29%) 0.0000 0.0005 0.3549 0.1453 -0.0076 0.2730 0.0097 -0.5832 -0.0208 0.4635 0.1324 -0.3105 0.2574 0.1923 -0.0753
280.	(0.00045)	RY	(4)	C 14	s(28.22%)p 0.68(19.18%)d 1.86(52.61%) 0.0000 0.0071 0.4811 -0.2251 0.0049 -0.2368 -0.0074 -0.0659 -0.0127 0.3621 0.1058 0.3325 -0.6121 -0.1721 -0.0014
281.	(0.00007)	RY	(5)	C 14	s(40.63%)p 1.08(43.89%)d 0.38(15.48%)
282.	(0.00003)	RY	(6)	C 14	s(3.70%)p 4.87(18.04%)d21.13(78.26%)
283.	(0.00003)	RY	(7)	C 14	s(3.03%)p 0.47(1.42%)d31.49(95.54%)
284.	(0.00001)	RY	(8)	C 14	s(31.48%)p 0.04(1.29%)d 2.14(67.24%)
285.	(0.00001)	RY	(9)	C 14	s(14.57%)p 0.25(3.60%)d 5.62(81.83%)
286.	(0.00000)	RY	(10)	C 14	s(50.10%)p 0.09(4.36%)d 0.91(45.54%)
287.	(0.00558)	RY	(1)	C 15	s(3.96%)p23.95(94.91%)d 0.28(1.12%) 0.0000 -0.0248 0.1944 0.0348 0.0210 -0.5606 -0.0052 0.4662 0.0248 -0.6453 0.0154 -0.0720 0.0654 -0.0087 -0.0384
288.	(0.00334)	RY	(2)	C 15	s(0.93%)p99.99(97.24%)d 1.97(1.83%) 0.0000 0.0036 0.0928 0.0255 -0.0026 -0.5735 -0.0047 -0.8002 0.0158 -0.0538 -0.0259 -0.0637 -0.0975 0.0631 -0.0100
289.	(0.00270)	RY	(3)	C 15	s(0.90%)p99.99(96.15%)d 3.25(2.94%) 0.0000 -0.0280 0.0883 0.0217 0.0199 0.5660 0.0026 -0.3413 -0.0075 -0.7241 -0.1163 0.0285 -0.0164 0.0380 0.1156
290.	(0.00113)	RY	(4)	C 15	s(0.21%)p 3.74(0.77%)d99.99(99.02%) 0.0000 0.0021 0.0454 0.0012 0.0049 -0.0108 0.0139 0.0632 0.0073 0.0579 -0.8998 -0.1264 -0.2236 -0.2016 -0.2721
291.	(0.00112)	RY	(5)	C 15	s(35.57%)p 0.12(4.19%)d 1.69(60.24%) 0.0000 0.0005 0.5961 -0.0208 0.0039 0.1711 -0.0075 0.0060 0.0230 0.1093 0.1419 -0.4226 0.0093 0.4216 -0.4752
292.	(0.00074)	RY	(6)	C 15	s(2.58%)p 0.34(0.87%)d37.40(96.55%) 0.0000 0.0018 0.1597 0.0177 -0.0441 0.0651 0.0069 -0.0399 -0.0104 0.0274 0.2037 -0.6118 -0.0505 -0.7122 0.1999
293.	(0.00058)	RY	(7)	C 15	s(35.09%)p 0.02(0.57%)d 1.83(64.35%) 0.0000 0.0030 0.5916 -0.0306 0.0011 0.0244 0.0006 0.0040 0.0177 0.0688 0.1293 0.6231 -0.3227 -0.3594 -0.0719
294.	(0.00044)	RY	(8)	C 15	s(19.38%)p 0.18(3.48%)d 3.98(77.14%) 0.0000 0.0039 0.4364 -0.0575 0.0011 -0.0341 -0.0081 0.0649 -0.0122 0.1709 -0.2880 -0.0487 0.1702 0.2593 0.7680
295.	(0.00035)	RY	(9)	C 15	s(2.04%)p 0.84(1.71%)d47.17(96.25%) 0.0000 0.0016 0.1415 -0.0196 -0.0003 0.0024 0.0162 -0.1253 -0.0039 0.0341 -0.1191 0.1706 0.8942 -0.2660 -0.2208
296.	(0.00003)	RY	(10)	C 15	s(99.43%)p 0.00(0.37%)d 0.00(0.21%)
297.	(0.00565)	RY	(1)	C 16	s(2.95%)p32.53(95.90%)d 0.39(1.15%) 0.0000 -0.0250 0.1667 0.0326 0.0223 -0.5444 0.0058 -0.5738 -0.0204 0.5766 -0.0276 0.0634 0.0751 -0.0260 -0.0204
298.	(0.00340)	RY	(2)	C 16	s(2.40%)p39.77(95.58%)d 0.84(2.01%) 0.0000 0.0047 0.1529 0.0251 -0.0050 -0.7031 0.0046 0.6780 -0.0206 -0.0361 -0.0004 0.1108 -0.0756 0.0439 -0.0146
299.	(0.00280)	RY	(3)	C 16	s(1.55%)p61.39(95.08%)d 2.18(3.37%) 0.0000 -0.0291 0.1183 0.0254 0.0221 0.3967 -0.0011 0.4293 0.0065 0.7801 0.1350 -0.0288 -0.0009 0.0563 0.1073
300.	(0.00113)	RY	(4)	C 16	s(33.58%)p 0.14(4.56%)d 1.84(61.86%)

		0.0000	0.0003	0.5790	-0.0247	0.0038
		0.1942	0.0106	-0.0302	-0.0194	-0.0801
		-0.3563	0.4318	0.0838	0.4458	-0.3156
301.	(0.00112) RY (5) C 16	s(5.29%)p 0.27(1.41%)d17.64(93.30%)	0.0000	0.0016	0.2300	-0.0011
			0.0076	0.0475	-0.0115	-0.0617
			-0.0134	-0.0879	0.8060	0.3054
			-0.1038	-0.2255	-0.3583	
302.	(0.00073) RY (6) C 16	s(5.00%)p 0.25(1.24%)d18.76(93.76%)	0.0000	0.0014	0.2233	0.0115
			-0.0433	0.0947	-0.0089	0.0255
			0.0072	-0.0275	-0.2828	0.4436
			-0.0241	-0.7267	0.3635	
303.	(0.00058) RY (7) C 16	s(34.89%)p 0.02(0.58%)d 1.85(64.53%)	0.0000	0.0031	0.5897	-0.0331
			0.0047	0.0282	-0.0003	-0.0213
			-0.0151	-0.0659	-0.0903	-0.6718
			-0.3355	-0.2404	-0.1243	
304.	(0.00043) RY (8) C 16	s(14.86%)p 0.26(3.83%)d 5.47(81.31%)	0.0000	0.0045	0.3813	-0.0570
			0.0025	-0.0270	0.0059	-0.0646
			0.0139	-0.1821	0.3354	-0.0991
			0.2604	0.6931		
305.	(0.00035) RY (9) C 16	s(0.16%)p10.56(1.69%)d99.99(98.15%)	0.0000	0.0008	0.0394	-0.0067
			0.0000	-0.0027	-0.0175	0.1288
			0.0024	-0.0010	-0.0572	-0.2101
			-0.2982	-0.3613		
306.	(0.00003) RY (10) C 16	s(99.42%)p 0.00(0.37%)d 0.00(0.20%)				
307.	(0.00221) RY (1) C 17	s(1.98%)p45.68(90.65%)d 3.71(7.36%)	0.0000	0.0016	0.1408	0.0049
			0.0034	0.4618	-0.0114	-0.8148
			-0.0058	-0.1711	-0.0061	0.0893
			-0.0425	-0.2172	-0.1290	
308.	(0.00184) RY (2) C 17	s(2.69%)p34.04(91.61%)d 2.12(5.70%)	0.0000	0.0129	0.1633	-0.0086
			-0.0059	0.4478	0.0010	0.0781
			0.0109	0.8422	-0.0906	-0.0528
			-0.0383	-0.0340	0.2083	
309.	(0.00075) RY (3) C 17	s(38.28%)p 1.55(59.45%)d 0.06(2.26%)	0.0000	0.0239	0.6177	0.0261
			0.0007	-0.6430	-0.0003	-0.3172
			0.0035	0.2835	-0.0050	0.0270
			0.0967	0.0517	-0.0992	
310.	(0.00013) RY (4) C 17	s(16.99%)p 1.16(19.78%)d 3.72(63.22%)	0.0000	-0.0155	0.3865	-0.1424
			-0.0220	0.3570	-0.0028	0.2270
			-0.0061	-0.1352	0.0204	0.2886
			0.3247	0.5439	-0.3839	
311.	(0.00006) RY (5) C 17	s(21.15%)p 0.96(20.36%)d 2.77(58.49%)				
312.	(0.00003) RY (6) C 17	s(15.18%)p 0.65(9.93%)d 4.93(74.89%)				
313.	(0.00002) RY (7) C 17	s(80.83%)p 0.01(0.61%)d 0.23(18.55%)				
314.	(0.00001) RY (8) C 17	s(8.72%)p 0.06(0.49%)d10.41(90.79%)				
315.	(0.00001) RY (9) C 17	s(0.01%)p99.99(3.13%)d99.99(96.86%)				
316.	(0.00000) RY (10) C 17	s(14.28%)p 0.29(4.10%)d 5.72(81.62%)				
317.	(0.00220) RY (1) C 18	s(0.40%)p99.99(92.59%)d17.50(7.01%)	0.0000	0.0047	0.0631	0.0020
			-0.0038	-0.3748	0.0011	-0.2341
			0.0147	0.8546	-0.1000	0.0037
			0.1973	0.0753	0.1244	
318.	(0.00185) RY (2) C 18	s(5.32%)p17.38(92.47%)d 0.42(2.21%)	0.0000	0.0155	0.2290	-0.0228
			-0.0019	0.7668	0.0080	0.3854
			0.0040	0.4338	0.1351	0.0171
			-0.0383	0.0424		
319.	(0.00105) RY (3) C 18	s(34.24%)p 1.81(62.03%)d 0.11(3.73%)	0.0000	0.0238	0.5832	0.0419
			0.0007	-0.4564	0.0030	0.6410
			-0.0005	-0.0327	-0.0509	0.0012
			-0.1463	0.0695	-0.0921	
320.	(0.00016) RY (4) C 18	s(7.19%)p 1.56(11.24%)d11.34(81.56%)	0.0000	-0.0116	0.2281	-0.1406
			-0.0236	0.2025	0.0070	-0.2660
			-0.0055	-0.0038	-0.5595	0.2258
			-0.3563	0.5360	-0.1934	
321.	(0.00010) RY (5) C 18	s(49.84%)p 0.61(30.56%)d 0.39(19.60%)	0.0000	-0.0219	0.7042	-0.0459
			0.0090	0.0641	0.0105	-0.5287
			0.0038	-0.1475	0.3225	-0.1244
			-0.0221	-0.1394	0.2378	
322.	(0.00003) RY (6) C 18	s(6.17%)p 0.56(3.43%)d14.64(90.39%)				
323.	(0.00001) RY (7) C 18	s(52.98%)p 0.02(1.09%)d 0.87(45.93%)				
324.	(0.00001) RY (8) C 18	s(7.57%)p 0.12(0.94%)d12.08(91.49%)				
325.	(0.00001) RY (9) C 18	s(3.13%)p 0.33(1.04%)d30.59(95.83%)				
326.	(0.00000) RY (10) C 18	s(33.28%)p 0.14(4.74%)d 1.86(61.98%)				
327.	(0.00220) RY (1) C 19	s(1.27%)p71.79(91.25%)d 5.88(7.47%)	0.0000	-0.0001	0.1127	0.0035
			0.0020	0.3896	0.0137	0.8413
			0.0085	0.2296	-0.0220	-0.0822
			-0.0553	-0.2087	-0.1446	
328.	(0.00186) RY (2) C 19	s(3.43%)p26.53(90.95%)d 1.64(5.62%)	0.0000	0.0104	0.1848	0.0008
			-0.0068			

				0.5356	-0.0026	-0.0322	-0.0107	-0.7883
				0.0891	0.0146	-0.0263	-0.0526	0.2111
329.	(0.00072)	RY	(3)	C 19	s(37.65%)	p 1.60(60.19%)	d 0.06(2.16%)	
					0.0000	0.0243	0.6122	0.0335
					-0.6350	0.0018	0.2942	-0.0026
					-0.0014	-0.0122	0.0897	0.0230
330.	(0.00013)	RY	(4)	C 19	s(17.62%)	p 1.02(17.97%)	d 3.66(64.42%)	
					0.0000	-0.0146	0.3909	-0.1522
					0.3421	0.0005	-0.1859	0.0045
					0.0390	-0.1628	0.3153	0.5648
331.	(0.00005)	RY	(5)	C 19	s(16.48%)	p 1.14(18.80%)	d 3.93(64.72%)	
332.	(0.00003)	RY	(6)	C 19	s(21.66%)	p 0.56(12.14%)	d 3.06(66.20%)	
333.	(0.00002)	RY	(7)	C 19	s(63.13%)	p 0.01(0.59%)	d 0.57(36.27%)	
334.	(0.00001)	RY	(8)	C 19	s(22.80%)	p 0.03(0.68%)	d 3.36(76.52%)	
335.	(0.00001)	RY	(9)	C 19	s(0.79%)	p 3.75(2.95%)	d99.99(96.26%)	
336.	(0.00000)	RY	(10)	C 19	s(15.30%)	p 0.30(4.60%)	d 5.24(80.10%)	
337.	(0.00222)	RY	(1)	C 20	s(0.15%)	p99.99(92.68%)	d48.56(7.17%)	
					0.0000	0.0054	0.0380	0.0011
					-0.3589	0.0006	0.2300	-0.0145
					0.0986	-0.0262	0.2089	0.0665
338.	(0.00201)	RY	(2)	C 20	s(4.33%)	p21.58(93.39%)	d 0.53(2.28%)	
					0.0000	0.0141	0.2064	-0.0217
					0.8334	-0.0081	-0.2673	-0.0055
					-0.1321	-0.0326	0.0285	-0.0174
339.	(0.00118)	RY	(3)	C 20	s(33.83%)	p 1.87(63.16%)	d 0.09(3.00%)	
					0.0000	0.0241	0.5800	0.0367
					-0.3686	-0.0026	-0.7028	0.0011
					0.0549	0.0203	-0.1339	0.0492
340.	(0.00017)	RY	(4)	C 20	s(16.45%)	p 1.02(16.80%)	d 4.06(66.74%)	
					0.0000	-0.0144	0.3822	-0.1352
					0.1671	-0.0092	0.3704	0.0017
					0.6004	-0.0837	-0.3247	0.4108
341.	(0.00011)	RY	(5)	C 20	s(42.97%)	p 0.56(23.90%)	d 0.77(33.13%)	
					0.0000	-0.0178	0.6543	0.0353
					-0.0341	-0.0066	0.4671	-0.0042
					-0.4450	0.0839	0.0262	-0.2261
342.	(0.00003)	RY	(6)	C 20	s(4.64%)	p 0.76(3.51%)	d19.79(91.85%)	
343.	(0.00001)	RY	(7)	C 20	s(60.55%)	p 0.02(0.95%)	d 0.64(38.50%)	
344.	(0.00001)	RY	(8)	C 20	s(1.91%)	p 0.44(0.85%)	d51.00(97.25%)	
345.	(0.00001)	RY	(9)	C 20	s(10.01%)	p 0.04(0.38%)	d 8.95(89.61%)	
346.	(0.00000)	RY	(10)	C 20	s(25.28%)	p 0.18(4.52%)	d 2.78(70.20%)	
347.	(0.00183)	RY	(1)	O 21	s(6.29%)	p14.06(88.52%)	d 0.82(5.19%)	
					0.0000	-0.0057	0.2506	0.0096
					0.0028	0.0011	-0.7275	0.0023
					-0.1481	-0.1253	-0.0254	-0.0146
348.	(0.00138)	RY	(2)	O 21	s(4.97%)	p17.36(86.28%)	d 1.76(8.75%)	
					0.0000	-0.0093	0.2180	-0.0456
					0.2945	-0.0003	0.6094	-0.0018
					0.1641	-0.1642	0.0296	0.1256
349.	(0.00068)	RY	(3)	O 21	s(15.14%)	p 5.46(82.72%)	d 0.14(2.14%)	
					0.0000	0.0083	0.3887	-0.0158
					0.8146	0.0007	-0.1340	0.0042
					-0.0818	-0.0777	-0.0133	-0.0655
350.	(0.00019)	RY	(4)	O 21	s(56.59%)	p 0.13(7.42%)	d 0.64(35.99%)	
					0.0000	-0.0004	0.7038	0.2656
					-0.2631	0.0029	0.0539	-0.0201
					0.2307	0.2199	-0.1309	-0.0379
351.	(0.00012)	RY	(5)	O 21	s(30.50%)	p 0.64(19.59%)	d 1.64(49.91%)	
					0.0000	0.0080	-0.3605	0.4182
					0.3471	-0.0080	-0.0091	-0.0147
					-0.1115	0.4335	0.2200	-0.3084
352.	(0.00007)	RY	(6)	O 21	s(20.15%)	p 0.02(0.39%)	d 3.94(79.46%)	
353.	(0.00004)	RY	(7)	O 21	s(8.65%)	p 0.88(7.61%)	d 9.69(83.74%)	
354.	(0.00003)	RY	(8)	O 21	s(4.32%)	p 0.74(3.22%)	d21.41(92.47%)	
355.	(0.00002)	RY	(9)	O 21	s(0.63%)	p 6.62(4.17%)	d99.99(95.20%)	
356.	(0.00002)	RY	(10)	O 21	s(52.81%)	p 0.01(0.62%)	d 0.88(46.57%)	
357.	(0.00161)	RY	(1)	O 22	s(7.89%)	p10.89(85.97%)	d 0.78(6.14%)	
					0.0000	-0.0074	0.2808	-0.0038
					-0.1087	-0.0033	0.6333	-0.0008
					0.1419	0.1738	-0.0033	-0.0296
358.	(0.00140)	RY	(2)	O 22	s(3.70%)	p23.92(88.49%)	d 2.11(7.81%)	
					0.0000	-0.0092	0.1862	-0.0474
					0.1710	0.0004	-0.7023	0.0021
					-0.1643	0.1607	0.0199	0.1368
359.	(0.00067)	RY	(3)	O 22	s(13.55%)	p 6.26(84.88%)	d 0.12(1.57%)	
					0.0000	0.0075	0.3676	-0.0181
					0.8819	-0.0004	0.1712	-0.0033

360.	(0.00018)	RY	(4)	O	22	-0.0281	0.1080	0.0021	-0.0224	-0.0523
						s(64.56%)p 0.13(8.66%)d 0.41(26.79%)				
						0.0000	-0.0008	0.7455	0.2998	-0.0052
						-0.2520	0.0008	-0.0939	0.0181	-0.1178
						-0.0199	-0.3026	-0.0664	0.0196	0.4137
361.	(0.00012)	RY	(5)	O	22	s(19.60%)p 1.06(20.85%)d 3.04(59.55%)				
						0.0000	-0.0088	0.3692	-0.2442	0.0054
						-0.2901	-0.0007	-0.0691	-0.0202	-0.3451
						0.1938	0.4343	0.0287	0.3901	-0.4651
362.	(0.00007)	RY	(6)	O	22	s(27.18%)p 0.06(1.54%)d 2.62(71.29%)				
363.	(0.00004)	RY	(7)	O	22	s(7.31%)p 0.29(2.09%)d12.39(90.60%)				
364.	(0.00004)	RY	(8)	O	22	s(4.07%)p 0.70(2.84%)d22.90(93.09%)				
365.	(0.00002)	RY	(9)	O	22	s(9.05%)p 0.36(3.30%)d 9.69(87.65%)				
366.	(0.00001)	RY	(10)	O	22	s(43.14%)p 0.05(1.94%)d 1.27(54.91%)				
367.	(0.01779)	RY	(1)	B	23	s(0.00%)p 1.00(96.22%)d 0.04(3.78%)				
						0.0000	-0.0030	0.0038	-0.0004	0.0088
						-0.0477	-0.0010	-0.1125	-0.1068	0.9674
						-0.0099	0.1934	0.0049	-0.0046	0.0151
368.	(0.00370)	RY	(2)	B	23	s(20.89%)p 2.86(59.82%)d 0.92(19.29%)				
						0.0000	0.0247	0.4562	0.0123	0.0314
						0.7720	0.0025	0.0112	0.0014	0.0321
						0.0823	0.0613	0.0831	0.2454	-0.3395
369.	(0.00278)	RY	(3)	B	23	s(0.20%)p99.99(96.80%)d15.06(3.00%)				
						0.0000	-0.0067	-0.0101	0.0429	0.0164
						0.0075	-0.0353	-0.9787	0.0028	-0.0929
						0.1177	-0.0913	-0.0207	-0.0536	-0.0670
370.	(0.00192)	RY	(4)	B	23	s(4.13%)p 0.69(2.84%)d22.50(93.02%)				
						0.0000	-0.0030	0.1949	-0.0581	0.0032
						-0.1615	0.0017	0.0467	0.0041	0.0102
						0.0774	-0.0142	-0.9036	-0.0236	-0.3271
371.	(0.00139)	RY	(5)	B	23	s(69.23%)p 0.27(19.01%)d 0.17(11.76%)				
						0.0000	-0.0179	0.8313	0.0311	-0.0173
						-0.4354	-0.0048	0.0029	0.0016	-0.0118
						0.1837	-0.0730	0.2026	-0.0167	0.1930
372.	(0.00107)	RY	(6)	B	23	s(0.27%)p22.14(5.91%)d99.99(93.82%)				
						0.0000	-0.0014	0.0510	0.0081	0.0049
						-0.0761	0.0055	-0.0727	-0.0543	-0.2122
						-0.0432	0.9658	0.0021	-0.0589	-0.0047
373.	(0.00100)	RY	(7)	B	23	s(0.93%)p19.08(17.79%)d87.17(81.28%)				
						0.0000	0.0009	0.0956	-0.0133	-0.0268
						0.4206	-0.0071	-0.0120	-0.0055	0.0051
						0.0895	0.0123	-0.3056	-0.3985	0.7432
374.	(0.00045)	RY	(8)	B	23	s(47.32%)p 0.00(0.23%)d 1.11(52.46%)				
						0.0000	0.0095	0.1538	0.6704	0.0007
						0.0172	0.0229	-0.0382	0.0010	0.0007
						-0.6984	-0.0568	-0.0529	-0.1695	-0.0455
375.	(0.00022)	RY	(9)	B	23	s(56.49%)p 0.02(1.18%)d 0.75(42.32%)				
						0.0000	-0.0008	-0.1640	0.7335	0.0189
						-0.0114	-0.0129	0.1052	-0.0006	0.0107
						0.6462	0.0442	-0.0173	0.0571	-0.0122
376.	(0.00011)	RY	(10)	B	23	s(0.68%)p 1.47(1.00%)d99.99(98.32%)				
						0.0000	-0.0250	-0.0203	0.0759	-0.0136
						-0.0387	0.0056	-0.0884	-0.0031	-0.0222
						-0.1524	0.0339	-0.1963	0.8610	0.4230
377.	(0.00425)	RY	(1)	N	24	s(7.58%)p11.81(89.45%)d 0.39(2.98%)				
						0.0000	-0.0133	0.2748	-0.0092	0.0104
						0.5504	-0.0292	-0.7177	0.0024	0.2747
						0.1438	-0.0490	0.0616	0.0096	0.0527
378.	(0.00093)	RY	(2)	N	24	s(1.60%)p55.20(88.59%)d 6.11(9.80%)				
						0.0000	-0.0101	0.1261	-0.0076	0.0023
						0.2910	-0.0009	0.5579	-0.0153	0.6998
						0.0486	-0.1460	-0.1022	0.2468	0.0547
379.	(0.00078)	RY	(3)	N	24	s(1.52%)p52.71(80.27%)d11.96(18.21%)				
						0.0000	-0.0109	0.1219	-0.0161	-0.0047
						0.5989	-0.0006	0.3028	0.0139	-0.5933
						0.2193	-0.1196	-0.0979	0.1414	-0.3002
380.	(0.00046)	RY	(4)	N	24	s(0.12%)p33.64(4.15%)d99.99(95.73%)				
						0.0000	0.0022	0.0345	-0.0061	-0.0053
						-0.1438	0.0025	-0.1257	0.0065	-0.0702
						-0.1435	-0.8549	-0.4407	-0.0460	0.0977
381.	(0.00036)	RY	(5)	N	24	s(8.67%)p 2.11(18.32%)d 8.43(73.01%)				
						0.0000	0.0047	0.2872	-0.0644	0.0164
						-0.3832	0.0134	-0.1237	-0.0072	0.1436
						0.4412	0.1312	-0.3835	0.1387	-0.5932
382.	(0.00026)	RY	(6)	N	24	s(34.18%)p 0.28(9.71%)d 1.64(56.12%)				
						0.0000	-0.0004	0.5845	-0.0080	0.0086
						-0.2538	0.0162	-0.0052	-0.0015	-0.1797

383.	(0.00018)	RY	(7)	N 24	-0.1287 -0.0994 0.3723 0.6006 0.1880 s(0.05%)p46.45(2.47%)d99.99(97.48%) 0.0000 0.0008 -0.0139 0.0183 0.0056 -0.0164 -0.0115 0.0196 -0.0347 0.1505 -0.2222 -0.3427 0.5918 -0.2185 -0.6403
384.	(0.00007)	RY	(8)	N 24	s(34.97%)p 0.16(5.55%)d 1.70(59.48%)
385.	(0.00005)	RY	(9)	N 24	s(14.54%)p 0.10(1.50%)d 5.77(83.96%)
386.	(0.00002)	RY	(10)	N 24	s(96.83%)p 0.00(0.23%)d 0.03(2.93%)
387.	(0.00116)	RY	(1)	H 25	s(99.32%)p 0.01(0.68%) -0.0006 0.9966 0.0513 0.0267 -0.0584 s(0.11%)p99.99(99.89%)
388.	(0.00009)	RY	(2)	H 25	s(0.55%)p99.99(99.45%)
389.	(0.00006)	RY	(3)	H 25	s(0.07%)p99.99(99.93%)
390.	(0.00000)	RY	(4)	H 25	s(99.16%)p 0.01(0.84%)
391.	(0.00119)	RY	(1)	H 26	-0.0001 0.9958 -0.0553 -0.0253 -0.0683 s(0.09%)p99.99(99.91%)
392.	(0.00009)	RY	(2)	H 26	s(0.64%)p99.99(99.36%)
393.	(0.00005)	RY	(3)	H 26	s(0.18%)p99.99(99.82%)
394.	(0.00001)	RY	(4)	H 26	s(99.44%)p 0.01(0.56%)
395.	(0.00118)	RY	(1)	H 27	-0.0003 0.9972 0.0380 0.0437 -0.0477 s(0.42%)p99.99(99.58%)
396.	(0.00009)	RY	(2)	H 27	s(0.10%)p99.99(99.90%)
397.	(0.00006)	RY	(3)	H 27	s(0.10%)p99.99(99.90%)
398.	(0.00000)	RY	(4)	H 27	s(99.20%)p 0.01(0.80%)
399.	(0.00122)	RY	(1)	H 28	-0.0004 0.9960 0.0552 0.0554 0.0438 s(0.68%)p99.99(99.32%)
400.	(0.00009)	RY	(2)	H 28	s(0.07%)p99.99(99.93%)
401.	(0.00006)	RY	(3)	H 28	s(0.11%)p99.99(99.89%)
402.	(0.00000)	RY	(4)	H 28	s(99.76%)p 0.00(0.24%)
403.	(0.00106)	RY	(1)	H 29	0.0023 0.9988 -0.0268 0.0403 0.0104 s(0.01%)p 1.00(99.99%)
404.	(0.00017)	RY	(2)	H 29	0.0002 0.0085 -0.0550 0.0100 -0.9984 s(0.02%)p99.99(99.98%)
405.	(0.00005)	RY	(3)	H 29	s(0.29%)p99.99(99.71%)
406.	(0.00001)	RY	(4)	H 29	s(99.50%)p 0.01(0.50%)
407.	(0.00112)	RY	(1)	H 30	0.0022 0.9975 -0.0268 0.0418 -0.0507 s(0.26%)p99.99(99.74%)
408.	(0.00018)	RY	(2)	H 30	0.0006 0.0514 0.0801 0.0304 0.9950 s(0.06%)p99.99(99.94%)
409.	(0.00005)	RY	(3)	H 30	s(0.26%)p99.99(99.74%)
410.	(0.00001)	RY	(4)	H 30	s(99.73%)p 0.00(0.27%)
411.	(0.00114)	RY	(1)	H 31	0.0022 0.9987 0.0430 -0.0109 0.0262 s(0.08%)p99.99(99.92%)
412.	(0.00017)	RY	(2)	H 31	0.0001 0.0275 -0.0126 0.0689 -0.9972 s(0.05%)p99.99(99.95%)
413.	(0.00005)	RY	(3)	H 31	s(0.21%)p99.99(99.79%)
414.	(0.00001)	RY	(4)	H 31	s(99.79%)p 0.00(0.21%)
415.	(0.00109)	RY	(1)	H 32	-0.0022 0.9990 0.0058 0.0414 -0.0183 s(0.04%)p99.99(99.96%)
416.	(0.00016)	RY	(2)	H 32	0.0000 0.0209 0.0486 -0.0686 0.9962 s(0.00%)p 1.00(100.00%)
417.	(0.00005)	RY	(3)	H 32	s(0.23%)p99.99(99.77%)
418.	(0.00001)	RY	(4)	H 32	s(99.32%)p 0.01(0.68%)
419.	(0.00114)	RY	(1)	H 33	-0.0002 0.9966 -0.0534 0.0393 0.0489 s(0.02%)p99.99(99.98%)
420.	(0.00006)	RY	(2)	H 33	s(0.52%)p99.99(99.48%)
421.	(0.00004)	RY	(3)	H 33	s(0.20%)p99.99(99.80%)
422.	(0.00001)	RY	(4)	H 33	s(99.59%)p 0.00(0.41%)
423.	(0.00273)	RY	(1)	H 34	-0.0048 0.9979 -0.0203 -0.0304 -0.0529 s(0.03%)p99.99(99.97%)
424.	(0.00007)	RY	(2)	H 34	s(0.38%)p99.99(99.62%)
425.	(0.00005)	RY	(3)	H 34	s(0.05%)p99.99(99.95%)
426.	(0.00001)	RY	(4)	H 34	s(99.60%)p 0.00(0.40%)
427.	(0.00091)	RY	(1)	H 35	-0.0002 0.9980 0.0226 -0.0582 0.0116 s(0.13%)p99.99(99.87%)
428.	(0.00006)	RY	(2)	H 35	s(0.25%)p99.99(99.75%)
429.	(0.00004)	RY	(3)	H 35	s(0.07%)p99.99(99.93%)
430.	(0.00000)	RY	(4)	H 35	s(99.60%)p 0.00(0.40%)
431.	(0.00135)	RY	(1)	H 36	0.0003 0.9980 -0.0329 -0.0107 -0.0532 s(0.02%)p99.99(99.98%)
432.	(0.00006)	RY	(2)	H 36	s(0.32%)p99.99(99.68%)
433.	(0.00004)	RY	(3)	H 36	s(0.13%)p99.99(99.87%)
434.	(0.00001)	RY	(4)	H 36	s(99.70%)p 0.00(0.30%)
435.	(0.00293)	RY	(1)	H 37	-0.0051 0.9985 -0.0269 0.0081 0.0471 s(0.00%)p 1.00(100.00%)
436.	(0.00007)	RY	(2)	H 37	s(0.30%)p99.99(99.70%)
437.	(0.00004)	RY	(3)	H 37	s(0.04%)p99.99(99.96%)
438.	(0.00000)	RY	(4)	H 37	

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439. (0.00086) RY ( 1) H 38      s( 99.94%)p 0.00( 0.06%)
                                  -0.0008 0.9997 -0.0207 0.0128 0.0017
440. (0.00007) RY ( 2) H 38      s( 0.05%)p99.99( 99.95%)
441. (0.00004) RY ( 3) H 38      s( 0.00%)p 1.00(100.00%)
442. (0.00001) RY ( 4) H 38      s( 0.06%)p99.99( 99.94%)
443. (0.00131) RY ( 1) H 39      s( 99.18%)p 0.01( 0.82%)
                                  0.0002 0.9959 0.0696 0.0568 -0.0121
444. (0.00007) RY ( 2) H 39      s( 0.82%)p99.99( 99.18%)
445. (0.00006) RY ( 3) H 39      s( 0.00%)p 1.00(100.00%)
446. (0.00001) RY ( 4) H 39      s( 0.06%)p99.99( 99.94%)
447. (0.00084) RY ( 1) H 40      s( 99.15%)p 0.01( 0.85%)
                                  0.0009 0.9957 -0.0049 -0.0673 0.0629
448. (0.00008) RY ( 2) H 40      s( 0.75%)p99.99( 99.25%)
449. (0.00007) RY ( 3) H 40      s( 0.04%)p99.99( 99.96%)
450. (0.00001) RY ( 4) H 40      s( 0.11%)p99.99( 99.89%)
451. (0.00117) RY ( 1) H 41      s( 99.61%)p 0.00( 0.39%)
                                  -0.0001 0.9981 -0.0563 -0.0213 0.0154
452. (0.00008) RY ( 2) H 41      s( 0.32%)p99.99( 99.68%)
453. (0.00007) RY ( 3) H 41      s( 0.07%)p99.99( 99.93%)
454. (0.00001) RY ( 4) H 41      s( 0.04%)p99.99( 99.96%)
455. (0.00139) RY ( 1) H 42      s( 99.20%)p 0.01( 0.80%)
                                  -0.0004 0.9960 -0.0290 0.0847 -0.0044
456. (0.00007) RY ( 2) H 42      s( 0.76%)p99.99( 99.24%)
457. (0.00005) RY ( 3) H 42      s( 0.04%)p99.99( 99.96%)
458. (0.00000) RY ( 4) H 42      s( 0.05%)p99.99( 99.95%)
459. (0.00100) RY ( 1) H 43      s( 98.61%)p 0.01( 1.39%)
                                  0.0010 0.9930 0.0445 0.0992 0.0454
460. (0.00009) RY ( 2) H 43      s( 1.16%)p85.53( 98.84%)
461. (0.00006) RY ( 3) H 43      s( 0.05%)p99.99( 99.95%)
462. (0.00001) RY ( 4) H 43      s( 0.23%)p99.99( 99.77%)
463. (0.00103) RY ( 1) H 44      s( 99.96%)p 0.00( 0.04%)
                                  -0.0008 0.9998 0.0096 0.0182 -0.0042
464. (0.00010) RY ( 2) H 44      s( 0.00%)p 1.00(100.00%)
465. (0.00007) RY ( 3) H 44      s( 0.00%)p 1.00(100.00%)
466. (0.00000) RY ( 4) H 44      s( 0.08%)p99.99( 99.92%)
467. (0.00129) RY ( 1) H 45      s( 99.16%)p 0.01( 0.84%)
                                  -0.0001 0.9958 -0.0675 0.0579 -0.0219
468. (0.00008) RY ( 2) H 45      s( 0.57%)p99.99( 99.43%)
469. (0.00006) RY ( 3) H 45      s( 0.27%)p99.99( 99.73%)
470. (0.00001) RY ( 4) H 45      s( 0.05%)p99.99( 99.95%)
471. (0.00092) RY ( 1) H 46      s( 99.30%)p 0.01( 0.70%)
                                  0.0014 0.9965 0.0103 0.0650 -0.0515
472. (0.00009) RY ( 2) H 46      s( 0.33%)p99.99( 99.67%)
473. (0.00007) RY ( 3) H 46      s( 0.23%)p99.99( 99.77%)
474. (0.00001) RY ( 4) H 46      s( 0.20%)p99.99( 99.80%)
475. (0.00104) RY ( 1) H 47      s( 99.75%)p 0.00( 0.25%)
                                  0.0001 0.9987 -0.0498 0.0060 -0.0030
476. (0.00007) RY ( 2) H 47      s( 0.05%)p99.99( 99.95%)
477. (0.00007) RY ( 3) H 47      s( 0.20%)p99.99( 99.80%)
478. (0.00000) RY ( 4) H 47      s( 0.04%)p99.99( 99.96%)
479. (0.00141) RY ( 1) H 48      s( 99.52%)p 0.00( 0.48%)
                                  -0.0002 0.9976 -0.0218 -0.0654 0.0030
480. (0.00007) RY ( 2) H 48      s( 0.38%)p99.99( 99.62%)
481. (0.00006) RY ( 3) H 48      s( 0.09%)p99.99( 99.91%)
482. (0.00000) RY ( 4) H 48      s( 0.05%)p99.99( 99.95%)
483. (0.00097) RY ( 1) H 49      s( 99.39%)p 0.01( 0.61%)
                                  0.0011 0.9970 0.0537 -0.0565 -0.0008
484. (0.00008) RY ( 2) H 49      s( 0.28%)p99.99( 99.72%)
485. (0.00007) RY ( 3) H 49      s( 0.16%)p99.99( 99.84%)
486. (0.00001) RY ( 4) H 49      s( 0.21%)p99.99( 99.79%)
487. (0.00129) RY ( 1) H 50      s( 99.95%)p 0.00( 0.05%)
                                  -0.0007 0.9997 -0.0074 -0.0050 0.0206
488. (0.00009) RY ( 2) H 50      s( 0.00%)p 1.00(100.00%)
489. (0.00008) RY ( 3) H 50      s( 0.03%)p99.99( 99.97%)
490. (0.00001) RY ( 4) H 50      s( 0.05%)p99.99( 99.95%)

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SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
1. CR (1) C 1	93. BD*(1) C 1- H 26	0.70	10.74	0.077
1. CR (1) C 1	112. BD*(1) C 8- C 11	1.07	10.65	0.095
1. CR (1) C 1	247. RY (1) C 11	1.09	11.33	0.099

2. CR (1) C 2	98. BD* (1) C 3- C 9	1.11	10.65	0.097
2. CR (1) C 2	227. RY (1) C 9	0.87	11.30	0.089
3. CR (1) C 3	94. BD* (1) C 2- C 9	1.63	10.43	0.116
3. CR (1) C 3	98. BD* (1) C 3- C 9	0.57	10.64	0.070
3. CR (1) C 3	101. BD* (1) C 4- C 5	0.84	10.61	0.084
3. CR (1) C 3	103. BD* (1) C 4- H 30	0.60	10.76	0.071
3. CR (1) C 3	115. BD* (1) C 9- C 12	0.78	10.59	0.081
3. CR (1) C 3	178. RY (2) C 4	0.90	10.88	0.088
3. CR (1) C 3	228. RY (2) C 9	2.13	11.23	0.138
3. CR (1) C 3	231. RY (5) C 9	0.52	11.53	0.069
4. CR (1) C 4	98. BD* (1) C 3- C 9	0.75	10.64	0.080
4. CR (1) C 4	100. BD* (1) C 3- H 29	0.58	10.78	0.071
4. CR (1) C 4	101. BD* (1) C 4- C 5	0.51	10.62	0.066
4. CR (1) C 4	104. BD* (1) C 5- C 10	1.07	10.57	0.095
4. CR (1) C 4	105. BD* (1) C 5- N 24	1.00	10.43	0.091
4. CR (1) C 4	168. RY (2) C 3	1.02	10.77	0.094
4. CR (1) C 4	187. RY (1) C 5	2.23	11.10	0.140
4. CR (1) C 4	188. RY (2) C 5	0.73	11.41	0.081
5. CR (1) C 5	97. BD* (1) C 3- C 4	0.87	10.62	0.086
5. CR (1) C 5	101. BD* (1) C 4- C 5	0.55	10.67	0.068
5. CR (1) C 5	103. BD* (1) C 4- H 30	0.56	10.82	0.070
5. CR (1) C 5	104. BD* (1) C 5- C 10	0.50	10.62	0.065
5. CR (1) C 5	108. BD* (1) C 6- C 10	1.13	10.64	0.098
5. CR (1) C 5	116. BD* (1) C 10- C 12	0.67	10.66	0.075
5. CR (1) C 5	118. BD* (1) C 13- N 24	0.57	10.42	0.069
5. CR (1) C 5	122. BD* (1) C 14- N 24	0.52	10.42	0.066
5. CR (1) C 5	178. RY (2) C 4	1.21	10.93	0.102
5. CR (1) C 5	237. RY (1) C 10	0.58	11.44	0.073
5. CR (1) C 5	238. RY (2) C 10	1.01	11.53	0.097
6. CR (1) C 6	104. BD* (1) C 5- C 10	1.15	10.56	0.098
6. CR (1) C 6	109. BD* (1) C 6- B 23	0.55	10.51	0.068
6. CR (1) C 6	110. BD* (1) C 7- C 8	0.89	10.56	0.086
6. CR (1) C 6	111. BD* (1) C 7- H 31	0.63	10.73	0.073
6. CR (1) C 6	116. BD* (1) C 10- C 12	0.77	10.60	0.080
6. CR (1) C 6	145. BD* (1) O 21- B 23	0.66	10.50	0.074
6. CR (1) C 6	208. RY (2) C 7	1.32	10.89	0.107
6. CR (1) C 6	238. RY (2) C 10	1.39	11.47	0.113
6. CR (1) C 6	368. RY (2) B 23	0.74	11.13	0.081
6. CR (1) C 6	371. RY (5) B 23	0.97	11.20	0.093
6. CR (1) C 6	373. RY (7) B 23	0.51	12.06	0.070
7. CR (1) C 7	108. BD* (1) C 6- C 10	0.84	10.59	0.084
7. CR (1) C 7	109. BD* (1) C 6- B 23	1.15	10.53	0.098
7. CR (1) C 7	112. BD* (1) C 8- C 11	0.73	10.65	0.079
7. CR (1) C 7	114. BD* (1) C 8- H 32	0.58	10.71	0.071
7. CR (1) C 7	197. RY (1) C 6	0.59	11.73	0.074
7. CR (1) C 7	198. RY (2) C 6	1.13	11.11	0.100
7. CR (1) C 7	218. RY (2) C 8	1.06	10.76	0.095
8. CR (1) C 8	91. BD* (1) C 1- C 11	1.64	10.43	0.117
8. CR (1) C 8	106. BD* (1) C 6- C 7	0.86	10.61	0.085
8. CR (1) C 8	112. BD* (1) C 8- C 11	0.59	10.64	0.071
8. CR (1) C 8	117. BD* (1) C 11- C 12	0.81	10.59	0.083
8. CR (1) C 8	208. RY (2) C 7	0.92	10.90	0.090
8. CR (1) C 8	211. RY (5) C 7	0.56	11.20	0.071
8. CR (1) C 8	248. RY (2) C 11	1.73	11.20	0.124
8. CR (1) C 8	251. RY (5) C 11	0.86	11.33	0.088
9. CR (1) C 9	97. BD* (1) C 3- C 4	0.69	10.59	0.076
9. CR (1) C 9	100. BD* (1) C 3- H 29	0.77	10.80	0.081
9. CR (1) C 9	115. BD* (1) C 9- C 12	0.82	10.61	0.083
9. CR (1) C 9	116. BD* (1) C 10- C 12	1.26	10.63	0.103
9. CR (1) C 9	117. BD* (1) C 11- C 12	0.67	10.62	0.075
9. CR (1) C 9	159. RY (3) C 2	0.62	10.74	0.073
9. CR (1) C 9	168. RY (2) C 3	1.11	10.79	0.098
9. CR (1) C 9	257. RY (1) C 12	1.20	11.42	0.104
10. CR (1) C 10	101. BD* (1) C 4- C 5	0.78	10.62	0.081
10. CR (1) C 10	105. BD* (1) C 5- N 24	0.66	10.44	0.074
10. CR (1) C 10	106. BD* (1) C 6- C 7	0.56	10.62	0.069
10. CR (1) C 10	109. BD* (1) C 6- B 23	1.08	10.53	0.095
10. CR (1) C 10	115. BD* (1) C 9- C 12	1.08	10.60	0.095
10. CR (1) C 10	116. BD* (1) C 10- C 12	0.56	10.62	0.069
10. CR (1) C 10	117. BD* (1) C 11- C 12	1.00	10.60	0.092
10. CR (1) C 10	187. RY (1) C 5	1.33	11.11	0.109
10. CR (1) C 10	198. RY (2) C 6	1.21	11.11	0.104
10. CR (1) C 10	258. RY (2) C 12	1.65	11.49	0.123
11. CR (1) C 11	110. BD* (1) C 7- C 8	0.63	10.59	0.073
11. CR (1) C 11	114. BD* (1) C 8- H 32	0.83	10.73	0.084
11. CR (1) C 11	115. BD* (1) C 9- C 12	0.66	10.61	0.075
11. CR (1) C 11	116. BD* (1) C 10- C 12	1.23	10.63	0.102

11. CR (1) C 11	117. BD* (1) C 11- C 12	0.82	10.62	0.083
11. CR (1) C 11	149. RY (3) C 1	0.61	10.75	0.072
11. CR (1) C 11	218. RY (2) C 8	1.30	10.78	0.106
11. CR (1) C 11	257. RY (1) C 12	1.16	11.42	0.103
12. CR (1) C 12	98. BD* (1) C 3- C 9	0.80	10.64	0.082
12. CR (1) C 12	104. BD* (1) C 5- C 10	0.77	10.57	0.081
12. CR (1) C 12	108. BD* (1) C 6- C 10	0.86	10.58	0.085
12. CR (1) C 12	112. BD* (1) C 8- C 11	0.85	10.64	0.085
12. CR (1) C 12	227. RY (1) C 9	1.18	11.28	0.103
12. CR (1) C 12	228. RY (2) C 9	0.78	11.23	0.083
12. CR (1) C 12	237. RY (1) C 10	1.84	11.39	0.129
12. CR (1) C 12	247. RY (1) C 11	0.81	11.32	0.085
12. CR (1) C 12	248. RY (2) C 11	1.16	11.19	0.102
13. CR (1) C 13	105. BD* (1) C 5- N 24	0.52	10.45	0.066
13. CR (1) C 13	119. BD* (1) C 13- H 33	0.54	10.71	0.068
13. CR (1) C 13	378. RY (2) N 24	0.63	11.36	0.076
14. CR (1) C 14	123. BD* (1) C 14- H 36	0.58	10.71	0.070
14. CR (1) C 14	379. RY (3) N 24	0.51	11.42	0.068
14. CR (1) C 14	439. RY (1) H 38	0.51	10.70	0.066
15. CR (1) C 15	129. BD* (1) C 15- O 21	0.96	10.39	0.089
15. CR (1) C 15	145. BD* (1) O 21- B 23	1.69	10.61	0.120
15. CR (1) C 15	299. RY (3) C 16	1.02	11.06	0.095
15. CR (1) C 15	309. RY (3) C 17	0.54	11.09	0.069
15. CR (1) C 15	319. RY (3) C 18	0.50	11.10	0.067
16. CR (1) C 16	126. BD* (1) C 15- C 16	0.51	10.46	0.065
16. CR (1) C 16	132. BD* (1) C 16- O 22	1.00	10.38	0.091
16. CR (1) C 16	146. BD* (1) O 22- B 23	1.64	10.61	0.118
16. CR (1) C 16	289. RY (3) C 15	0.97	11.05	0.093
16. CR (1) C 16	329. RY (3) C 19	0.54	11.07	0.069
16. CR (1) C 16	339. RY (3) C 20	0.54	11.09	0.069
17. CR (1) C 17	288. RY (2) C 15	1.23	11.00	0.104
17. CR (1) C 17	289. RY (3) C 15	0.61	10.92	0.073
18. CR (1) C 18	288. RY (2) C 15	1.00	11.00	0.094
18. CR (1) C 18	289. RY (3) C 15	0.95	10.92	0.091
19. CR (1) C 19	298. RY (2) C 16	1.14	11.04	0.100
20. CR (1) C 20	298. RY (2) C 16	0.80	11.03	0.084
20. CR (1) C 20	299. RY (3) C 16	1.13	10.92	0.099
21. CR (1) O 21	287. RY (1) C 15	1.83	19.76	0.170
21. CR (1) O 21	367. RY (1) B 23	2.85	19.60	0.211
21. CR (1) O 21	368. RY (2) B 23	0.53	20.01	0.092
22. CR (1) O 22	297. RY (1) C 16	1.64	19.78	0.161
22. CR (1) O 22	298. RY (2) C 16	0.56	19.94	0.094
22. CR (1) O 22	367. RY (1) B 23	2.81	19.60	0.209
22. CR (1) O 22	368. RY (2) B 23	0.50	20.01	0.089
23. CR (1) B 23	106. BD* (1) C 6- C 7	0.60	7.28	0.059
23. CR (1) B 23	108. BD* (1) C 6- C 10	1.04	7.25	0.078
23. CR (1) B 23	129. BD* (1) C 15- O 21	1.58	6.95	0.094
23. CR (1) B 23	132. BD* (1) C 16- O 22	1.53	6.95	0.092
24. CR (1) N 24	101. BD* (1) C 4- C 5	0.79	14.77	0.096
24. CR (1) N 24	188. RY (2) C 5	1.80	15.57	0.149
24. CR (1) N 24	270. RY (4) C 13	0.69	15.00	0.091
25. LP (1) C 12	99. BD* (2) C 3- C 9	98.15	0.14	0.106
25. LP (1) C 12	102. BD* (2) C 4- C 5	0.98	0.13	0.010
25. LP (1) C 12	107. BD* (2) C 6- C 7	1.06	0.14	0.011
25. LP (1) C 12	113. BD* (2) C 8- C 11	98.50	0.14	0.106
25. LP (1) C 12	229. RY (3) C 9	1.95	0.99	0.039
25. LP (1) C 12	230. RY (4) C 9	0.84	1.78	0.034
25. LP (1) C 12	232. RY (6) C 9	0.76	1.93	0.034
25. LP (1) C 12	239. RY (3) C 10	1.25	1.59	0.040
25. LP (1) C 12	241. RY (5) C 10	1.78	1.57	0.047
25. LP (1) C 12	242. RY (6) C 10	0.54	1.81	0.028
25. LP (1) C 12	249. RY (3) C 11	2.04	0.97	0.040
25. LP (1) C 12	250. RY (4) C 11	1.08	1.98	0.041
25. LP (1) C 12	253. RY (7) C 11	0.77	1.95	0.035
25. LP (1) C 12	262. RY (6) C 12	6.03	0.84	0.064
26. LP (1) O 21	109. BD* (1) C 6- B 23	0.89	1.00	0.027
26. LP (1) O 21	126. BD* (1) C 15- C 16	3.48	0.83	0.048
26. LP (1) O 21	127. BD* (1) C 15- C 17	0.85	0.88	0.024
26. LP (1) O 21	146. BD* (1) O 22- B 23	4.64	0.98	0.060
26. LP (1) O 21	287. RY (1) C 15	2.54	1.36	0.052
26. LP (1) O 21	288. RY (2) C 15	0.69	1.50	0.029
26. LP (1) O 21	291. RY (5) C 15	0.62	2.41	0.035
26. LP (1) O 21	367. RY (1) B 23	5.16	1.19	0.070
26. LP (1) O 21	368. RY (2) B 23	1.64	1.61	0.046
27. LP (2) O 21	89. LV (1) B 23	59.60	0.32	0.124
27. LP (2) O 21	109. BD* (1) C 6- B 23	0.59	0.80	0.019
27. LP (2) O 21	126. BD* (1) C 15- C 16	0.52	0.63	0.016

27. LP (2) O 21	127. BD* (1) C 15- C 17	2.78	0.68	0.039
27. LP (2) O 21	128. BD* (1) C 15- C 18	6.03	0.67	0.057
27. LP (2) O 21	137. BD* (1) C 18- H 43	0.87	0.92	0.025
27. LP (2) O 21	290. RY (4) C 15	0.93	2.45	0.043
27. LP (2) O 21	370. RY (4) B 23	1.21	2.07	0.045
28. LP (1) O 22	109. BD* (1) C 6- B 23	0.86	1.00	0.026
28. LP (1) O 22	126. BD* (1) C 15- C 16	3.16	0.84	0.046
28. LP (1) O 22	130. BD* (1) C 16- C 19	0.92	0.88	0.025
28. LP (1) O 22	145. BD* (1) O 21- B 23	4.57	0.98	0.060
28. LP (1) O 22	297. RY (1) C 16	2.21	1.38	0.049
28. LP (1) O 22	298. RY (2) C 16	1.04	1.54	0.036
28. LP (1) O 22	367. RY (1) B 23	5.33	1.20	0.071
28. LP (1) O 22	368. RY (2) B 23	1.65	1.61	0.046
29. LP (2) O 22	89. LV (1) B 23	62.66	0.32	0.126
29. LP (2) O 22	126. BD* (1) C 15- C 16	0.70	0.63	0.019
29. LP (2) O 22	130. BD* (1) C 16- C 19	2.41	0.67	0.036
29. LP (2) O 22	131. BD* (1) C 16- C 20	6.22	0.67	0.058
29. LP (2) O 22	143. BD* (1) C 20- H 49	0.82	0.93	0.025
29. LP (2) O 22	301. RY (5) C 16	0.78	2.40	0.039
29. LP (2) O 22	370. RY (4) B 23	0.98	2.06	0.040
30. LP (1) N 24	89. LV (1) B 23	10.88	0.31	0.052
30. LP (1) N 24	101. BD* (1) C 4- C 5	8.09	0.88	0.075
30. LP (1) N 24	102. BD* (2) C 4- C 5	3.34	0.33	0.029
30. LP (1) N 24	104. BD* (1) C 5- C 10	2.82	0.84	0.043
30. LP (1) N 24	119. BD* (1) C 13- H 33	1.39	0.96	0.033
30. LP (1) N 24	120. BD* (1) C 13- H 34	6.35	0.89	0.067
30. LP (1) N 24	121. BD* (1) C 13- H 35	0.58	0.90	0.020
30. LP (1) N 24	123. BD* (1) C 14- H 36	1.18	0.97	0.030
30. LP (1) N 24	124. BD* (1) C 14- H 37	6.25	0.87	0.066
30. LP (1) N 24	125. BD* (1) C 14- H 38	0.75	0.96	0.024
30. LP (1) N 24	188. RY (2) C 5	0.78	1.68	0.032
30. LP (1) N 24	190. RY (4) C 5	0.75	2.14	0.036
30. LP (1) N 24	268. RY (2) C 13	0.82	1.49	0.031
30. LP (1) N 24	278. RY (2) C 14	0.54	1.45	0.025
31. BD (1) C 1- C 2	91. BD* (1) C 1- C 11	0.78	0.98	0.025
31. BD (1) C 1- C 2	92. BD* (1) C 1- H 25	0.96	1.18	0.030
31. BD (1) C 1- C 2	93. BD* (1) C 1- H 26	1.25	1.27	0.036
31. BD (1) C 1- C 2	94. BD* (1) C 2- C 9	0.84	0.98	0.025
31. BD (1) C 1- C 2	95. BD* (1) C 2- H 27	1.06	1.22	0.032
31. BD (1) C 1- C 2	96. BD* (1) C 2- H 28	0.97	1.19	0.030
31. BD (1) C 1- C 2	98. BD* (1) C 3- C 9	4.44	1.19	0.065
31. BD (1) C 1- C 2	112. BD* (1) C 8- C 11	4.23	1.19	0.063
31. BD (1) C 1- C 2	117. BD* (1) C 11- C 12	0.51	1.14	0.022
32. BD (1) C 1- C 11	92. BD* (1) C 1- H 25	1.38	1.22	0.037
32. BD (1) C 1- C 11	93. BD* (1) C 1- H 26	1.72	1.32	0.042
32. BD (1) C 1- C 11	94. BD* (1) C 2- C 9	0.76	1.02	0.025
32. BD (1) C 1- C 11	95. BD* (1) C 2- H 27	0.62	1.26	0.025
32. BD (1) C 1- C 11	96. BD* (1) C 2- H 28	0.57	1.23	0.024
32. BD (1) C 1- C 11	110. BD* (1) C 7- C 8	1.95	1.15	0.042
32. BD (1) C 1- C 11	112. BD* (1) C 8- C 11	2.59	1.23	0.050
32. BD (1) C 1- C 11	116. BD* (1) C 10- C 12	4.53	1.19	0.066
32. BD (1) C 1- C 11	117. BD* (1) C 11- C 12	1.75	1.18	0.041
32. BD (1) C 1- C 11	217. RY (1) C 8	0.65	1.93	0.032
32. BD (1) C 1- C 11	258. RY (2) C 12	0.53	2.07	0.029
33. BD (1) C 1- H 25	91. BD* (1) C 1- C 11	0.73	0.95	0.024
33. BD (1) C 1- H 25	93. BD* (1) C 1- H 26	1.15	1.25	0.034
33. BD (1) C 1- H 25	94. BD* (1) C 2- C 9	0.56	0.95	0.021
33. BD (1) C 1- H 25	96. BD* (1) C 2- H 28	0.83	1.17	0.028
33. BD (1) C 1- H 25	113. BD* (2) C 8- C 11	3.16	0.59	0.039
33. BD (1) C 1- H 25	117. BD* (1) C 11- C 12	1.07	1.11	0.031
33. BD (1) C 1- H 25	157. RY (1) C 2	0.64	1.57	0.028
33. BD (1) C 1- H 25	249. RY (3) C 11	0.75	1.42	0.029
34. BD (1) C 1- H 26	91. BD* (1) C 1- C 11	0.85	0.97	0.026
34. BD (1) C 1- H 26	92. BD* (1) C 1- H 25	1.06	1.17	0.031
34. BD (1) C 1- H 26	94. BD* (1) C 2- C 9	0.67	0.97	0.023
34. BD (1) C 1- H 26	95. BD* (1) C 2- H 27	0.69	1.22	0.026
34. BD (1) C 1- H 26	113. BD* (2) C 8- C 11	3.18	0.61	0.039
34. BD (1) C 1- H 26	117. BD* (1) C 11- C 12	1.07	1.13	0.031
34. BD (1) C 1- H 26	249. RY (3) C 11	0.69	1.44	0.028
35. BD (1) C 2- C 9	91. BD* (1) C 1- C 11	0.73	1.02	0.024
35. BD (1) C 2- C 9	93. BD* (1) C 1- H 26	0.54	1.31	0.024
35. BD (1) C 2- C 9	95. BD* (1) C 2- H 27	1.53	1.26	0.039
35. BD (1) C 2- C 9	96. BD* (1) C 2- H 28	1.40	1.23	0.037
35. BD (1) C 2- C 9	97. BD* (1) C 3- C 4	2.08	1.15	0.044
35. BD (1) C 2- C 9	98. BD* (1) C 3- C 9	2.60	1.22	0.050
35. BD (1) C 2- C 9	115. BD* (1) C 9- C 12	1.71	1.17	0.040
35. BD (1) C 2- C 9	116. BD* (1) C 10- C 12	4.64	1.19	0.066

35. BD (1) C 2- C 9	167. RY (1) C 3	0.74	1.95	0.034
35. BD (1) C 2- C 9	257. RY (1) C 12	0.64	1.98	0.032
35. BD (1) C 2- C 9	258. RY (2) C 12	0.56	2.06	0.030
36. BD (1) C 2- H 27	91. BD* (1) C 1- C 11	0.63	0.96	0.022
36. BD (1) C 2- H 27	94. BD* (1) C 2- C 9	0.79	0.96	0.025
36. BD (1) C 2- H 27	96. BD* (1) C 2- H 28	1.01	1.18	0.031
36. BD (1) C 2- H 27	99. BD* (2) C 3- C 9	2.94	0.60	0.037
36. BD (1) C 2- H 27	115. BD* (1) C 9- C 12	1.17	1.12	0.032
36. BD (1) C 2- H 27	147. RY (1) C 1	0.59	1.58	0.027
36. BD (1) C 2- H 27	229. RY (3) C 9	0.67	1.45	0.028
37. BD (1) C 2- H 28	91. BD* (1) C 1- C 11	0.53	0.96	0.020
37. BD (1) C 2- H 28	92. BD* (1) C 1- H 25	0.66	1.16	0.025
37. BD (1) C 2- H 28	94. BD* (1) C 2- C 9	0.78	0.95	0.024
37. BD (1) C 2- H 28	95. BD* (1) C 2- H 27	1.02	1.20	0.031
37. BD (1) C 2- H 28	99. BD* (2) C 3- C 9	3.63	0.59	0.041
37. BD (1) C 2- H 28	115. BD* (1) C 9- C 12	1.06	1.11	0.031
37. BD (1) C 2- H 28	147. RY (1) C 1	0.52	1.57	0.026
37. BD (1) C 2- H 28	229. RY (3) C 9	0.70	1.44	0.028
38. BD (1) C 3- C 4	94. BD* (1) C 2- C 9	5.59	1.07	0.069
38. BD (1) C 3- C 4	98. BD* (1) C 3- C 9	3.54	1.28	0.060
38. BD (1) C 3- C 4	100. BD* (1) C 3- H 29	2.54	1.43	0.054
38. BD (1) C 3- C 4	101. BD* (1) C 4- C 5	3.48	1.26	0.059
38. BD (1) C 3- C 4	103. BD* (1) C 4- H 30	2.64	1.41	0.054
38. BD (1) C 3- C 4	105. BD* (1) C 5- N 24	4.48	1.07	0.062
38. BD (1) C 3- C 4	187. RY (1) C 5	2.04	1.74	0.053
38. BD (1) C 3- C 4	188. RY (2) C 5	0.60	2.06	0.031
38. BD (1) C 3- C 4	227. RY (1) C 9	1.69	1.93	0.051
38. BD (1) C 3- C 4	228. RY (2) C 9	0.64	1.88	0.031
39. BD (1) C 3- C 9	94. BD* (1) C 2- C 9	2.13	1.12	0.044
39. BD (1) C 3- C 9	97. BD* (1) C 3- C 4	2.52	1.26	0.050
39. BD (1) C 3- C 9	100. BD* (1) C 3- H 29	3.94	1.47	0.068
39. BD (1) C 3- C 9	103. BD* (1) C 4- H 30	1.70	1.45	0.044
39. BD (1) C 3- C 9	115. BD* (1) C 9- C 12	4.11	1.28	0.065
39. BD (1) C 3- C 9	117. BD* (1) C 11- C 12	2.38	1.28	0.049
39. BD (1) C 3- C 9	177. RY (1) C 4	0.70	2.02	0.034
39. BD (1) C 3- C 9	178. RY (2) C 4	1.00	1.57	0.035
39. BD (1) C 3- C 9	258. RY (2) C 12	1.12	2.17	0.044
40. BD (2) C 3- C 9	95. BD* (1) C 2- H 27	1.47	0.91	0.033
40. BD (2) C 3- C 9	96. BD* (1) C 2- H 28	1.51	0.88	0.033
40. BD (2) C 3- C 9	102. BD* (2) C 4- C 5	18.49	0.29	0.066
40. BD (2) C 3- C 9	179. RY (3) C 4	1.79	1.18	0.041
40. BD (2) C 3- C 9	260. RY (4) C 12	0.52	2.16	0.030
40. BD (2) C 3- C 9	262. RY (6) C 12	0.83	1.00	0.026
41. BD (1) C 3- H 29	97. BD* (1) C 3- C 4	1.10	1.13	0.032
41. BD (1) C 3- H 29	98. BD* (1) C 3- C 9	2.11	1.20	0.045
41. BD (1) C 3- H 29	101. BD* (1) C 4- C 5	3.42	1.18	0.057
41. BD (1) C 3- H 29	115. BD* (1) C 9- C 12	4.13	1.15	0.062
41. BD (1) C 3- H 29	177. RY (1) C 4	0.78	1.89	0.034
41. BD (1) C 3- H 29	227. RY (1) C 9	1.37	1.85	0.045
42. BD (1) C 4- C 5	97. BD* (1) C 3- C 4	2.87	1.25	0.053
42. BD (1) C 4- C 5	100. BD* (1) C 3- H 29	1.50	1.46	0.042
42. BD (1) C 4- C 5	103. BD* (1) C 4- H 30	3.25	1.45	0.061
42. BD (1) C 4- C 5	104. BD* (1) C 5- C 10	3.89	1.25	0.062
42. BD (1) C 4- C 5	105. BD* (1) C 5- N 24	1.05	1.11	0.031
42. BD (1) C 4- C 5	108. BD* (1) C 6- C 10	3.27	1.27	0.057
42. BD (1) C 4- C 5	122. BD* (1) C 14- N 24	0.52	1.05	0.021
42. BD (1) C 4- C 5	168. RY (2) C 3	1.05	1.45	0.035
42. BD (1) C 4- C 5	237. RY (1) C 10	1.33	2.07	0.047
43. BD (2) C 4- C 5	88. LV (1) C 10	56.10	0.17	0.086
43. BD (2) C 4- C 5	99. BD* (2) C 3- C 9	15.96	0.31	0.063
43. BD (2) C 4- C 5	118. BD* (1) C 13- N 24	0.90	0.61	0.021
43. BD (2) C 4- C 5	122. BD* (1) C 14- N 24	2.46	0.60	0.034
43. BD (2) C 4- C 5	123. BD* (1) C 14- H 36	0.63	0.94	0.022
43. BD (2) C 4- C 5	169. RY (3) C 3	1.89	1.04	0.040
43. BD (2) C 4- C 5	239. RY (3) C 10	0.86	1.76	0.035
44. BD (1) C 4- H 30	97. BD* (1) C 3- C 4	1.02	1.13	0.030
44. BD (1) C 4- H 30	98. BD* (1) C 3- C 9	3.10	1.20	0.054
44. BD (1) C 4- H 30	101. BD* (1) C 4- C 5	1.91	1.17	0.042
44. BD (1) C 4- H 30	104. BD* (1) C 5- C 10	5.19	1.13	0.068
44. BD (1) C 4- H 30	167. RY (1) C 3	0.82	1.92	0.035
44. BD (1) C 4- H 30	188. RY (2) C 5	1.51	1.97	0.049
45. BD (1) C 5- C 10	101. BD* (1) C 4- C 5	3.19	1.26	0.057
45. BD (1) C 5- C 10	103. BD* (1) C 4- H 30	1.71	1.42	0.044
45. BD (1) C 5- C 10	105. BD* (1) C 5- N 24	0.89	1.08	0.028
45. BD (1) C 5- C 10	106. BD* (1) C 6- C 7	1.36	1.26	0.037
45. BD (1) C 5- C 10	108. BD* (1) C 6- C 10	4.18	1.23	0.064
45. BD (1) C 5- C 10	116. BD* (1) C 10- C 12	3.61	1.26	0.060

45. BD (1) C 5- C 10	117. BD* (1) C 11- C 12	3.26	1.24	0.057
45. BD (1) C 5- C 10	118. BD* (1) C 13- N 24	1.72	1.02	0.037
45. BD (1) C 5- C 10	122. BD* (1) C 14- N 24	0.52	1.01	0.021
45. BD (1) C 5- C 10	178. RY (2) C 4	0.79	1.53	0.031
45. BD (1) C 5- C 10	197. RY (1) C 6	0.98	2.38	0.043
45. BD (1) C 5- C 10	257. RY (1) C 12	1.47	2.05	0.049
45. BD (1) C 5- C 10	377. RY (1) N 24	0.74	1.79	0.032
46. BD (1) C 5- N 24	97. BD* (1) C 3- C 4	1.69	1.28	0.042
46. BD (1) C 5- N 24	101. BD* (1) C 4- C 5	2.02	1.33	0.046
46. BD (1) C 5- N 24	104. BD* (1) C 5- C 10	1.52	1.29	0.040
46. BD (1) C 5- N 24	116. BD* (1) C 10- C 12	2.00	1.33	0.046
46. BD (1) C 5- N 24	119. BD* (1) C 13- H 33	0.80	1.41	0.030
46. BD (1) C 5- N 24	122. BD* (1) C 14- N 24	0.52	1.08	0.021
46. BD (1) C 5- N 24	123. BD* (1) C 14- H 36	0.94	1.42	0.033
46. BD (1) C 5- N 24	237. RY (1) C 10	0.97	2.11	0.040
46. BD (1) C 5- N 24	238. RY (2) C 10	0.55	2.20	0.031
46. BD (1) C 5- N 24	278. RY (2) C 14	0.71	1.91	0.033
47. BD (1) C 6- C 7	89. LV (1) B 23	2.42	0.71	0.037
47. BD (1) C 6- C 7	104. BD* (1) C 5- C 10	4.12	1.23	0.064
47. BD (1) C 6- C 7	108. BD* (1) C 6- C 10	3.46	1.24	0.059
47. BD (1) C 6- C 7	109. BD* (1) C 6- B 23	4.28	1.18	0.063
47. BD (1) C 6- C 7	110. BD* (1) C 7- C 8	2.51	1.23	0.050
47. BD (1) C 6- C 7	111. BD* (1) C 7- H 31	2.96	1.40	0.057
47. BD (1) C 6- C 7	114. BD* (1) C 8- H 32	1.51	1.37	0.040
47. BD (1) C 6- C 7	145. BD* (1) O 21- B 23	0.76	1.17	0.027
47. BD (1) C 6- C 7	218. RY (2) C 8	1.25	1.41	0.038
47. BD (1) C 6- C 7	237. RY (1) C 10	2.04	2.05	0.058
48. BD (2) C 6- C 7	88. LV (1) C 10	66.65	0.15	0.089
48. BD (2) C 6- C 7	113. BD* (2) C 8- C 11	16.65	0.29	0.062
48. BD (2) C 6- C 7	145. BD* (1) O 21- B 23	4.83	0.73	0.053
48. BD (2) C 6- C 7	146. BD* (1) O 22- B 23	4.94	0.73	0.054
48. BD (2) C 6- C 7	219. RY (3) C 8	1.65	0.92	0.035
48. BD (2) C 6- C 7	241. RY (5) C 10	0.72	1.72	0.031
49. BD (1) C 6- C 10	101. BD* (1) C 4- C 5	1.70	1.26	0.041
49. BD (1) C 6- C 10	104. BD* (1) C 5- C 10	3.98	1.22	0.062
49. BD (1) C 6- C 10	106. BD* (1) C 6- C 7	2.91	1.26	0.054
49. BD (1) C 6- C 10	109. BD* (1) C 6- B 23	4.08	1.17	0.062
49. BD (1) C 6- C 10	111. BD* (1) C 7- H 31	2.12	1.38	0.048
49. BD (1) C 6- C 10	115. BD* (1) C 9- C 12	3.19	1.24	0.056
49. BD (1) C 6- C 10	116. BD* (1) C 10- C 12	4.10	1.25	0.064
49. BD (1) C 6- C 10	188. RY (2) C 5	1.20	2.06	0.044
49. BD (1) C 6- C 10	208. RY (2) C 7	0.68	1.55	0.029
49. BD (1) C 6- C 10	257. RY (1) C 12	1.26	2.05	0.045
50. BD (1) C 6- B 23	106. BD* (1) C 6- C 7	2.66	1.12	0.049
50. BD (1) C 6- B 23	108. BD* (1) C 6- C 10	3.11	1.09	0.052
50. BD (1) C 6- B 23	110. BD* (1) C 7- C 8	4.89	1.07	0.065
50. BD (1) C 6- B 23	116. BD* (1) C 10- C 12	4.12	1.11	0.060
50. BD (1) C 6- B 23	129. BD* (1) C 15- O 21	2.45	0.79	0.039
50. BD (1) C 6- B 23	132. BD* (1) C 16- O 22	2.51	0.79	0.040
50. BD (1) C 6- B 23	207. RY (1) C 7	1.48	1.85	0.047
50. BD (1) C 6- B 23	237. RY (1) C 10	2.06	1.90	0.056
50. BD (1) C 6- B 23	238. RY (2) C 10	0.75	1.98	0.034
51. BD (1) C 7- C 8	91. BD* (1) C 1- C 11	5.89	1.07	0.071
51. BD (1) C 7- C 8	106. BD* (1) C 6- C 7	2.96	1.25	0.054
51. BD (1) C 7- C 8	109. BD* (1) C 6- B 23	2.50	1.16	0.048
51. BD (1) C 7- C 8	111. BD* (1) C 7- H 31	2.01	1.38	0.047
51. BD (1) C 7- C 8	112. BD* (1) C 8- C 11	3.45	1.28	0.059
51. BD (1) C 7- C 8	114. BD* (1) C 8- H 32	2.16	1.34	0.048
51. BD (1) C 7- C 8	197. RY (1) C 6	0.77	2.37	0.038
51. BD (1) C 7- C 8	198. RY (2) C 6	1.85	1.74	0.051
51. BD (1) C 7- C 8	247. RY (1) C 11	1.38	1.96	0.046
51. BD (1) C 7- C 8	248. RY (2) C 11	0.95	1.84	0.037
52. BD (1) C 7- H 31	106. BD* (1) C 6- C 7	1.63	1.16	0.039
52. BD (1) C 7- H 31	108. BD* (1) C 6- C 10	4.07	1.13	0.060
52. BD (1) C 7- H 31	110. BD* (1) C 7- C 8	0.81	1.11	0.027
52. BD (1) C 7- H 31	112. BD* (1) C 8- C 11	3.38	1.18	0.056
52. BD (1) C 7- H 31	197. RY (1) C 6	0.81	2.27	0.038
52. BD (1) C 7- H 31	217. RY (1) C 8	0.73	1.89	0.033
53. BD (1) C 8- C 11	91. BD* (1) C 1- C 11	2.27	1.12	0.045
53. BD (1) C 8- C 11	110. BD* (1) C 7- C 8	2.48	1.26	0.050
53. BD (1) C 8- C 11	111. BD* (1) C 7- H 31	1.38	1.42	0.040
53. BD (1) C 8- C 11	114. BD* (1) C 8- H 32	3.31	1.39	0.061
53. BD (1) C 8- C 11	115. BD* (1) C 9- C 12	2.28	1.28	0.048
53. BD (1) C 8- C 11	117. BD* (1) C 11- C 12	4.02	1.28	0.064
53. BD (1) C 8- C 11	207. RY (1) C 7	0.75	2.03	0.035
53. BD (1) C 8- C 11	208. RY (2) C 7	0.99	1.59	0.035
53. BD (1) C 8- C 11	258. RY (2) C 12	1.33	2.17	0.048

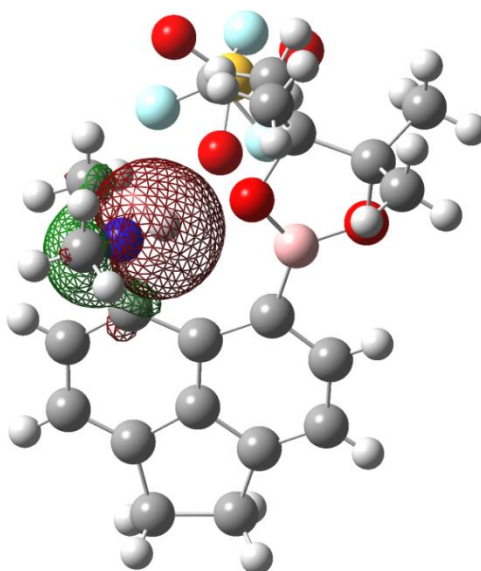
54. BD (2) C 8- C 11	92. BD* (1) C 1- H 25	1.71	0.87	0.034
54. BD (2) C 8- C 11	93. BD* (1) C 1- H 26	1.55	0.96	0.034
54. BD (2) C 8- C 11	107. BD* (2) C 6- C 7	18.35	0.30	0.067
54. BD (2) C 8- C 11	209. RY (3) C 7	1.47	1.59	0.043
54. BD (2) C 8- C 11	262. RY (6) C 12	1.06	1.00	0.029
55. BD (1) C 8- H 32	106. BD* (1) C 6- C 7	3.38	1.16	0.056
55. BD (1) C 8- H 32	110. BD* (1) C 7- C 8	0.98	1.11	0.030
55. BD (1) C 8- H 32	112. BD* (1) C 8- C 11	1.85	1.19	0.042
55. BD (1) C 8- H 32	117. BD* (1) C 11- C 12	4.03	1.14	0.060
55. BD (1) C 8- H 32	207. RY (1) C 7	0.69	1.89	0.032
55. BD (1) C 8- H 32	247. RY (1) C 11	1.47	1.87	0.047
56. BD (1) C 9- C 12	94. BD* (1) C 2- C 9	1.08	1.08	0.030
56. BD (1) C 9- C 12	95. BD* (1) C 2- H 27	0.56	1.32	0.024
56. BD (1) C 9- C 12	98. BD* (1) C 3- C 9	3.75	1.29	0.062
56. BD (1) C 9- C 12	100. BD* (1) C 3- H 29	2.66	1.43	0.055
56. BD (1) C 9- C 12	108. BD* (1) C 6- C 10	2.50	1.23	0.050
56. BD (1) C 9- C 12	112. BD* (1) C 8- C 11	2.79	1.29	0.053
56. BD (1) C 9- C 12	116. BD* (1) C 10- C 12	4.71	1.25	0.069
56. BD (1) C 9- C 12	117. BD* (1) C 11- C 12	3.43	1.24	0.058
56. BD (1) C 9- C 12	168. RY (2) C 3	0.75	1.42	0.029
56. BD (1) C 9- C 12	238. RY (2) C 10	1.32	2.12	0.047
56. BD (1) C 9- C 12	247. RY (1) C 11	1.34	1.97	0.046
57. BD (1) C 10- C 12	91. BD* (1) C 1- C 11	1.65	1.09	0.038
57. BD (1) C 10- C 12	94. BD* (1) C 2- C 9	1.57	1.09	0.037
57. BD (1) C 10- C 12	104. BD* (1) C 5- C 10	3.39	1.23	0.058
57. BD (1) C 10- C 12	105. BD* (1) C 5- N 24	3.42	1.09	0.054
57. BD (1) C 10- C 12	108. BD* (1) C 6- C 10	3.83	1.24	0.062
57. BD (1) C 10- C 12	109. BD* (1) C 6- B 23	2.60	1.18	0.049
57. BD (1) C 10- C 12	115. BD* (1) C 9- C 12	4.66	1.25	0.068
57. BD (1) C 10- C 12	117. BD* (1) C 11- C 12	4.49	1.25	0.067
57. BD (1) C 10- C 12	187. RY (1) C 5	0.85	1.76	0.035
57. BD (1) C 10- C 12	188. RY (2) C 5	0.66	2.07	0.033
57. BD (1) C 10- C 12	197. RY (1) C 6	1.14	2.38	0.047
57. BD (1) C 10- C 12	228. RY (2) C 9	1.14	1.89	0.041
57. BD (1) C 10- C 12	248. RY (2) C 11	1.09	1.86	0.040
58. BD (1) C 11- C 12	91. BD* (1) C 1- C 11	1.12	1.08	0.031
58. BD (1) C 11- C 12	92. BD* (1) C 1- H 25	0.60	1.28	0.025
58. BD (1) C 11- C 12	93. BD* (1) C 1- H 26	0.52	1.38	0.024
58. BD (1) C 11- C 12	98. BD* (1) C 3- C 9	2.76	1.29	0.053
58. BD (1) C 11- C 12	104. BD* (1) C 5- C 10	2.46	1.22	0.049
58. BD (1) C 11- C 12	112. BD* (1) C 8- C 11	3.76	1.29	0.062
58. BD (1) C 11- C 12	114. BD* (1) C 8- H 32	2.82	1.35	0.055
58. BD (1) C 11- C 12	115. BD* (1) C 9- C 12	3.34	1.24	0.057
58. BD (1) C 11- C 12	116. BD* (1) C 10- C 12	4.75	1.25	0.069
58. BD (1) C 11- C 12	217. RY (1) C 8	0.54	1.99	0.029
58. BD (1) C 11- C 12	218. RY (2) C 8	0.85	1.40	0.031
58. BD (1) C 11- C 12	227. RY (1) C 9	1.08	1.93	0.041
58. BD (1) C 11- C 12	228. RY (2) C 9	0.55	1.88	0.029
58. BD (1) C 11- C 12	238. RY (2) C 10	1.64	2.12	0.053
59. BD (1) C 13- N 24	102. BD* (2) C 4- C 5	1.32	0.73	0.028
59. BD (1) C 13- N 24	104. BD* (1) C 5- C 10	2.25	1.24	0.047
59. BD (1) C 13- N 24	105. BD* (1) C 5- N 24	0.76	1.10	0.026
59. BD (1) C 13- N 24	119. BD* (1) C 13- H 33	0.85	1.36	0.030
59. BD (1) C 13- N 24	121. BD* (1) C 13- H 35	0.59	1.30	0.025
59. BD (1) C 13- N 24	125. BD* (1) C 14- H 38	1.27	1.36	0.037
59. BD (1) C 13- N 24	187. RY (1) C 5	1.61	1.77	0.048
59. BD (1) C 13- N 24	277. RY (1) C 14	0.89	1.71	0.035
60. BD (1) C 13- H 33	105. BD* (1) C 5- N 24	3.26	0.98	0.050
60. BD (1) C 13- H 33	120. BD* (1) C 13- H 34	0.92	1.17	0.029
60. BD (1) C 13- H 33	121. BD* (1) C 13- H 35	1.18	1.18	0.033
61. BD (1) C 13- H 34	119. BD* (1) C 13- H 33	1.11	1.23	0.033
61. BD (1) C 13- H 34	121. BD* (1) C 13- H 35	0.88	1.18	0.029
62. BD (1) C 13- H 35	119. BD* (1) C 13- H 33	1.41	1.22	0.037
62. BD (1) C 13- H 35	120. BD* (1) C 13- H 34	0.79	1.15	0.027
62. BD (1) C 13- H 35	122. BD* (1) C 14- N 24	3.16	0.90	0.048
63. BD (1) C 14- N 24	101. BD* (1) C 4- C 5	0.73	1.27	0.027
63. BD (1) C 14- N 24	102. BD* (2) C 4- C 5	3.77	0.72	0.046
63. BD (1) C 14- N 24	104. BD* (1) C 5- C 10	0.56	1.23	0.023
63. BD (1) C 14- N 24	105. BD* (1) C 5- N 24	0.76	1.09	0.026
63. BD (1) C 14- N 24	121. BD* (1) C 13- H 35	1.37	1.29	0.038
63. BD (1) C 14- N 24	123. BD* (1) C 14- H 36	0.72	1.36	0.028
63. BD (1) C 14- N 24	125. BD* (1) C 14- H 38	0.69	1.35	0.027
63. BD (1) C 14- N 24	189. RY (3) C 5	1.55	1.61	0.045
63. BD (1) C 14- N 24	267. RY (1) C 13	1.06	1.66	0.037
64. BD (1) C 14- H 36	105. BD* (1) C 5- N 24	3.04	0.97	0.049
64. BD (1) C 14- H 36	124. BD* (1) C 14- H 37	0.81	1.15	0.027
64. BD (1) C 14- H 36	125. BD* (1) C 14- H 38	1.40	1.24	0.037

65. BD (1) C 14- H 37	123. BD* (1) C 14- H 36	1.09	1.24	0.033
65. BD (1) C 14- H 37	125. BD* (1) C 14- H 38	1.05	1.22	0.032
66. BD (1) C 14- H 38	118. BD* (1) C 13- N 24	2.98	0.90	0.046
66. BD (1) C 14- H 38	123. BD* (1) C 14- H 36	1.60	1.24	0.040
66. BD (1) C 14- H 38	124. BD* (1) C 14- H 37	0.88	1.14	0.028
67. BD (1) C 15- C 16	109. BD* (1) C 6- B 23	1.47	1.12	0.036
67. BD (1) C 15- C 16	127. BD* (1) C 15- C 17	0.81	1.00	0.025
67. BD (1) C 15- C 16	128. BD* (1) C 15- C 18	0.63	0.99	0.022
67. BD (1) C 15- C 16	130. BD* (1) C 16- C 19	0.78	1.00	0.025
67. BD (1) C 15- C 16	131. BD* (1) C 16- C 20	0.66	1.00	0.023
67. BD (1) C 15- C 16	133. BD* (1) C 17- H 39	1.12	1.30	0.034
67. BD (1) C 15- C 16	136. BD* (1) C 18- H 42	1.09	1.24	0.033
67. BD (1) C 15- C 16	139. BD* (1) C 19- H 45	1.09	1.28	0.033
67. BD (1) C 15- C 16	142. BD* (1) C 20- H 48	1.18	1.28	0.035
67. BD (1) C 15- C 16	145. BD* (1) O 21- B 23	0.93	1.10	0.029
67. BD (1) C 15- C 16	146. BD* (1) O 22- B 23	0.94	1.10	0.029
67. BD (1) C 15- C 16	308. RY (2) C 17	0.61	1.47	0.027
67. BD (1) C 15- C 16	317. RY (1) C 18	0.61	1.49	0.027
67. BD (1) C 15- C 16	328. RY (2) C 19	0.58	1.46	0.026
67. BD (1) C 15- C 16	337. RY (1) C 20	0.53	1.48	0.025
68. BD (1) C 15- C 17	126. BD* (1) C 15- C 16	0.83	0.95	0.025
68. BD (1) C 15- C 17	128. BD* (1) C 15- C 18	0.62	0.99	0.022
68. BD (1) C 15- C 17	132. BD* (1) C 16- O 22	1.09	0.87	0.028
68. BD (1) C 15- C 17	133. BD* (1) C 17- H 39	2.01	1.30	0.046
68. BD (1) C 15- C 17	134. BD* (1) C 17- H 40	1.44	1.24	0.038
68. BD (1) C 15- C 17	135. BD* (1) C 17- H 41	1.64	1.22	0.040
68. BD (1) C 15- C 17	138. BD* (1) C 18- H 44	1.43	1.24	0.038
68. BD (1) C 15- C 17	145. BD* (1) O 21- B 23	1.63	1.10	0.038
68. BD (1) C 15- C 17	299. RY (3) C 16	0.82	1.55	0.032
68. BD (1) C 15- C 17	348. RY (2) O 21	0.86	1.92	0.036
69. BD (1) C 15- C 18	126. BD* (1) C 15- C 16	0.78	0.95	0.024
69. BD (1) C 15- C 18	127. BD* (1) C 15- C 17	0.59	0.99	0.022
69. BD (1) C 15- C 18	131. BD* (1) C 16- C 20	1.70	0.99	0.037
69. BD (1) C 15- C 18	135. BD* (1) C 17- H 41	1.56	1.21	0.039
69. BD (1) C 15- C 18	136. BD* (1) C 18- H 42	1.58	1.23	0.039
69. BD (1) C 15- C 18	137. BD* (1) C 18- H 43	1.57	1.23	0.039
69. BD (1) C 15- C 18	138. BD* (1) C 18- H 44	1.47	1.23	0.038
69. BD (1) C 15- C 18	145. BD* (1) O 21- B 23	1.28	1.09	0.033
69. BD (1) C 15- C 18	297. RY (1) C 16	0.69	1.49	0.029
69. BD (1) C 15- C 18	298. RY (2) C 16	0.55	1.65	0.027
69. BD (1) C 15- C 18	307. RY (1) C 17	0.80	1.43	0.030
69. BD (1) C 15- C 18	347. RY (1) O 21	0.64	1.82	0.030
70. BD (1) C 15- O 21	89. LV (1) B 23	0.58	0.80	0.019
70. BD (1) C 15- O 21	109. BD* (1) C 6- B 23	3.53	1.28	0.060
70. BD (1) C 15- O 21	130. BD* (1) C 16- C 19	1.18	1.16	0.033
70. BD (1) C 15- O 21	132. BD* (1) C 16- O 22	1.23	1.03	0.032
70. BD (1) C 15- O 21	134. BD* (1) C 17- H 40	1.06	1.40	0.034
70. BD (1) C 15- O 21	137. BD* (1) C 18- H 43	1.14	1.40	0.036
70. BD (1) C 15- O 21	145. BD* (1) O 21- B 23	1.51	1.26	0.039
70. BD (1) C 15- O 21	146. BD* (1) O 22- B 23	1.28	1.26	0.036
70. BD (1) C 15- O 21	367. RY (1) B 23	2.83	1.47	0.058
71. BD (1) C 16- C 19	126. BD* (1) C 15- C 16	0.85	0.95	0.025
71. BD (1) C 16- C 19	129. BD* (1) C 15- O 21	1.13	0.88	0.028
71. BD (1) C 16- C 19	131. BD* (1) C 16- C 20	0.62	1.00	0.022
71. BD (1) C 16- C 19	139. BD* (1) C 19- H 45	1.86	1.27	0.043
71. BD (1) C 16- C 19	140. BD* (1) C 19- H 46	1.59	1.28	0.040
71. BD (1) C 16- C 19	141. BD* (1) C 19- H 47	1.52	1.21	0.038
71. BD (1) C 16- C 19	144. BD* (1) C 20- H 50	1.49	1.26	0.039
71. BD (1) C 16- C 19	146. BD* (1) O 22- B 23	1.60	1.10	0.037
71. BD (1) C 16- C 19	289. RY (3) C 15	0.76	1.54	0.031
71. BD (1) C 16- C 19	358. RY (2) O 22	0.79	1.86	0.034
72. BD (1) C 16- C 20	126. BD* (1) C 15- C 16	0.80	0.95	0.025
72. BD (1) C 16- C 20	128. BD* (1) C 15- C 18	1.72	0.99	0.037
72. BD (1) C 16- C 20	130. BD* (1) C 16- C 19	0.62	0.99	0.022
72. BD (1) C 16- C 20	141. BD* (1) C 19- H 47	1.69	1.21	0.040
72. BD (1) C 16- C 20	142. BD* (1) C 20- H 48	1.91	1.28	0.044
72. BD (1) C 16- C 20	143. BD* (1) C 20- H 49	1.62	1.25	0.040
72. BD (1) C 16- C 20	144. BD* (1) C 20- H 50	1.66	1.26	0.041
72. BD (1) C 16- C 20	146. BD* (1) O 22- B 23	1.20	1.10	0.032
72. BD (1) C 16- C 20	287. RY (1) C 15	0.58	1.48	0.026
72. BD (1) C 16- C 20	288. RY (2) C 15	0.61	1.62	0.028
72. BD (1) C 16- C 20	327. RY (1) C 19	0.76	1.47	0.030
72. BD (1) C 16- C 20	357. RY (1) O 22	0.52	1.81	0.027
73. BD (1) C 16- O 22	109. BD* (1) C 6- B 23	3.55	1.27	0.060
73. BD (1) C 16- O 22	127. BD* (1) C 15- C 17	1.27	1.15	0.034
73. BD (1) C 16- O 22	129. BD* (1) C 15- O 21	1.28	1.03	0.032
73. BD (1) C 16- O 22	140. BD* (1) C 19- H 46	1.02	1.43	0.034

73. BD (1) C 16- O 22	143. BD* (1) C 20- H 49	1.21	1.40	0.037
73. BD (1) C 16- O 22	145. BD* (1) O 21- B 23	1.28	1.25	0.036
73. BD (1) C 16- O 22	146. BD* (1) O 22- B 23	1.38	1.25	0.037
73. BD (1) C 16- O 22	367. RY (1) B 23	2.72	1.46	0.056
74. BD (1) C 17- H 39	126. BD* (1) C 15- C 16	3.56	0.90	0.051
74. BD (1) C 17- H 39	127. BD* (1) C 15- C 17	1.01	0.94	0.028
74. BD (1) C 17- H 39	134. BD* (1) C 17- H 40	1.24	1.18	0.034
74. BD (1) C 17- H 39	135. BD* (1) C 17- H 41	1.34	1.17	0.035
74. BD (1) C 17- H 39	288. RY (2) C 15	0.63	1.57	0.028
75. BD (1) C 17- H 40	127. BD* (1) C 15- C 17	0.66	0.94	0.022
75. BD (1) C 17- H 40	129. BD* (1) C 15- O 21	4.78	0.82	0.056
75. BD (1) C 17- H 40	133. BD* (1) C 17- H 39	1.32	1.25	0.036
75. BD (1) C 17- H 40	135. BD* (1) C 17- H 41	0.96	1.16	0.030
75. BD (1) C 17- H 40	287. RY (1) C 15	0.77	1.42	0.029
76. BD (1) C 17- H 41	127. BD* (1) C 15- C 17	0.82	0.93	0.025
76. BD (1) C 17- H 41	128. BD* (1) C 15- C 18	3.00	0.92	0.047
76. BD (1) C 17- H 41	129. BD* (1) C 15- O 21	0.85	0.81	0.023
76. BD (1) C 17- H 41	133. BD* (1) C 17- H 39	1.37	1.23	0.037
76. BD (1) C 17- H 41	134. BD* (1) C 17- H 40	1.07	1.17	0.032
76. BD (1) C 17- H 41	289. RY (3) C 15	0.69	1.47	0.028
77. BD (1) C 18- H 42	126. BD* (1) C 15- C 16	3.61	0.89	0.050
77. BD (1) C 18- H 42	128. BD* (1) C 15- C 18	0.96	0.92	0.027
77. BD (1) C 18- H 42	129. BD* (1) C 15- O 21	0.80	0.81	0.023
77. BD (1) C 18- H 42	137. BD* (1) C 18- H 43	1.16	1.17	0.033
77. BD (1) C 18- H 42	138. BD* (1) C 18- H 44	1.19	1.18	0.033
78. BD (1) C 18- H 43	128. BD* (1) C 15- C 18	0.62	0.93	0.021
78. BD (1) C 18- H 43	129. BD* (1) C 15- O 21	4.32	0.82	0.053
78. BD (1) C 18- H 43	136. BD* (1) C 18- H 42	1.01	1.17	0.031
78. BD (1) C 18- H 43	138. BD* (1) C 18- H 44	1.05	1.18	0.031
78. BD (1) C 18- H 43	288. RY (2) C 15	0.79	1.56	0.031
79. BD (1) C 18- H 44	127. BD* (1) C 15- C 17	3.05	0.93	0.048
79. BD (1) C 18- H 44	128. BD* (1) C 15- C 18	0.86	0.92	0.025
79. BD (1) C 18- H 44	136. BD* (1) C 18- H 42	1.12	1.17	0.032
79. BD (1) C 18- H 44	137. BD* (1) C 18- H 43	1.06	1.18	0.032
79. BD (1) C 18- H 44	289. RY (3) C 15	1.00	1.48	0.034
80. BD (1) C 19- H 45	126. BD* (1) C 15- C 16	3.71	0.89	0.051
80. BD (1) C 19- H 45	130. BD* (1) C 16- C 19	0.92	0.93	0.026
80. BD (1) C 19- H 45	140. BD* (1) C 19- H 46	1.41	1.22	0.037
80. BD (1) C 19- H 45	141. BD* (1) C 19- H 47	1.21	1.14	0.033
80. BD (1) C 19- H 45	298. RY (2) C 16	0.51	1.60	0.026
81. BD (1) C 19- H 46	130. BD* (1) C 16- C 19	0.65	0.94	0.022
81. BD (1) C 19- H 46	132. BD* (1) C 16- O 22	4.71	0.82	0.056
81. BD (1) C 19- H 46	139. BD* (1) C 19- H 45	1.37	1.22	0.037
81. BD (1) C 19- H 46	141. BD* (1) C 19- H 47	0.95	1.16	0.030
81. BD (1) C 19- H 46	297. RY (1) C 16	0.89	1.44	0.032
82. BD (1) C 19- H 47	130. BD* (1) C 16- C 19	0.79	0.92	0.024
82. BD (1) C 19- H 47	131. BD* (1) C 16- C 20	2.66	0.93	0.044
82. BD (1) C 19- H 47	132. BD* (1) C 16- O 22	0.81	0.80	0.023
82. BD (1) C 19- H 47	139. BD* (1) C 19- H 45	1.28	1.20	0.035
82. BD (1) C 19- H 47	140. BD* (1) C 19- H 46	1.22	1.21	0.034
82. BD (1) C 19- H 47	299. RY (3) C 16	0.70	1.48	0.029
83. BD (1) C 20- H 48	126. BD* (1) C 15- C 16	3.58	0.89	0.050
83. BD (1) C 20- H 48	131. BD* (1) C 16- C 20	1.04	0.93	0.028
83. BD (1) C 20- H 48	132. BD* (1) C 16- O 22	0.84	0.81	0.023
83. BD (1) C 20- H 48	143. BD* (1) C 20- H 49	1.33	1.19	0.035
83. BD (1) C 20- H 48	144. BD* (1) C 20- H 50	1.43	1.19	0.037
83. BD (1) C 20- H 48	297. RY (1) C 16	0.53	1.43	0.024
84. BD (1) C 20- H 49	131. BD* (1) C 16- C 20	0.66	0.94	0.022
84. BD (1) C 20- H 49	132. BD* (1) C 16- O 22	4.26	0.81	0.053
84. BD (1) C 20- H 49	142. BD* (1) C 20- H 48	1.27	1.22	0.035
84. BD (1) C 20- H 49	144. BD* (1) C 20- H 50	1.17	1.20	0.033
84. BD (1) C 20- H 49	298. RY (2) C 16	0.90	1.60	0.034
85. BD (1) C 20- H 50	130. BD* (1) C 16- C 19	3.10	0.93	0.048
85. BD (1) C 20- H 50	131. BD* (1) C 16- C 20	0.92	0.93	0.026
85. BD (1) C 20- H 50	142. BD* (1) C 20- H 48	1.42	1.21	0.037
85. BD (1) C 20- H 50	143. BD* (1) C 20- H 49	1.15	1.19	0.033
85. BD (1) C 20- H 50	299. RY (3) C 16	1.12	1.48	0.036
86. BD (1) O 21- B 23	107. BD* (2) C 6- C 7	0.53	0.94	0.020
86. BD (1) O 21- B 23	127. BD* (1) C 15- C 17	1.39	1.27	0.037
86. BD (1) O 21- B 23	129. BD* (1) C 15- O 21	1.06	1.15	0.031
86. BD (1) O 21- B 23	197. RY (1) C 6	0.74	2.59	0.039
86. BD (1) O 21- B 23	287. RY (1) C 15	3.56	1.75	0.070
86. BD (1) O 21- B 23	367. RY (1) B 23	0.98	1.58	0.035
87. BD (1) O 22- B 23	107. BD* (2) C 6- C 7	0.75	0.93	0.024
87. BD (1) O 22- B 23	130. BD* (1) C 16- C 19	1.37	1.26	0.037
87. BD (1) O 22- B 23	132. BD* (1) C 16- O 22	1.01	1.14	0.030
87. BD (1) O 22- B 23	197. RY (1) C 6	0.96	2.59	0.044

87. BD (1) O 22- B 23	297. RY (1) C 16	3.41	1.76	0.069
87. BD (1) O 22- B 23	367. RY (1) B 23	1.01	1.58	0.036

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Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.9962	0.0061	0.0004	0.0006	0.0016	0.0111	0.0113	0.0066
2. C	0.9962	0.0000	0.0112	0.0108	0.0018	0.0005	0.0005	0.0065	1.0047
3. C	0.0061	0.0112	0.0000	1.3139	0.0195	0.0038	0.0227	0.0018	1.5002
4. C	0.0004	0.0108	1.3139	0.0000	1.4998	0.0299	0.0027	0.0295	0.0139
5. C	0.0006	0.0018	0.0195	1.4998	0.0000	0.0138	0.0279	0.0005	0.1014
6. C	0.0016	0.0005	0.0038	0.0299	0.0138	0.0000	1.4955	0.0109	0.0089
7. C	0.0111	0.0005	0.0227	0.0027	0.0279	1.4955	0.0000	1.3039	0.0036
8. C	0.0113	0.0065	0.0018	0.0295	0.0005	0.0109	1.3039	0.0000	0.0343
9. C	0.0066	1.0047	1.5002	0.0139	0.1014	0.0089	0.0036	0.0343	0.0000
10. C	0.0080	0.0079	0.0625	0.0166	1.2710	1.2161	0.0108	0.0612	0.0103
11. C	1.0040	0.0060	0.0289	0.0013	0.0075	0.1003	0.0176	1.5112	0.0168
12. C	0.0090	0.0091	0.0110	0.0657	0.0142	0.0118	0.0528	0.0115	1.2525
13. C	0.0000	0.0001	0.0006	0.0051	0.0101	0.0001	0.0004	0.0000	0.0020
14. C	0.0000	0.0001	0.0006	0.0057	0.0094	0.0002	0.0004	0.0001	0.0023
15. C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0115	0.0009	0.0004	0.0000
16. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0100	0.0006	0.0001	0.0000
17. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0004	0.0000	0.0000
18. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000
19. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
20. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0003	0.0000	0.0000
21. O	0.0001	0.0000	0.0002	0.0006	0.0008	0.0061	0.0131	0.0003	0.0001
22. O	0.0001	0.0000	0.0005	0.0009	0.0006	0.0081	0.0105	0.0005	0.0002
23. B	0.0007	0.0003	0.0011	0.0012	0.0025	0.9040	0.0320	0.0104	0.0005
24. N	0.0004	0.0005	0.0085	0.0067	0.8978	0.0014	0.0002	0.0000	0.0005
25. H	0.9179	0.0026	0.0004	0.0003	0.0001	0.0022	0.0001	0.0048	0.0039
26. H	0.9078	0.0031	0.0011	0.0002	0.0002	0.0036	0.0002	0.0088	0.0015
27. H	0.0032	0.9126	0.0079	0.0001	0.0034	0.0002	0.0004	0.0012	0.0043
28. H	0.0027	0.9143	0.0049	0.0001	0.0022	0.0001	0.0004	0.0005	0.0037
29. H	0.0001	0.0020	0.9234	0.0048	0.0058	0.0003	0.0000	0.0002	0.0075
30. H	0.0002	0.0002	0.0064	0.9273	0.0057	0.0002	0.0002	0.0000	0.0055
31. H	0.0002	0.0002	0.0000	0.0002	0.0001	0.0077	0.9196	0.0042	0.0003
32. H	0.0018	0.0001	0.0002	0.0000	0.0003	0.0058	0.0052	0.9261	0.0001
33. H	0.0000	0.0000	0.0001	0.0010	0.0071	0.0001	0.0001	0.0000	0.0004
34. H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
35. H	0.0000	0.0000	0.0000	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000
36. H	0.0000	0.0000	0.0001	0.0012	0.0071	0.0001	0.0000	0.0001	0.0005
37. H	0.0000	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000
38. H	0.0000	0.0000	0.0000	0.0004	0.0005	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
41. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000

44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0032	0.0044	0.0006	0.0001	0.0000	0.0000
52.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	S	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	O	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0002	0.0000	0.0000

	Atom	10	11	12	13	14	15	16	17	18
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1.	C	0.0080	1.0040	0.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0079	0.0060	0.0091	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
3.	C	0.0625	0.0289	0.0110	0.0006	0.0006	0.0000	0.0000	0.0000	0.0000
4.	C	0.0166	0.0013	0.0657	0.0051	0.0057	0.0000	0.0000	0.0000	0.0000
5.	C	1.2710	0.0075	0.0142	0.0101	0.0094	0.0002	0.0001	0.0000	0.0000
6.	C	1.2161	0.1003	0.0118	0.0001	0.0002	0.0115	0.0100	0.0003	0.0002
7.	C	0.0108	0.0176	0.0528	0.0004	0.0004	0.0009	0.0006	0.0004	0.0002
8.	C	0.0612	1.5112	0.0115	0.0000	0.0001	0.0004	0.0001	0.0000	0.0000
9.	C	0.0103	0.0168	1.2525	0.0020	0.0023	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0114	1.2418	0.0063	0.0062	0.0002	0.0005	0.0001	0.0001
11.	C	0.0114	0.0000	1.2373	0.0001	0.0001	0.0002	0.0002	0.0002	0.0000
12.	C	1.2418	1.2373	0.0000	0.0003	0.0003	0.0001	0.0003	0.0000	0.0000
13.	C	0.0063	0.0001	0.0003	0.0000	0.0110	0.0002	0.0001	0.0002	0.0000
14.	C	0.0062	0.0001	0.0003	0.0110	0.0000	0.0001	0.0001	0.0000	0.0000
15.	C	0.0002	0.0002	0.0001	0.0002	0.0001	0.0000	0.9527	1.0009	1.0070
16.	C	0.0005	0.0002	0.0003	0.0001	0.0001	0.9527	0.0000	0.0072	0.0076
17.	C	0.0001	0.0002	0.0000	0.0002	0.0000	1.0009	0.0072	0.0000	0.0085
18.	C	0.0001	0.0000	0.0000	0.0000	0.0000	1.0070	0.0076	0.0085	0.0000
19.	C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0084	0.9959	0.0031	0.0013
20.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0070	1.0037	0.0074	0.0028
21.	O	0.0038	0.0035	0.0001	0.0015	0.0020	0.8083	0.0139	0.0157	0.0133
22.	O	0.0083	0.0044	0.0004	0.0001	0.0001	0.0179	0.8440	0.0015	0.0055
23.	B	0.0130	0.0090	0.0071	0.0001	0.0001	0.0075	0.0073	0.0057	0.0072
24.	N	0.0057	0.0003	0.0085	0.8935	0.9112	0.0008	0.0004	0.0001	0.0000
25.	H	0.0001	0.0038	0.0060	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0043	0.0050	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0001	0.0015	0.0055	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
28.	H	0.0001	0.0039	0.0065	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
29.	H	0.0001	0.0002	0.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0067	0.0002	0.0004	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
31.	H	0.0079	0.0054	0.0003	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000
32.	H	0.0001	0.0067	0.0083	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0003	0.0000	0.0002	0.9331	0.0003	0.0000	0.0001	0.0001	0.0000
34.	H	0.0001	0.0000	0.0000	0.8980	0.0067	0.0000	0.0000	0.0000	0.0000
35.	H	0.0001	0.0000	0.0000	0.9412	0.0005	0.0000	0.0000	0.0001	0.0000
36.	H	0.0004	0.0000	0.0002	0.0003	0.9329	0.0000	0.0000	0.0000	0.0000
37.	H	0.0001	0.0000	0.0000	0.0072	0.9299	0.0000	0.0000	0.0000	0.0000
38.	H	0.0001	0.0000	0.0000	0.0005	0.9386	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0040	0.0080	0.9277	0.0009
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0004	0.9221	0.0006
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0035	0.0009	0.9112	0.0072
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0050	0.0090	0.0017	0.9285
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0006	0.0004	0.9211
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0008	0.0095	0.9279
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0084	0.0042	0.0002	0.0001
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0069	0.0001	0.0001
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0039	0.0006	0.0002
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0093	0.0052	0.0003	0.0003
49.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0004	0.0073	0.0000	0.0002
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0040	0.0004	0.0002
51.	H	0.0007	0.0000	0.0002	0.0057	0.0049	0.0006	0.0011	0.0003	0.0001
52.	C	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0012	0.0000
53.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
54.	F	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000
55.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
56.	S	0.0000	0.0000	0.0000	0.0005	0.0000	0.0001	0.0000	0.0009	0.0000
57.	O	0.0000	0.0000	0.0000	0.0004	0.0000	0.0002	0.0000	0.0018	0.0000
58.	O	0.0000	0.0000	0.0000	0.0010	0.0000	0.0002	0.0000	0.0012	0.0000

59.	O	0.0001	0.0001	0.0000	0.0048	0.0001	0.0001	0.0000	0.0020	0.0001
	Atom	19	20	21	22	23	24	25	26	27
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1.	C	0.0000	0.0000	0.0001	0.0001	0.0007	0.0004	0.9179	0.9078	0.0032
2.	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0005	0.0026	0.0031	0.9126
3.	C	0.0000	0.0000	0.0002	0.0005	0.0011	0.0085	0.0004	0.0011	0.0079
4.	C	0.0000	0.0000	0.0006	0.0009	0.0012	0.0067	0.0003	0.0002	0.0001
5.	C	0.0000	0.0000	0.0008	0.0006	0.0025	0.8978	0.0001	0.0002	0.0034
6.	C	0.0003	0.0004	0.0061	0.0081	0.9040	0.0014	0.0022	0.0036	0.0002
7.	C	0.0001	0.0003	0.0131	0.0105	0.0320	0.0002	0.0001	0.0002	0.0004
8.	C	0.0000	0.0000	0.0003	0.0005	0.0104	0.0000	0.0048	0.0088	0.0012
9.	C	0.0000	0.0000	0.0001	0.0002	0.0005	0.0005	0.0039	0.0015	0.0043
10.	C	0.0002	0.0002	0.0038	0.0083	0.0130	0.0057	0.0001	0.0000	0.0001
11.	C	0.0001	0.0002	0.0035	0.0044	0.0090	0.0003	0.0038	0.0043	0.0015
12.	C	0.0000	0.0000	0.0001	0.0004	0.0071	0.0085	0.0060	0.0050	0.0055
13.	C	0.0000	0.0000	0.0015	0.0001	0.0001	0.8935	0.0000	0.0000	0.0001
14.	C	0.0000	0.0000	0.0020	0.0001	0.0001	0.9112	0.0000	0.0000	0.0001
15.	C	0.0084	0.0070	0.8083	0.0179	0.0075	0.0008	0.0000	0.0000	0.0000
16.	C	0.9959	1.0037	0.0139	0.8440	0.0073	0.0004	0.0000	0.0000	0.0000
17.	C	0.0031	0.0074	0.0157	0.0015	0.0057	0.0001	0.0000	0.0000	0.0000
18.	C	0.0013	0.0028	0.0133	0.0055	0.0072	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0084	0.0056	0.0153	0.0086	0.0001	0.0000	0.0000	0.0000
20.	C	0.0084	0.0000	0.0015	0.0173	0.0065	0.0000	0.0000	0.0000	0.0000
21.	O	0.0056	0.0015	0.0000	0.0501	0.8808	0.0124	0.0001	0.0001	0.0000
22.	O	0.0153	0.0173	0.0501	0.0000	0.9505	0.0004	0.0001	0.0002	0.0000
23.	B	0.0086	0.0065	0.8808	0.9505	0.0000	0.0009	0.0002	0.0004	0.0000
24.	N	0.0001	0.0000	0.0124	0.0004	0.0009	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000	0.0027	0.0016
26.	H	0.0000	0.0000	0.0001	0.0002	0.0004	0.0000	0.0027	0.0000	0.0027
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0027	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0017	0.0027
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0027	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0011	0.0023	0.0020	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
33.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0004	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0005	0.0000	0.0000	0.0015	0.0000	0.0000	0.0000
39.	H	0.0004	0.0002	0.0022	0.0004	0.0002	0.0001	0.0000	0.0000	0.0000
40.	H	0.0002	0.0000	0.0102	0.0002	0.0007	0.0000	0.0000	0.0000	0.0000
41.	H	0.0002	0.0003	0.0014	0.0003	0.0009	0.0000	0.0000	0.0000	0.0000
42.	H	0.0001	0.0002	0.0014	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000
43.	H	0.0001	0.0001	0.0106	0.0007	0.0003	0.0000	0.0000	0.0000	0.0000
44.	H	0.0002	0.0004	0.0022	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000
45.	H	0.9263	0.0010	0.0007	0.0018	0.0001	0.0000	0.0000	0.0000	0.0000
46.	H	0.9308	0.0004	0.0005	0.0095	0.0004	0.0000	0.0000	0.0000	0.0000
47.	H	0.9194	0.0075	0.0001	0.0014	0.0001	0.0000	0.0000	0.0000	0.0000
48.	H	0.0009	0.9206	0.0003	0.0030	0.0003	0.0000	0.0000	0.0000	0.0000
49.	H	0.0009	0.9238	0.0002	0.0112	0.0007	0.0000	0.0000	0.0000	0.0000
50.	H	0.0093	0.9301	0.0006	0.0013	0.0009	0.0000	0.0000	0.0000	0.0000
51.	H	0.0001	0.0001	0.0307	0.0013	0.0010	0.7581	0.0000	0.0000	0.0000
52.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
53.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	S	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	O	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
58.	O	0.0000	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
59.	O	0.0000	0.0000	0.0003	0.0002	0.0029	0.0001	0.0000	0.0000	0.0000
	Atom	28	29	30	31	32	33	34	35	36
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1.	C	0.0027	0.0001	0.0002	0.0002	0.0018	0.0000	0.0000	0.0000	0.0000
2.	C	0.9143	0.0020	0.0002	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
3.	C	0.0049	0.9234	0.0064	0.0000	0.0002	0.0001	0.0000	0.0000	0.0001
4.	C	0.0001	0.0048	0.9273	0.0002	0.0000	0.0010	0.0001	0.0003	0.0012
5.	C	0.0022	0.0058	0.0057	0.0001	0.0003	0.0071	0.0003	0.0006	0.0071
6.	C	0.0001	0.0003	0.0002	0.0077	0.0058	0.0001	0.0000	0.0000	0.0001
7.	C	0.0004	0.0000	0.0002	0.9196	0.0052	0.0001	0.0000	0.0000	0.0000
8.	C	0.0005	0.0002	0.0000	0.0042	0.9261	0.0000	0.0000	0.0000	0.0001
9.	C	0.0037	0.0075	0.0055	0.0003	0.0001	0.0004	0.0000	0.0000	0.0005
10.	C	0.0001	0.0001	0.0067	0.0079	0.0001	0.0003	0.0001	0.0001	0.0004
11.	C	0.0039	0.0002	0.0002	0.0054	0.0067	0.0000	0.0000	0.0000	0.0000

[illegible]

27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0028	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0033	0.0032	0.0001	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0033	0.0000	0.0034	0.0000	0.0000	0.0002	0.0000
41.	H	0.0000	0.0000	0.0032	0.0034	0.0000	0.0002	0.0001	0.0005	0.0000
42.	H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0034	0.0028	0.0001
43.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0034	0.0000	0.0032	0.0000
44.	H	0.0000	0.0000	0.0000	0.0002	0.0005	0.0028	0.0032	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0030
47.	H	0.0000	0.0000	0.0001	0.0001	0.0003	0.0000	0.0000	0.0000	0.0029
48.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
51.	H	0.0003	0.0044	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	C	0.0000	0.0000	0.0001	0.0000	0.0015	0.0000	0.0000	0.0000	0.0000
53.	F	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
54.	F	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
55.	F	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
56.	S	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
57.	O	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	0.0000	0.0000	0.0000
58.	O	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	O	0.0000	0.0000	0.0001	0.0002	0.0038	0.0000	0.0000	0.0000	0.0000

	Atom	46	47	48	49	50	51	52	53	54
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1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0032	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0000	0.0000	0.0000
6.	C	0.0003	0.0000	0.0001	0.0003	0.0001	0.0006	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0007	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0057	0.0003	0.0000	0.0001
14.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	0.0000	0.0000
15.	C	0.0004	0.0010	0.0093	0.0004	0.0012	0.0006	0.0001	0.0000	0.0000
16.	C	0.0069	0.0039	0.0052	0.0073	0.0040	0.0011	0.0000	0.0000	0.0000
17.	C	0.0001	0.0006	0.0003	0.0000	0.0004	0.0003	0.0012	0.0001	0.0002
18.	C	0.0001	0.0002	0.0003	0.0002	0.0002	0.0001	0.0000	0.0000	0.0000
19.	C	0.9308	0.9194	0.0009	0.0009	0.0093	0.0001	0.0000	0.0000	0.0000
20.	C	0.0004	0.0075	0.9206	0.9238	0.9301	0.0001	0.0000	0.0000	0.0000
21.	O	0.0005	0.0001	0.0003	0.0002	0.0006	0.0307	0.0000	0.0000	0.0000
22.	O	0.0095	0.0014	0.0030	0.0112	0.0013	0.0013	0.0000	0.0000	0.0000
23.	B	0.0004	0.0001	0.0003	0.0007	0.0009	0.0010	0.0002	0.0000	0.0000
24.	N	0.0000	0.0000	0.0000	0.0000	0.0000	0.7581	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0005	0.0000	0.0001
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0000	0.0000	0.0000
39.	H	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
40.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0015	0.0001	0.0003

42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000
45.	H	0.0030	0.0029	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0030	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
47.	H	0.0030	0.0000	0.0000	0.0002	0.0004	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0033	0.0029	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0002	0.0033	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000
50.	H	0.0001	0.0004	0.0029	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9747
53.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7598	0.0000	0.0556
54.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9747	0.0556	0.0000
55.	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9241	0.0524	0.0632
56.	S	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6407	0.0238	0.0355
57.	O	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.1142	0.0034	0.0050
58.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1044	0.0171	0.0057
59.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.1003	0.0034	0.0161

	Atom	55	56	57	58	59
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0002
6.	C	0.0000	0.0000	0.0000	0.0000	0.0001
7.	C	0.0000	0.0000	0.0000	0.0000	0.0002
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000	0.0000	0.0001
11.	C	0.0000	0.0000	0.0000	0.0000	0.0001
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0005	0.0004	0.0010	0.0048
14.	C	0.0000	0.0000	0.0000	0.0000	0.0001
15.	C	0.0000	0.0001	0.0002	0.0002	0.0001
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0001	0.0009	0.0018	0.0012	0.0020
18.	C	0.0000	0.0000	0.0000	0.0000	0.0001
19.	C	0.0000	0.0000	0.0001	0.0000	0.0000
20.	C	0.0000	0.0000	0.0000	0.0000	0.0000
21.	O	0.0000	0.0000	0.0000	0.0000	0.0003
22.	O	0.0000	0.0000	0.0000	0.0000	0.0002
23.	B	0.0000	0.0000	0.0001	0.0002	0.0029
24.	N	0.0000	0.0000	0.0000	0.0001	0.0001
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0001	0.0001
34.	H	0.0001	0.0003	0.0009	0.0015	0.0122
35.	H	0.0000	0.0000	0.0000	0.0000	0.0002
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0001	0.0000	0.0005	0.0001
40.	H	0.0000	0.0000	0.0000	0.0000	0.0002
41.	H	0.0003	0.0004	0.0028	0.0000	0.0038
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0006	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0003
52.	C	0.9241	0.6407	0.1142	0.1044	0.1003
53.	F	0.0524	0.0238	0.0034	0.0171	0.0034
54.	F	0.0632	0.0355	0.0050	0.0057	0.0161
55.	F	0.0000	0.0325	0.0173	0.0042	0.0051
56.	S	0.0325	0.0000	1.1479	1.1242	1.0233

57. O 0.0173 1.1479 0.0000 0.1502 0.1384
 58. O 0.0042 1.1242 0.1502 0.0000 0.1268
 59. O 0.0051 1.0233 0.1384 0.1268 0.0000

(Occupancy)		Bond orbital /		Coefficients /		Hybrids	
		Lewis					
1.	(1.99910)	CR	(1) C 1	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
2.	(1.99910)	CR	(1) C 2	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
3.	(1.99892)	CR	(1) C 3	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
4.	(1.99901)	CR	(1) C 4	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
5.	(1.99882)	CR	(1) C 5	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
6.	(1.99882)	CR	(1) C 6	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
7.	(1.99908)	CR	(1) C 7	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
8.	(1.99895)	CR	(1) C 8	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
9.	(1.99896)	CR	(1) C 9	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
10.	(1.99884)	CR	(1) C 10	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
11.	(1.99895)	CR	(1) C 11	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
12.	(1.99884)	CR	(1) C 12	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
13.	(1.99909)	CR	(1) C 13	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
14.	(1.99909)	CR	(1) C 14	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
15.	(1.99890)	CR	(1) C 15	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
16.	(1.99888)	CR	(1) C 16	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
17.	(1.99909)	CR	(1) C 17	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
18.	(1.99906)	CR	(1) C 18	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
19.	(1.99910)	CR	(1) C 19	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
20.	(1.99909)	CR	(1) C 20	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
21.	(1.99973)	CR	(1) O 21	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
22.	(1.99972)	CR	(1) O 22	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
23.	(1.99912)	CR	(1) B 23	s(100.00%)			
				1.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000
24.	(1.99915)	CR	(1) N 24	s(100.00%)			

		1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
25. (1.99974) CR (1) C 52	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
26. (1.99996) CR (1) F 53	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
27. (1.99986) CR (1) F 54	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
28. (1.99989) CR (1) F 55	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
29. (2.00000) CR (1) S 56	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000		
30. (1.99922) CR (2) S 56	s(100.00%)	0.0000	1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000		
31. (1.99993) CR (3) S 56	s(0.00%)p 1.00(100.00%)	0.0000	0.0000	0.0000	0.0000	1.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000		
32. (1.99988) CR (4) S 56	s(0.00%)p 1.00(100.00%)	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	1.0000	0.0000	0.0000
		0.0000	0.0000	0.0000		
33. (1.99990) CR (5) S 56	s(0.00%)p 1.00(100.00%)	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		1.0000	0.0000	0.0000		
34. (1.99990) CR (1) O 57	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
35. (1.99989) CR (1) O 58	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
36. (1.99992) CR (1) O 59	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	
37. (0.99887) LP (1) C 12	s(0.00%)p 1.00(100.00%)	0.0000	0.0056	0.0025	-0.8064	-0.0067
		-0.5530	-0.0118	-0.2089	-0.0075	
38. (1.94335) LP (1) O 21	s(28.46%)p 2.51(71.54%)	0.0000	0.5335	0.0001	0.2170	-0.0017
		-0.1430	0.0063	0.8048	-0.0041	
39. (1.81809) LP (2) O 21	s(0.07%)p99.99(99.93%)	0.0000	0.0259	0.0026	0.6863	0.0049
		0.7231	-0.0005	-0.0737	0.0048	
40. (1.95355) LP (1) O 22	s(29.13%)p 2.43(70.87%)	0.0000	0.5397	0.0003	0.0098	-0.0008
		-0.0741	-0.0011	-0.8385	0.0023	
41. (1.78643) LP (2) O 22	s(0.27%)p99.99(99.73%)	0.0000	0.0518	-0.0012	-0.8385	-0.0001
		-0.5377	-0.0022	0.0710	-0.0021	
42. (1.99307) LP (1) F 53	s(79.47%)p 0.26(20.53%)	0.0000	0.8914	0.0000	0.2924	-0.0027
		-0.0227	0.0004	-0.3454	0.0032	
43. (1.96714) LP (2) F 53	s(1.54%)p64.00(98.46%)	0.0000	0.1240	-0.0021	-0.8921	0.0017
		-0.0471	-0.0010	-0.4320	0.0019	
44. (1.96167) LP (3) F 53	s(0.83%)p99.99(99.17%)	0.0000	0.0910	-0.0010	-0.0573	-0.0008
		-0.9624	-0.0004	0.2494	-0.0010	
45. (1.98373) LP (1) F 54	s(62.41%)p 0.60(37.59%)	0.0000	0.7900	-0.0015	-0.5956	0.0050
		-0.0088	0.0006	-0.1451	0.0029	
46. (1.91887) LP (2) F 54	s(0.08%)p99.99(99.92%)	0.0000	0.0291	-0.0006	0.0817	-0.0012
		-0.9893	-0.0065	-0.1174	-0.0012	
47. (1.89408) LP (3) F 54	s(0.77%)p99.99(99.23%)	0.0000	0.0880	-0.0018	0.3401	0.0015
		0.1405	-0.0002	-0.9256	-0.0019	
48. (1.98654) LP (1) F 55	s(68.49%)p 0.46(31.51%)					

				0.0000	0.8276	-0.0002	0.1646	-0.0017	
				-0.3859	0.0033	0.3729	-0.0019		
49.	(1.93545)	LP (2)	F 55	s(0.07%)	p99.99(99.93%)				
				0.0000	0.0262	-0.0007	-0.6034	-0.0017	
				-0.6487	-0.0037	-0.4630	-0.0010		
50.	(1.90972)	LP (3)	F 55	s(0.62%)	p99.99(99.38%)				
				0.0000	0.0787	-0.0015	0.7125	-0.0005	
				-0.1785	0.0004	-0.6740	-0.0005		
51.	(1.98200)	LP (1)	O 57	s(77.21%)	p 0.30(22.79%)				
				0.0000	0.8787	-0.0031	-0.1987	-0.0027	
				0.2712	0.0034	-0.3389	-0.0047		
52.	(1.83783)	LP (2)	O 57	s(0.00%)	p 1.00(100.00%)				
				0.0000	0.0020	0.0002	-0.7993	0.0064	
				0.1384	-0.0005	0.5847	-0.0050		
53.	(1.81291)	LP (3)	O 57	s(0.27%)	p99.99(99.73%)				
				0.0000	0.0520	-0.0009	0.4680	-0.0061	
				0.7515	-0.0116	0.4619	-0.0042		
54.	(1.98237)	LP (1)	O 58	s(74.72%)	p 0.34(25.28%)				
				0.0000	0.8644	-0.0044	-0.1577	-0.0021	
				0.0535	0.0007	0.4744	0.0074		
55.	(1.84527)	LP (2)	O 58	s(0.29%)	p99.99(99.71%)				
				0.0000	0.0543	-0.0015	0.8714	-0.0080	
				-0.4251	0.0036	0.2386	-0.0045		
56.	(1.82440)	LP (3)	O 58	s(0.09%)	p99.99(99.91%)				
				0.0000	0.0298	0.0002	0.4388	-0.0067	
				0.8979	-0.0139	-0.0096	-0.0017		
57.	(1.98567)	LP (1)	O 59	s(82.17%)	p 0.22(17.83%)				
				0.0000	0.9065	0.0002	0.4003	0.0046	
				-0.0785	-0.0023	-0.1088	-0.0016		
58.	(1.89426)	LP (2)	O 59	s(0.85%)	p99.99(99.15%)				
				0.0000	0.0919	-0.0031	-0.0010	-0.0015	
				-0.2717	0.0012	0.9580	-0.0033		
59.	(1.84204)	LP (3)	O 59	s(0.71%)	p99.99(99.29%)				
				0.0000	0.0841	-0.0031	0.0690	-0.0033	
				0.9584	-0.0080	0.2639	-0.0017		
60.	(1.97999)	BD (1)	C 1- C 2						
	(49.75%)		0.7053* C 1	s(23.73%)	p 3.21(76.27%)				
				0.0000	0.4871	-0.0021	0.1710	0.0120	
				-0.3425	-0.0101	0.7845	-0.0207		
	(50.25%)		0.7089* C 2	s(24.09%)	p 3.15(75.91%)				
				0.0000	0.4908	-0.0030	-0.1384	0.0147	
				0.3034	-0.0228	-0.8045	0.0033		
61.	(1.97671)	BD (1)	C 1- C 11						
	(49.18%)		0.7013* C 1	s(24.71%)	p 3.05(75.29%)				
				0.0000	0.4971	-0.0012	-0.4549	0.0085	
				0.7306	-0.0046	0.1088	-0.0186		
	(50.82%)		0.7129* C 11	s(30.91%)	p 2.24(69.09%)				
				0.0000	0.5559	-0.0069	0.4610	-0.0072	
				-0.6578	0.0211	-0.2111	-0.0258		
62.	(1.97851)	BD (1)	C 1- H 25						
	(61.65%)		0.7852* C 1	s(25.83%)	p 2.87(74.17%)				
				0.0000	0.5082	0.0028	0.7415	0.0034	
				0.1752	-0.0110	-0.4012	-0.0129		
	(38.35%)		0.6192* H 25	s(100.00%)					
				1.0000	-0.0002				
63.	(1.97224)	BD (1)	C 1- H 26						
	(62.01%)		0.7874* C 1	s(25.57%)	p 2.91(74.43%)				
				0.0000	0.5057	0.0001	-0.4626	0.0092	
				-0.5641	-0.0080	-0.4600	-0.0158		
	(37.99%)		0.6164* H 26	s(100.00%)					
				1.0000	0.0003				
64.	(1.97686)	BD (1)	C 2- C 9						
	(48.93%)		0.6995* C 2	s(24.62%)	p 3.06(75.38%)				
				0.0000	0.4962	-0.0002	-0.5094	0.0104	
				0.4323	-0.0166	0.5541	0.0092		
	(51.07%)		0.7146* C 9	s(31.27%)	p 2.20(68.73%)				
				0.0000	0.5592	-0.0065	0.4982	-0.0037	
				-0.4958	-0.0040	-0.4384	0.0319		
65.	(1.97298)	BD (1)	C 2- H 27						
	(61.60%)		0.7848* C 2	s(25.50%)	p 2.92(74.50%)				
				0.0000	0.5049	0.0014	0.8274	0.0121	
				0.1222	-0.0162	0.2125	0.0017		
	(38.40%)		0.6197* H 27	s(100.00%)					
				1.0000	0.0001				
66.	(1.97786)	BD (1)	C 2- H 28						
	(61.95%)		0.7871* C 2	s(25.63%)	p 2.90(74.37%)				
				0.0000	0.5062	0.0015	-0.1918	0.0134	

	(38.05%)	0.6168*	H 28	s(100.00%)	-0.8403 -0.0080 0.0254 -0.0004 1.0000 0.0000			
67.	(1.96792)	BD (1) C	3- C 4					
	(49.24%)	0.7017*	C 3	s(32.54%)p 2.07(67.46%)	0.0000 0.5704 0.0052 -0.4949 -0.0004 0.5456 -0.0136 0.3611 0.0365			
	(50.76%)	0.7124*	C 4	s(34.28%)p 1.92(65.72%)	0.0000 0.5855 0.0036 0.4778 0.0026 -0.5524 -0.0149 -0.3503 0.0283			
68.	(1.97724)	BD (1) C	3- C 9					
	(49.29%)	0.7021*	C 3	s(35.08%)p 1.85(64.92%)	0.0000 0.5923 -0.0007 0.1755 0.0147 0.0579 -0.0246 -0.7837 0.0010			
	(50.71%)	0.7121*	C 9	s(37.43%)p 1.67(62.57%)	0.0000 0.6117 0.0123 -0.1245 0.0116 -0.1166 -0.0258 0.7717 0.0168			
69.	(1.70106)	BD (2) C	3- C 9					
	(53.12%)	0.7288*	C 3	s(0.00%)p 1.00(100.00%)	0.0000 -0.0009 0.0038 -0.7909 0.0184 -0.5707 0.0103 -0.2200 0.0013			
	(46.88%)	0.6847*	C 9	s(0.01%)p 1.00(99.99%)	0.0000 0.0087 0.0011 -0.7828 0.0036 -0.5816 0.0023 -0.2210 -0.0027			
70.	(1.98102)	BD (1) C	3- H 29					
	(60.86%)	0.7802*	C 3	s(32.22%)p 2.10(67.78%)	0.0000 0.5676 -0.0027 0.3135 0.0015 -0.6106 -0.0084 0.4544 0.0117			
	(39.14%)	0.6256*	H 29	s(100.00%) 1.0000 -0.0010				
71.	(1.97697)	BD (1) C	4- C 5					
	(49.13%)	0.7009*	C 4	s(34.06%)p 1.94(65.94%)	0.0000 0.5836 0.0020 -0.3121 -0.0074 0.6180 0.0046 -0.4241 0.0115			
	(50.87%)	0.7133*	C 5	s(37.55%)p 1.66(62.45%)	0.0000 0.6128 0.0031 0.3021 -0.0026 -0.6018 -0.0061 0.4131 0.0164			
72.	(1.77932)	BD (2) C	4- C 5					
	(46.03%)	0.6785*	C 4	s(0.00%)p 1.00(100.00%)	0.0000 0.0019 0.0044 -0.8029 0.0122 -0.5554 0.0068 -0.2160 0.0034			
	(53.97%)	0.7346*	C 5	s(0.02%)p99.99(99.98%)	0.0000 0.0110 0.0083 -0.8117 0.0133 -0.5432 0.0057 -0.2139 0.0008			
73.	(1.97914)	BD (1) C	4- H 30					
	(60.40%)	0.7772*	C 4	s(31.52%)p 2.17(68.48%)	0.0000 0.5614 -0.0035 -0.1717 0.0055 -0.0635 -0.0192 0.8066 0.0178			
	(39.60%)	0.6293*	H 30	s(100.00%) 1.0000 -0.0002				
74.	(1.97443)	BD (1) C	5- C 10					
	(49.90%)	0.7064*	C 5	s(38.29%)p 1.61(61.71%)	0.0000 0.6188 -0.0057 0.1030 -0.0097 0.1586 0.0050 -0.7623 0.0082			
	(50.10%)	0.7078*	C 10	s(33.67%)p 1.97(66.33%)	0.0000 0.5803 0.0048 -0.1804 -0.0102 -0.0465 0.0121 0.7927 -0.0013			
75.	(1.98270)	BD (1) C	5- N 24					
	(35.42%)	0.5951*	C 5	s(24.12%)p 3.15(75.88%)	0.0000 0.4910 0.0101 -0.4889 -0.0094 0.5634 0.0079 0.4498 0.0027			
	(64.58%)	0.8036*	N 24	s(25.35%)p 2.94(74.65%)	0.0000 0.5035 -0.0024 0.4832 -0.0112 -0.5957 0.0107 -0.3975 0.0035			
76.	(1.97201)	BD (1) C	6- C 7					
	(51.35%)	0.7166*	C 6	s(33.17%)p 2.01(66.83%)	0.0000 0.5759 0.0091 0.2686 0.0079 -0.0721 0.0003 -0.7684 -0.0221			
	(48.65%)	0.6975*	C 7	s(35.48%)p 1.82(64.52%)	0.0000 0.5956 -0.0016 -0.2409 -0.0037 0.0138 0.0094 0.7661 -0.0056			
77.	(1.70277)	BD (2) C	6- C 7					
	(54.42%)	0.7377*	C 6	s(0.00%)p 1.00(100.00%)	0.0000 -0.0002 0.0069 -0.8103 -0.0029 -0.5376 -0.0132 -0.2328 -0.0040			
	(45.58%)	0.6751*	C 7	s(0.00%)p 1.00(100.00%)	0.0000 0.0003 0.0027 -0.8105 0.0102			

					-0.5317	0.0050	-0.2455	-0.0013	
78.	(1.97083)	BD (1) C	6- C 10						
	(48.59%)		0.6971* C 6	s(32.96%)p 2.03(67.04%)					
				0.0000 0.5741 0.0065 0.2123 -0.0051					
				-0.5613 -0.0008 0.5569 0.0090					
	(51.41%)		0.7170* C 10	s(34.87%)p 1.87(65.13%)					
				0.0000 0.5905 -0.0033 -0.2645 0.0006					
				0.6106 -0.0074 -0.4565 0.0110					
79.	(1.96214)	BD (1) C	6- B 23						
	(68.29%)		0.8264* C 6	s(33.85%)p 1.95(66.15%)					
				0.0000 0.5817 -0.0098 -0.4750 0.0158					
				0.6247 -0.0275 0.2114 -0.0025					
	(31.71%)		0.5631* B 23	s(39.38%)p 1.54(60.62%)					
				0.0000 0.6275 -0.0082 0.4663 -0.0116					
				-0.6188 0.0084 -0.0750 -0.0062					
80.	(1.97429)	BD (1) C	7- C 8						
	(49.85%)		0.7060* C 7	s(33.13%)p 2.02(66.87%)					
				0.0000 0.5756 0.0057 0.4787 -0.0010					
				-0.5967 0.0140 -0.2866 -0.0328					
	(50.15%)		0.7082* C 8	s(32.54%)p 2.07(67.46%)					
				0.0000 0.5704 0.0024 -0.4658 -0.0030					
				0.6063 0.0165 0.2981 -0.0298					
81.	(1.97943)	BD (1) C	7- H 31						
	(61.25%)		0.7826* C 7	s(31.28%)p 2.20(68.72%)					
				0.0000 0.5592 -0.0032 -0.2362 0.0005					
				0.6006 0.0020 -0.5201 -0.0159					
	(38.75%)		0.6225* H 31	s(100.00%)					
				1.0000 -0.0024					
82.	(1.97742)	BD (1) C	8- C 11						
	(48.88%)		0.6991* C 8	s(34.42%)p 1.91(65.58%)					
				0.0000 0.5866 0.0034 0.2416 0.0133					
				-0.6038 -0.0132 0.4818 -0.0200					
	(51.12%)		0.7150* C 11	s(37.31%)p 1.68(62.69%)					
				0.0000 0.6107 0.0116 -0.2013 0.0104					
				0.5473 -0.0056 -0.5345 -0.0305					
83.	(1.69986)	BD (2) C	8- C 11						
	(52.18%)		0.7224* C 8	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0049 -0.0033 0.8212 -0.0170					
				0.5166 -0.0087 0.2415 -0.0070					
	(47.82%)		0.6915* C 11	s(0.01%)p 1.00(99.99%)					
				0.0000 0.0068 -0.0023 0.8278 -0.0077					
				0.5147 0.0031 0.2229 -0.0014					
84.	(1.98207)	BD (1) C	8- H 32						
	(60.72%)		0.7792* C 8	s(32.89%)p 2.04(67.11%)					
				0.0000 0.5735 -0.0036 0.2234 0.0010					
				0.0185 0.0057 -0.7877 -0.0166					
	(39.28%)		0.6267* H 32	s(100.00%)					
				1.0000 -0.0008					
85.	(1.96941)	BD (1) C	9- C 12						
	(49.00%)		0.7000* C 9	s(31.20%)p 2.21(68.80%)					
				0.0000 0.5585 -0.0050 -0.3509 0.0022					
				0.6341 -0.0033 -0.4035 -0.0018					
	(51.00%)		0.7141* C 12	s(32.51%)p 2.08(67.49%)					
				0.0000 0.5702 -0.0004 0.2972 -0.0052					
				-0.6050 0.0063 0.4695 0.0022					
86.	(1.95938)	BD (1) C	10- C 12						
	(50.18%)		0.7084* C 10	s(31.43%)p 2.18(68.57%)					
				0.0000 0.5607 0.0010 0.4833 -0.0047					
				-0.5830 0.0073 -0.3348 -0.0056					
	(49.82%)		0.7058* C 12	s(34.46%)p 1.90(65.54%)					
				0.0000 0.5871 0.0021 -0.4721 0.0055					
				0.5724 -0.0096 0.3237 -0.0044					
87.	(1.96914)	BD (1) C	11- C 12						
	(48.73%)		0.6981* C 11	s(31.67%)p 2.16(68.33%)					
				0.0000 0.5627 -0.0040 -0.2475 -0.0012					
				0.0497 0.0020 0.7872 -0.0020					
	(51.27%)		0.7160* C 12	s(33.02%)p 2.03(66.98%)					
				0.0000 0.5746 -0.0003 0.1953 -0.0031					
				0.0211 0.0027 -0.7945 0.0019					
88.	(1.98441)	BD (1) C	13- N 24						
	(33.98%)		0.5829* C 13	s(19.02%)p 4.26(80.98%)					
				0.0000 0.4358 0.0149 0.7427 0.0174					
				0.3658 0.0161 -0.3519 -0.0087					
	(66.02%)		0.8125* N 24	s(23.88%)p 3.19(76.12%)					
				0.0000 0.4887 -0.0031 -0.6787 0.0007					
				-0.3926 0.0085 0.3825 -0.0090					
89.	(1.98825)	BD (1) C	13- H 33						

	(61.30%)	0.7829*	C 13	s(26.44%)p 2.78(73.56%)					
				0.0000 0.5142 0.0005 -0.4365 -0.0188					
				0.6356 -0.0156 0.3747 0.0009					
	(38.70%)	0.6221*	H 33	s(100.00%)					
				1.0000 0.0002					
90. (1.98769)	BD (1) C 13-		H 34						
	(64.21%)	0.8013*	C 13	s(28.30%)p 2.53(71.70%)					
				0.0000 0.5320 -0.0040 -0.4353 -0.0115					
				-0.3569 0.0020 -0.6321 0.0221					
	(35.79%)	0.5983*	H 34	s(100.00%)					
				1.0000 0.0053					
91. (1.99247)	BD (1) C 13-		H 35						
	(60.88%)	0.7803*	C 13	s(26.20%)p 2.82(73.80%)					
				0.0000 0.5119 -0.0027 0.2597 -0.0260					
				-0.5782 -0.0077 0.5792 0.0045					
	(39.12%)	0.6254*	H 35	s(100.00%)					
				1.0000 -0.0007					
92. (1.98509)	BD (1) C 14-		N 24						
	(35.64%)	0.5970*	C 14	s(20.23%)p 3.94(79.77%)					
				0.0000 0.4497 0.0107 -0.4837 -0.0130					
				-0.4425 -0.0007 -0.6063 -0.0098					
	(64.36%)	0.8022*	N 24	s(23.09%)p 3.33(76.91%)					
				0.0000 0.4805 -0.0010 0.4815 -0.0038					
				0.3778 0.0066 0.6280 -0.0039					
93. (1.98937)	BD (1) C 14-		H 36						
	(61.40%)	0.7836*	C 14	s(26.73%)p 2.74(73.27%)					
				0.0000 0.5170 0.0007 -0.5059 0.0162					
				0.5924 0.0062 0.3543 0.0062					
	(38.60%)	0.6213*	H 36	s(100.00%)					
				1.0000 -0.0001					
94. (1.99001)	BD (1) C 14-		H 37						
	(61.87%)	0.7866*	C 14	s(26.55%)p 2.77(73.45%)					
				0.0000 0.5153 -0.0018 0.6618 0.0001					
				0.3595 0.0084 -0.4085 0.0176					
	(38.13%)	0.6175*	H 37	s(100.00%)					
				1.0000 0.0004					
95. (1.99280)	BD (1) C 14-		H 38						
	(61.18%)	0.7822*	C 14	s(26.45%)p 2.78(73.55%)					
				0.0000 0.5143 -0.0034 0.2678 0.0106					
				-0.5691 0.0175 0.5826 0.0115					
	(38.82%)	0.6231*	H 38	s(100.00%)					
				1.0000 0.0006					
96. (1.97685)	BD (1) C 15-		C 16						
	(50.46%)	0.7104*	C 15	s(28.02%)p 2.57(71.98%)					
				0.0000 0.5292 -0.0138 0.1013 -0.0143					
				0.2313 0.0129 -0.8096 0.0161					
	(49.54%)	0.7038*	C 16	s(26.59%)p 2.76(73.41%)					
				0.0000 0.5155 -0.0157 -0.1379 -0.0135					
				-0.1914 0.0178 0.8233 -0.0111					
97. (1.97917)	BD (1) C 15-		C 17						
	(51.97%)	0.7209*	C 15	s(28.10%)p 2.56(71.90%)					
				0.0000 0.5301 -0.0026 -0.7145 -0.0002					
				-0.4367 0.0040 0.1327 0.0123					
	(48.03%)	0.6931*	C 17	s(24.85%)p 3.02(75.15%)					
				0.0000 0.4985 -0.0009 0.7328 -0.0031					
				0.4309 -0.0107 -0.1691 0.0082					
98. (1.97918)	BD (1) C 15-		C 18						
	(50.47%)	0.7105*	C 15	s(28.53%)p 2.51(71.47%)					
				0.0000 0.5339 0.0134 0.1077 0.0059					
				0.6376 -0.0030 0.5445 0.0123					
	(49.53%)	0.7037*	C 18	s(26.33%)p 2.80(73.67%)					
				0.0000 0.5131 -0.0036 -0.0777 0.0066					
				-0.6437 0.0058 -0.5621 0.0173					
99. (1.97994)	BD (1) C 15-		O 21						
	(29.77%)	0.5457*	C 15	s(15.26%)p 5.55(84.74%)					
				0.0000 0.3904 0.0118 0.6833 0.0133					
				-0.5907 -0.0048 0.1723 0.0414					
	(70.23%)	0.8380*	O 21	s(26.64%)p 2.75(73.36%)					
				0.0000 0.5161 -0.0004 -0.6317 -0.0011					
				0.5739 -0.0035 -0.0697 0.0179					
100. (1.97641)	BD (1) C 16-		C 19						
	(51.70%)	0.7190*	C 16	s(27.79%)p 2.60(72.21%)					
				0.0000 0.5271 0.0088 -0.7270 0.0092					
				0.0999 -0.0072 -0.4282 -0.0112					
	(48.30%)	0.6950*	C 19	s(24.44%)p 3.09(75.56%)					
				0.0000 0.4943 -0.0012 0.7432 -0.0070					
				-0.1097 -0.0022 0.4370 -0.0169					

101.	(1.98035)	BD (1) C 16- C 20	(50.40%)	0.7099*	C 16	s(28.81%)p 2.47(71.19%)	0.0000	0.5368	0.0028	0.5351	-0.0012
							0.6448	0.0077	-0.0969	-0.0172	
			(49.60%)	0.7043*	C 20	s(26.08%)p 2.83(73.92%)	0.0000	0.5107	-0.0042	-0.5348	0.0145
							-0.6618	0.0078	0.1215	-0.0113	
102.	(1.97997)	BD (1) C 16- O 22	(31.26%)	0.5591*	C 16	s(16.69%)p 4.99(83.31%)	0.0000	0.4084	0.0105	0.4072	-0.0036
							-0.7328	-0.0065	-0.3582	-0.0451	
			(68.74%)	0.8291*	O 22	s(26.72%)p 2.74(73.28%)	0.0000	0.5169	-0.0014	-0.4000	-0.0009
							0.7087	0.0022	0.2653	-0.0140	
103.	(1.98276)	BD (1) C 17- H 39	(61.23%)	0.7825*	C 17	s(25.43%)p 2.93(74.57%)	0.0000	0.5043	0.0034	0.0274	-0.0216
							-0.3154	-0.0129	0.8030	-0.0026	
			(38.77%)	0.6227*	H 39	s(100.00%)	1.0000	-0.0009			
104.	(1.97765)	BD (1) C 17- H 40	(61.29%)	0.7829*	C 17	s(24.46%)p 3.09(75.54%)	0.0000	0.4945	0.0004	-0.6736	-0.0232
							0.5434	-0.0132	-0.0750	0.0061	
			(38.71%)	0.6221*	H 40	s(100.00%)	1.0000	-0.0013			
105.	(1.98328)	BD (1) C 17- H 41	(62.69%)	0.7917*	C 17	s(25.08%)p 2.99(74.92%)	0.0000	0.5008	-0.0021	-0.0909	-0.0198
							-0.6477	-0.0059	-0.5663	0.0161	
			(37.31%)	0.6109*	H 41	s(100.00%)	1.0000	0.0022			
106.	(1.98392)	BD (1) C 18- H 42	(61.11%)	0.7817*	C 18	s(25.20%)p 2.97(74.80%)	0.0000	0.5020	0.0036	-0.1482	0.0046
							-0.2832	0.0171	0.8034	0.0090	
			(38.89%)	0.6236*	H 42	s(100.00%)	1.0000	0.0007			
107.	(1.97577)	BD (1) C 18- H 43	(61.22%)	0.7824*	C 18	s(24.21%)p 3.13(75.79%)	0.0000	0.4920	0.0000	-0.5703	0.0000
							0.6288	0.0162	-0.1915	0.0175	
			(38.78%)	0.6228*	H 43	s(100.00%)	1.0000	0.0016			
108.	(1.98393)	BD (1) C 18- H 44	(61.15%)	0.7820*	C 18	s(24.11%)p 3.15(75.89%)	0.0000	0.4910	0.0005	0.8042	-0.0016
							0.3316	0.0098	-0.0420	0.0183	
			(38.85%)	0.6233*	H 44	s(100.00%)	1.0000	-0.0008			
109.	(1.98403)	BD (1) C 19- H 45	(61.51%)	0.7843*	C 19	s(25.40%)p 2.94(74.60%)	0.0000	0.5040	0.0030	0.1758	-0.0189
							0.1527	-0.0044	-0.8314	-0.0055	
			(38.49%)	0.6204*	H 45	s(100.00%)	1.0000	-0.0007			
110.	(1.97938)	BD (1) C 19- H 46	(60.63%)	0.7786*	C 19	s(24.54%)p 3.08(75.46%)	0.0000	0.4954	0.0004	-0.4269	-0.0225
							0.6778	0.0068	0.3351	-0.0125	
			(39.37%)	0.6275*	H 46	s(100.00%)	1.0000	-0.0018			
111.	(1.98438)	BD (1) C 19- H 47	(62.27%)	0.7891*	C 19	s(25.46%)p 2.93(74.54%)	0.0000	0.5046	-0.0012	-0.4842	-0.0107
							-0.7107	0.0074	0.0732	-0.0191	
			(37.73%)	0.6142*	H 47	s(100.00%)	1.0000	-0.0006			
112.	(1.98162)	BD (1) C 20- H 48	(61.81%)	0.7862*	C 20	s(24.85%)p 3.02(75.15%)	0.0000	0.4984	0.0035	0.2263	0.0133
							0.0489	0.0128	-0.8352	0.0028	
			(38.19%)	0.6180*	H 48	s(100.00%)	1.0000	0.0007			
113.	(1.97860)	BD (1) C 20- H 49	(61.15%)	0.7820*	C 20	s(24.21%)p 3.13(75.79%)	0.0000	0.4921	0.0000	-0.3938	0.0137

				0.7409	0.0176	0.2308	-0.0064	
	(38.85%)	0.6233*	H 49	s(100.00%)				
				1.0000	-0.0011			
114.	(1.98441)	BD (1) C 20-	H 50					
	(60.97%)	0.7808*	C 20	s(24.69%)p 3.05(75.31%)				
				0.0000	0.4969	0.0012	0.7125	0.0135
				-0.1028	0.0163	0.4840	-0.0098	
	(39.03%)	0.6248*	H 50	s(100.00%)				
				1.0000	-0.0005			
115.	(1.99046)	BD (1) O 21-	B 23					
	(81.02%)	0.9001*	O 21	s(44.83%)p 1.23(55.17%)				
				0.0000	0.6695	0.0018	0.2876	0.0096
				-0.3566	-0.0036	-0.5846	-0.0011	
	(18.98%)	0.4357*	B 23	s(29.18%)p 2.43(70.82%)				
				0.0000	0.5401	0.0062	-0.1977	0.0215
				0.3059	-0.0104	0.7566	0.0515	
116.	(1.98947)	BD (1) O 22-	B 23					
	(80.38%)	0.8965*	O 22	s(43.88%)p 1.28(56.12%)				
				0.0000	0.6624	0.0022	0.3698	0.0024
				-0.4506	-0.0088	0.4704	-0.0053	
	(19.62%)	0.4429*	B 23	s(31.42%)p 2.18(68.58%)				
				0.0000	0.5605	0.0078	-0.3070	-0.0039
				0.4154	-0.0144	-0.6444	-0.0594	
117.	(1.98272)	BD (1) N 24-	H 51					
	(72.66%)	0.8524*	N 24	s(27.61%)p 2.62(72.39%)				
				0.0000	0.5254	0.0060	-0.2720	-0.0140
				0.5901	0.0192	-0.5487	-0.0062	
	(27.34%)	0.5229*	H 51	s(100.00%)				
				0.9999	-0.0119			
118.	(1.99336)	BD (1) C 52-	F 53					
	(27.57%)	0.5250*	C 52	s(16.25%)p 5.15(83.75%)				
				0.0000	0.4025	0.0233	0.4362	0.0235
				-0.2013	-0.0111	-0.7773	-0.0415	
	(72.43%)	0.8511*	F 53	s(18.17%)p 4.50(81.83%)				
				0.0000	0.4262	0.0057	-0.3398	-0.0004
				0.2665	0.0013	0.7949	0.0015	
119.	(1.99691)	BD (1) C 52-	F 54					
	(26.45%)	0.5142*	C 52	s(26.04%)p 2.84(73.96%)				
				0.0000	0.5050	0.0733	-0.8323	-0.0835
				-0.0493	-0.0074	-0.1917	-0.0238	
	(73.55%)	0.8576*	F 54	s(36.73%)p 1.72(63.27%)				
				0.0000	0.6060	0.0066	0.7231	-0.0091
				0.0385	-0.0006	0.3291	-0.0043	
120.	(1.99550)	BD (1) C 52-	F 55					
	(27.17%)	0.5212*	C 52	s(25.17%)p 2.97(74.83%)				
				0.0000	0.4978	0.0627	0.2167	0.0227
				-0.6318	-0.0609	0.5441	0.0439	
	(72.83%)	0.8534*	F 55	s(30.82%)p 2.24(69.18%)				
				0.0000	0.5551	0.0048	-0.3180	0.0017
				0.6312	-0.0038	-0.4385	0.0021	
121.	(1.97804)	BD (1) C 52-	S 56					
	(55.81%)	0.7471*	C 52	s(33.02%)p 2.03(66.98%)				
				0.0000	0.5729	-0.0439	0.2458	-0.0119
				0.7415	-0.0308	0.2417	-0.0068	
	(44.19%)	0.6647*	S 56	s(19.27%)p 4.19(80.73%)				
				0.0000	0.0000	0.4373	0.0382	0.0000
				-0.3307	0.0106	0.0000	-0.8070	0.0301
				0.0000	-0.2134	0.0117		
122.	(1.98721)	BD (1) S 56-	O 57					
	(36.56%)	0.6047*	S 56	s(27.88%)p 2.59(72.12%)				
				0.0000	0.0000	0.5276	-0.0207	0.0000
				-0.3231	0.0203	0.0000	0.5603	-0.0558
				0.0000	-0.5458	0.0372		
	(63.44%)	0.7965*	O 57	s(22.55%)p 3.44(77.45%)				
				0.0000	0.4744	0.0209	0.3197	0.0146
				-0.5847	-0.0199	0.5739	0.0242	
123.	(1.98937)	BD (1) S 56-	O 58					
	(35.40%)	0.5949*	S 56	s(27.31%)p 2.66(72.69%)				
				0.0000	0.0000	0.5219	-0.0266	0.0000
				-0.2267	0.0119	0.0000	0.1604	-0.0250
				0.0000	0.8027	-0.0681		
	(64.60%)	0.8038*	O 58	s(24.93%)p 3.01(75.07%)				
				0.0000	0.4988	0.0231	0.1519	0.0102
				-0.0999	-0.0025	-0.8463	-0.0370	
124.	(1.98486)	BD (1) S 56-	O 59					
	(38.47%)	0.6203*	S 56	s(25.66%)p 2.90(74.34%)				
				0.0000	0.0000	0.5066	0.0005	0.0000

				0.8543	-0.0674	0.0000	-0.0564	-0.0036
				0.0000	-0.0761	-0.0013		
(61.53%)	0.7844*	O 59	s(16.29%)	p 5.14(83.71%)				
				0.0000	0.4034	0.0151	-0.9134	-0.0227
				0.0383	0.0060	-0.0288	0.0032	
----- non-Lewis -----								
125. (0.98373)	LV (1)	C 10	s(0.02%)	p99.99(99.98%)				
				0.0000	0.0125	0.0070	-0.8147	-0.0064
				-0.5338	-0.0106	-0.2258	-0.0069	
126. (0.42275)	LV (1)	B 23	s(0.04%)	p99.99(99.96%)				
				0.0000	0.0167	0.0114	-0.8051	0.0202
				-0.5921	0.0083	0.0172	-0.0093	
127. (0.00904)	BD*(1)	C 1- C 2						
(50.25%)	0.7089*	C 1	s(23.73%)	p 3.21(76.27%)				
				0.0000	-0.4871	0.0021	-0.1710	-0.0120
				0.3425	0.0101	-0.7845	0.0207	
(49.75%)	-0.7053*	C 2	s(24.09%)	p 3.15(75.91%)				
				0.0000	-0.4908	0.0030	0.1384	-0.0147
				-0.3034	0.0228	0.8045	-0.0033	
128. (0.02344)	BD*(1)	C 1- C 11						
(50.82%)	0.7129*	C 1	s(24.71%)	p 3.05(75.29%)				
				0.0000	-0.4971	0.0012	0.4549	-0.0085
				-0.7306	0.0046	-0.1088	0.0186	
(49.18%)	-0.7013*	C 11	s(30.91%)	p 2.24(69.09%)				
				0.0000	-0.5559	0.0069	-0.4610	0.0072
				0.6578	-0.0211	0.2111	0.0258	
129. (0.00956)	BD*(1)	C 1- H 25						
(38.35%)	0.6192*	C 1	s(25.83%)	p 2.87(74.17%)				
				0.0000	-0.5082	-0.0028	-0.7415	-0.0034
				-0.1752	0.0110	0.4012	0.0129	
(61.65%)	-0.7852*	H 25	s(100.00%)					
				-1.0000	0.0002			
130. (0.01079)	BD*(1)	C 1- H 26						
(37.99%)	0.6164*	C 1	s(25.57%)	p 2.91(74.43%)				
				0.0000	-0.5057	-0.0001	0.4626	-0.0092
				0.5641	0.0080	0.4600	0.0158	
(62.01%)	-0.7874*	H 26	s(100.00%)					
				-1.0000	-0.0003			
131. (0.02288)	BD*(1)	C 2- C 9						
(51.07%)	0.7146*	C 2	s(24.62%)	p 3.06(75.38%)				
				0.0000	-0.4962	0.0002	0.5094	-0.0104
				-0.4323	0.0166	-0.5541	-0.0092	
(48.93%)	-0.6995*	C 9	s(31.27%)	p 2.20(68.73%)				
				0.0000	-0.5592	0.0065	-0.4982	0.0037
				0.4958	0.0040	0.4384	-0.0319	
132. (0.01049)	BD*(1)	C 2- H 27						
(38.40%)	0.6197*	C 2	s(25.50%)	p 2.92(74.50%)				
				0.0000	-0.5049	-0.0014	-0.8274	-0.0121
				-0.1222	0.0162	-0.2125	-0.0017	
(61.60%)	-0.7848*	H 27	s(100.00%)					
				-1.0000	-0.0001			
133. (0.00984)	BD*(1)	C 2- H 28						
(38.05%)	0.6168*	C 2	s(25.63%)	p 2.90(74.37%)				
				0.0000	-0.5062	-0.0015	0.1918	-0.0134
				0.8403	0.0080	-0.0254	0.0004	
(61.95%)	-0.7871*	H 28	s(100.00%)					
				-1.0000	0.0000			
134. (0.01705)	BD*(1)	C 3- C 4						
(50.76%)	0.7124*	C 3	s(32.54%)	p 2.07(67.46%)				
				0.0000	-0.5704	-0.0052	0.4949	0.0004
				-0.5456	0.0136	-0.3611	-0.0365	
(49.24%)	-0.7017*	C 4	s(34.28%)	p 1.92(65.72%)				
				0.0000	-0.5855	-0.0036	-0.4778	-0.0026
				0.5524	0.0149	0.3503	-0.0283	
135. (0.02278)	BD*(1)	C 3- C 9						
(50.71%)	0.7121*	C 3	s(35.08%)	p 1.85(64.92%)				
				0.0000	-0.5923	0.0007	-0.1755	-0.0147
				-0.0579	0.0246	0.7837	-0.0010	
(49.29%)	-0.7021*	C 9	s(37.43%)	p 1.67(62.57%)				
				0.0000	-0.6117	-0.0123	0.1245	-0.0116
				0.1166	0.0258	-0.7717	-0.0168	
136. (0.25910)	BD*(2)	C 3- C 9						
(46.88%)	0.6847*	C 3	s(0.00%)	p 1.00(100.00%)				
				0.0000	0.0009	-0.0038	0.7909	-0.0184
				0.5707	-0.0103	0.2200	-0.0013	
(53.12%)	-0.7288*	C 9	s(0.01%)	p 1.00(99.99%)				
				0.0000	-0.0087	-0.0011	0.7828	-0.0036

					0.5816	-0.0023	0.2210	0.0027	
137.	(0.01280)	BD*(1) C	3- H 29						
	(39.14%)	0.6256*	C 3	s(32.22%)p 2.10(67.78%)					
				0.0000	-0.5676	0.0027	-0.3135	-0.0015	
				0.6106	0.0084	-0.4544	-0.0117		
	(60.86%)	-0.7802*	H 29	s(100.00%)					
				-1.0000	0.0010				
138.	(0.01992)	BD*(1) C	4- C 5						
	(50.87%)	0.7133*	C 4	s(34.06%)p 1.94(65.94%)					
				0.0000	-0.5836	-0.0020	0.3121	0.0074	
				-0.6180	-0.0046	0.4241	-0.0115		
	(49.13%)	-0.7009*	C 5	s(37.55%)p 1.66(62.45%)					
				0.0000	-0.6128	-0.0031	-0.3021	0.0026	
				0.6018	0.0061	-0.4131	-0.0164		
139.	(0.33828)	BD*(2) C	4- C 5						
	(53.97%)	0.7346*	C 4	s(0.00%)p 1.00(100.00%)					
				0.0000	-0.0019	-0.0044	0.8029	-0.0122	
				0.5554	-0.0068	0.2160	-0.0034		
	(46.03%)	-0.6785*	C 5	s(0.02%)p 99.99(99.98%)					
				0.0000	-0.0110	-0.0083	0.8117	-0.0133	
				0.5432	-0.0057	0.2139	-0.0008		
140.	(0.01089)	BD*(1) C	4- H 30						
	(39.60%)	0.6293*	C 4	s(31.52%)p 2.17(68.48%)					
				0.0000	-0.5614	0.0035	0.1717	-0.0055	
				0.0635	0.0192	-0.8066	-0.0178		
	(60.40%)	-0.7772*	H 30	s(100.00%)					
				-1.0000	0.0002				
141.	(0.02972)	BD*(1) C	5- C 10						
	(50.10%)	0.7078*	C 5	s(38.29%)p 1.61(61.71%)					
				0.0000	0.6188	-0.0057	0.1030	-0.0097	
				0.1586	0.0050	-0.7623	0.0082		
	(49.90%)	-0.7064*	C 10	s(33.67%)p 1.97(66.33%)					
				0.0000	0.5803	0.0048	-0.1804	-0.0102	
				-0.0465	0.0121	0.7927	-0.0013		
142.	(0.04305)	BD*(1) C	5- N 24						
	(64.58%)	0.8036*	C 5	s(24.12%)p 3.15(75.88%)					
				0.0000	0.4910	0.0101	-0.4889	-0.0094	
				0.5634	0.0079	0.4498	0.0027		
	(35.42%)	-0.5951*	N 24	s(25.35%)p 2.94(74.65%)					
				0.0000	0.5035	-0.0024	0.4832	-0.0112	
				-0.5957	0.0107	-0.3975	0.0035		
143.	(0.01881)	BD*(1) C	6- C 7						
	(48.65%)	0.6975*	C 6	s(33.17%)p 2.01(66.83%)					
				0.0000	-0.5759	-0.0091	-0.2686	-0.0079	
				0.0721	-0.0003	0.7684	0.0221		
	(51.35%)	-0.7166*	C 7	s(35.48%)p 1.82(64.52%)					
				0.0000	-0.5956	0.0016	0.2409	0.0037	
				-0.0138	-0.0094	-0.7661	0.0056		
144.	(0.26032)	BD*(2) C	6- C 7						
	(45.58%)	0.6751*	C 6	s(0.00%)p 1.00(100.00%)					
				0.0000	-0.0002	0.0069	-0.8103	-0.0029	
				-0.5376	-0.0132	-0.2328	-0.0040		
	(54.42%)	-0.7377*	C 7	s(0.00%)p 1.00(100.00%)					
				0.0000	0.0003	0.0027	-0.8105	0.0102	
				-0.5317	0.0050	-0.2455	-0.0013		
145.	(0.03111)	BD*(1) C	6- C 10						
	(51.41%)	0.7170*	C 6	s(32.96%)p 2.03(67.04%)					
				0.0000	-0.5741	-0.0065	-0.2123	0.0051	
				0.5613	0.0008	-0.5569	-0.0090		
	(48.59%)	-0.6971*	C 10	s(34.87%)p 1.87(65.13%)					
				0.0000	-0.5905	0.0033	0.2645	-0.0006	
				-0.6106	0.0074	0.4565	-0.0110		
146.	(0.02706)	BD*(1) C	6- B 23						
	(31.71%)	0.5631*	C 6	s(33.85%)p 1.95(66.15%)					
				0.0000	-0.5817	0.0098	0.4750	-0.0158	
				-0.6247	0.0275	-0.2114	0.0025		
	(68.29%)	-0.8264*	B 23	s(39.38%)p 1.54(60.62%)					
				0.0000	-0.6275	0.0082	-0.4663	0.0116	
				0.6188	-0.0084	0.0750	0.0062		
147.	(0.02041)	BD*(1) C	7- C 8						
	(50.15%)	0.7082*	C 7	s(33.13%)p 2.02(66.87%)					
				0.0000	0.5756	0.0057	0.4787	-0.0010	
				-0.5967	0.0140	-0.2866	-0.0328		
	(49.85%)	-0.7060*	C 8	s(32.54%)p 2.07(67.46%)					
				0.0000	0.5704	0.0024	-0.4658	-0.0030	
				0.6063	0.0165	0.2981	-0.0298		
148.	(0.01167)	BD*(1) C	7- H 31						

	(38.75%)	0.6225*	C 7	s(31.28%)p 2.20(68.72%)					
				0.0000 -0.5592 0.0032 0.2362 -0.0005					
				-0.6006 -0.0020 0.5201 0.0159					
	(61.25%)	-0.7826*	H 31	s(100.00%)					
				-1.0000 0.0024					
149. (0.02275)	BD*(1) C 8-	C 11							
	(51.12%)	0.7150*	C 8	s(34.42%)p 1.91(65.58%)					
				0.0000 -0.5866 -0.0034 -0.2416 -0.0133					
				0.6038 0.0132 -0.4818 0.0200					
	(48.88%)	-0.6991*	C 11	s(37.31%)p 1.68(62.69%)					
				0.0000 -0.6107 -0.0116 0.2013 -0.0104					
				-0.5473 0.0056 0.5345 0.0305					
150. (0.24394)	BD*(2) C 8-	C 11							
	(47.82%)	0.6915*	C 8	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0049 0.0033 -0.8212 0.0170					
				-0.5166 0.0087 -0.2415 0.0070					
	(52.18%)	-0.7224*	C 11	s(0.01%)p 1.00(99.99%)					
				0.0000 -0.0068 0.0023 -0.8278 0.0077					
				-0.5147 -0.0031 -0.2229 0.0014					
151. (0.01224)	BD*(1) C 8-	H 32							
	(39.28%)	0.6267*	C 8	s(32.89%)p 2.04(67.11%)					
				0.0000 -0.5735 0.0036 -0.2234 -0.0010					
				-0.0185 -0.0057 0.7877 0.0166					
	(60.72%)	-0.7792*	H 32	s(100.00%)					
				-1.0000 0.0008					
152. (0.02909)	BD*(1) C 9-	C 12							
	(51.00%)	0.7141*	C 9	s(31.20%)p 2.21(68.80%)					
				0.0000 -0.5585 0.0050 0.3509 -0.0022					
				-0.6341 0.0033 0.4035 0.0018					
	(49.00%)	-0.7000*	C 12	s(32.51%)p 2.08(67.49%)					
				0.0000 -0.5702 0.0004 -0.2972 0.0052					
				0.6050 -0.0063 -0.4695 -0.0022					
153. (0.03142)	BD*(1) C 10-	C 12							
	(49.82%)	0.7058*	C 10	s(31.43%)p 2.18(68.57%)					
				0.0000 -0.5607 -0.0010 -0.4833 0.0047					
				0.5830 -0.0073 0.3348 0.0056					
	(50.18%)	-0.7084*	C 12	s(34.46%)p 1.90(65.54%)					
				0.0000 -0.5871 -0.0021 0.4721 -0.0055					
				-0.5724 0.0096 -0.3237 0.0044					
154. (0.02934)	BD*(1) C 11-	C 12							
	(51.27%)	0.7160*	C 11	s(31.67%)p 2.16(68.33%)					
				0.0000 0.5627 -0.0040 -0.2475 -0.0012					
				0.0497 0.0020 0.7872 -0.0020					
	(48.73%)	-0.6981*	C 12	s(33.02%)p 2.03(66.98%)					
				0.0000 0.5746 -0.0003 0.1953 -0.0031					
				0.0211 0.0027 -0.7945 0.0019					
155. (0.01583)	BD*(1) C 13-	N 24							
	(66.02%)	0.8125*	C 13	s(19.02%)p 4.26(80.98%)					
				0.0000 0.4358 0.0149 0.7427 0.0174					
				0.3658 0.0161 -0.3519 -0.0087					
	(33.98%)	-0.5829*	N 24	s(23.88%)p 3.19(76.12%)					
				0.0000 0.4887 -0.0031 -0.6787 0.0007					
				-0.3926 0.0085 0.3825 -0.0090					
156. (0.00614)	BD*(1) C 13-	H 33							
	(38.70%)	0.6221*	C 13	s(26.44%)p 2.78(73.56%)					
				0.0000 -0.5142 -0.0005 0.4365 0.0188					
				-0.6356 0.0156 -0.3747 -0.0009					
	(61.30%)	-0.7829*	H 33	s(100.00%)					
				-1.0000 -0.0002					
157. (0.01200)	BD*(1) C 13-	H 34							
	(35.79%)	0.5983*	C 13	s(28.30%)p 2.53(71.70%)					
				0.0000 -0.5320 0.0040 0.4353 0.0115					
				0.3569 -0.0020 0.6321 -0.0221					
	(64.21%)	-0.8013*	H 34	s(100.00%)					
				-1.0000 -0.0053					
158. (0.00565)	BD*(1) C 13-	H 35							
	(39.12%)	0.6254*	C 13	s(26.20%)p 2.82(73.80%)					
				0.0000 -0.5119 0.0027 -0.2597 0.0260					
				0.5782 0.0077 -0.5792 -0.0045					
	(60.88%)	-0.7803*	H 35	s(100.00%)					
				-1.0000 0.0007					
159. (0.01741)	BD*(1) C 14-	N 24							
	(64.36%)	0.8022*	C 14	s(20.23%)p 3.94(79.77%)					
				0.0000 0.4497 0.0107 -0.4837 -0.0130					
				-0.4425 -0.0007 -0.6063 -0.0098					
	(35.64%)	-0.5970*	N 24	s(23.09%)p 3.33(76.91%)					
				0.0000 0.4805 -0.0010 0.4815 -0.0038					

				0.3778	0.0066	0.6280	-0.0039	
160.	(0.00651)	BD*(1) C 14- H 36						
	(38.60%)	0.6213* C 14	s(26.73%)p 2.74(73.27%)					
			0.0000 -0.5170 -0.0007 0.5059 -0.0162					
			-0.5924 -0.0062 -0.3543 -0.0062					
	(61.40%)	-0.7836* H 36	s(100.00%)					
			-1.0000 0.0001					
161.	(0.00564)	BD*(1) C 14- H 37						
	(38.13%)	0.6175* C 14	s(26.55%)p 2.77(73.45%)					
			0.0000 -0.5153 0.0018 -0.6618 -0.0001					
			-0.3595 -0.0084 0.4085 -0.0176					
	(61.87%)	-0.7866* H 37	s(100.00%)					
			-1.0000 -0.0004					
162.	(0.00590)	BD*(1) C 14- H 38						
	(38.82%)	0.6231* C 14	s(26.45%)p 2.78(73.55%)					
			0.0000 -0.5143 0.0034 -0.2678 -0.0106					
			0.5691 -0.0175 -0.5826 -0.0115					
	(61.18%)	-0.7822* H 38	s(100.00%)					
			-1.0000 -0.0006					
163.	(0.05754)	BD*(1) C 15- C 16						
	(49.54%)	0.7038* C 15	s(28.02%)p 2.57(71.98%)					
			0.0000 0.5292 -0.0138 0.1013 -0.0143					
			0.2313 0.0129 -0.8096 0.0161					
	(50.46%)	-0.7104* C 16	s(26.59%)p 2.76(73.41%)					
			0.0000 0.5155 -0.0157 -0.1379 -0.0135					
			-0.1914 0.0178 0.8233 -0.0111					
164.	(0.02534)	BD*(1) C 15- C 17						
	(48.03%)	0.6931* C 15	s(28.10%)p 2.56(71.90%)					
			0.0000 0.5301 -0.0026 -0.7145 -0.0002					
			-0.4367 0.0040 0.1327 0.0123					
	(51.97%)	-0.7209* C 17	s(24.85%)p 3.02(75.15%)					
			0.0000 0.4985 -0.0009 0.7328 -0.0031					
			0.4309 -0.0107 -0.1691 0.0082					
165.	(0.02502)	BD*(1) C 15- C 18						
	(49.53%)	0.7037* C 15	s(28.53%)p 2.51(71.47%)					
			0.0000 0.5339 0.0134 0.1077 0.0059					
			0.6376 -0.0030 0.5445 0.0123					
	(50.47%)	-0.7105* C 18	s(26.33%)p 2.80(73.67%)					
			0.0000 0.5131 -0.0036 -0.0777 0.0066					
			-0.6437 0.0058 -0.5621 0.0173					
166.	(0.06222)	BD*(1) C 15- O 21						
	(70.23%)	0.8380* C 15	s(15.26%)p 5.55(84.74%)					
			0.0000 0.3904 0.0118 0.6833 0.0133					
			-0.5907 -0.0048 0.1723 0.0414					
	(29.77%)	-0.5457* O 21	s(26.64%)p 2.75(73.36%)					
			0.0000 0.5161 -0.0004 -0.6317 -0.0011					
			0.5739 -0.0035 -0.0697 0.0179					
167.	(0.02580)	BD*(1) C 16- C 19						
	(48.30%)	0.6950* C 16	s(27.79%)p 2.60(72.21%)					
			0.0000 0.5271 0.0088 -0.7270 0.0092					
			0.0999 -0.0072 -0.4282 -0.0112					
	(51.70%)	-0.7190* C 19	s(24.44%)p 3.09(75.56%)					
			0.0000 0.4943 -0.0012 0.7432 -0.0070					
			-0.1097 -0.0022 0.4370 -0.0169					
168.	(0.02794)	BD*(1) C 16- C 20						
	(49.60%)	0.7043* C 16	s(28.81%)p 2.47(71.19%)					
			0.0000 0.5368 0.0028 0.5351 -0.0012					
			0.6448 0.0077 -0.0969 -0.0172					
	(50.40%)	-0.7099* C 20	s(26.08%)p 2.83(73.92%)					
			0.0000 0.5107 -0.0042 -0.5348 0.0145					
			-0.6618 0.0078 0.1215 -0.0113					
169.	(0.05358)	BD*(1) C 16- O 22						
	(68.74%)	0.8291* C 16	s(16.69%)p 4.99(83.31%)					
			0.0000 0.4084 0.0105 0.4072 -0.0036					
			-0.7328 -0.0065 -0.3582 -0.0451					
	(31.26%)	-0.5591* O 22	s(26.72%)p 2.74(73.28%)					
			0.0000 0.5169 -0.0014 -0.4000 -0.0009					
			0.7087 0.0022 0.2653 -0.0140					
170.	(0.00724)	BD*(1) C 17- H 39						
	(38.77%)	0.6227* C 17	s(25.43%)p 2.93(74.57%)					
			0.0000 -0.5043 -0.0034 -0.0274 0.0216					
			0.3154 0.0129 -0.8030 0.0026					
	(61.23%)	-0.7825* H 39	s(100.00%)					
			-1.0000 0.0009					
171.	(0.00756)	BD*(1) C 17- H 40						
	(38.71%)	0.6221* C 17	s(24.46%)p 3.09(75.54%)					
			0.0000 -0.4945 -0.0004 0.6736 0.0232					

	(61.29%)	-0.7829*	H 40	s(100.00%) -1.0000 0.0013	-0.5434 0.0132 0.0750 -0.0061	
172.	(0.01055)	BD*(1) C 17-	H 41	s(25.08%)p 2.99(74.92%) 0.0000 -0.5008 0.0021 0.0909 0.0198 0.6477 0.0059 0.5663 -0.0161		
	(37.31%)	0.6109*	C 17	s(100.00%) -1.0000 -0.0022		
173.	(0.00854)	BD*(1) C 18-	H 42	s(25.20%)p 2.97(74.80%) 0.0000 -0.5020 -0.0036 0.1482 -0.0046 0.2832 -0.0171 -0.8034 -0.0090		
	(38.89%)	0.6236*	C 18	s(100.00%) -1.0000 -0.0007		
174.	(0.00748)	BD*(1) C 18-	H 43	s(24.21%)p 3.13(75.79%) 0.0000 -0.4920 0.0000 0.5703 0.0000 -0.6288 -0.0162 0.1915 -0.0175		
	(38.78%)	0.6228*	C 18	s(100.00%) -1.0000 -0.0016		
175.	(0.00890)	BD*(1) C 18-	H 44	s(24.11%)p 3.15(75.89%) 0.0000 -0.4910 -0.0005 -0.8042 0.0016 -0.3316 -0.0098 0.0420 -0.0183		
	(38.85%)	0.6233*	C 18	s(100.00%) -1.0000 0.0008		
176.	(0.00723)	BD*(1) C 19-	H 45	s(25.40%)p 2.94(74.60%) 0.0000 -0.5040 -0.0030 -0.1758 0.0189 -0.1527 0.0044 0.8314 0.0055		
	(38.49%)	0.6204*	C 19	s(100.00%) -1.0000 0.0007		
177.	(0.00632)	BD*(1) C 19-	H 46	s(24.54%)p 3.08(75.46%) 0.0000 -0.4954 -0.0004 0.4269 0.0225 -0.6778 -0.0068 -0.3351 0.0125		
	(39.37%)	0.6275*	C 19	s(100.00%) -1.0000 0.0018		
178.	(0.00716)	BD*(1) C 19-	H 47	s(25.46%)p 2.93(74.54%) 0.0000 -0.5046 0.0012 0.4842 0.0107 0.7107 -0.0074 -0.0732 0.0191		
	(37.73%)	0.6142*	C 19	s(100.00%) -1.0000 0.0006		
179.	(0.00801)	BD*(1) C 20-	H 48	s(24.85%)p 3.02(75.15%) 0.0000 -0.4984 -0.0035 -0.2263 -0.0133 -0.0489 -0.0128 0.8352 -0.0028		
	(38.19%)	0.6180*	C 20	s(100.00%) -1.0000 -0.0007		
180.	(0.00799)	BD*(1) C 20-	H 49	s(24.21%)p 3.13(75.79%) 0.0000 -0.4921 0.0000 0.3938 -0.0137 -0.7409 -0.0176 -0.2308 0.0064		
	(38.85%)	0.6233*	C 20	s(100.00%) -1.0000 0.0011		
181.	(0.00851)	BD*(1) C 20-	H 50	s(24.69%)p 3.05(75.31%) 0.0000 -0.4969 -0.0012 -0.7125 -0.0135 0.1028 -0.0163 -0.4840 0.0098		
	(39.03%)	0.6248*	C 20	s(100.00%) -1.0000 0.0005		
182.	(0.02739)	BD*(1) O 21-	B 23	s(44.83%)p 1.23(55.17%) 0.0000 -0.6695 -0.0018 -0.2876 -0.0096 0.3566 0.0036 0.5846 0.0011		
	(18.98%)	0.4357*	O 21	s(29.18%)p 2.43(70.82%) 0.0000 -0.5401 -0.0062 0.1977 -0.0215 -0.3059 0.0104 -0.7566 -0.0515		
183.	(0.02191)	BD*(1) O 22-	B 23	s(43.88%)p 1.28(56.12%) 0.0000 -0.6624 -0.0022 -0.3698 -0.0024 0.4506 0.0088 -0.4704 0.0053		
	(19.62%)	0.4429*	O 22	s(31.42%)p 2.18(68.58%) 0.0000 -0.5605 -0.0078 0.3070 0.0039 -0.4154 0.0144 0.6444 0.0594		
	(80.38%)	-0.8965*	B 23			

184.	(0.03194)	BD*(1) N 24- H 51	(27.34%)	0.5229*	N 24	s(27.61%)p 2.62(72.39%)	0.0000	-0.5254	-0.0060	0.2720	0.0140
							-0.5901	-0.0192	0.5487	0.0062	
			(72.66%)	-0.8524*	H 51	s(100.00%)	-0.9999	0.0119			
185.	(0.17979)	BD*(1) C 52- F 53	(72.43%)	0.8511*	C 52	s(16.25%)p 5.15(83.75%)	0.0000	0.4025	0.0233	0.4362	0.0235
							-0.2013	-0.0111	-0.7773	-0.0415	
			(27.57%)	-0.5250*	F 53	s(18.17%)p 4.50(81.83%)	0.0000	0.4262	0.0057	-0.3398	-0.0004
							0.2665	0.0013	0.7949	0.0015	
186.	(0.08366)	BD*(1) C 52- F 54	(73.55%)	0.8576*	C 52	s(26.04%)p 2.84(73.96%)	0.0000	0.5050	0.0733	-0.8323	-0.0835
							-0.0493	-0.0074	-0.1917	-0.0238	
			(26.45%)	-0.5142*	F 54	s(36.73%)p 1.72(63.27%)	0.0000	0.6060	0.0066	0.7231	-0.0091
							0.0385	-0.0006	0.3291	-0.0043	
187.	(0.10593)	BD*(1) C 52- F 55	(72.83%)	0.8534*	C 52	s(25.17%)p 2.97(74.83%)	0.0000	0.4978	0.0627	0.2167	0.0227
							-0.6318	-0.0609	0.5441	0.0439	
			(27.17%)	-0.5212*	F 55	s(30.82%)p 2.24(69.18%)	0.0000	0.5551	0.0048	-0.3180	0.0017
							0.6312	-0.0038	-0.4385	0.0021	
188.	(0.40352)	BD*(1) C 52- S 56	(44.19%)	0.6647*	C 52	s(33.02%)p 2.03(66.98%)	0.0000	0.5729	-0.0439	0.2458	-0.0119
							0.7415	-0.0308	0.2417	-0.0068	
			(55.81%)	-0.7471*	S 56	s(19.27%)p 4.19(80.73%)	0.0000	0.0000	0.4373	0.0382	0.0000
							-0.3307	0.0106	0.0000	-0.8070	0.0301
							0.0000	-0.2134	0.0117		
189.	(0.16992)	BD*(1) S 56- O 57	(63.44%)	0.7965*	S 56	s(27.88%)p 2.59(72.12%)	0.0000	0.0000	0.5276	-0.0207	0.0000
							-0.3231	0.0203	0.0000	0.5603	-0.0558
							0.0000	-0.5458	0.0372		
			(36.56%)	-0.6047*	O 57	s(22.55%)p 3.44(77.45%)	0.0000	0.4744	0.0209	0.3197	0.0146
							-0.5847	-0.0199	0.5739	0.0242	
190.	(0.16459)	BD*(1) S 56- O 58	(64.60%)	0.8038*	S 56	s(27.31%)p 2.66(72.69%)	0.0000	0.0000	0.5219	-0.0266	0.0000
							-0.2267	0.0119	0.0000	0.1604	-0.0250
							0.0000	0.8027	-0.0681		
			(35.40%)	-0.5949*	O 58	s(24.93%)p 3.01(75.07%)	0.0000	0.4988	0.0231	0.1519	0.0102
							-0.0999	-0.0025	-0.8463	-0.0370	
191.	(0.21129)	BD*(1) S 56- O 59	(61.53%)	0.7844*	S 56	s(25.66%)p 2.90(74.34%)	0.0000	0.0000	0.5066	0.0005	0.0000
							0.8543	-0.0674	0.0000	-0.0564	-0.0036
							0.0000	-0.0761	-0.0013		
			(38.47%)	-0.6203*	O 59	s(16.29%)p 5.14(83.71%)	0.0000	0.4034	0.0151	-0.9134	-0.0227
							0.0383	0.0060	-0.0288	0.0032	
192.	(0.00223)	RY (1) C 1				s(0.69%)p99.99(99.31%)	0.0000	0.0252	0.0794	-0.0058	-0.7139
							-0.0009	-0.3799	0.0069	0.5822	
193.	(0.00140)	RY (2) C 1				s(0.69%)p99.99(99.31%)	0.0000	0.0296	0.0775	0.0012	0.3309
							-0.0008	0.5570	0.0032	0.7572	
194.	(0.00095)	RY (3) C 1				s(3.56%)p27.07(96.44%)	0.0000	0.0122	0.1883	0.0012	-0.5990
							-0.0034	0.7223	0.0020	-0.2894	
195.	(0.00020)	RY (4) C 1				s(95.22%)p 0.05(4.78%)	0.0000	-0.0066	0.9758	-0.0021	0.1475
							0.0005	-0.1527	0.0018	-0.0517	
196.	(0.00216)	RY (1) C 2				s(0.61%)p99.99(99.39%)	0.0000	0.0240	0.0742	-0.0009	0.2746
							0.0105	0.9182	-0.0036	-0.2742	
197.	(0.00134)	RY (2) C 2				s(0.52%)p99.99(99.48%)	0.0000	-0.0235	0.0685	0.0023	0.7231
							-0.0032	-0.0160	0.0003	0.6868	

198.	(0.00104)	RY	(3)	C	2	s(5.64%)p16.73(94.36%) 0.0000 0.0229 0.2364 0.0022 -0.6281 -0.0002 0.3614 -0.0064 0.6469
199.	(0.00022)	RY	(4)	C	2	s(93.39%)p 0.07(6.61%) 0.0000 -0.0057 0.9664 -0.0020 0.0813 0.0016 -0.1578 -0.0009 -0.1859
200.	(0.00444)	RY	(1)	C	3	s(0.17%)p99.99(99.83%) 0.0000 0.0400 -0.0090 -0.0079 -0.3191 0.0110 0.6860 0.0009 -0.6525
201.	(0.00227)	RY	(2)	C	3	s(0.43%)p99.99(99.57%) 0.0000 -0.0034 0.0654 0.0095 -0.5104 -0.0101 0.4549 -0.0242 0.7263
202.	(0.00093)	RY	(3)	C	3	s(0.28%)p99.99(99.72%) 0.0000 0.0021 0.0532 0.0172 0.7981 0.0114 0.5645 0.0038 0.2026
203.	(0.00024)	RY	(4)	C	3	s(99.28%)p 0.01(0.72%) 0.0000 -0.0005 0.9964 0.0049 -0.0121 -0.0022 -0.0538 0.0010 -0.0645
204.	(0.00377)	RY	(1)	C	4	s(0.11%)p99.99(99.89%) 0.0000 0.0331 0.0025 0.0060 0.2161 -0.0087 0.0364 -0.0015 -0.9751
205.	(0.00210)	RY	(2)	C	4	s(2.83%)p34.35(97.17%) 0.0000 0.0168 0.1674 0.0059 -0.5137 -0.0144 0.8371 0.0144 -0.0814
206.	(0.00084)	RY	(3)	C	4	s(0.10%)p99.99(99.90%) 0.0000 -0.0020 0.0319 -0.0107 -0.8224 -0.0085 -0.5306 -0.0040 -0.2021
207.	(0.00044)	RY	(4)	C	4	s(97.09%)p 0.03(2.91%) 0.0000 -0.0042 0.9854 0.0012 0.1133 0.0058 -0.1252 0.0037 0.0228
208.	(0.00480)	RY	(1)	C	5	s(0.94%)p99.99(99.06%) 0.0000 -0.0139 0.0958 -0.0057 0.0409 0.0097 -0.3628 -0.0037 0.9259
209.	(0.00368)	RY	(2)	C	5	s(3.01%)p32.26(96.99%) 0.0000 0.0140 0.1728 0.0003 0.5497 0.0089 -0.7456 -0.0035 -0.3342
210.	(0.00326)	RY	(3)	C	5	s(0.11%)p99.99(99.89%) 0.0000 0.0052 0.0326 0.0116 0.8242 0.0085 0.5386 0.0022 0.1713
211.	(0.00134)	RY	(4)	C	5	s(95.97%)p 0.04(4.03%) 0.0000 -0.0048 0.9796 0.0117 -0.1285 -0.0012 0.1491 -0.0077 -0.0373
212.	(0.00425)	RY	(1)	C	6	s(2.14%)p45.75(97.86%) 0.0000 0.0197 0.1449 -0.0155 -0.4913 0.0159 0.5411 -0.0144 0.6662
213.	(0.00278)	RY	(2)	C	6	s(5.37%)p17.61(94.63%) 0.0000 0.0053 0.2318 -0.0162 -0.1992 0.0100 0.6324 0.0187 -0.7113
214.	(0.00142)	RY	(3)	C	6	s(92.49%)p 0.08(7.51%) 0.0000 -0.0077 0.9617 0.0033 0.1122 0.0099 -0.2400 0.0050 0.0687
215.	(0.00079)	RY	(4)	C	6	s(0.01%)p99.99(99.99%) 0.0000 0.0009 0.0114 -0.0085 0.8402 -0.0059 0.4988 0.0012 0.2120
216.	(0.00494)	RY	(1)	C	7	s(0.42%)p99.99(99.58%) 0.0000 -0.0311 0.0568 -0.0085 -0.2946 0.0127 0.7105 0.0066 -0.6355
217.	(0.00209)	RY	(2)	C	7	s(1.94%)p50.57(98.06%) 0.0000 0.0150 0.1384 0.0028 -0.5078 -0.0050 0.4334 -0.0129 0.7313
218.	(0.00052)	RY	(3)	C	7	s(90.72%)p 0.10(9.28%) 0.0000 -0.0005 0.9525 0.0008 0.3007 0.0083 0.0483 0.0033 0.0000
219.	(0.00045)	RY	(4)	C	7	s(7.04%)p13.21(92.96%) 0.0000 -0.0015 0.2653 -0.0088 -0.7516 -0.0044 -0.5520 0.0004 -0.2449
220.	(0.00413)	RY	(1)	C	8	s(0.16%)p99.99(99.84%) 0.0000 0.0387 -0.0108 -0.0022 -0.2712 0.0045 -0.0031 0.0071 0.9616
221.	(0.00204)	RY	(2)	C	8	s(0.66%)p99.99(99.34%) 0.0000 -0.0062 0.0812 0.0108 -0.4581 -0.0215 0.8759 0.0061 -0.1252
222.	(0.00066)	RY	(3)	C	8	s(0.10%)p99.99(99.90%) 0.0000 -0.0011 0.0316 -0.0157 -0.8440 -0.0114 -0.4786 -0.0052 -0.2391
223.	(0.00032)	RY	(4)	C	8	s(99.23%)p 0.01(0.77%) 0.0000 -0.0004 0.9961 0.0034 0.0611

224.	(0.00398)	RY	(1)	C	9	0.0045 -0.0563 -0.0047 0.0283 s(0.05%)p99.99(99.95%) 0.0000 0.0098 0.0206 0.0162 0.4006 -0.0129 -0.4590 -0.0115 -0.7923
225.	(0.00348)	RY	(2)	C	9	s(3.14%)p30.87(96.86%) 0.0000 0.0319 0.1742 0.0075 -0.3643 -0.0110 0.7018 0.0132 -0.5857
226.	(0.00155)	RY	(3)	C	9	s(1.32%)p74.59(98.68%) 0.0000 -0.0029 0.1150 -0.0032 -0.8265 -0.0008 -0.5417 -0.0037 -0.1011
227.	(0.00072)	RY	(4)	C	9	s(95.58%)p 0.05(4.42%) 0.0000 -0.0067 0.9776 0.0027 0.1535 0.0045 -0.0514 -0.0161 0.1329
228.	(0.00576)	RY	(1)	C	10	s(1.04%)p95.35(98.96%) 0.0000 0.0082 0.1015 0.0034 0.4539 0.0068 -0.4003 0.0052 -0.7895
229.	(0.00399)	RY	(2)	C	10	s(0.04%)p99.99(99.96%) 0.0000 -0.0064 0.0198 -0.0069 -0.3596 0.0132 0.7334 -0.0130 -0.5761
230.	(0.00075)	RY	(3)	C	10	s(1.70%)p57.92(98.30%) 0.0000 -0.0029 0.1302 0.0110 -0.8123 0.0070 -0.5403 0.0018 -0.1762
231.	(0.00053)	RY	(4)	C	10	s(97.23%)p 0.03(2.77%) 0.0000 -0.0018 0.9860 0.0037 0.0679 0.0047 0.0978 -0.0039 0.1162
232.	(0.00396)	RY	(1)	C	11	s(0.49%)p99.99(99.51%) 0.0000 0.0071 0.0694 -0.0131 -0.5835 0.0142 0.7148 -0.0115 0.3785
233.	(0.00323)	RY	(2)	C	11	s(1.90%)p51.65(98.10%) 0.0000 0.0342 0.1335 0.0130 0.1008 -0.0076 -0.4061 -0.0158 0.8975
234.	(0.00168)	RY	(3)	C	11	s(2.09%)p46.83(97.91%) 0.0000 -0.0019 0.1446 0.0037 0.8006 0.0021 0.5635 0.0033 0.1436
235.	(0.00069)	RY	(4)	C	11	s(95.63%)p 0.05(4.37%) 0.0000 -0.0059 0.9779 0.0051 -0.0909 -0.0100 -0.0784 0.0111 -0.1705
236.	(0.00514)	RY	(1)	C	12	s(0.33%)p99.99(99.67%) 0.0000 -0.0001 0.0577 -0.0017 -0.0256 -0.0011 -0.3937 0.0005 0.9171
237.	(0.00256)	RY	(2)	C	12	s(3.79%)p25.39(96.21%) 0.0000 -0.0005 0.1947 -0.0143 -0.5430 0.0073 0.7601 0.0017 0.2989
238.	(0.00077)	RY	(3)	C	12	s(95.88%)p 0.04(4.12%) 0.0000 -0.0008 0.9792 0.0061 0.1124 -0.0015 -0.1261 -0.0006 -0.1126
239.	(0.00038)	RY	(4)	C	12	s(0.00%)p 1.00(100.00%) 0.0000 -0.0017 0.0035 0.0110 -0.8317 0.0069 -0.5011 0.0027 -0.2385
240.	(0.00284)	RY	(1)	C	13	s(0.01%)p 1.00(99.99%) 0.0000 0.0014 0.0076 0.0036 0.4988 0.0045 -0.0096 0.0172 0.8664
241.	(0.00245)	RY	(2)	C	13	s(0.50%)p99.99(99.50%) 0.0000 -0.0045 0.0703 -0.0077 -0.2822 0.0058 0.9410 0.0119 0.1720
242.	(0.00133)	RY	(3)	C	13	s(30.41%)p 2.29(69.59%) 0.0000 0.0183 0.5511 -0.0299 0.6908 -0.0194 0.2389 0.0177 -0.4000
243.	(0.00024)	RY	(4)	C	13	s(69.13%)p 0.45(30.87%) 0.0000 -0.0157 0.8313 0.0061 -0.4391 0.0017 -0.2381 -0.0080 0.2430
244.	(0.00232)	RY	(1)	C	14	s(0.07%)p99.99(99.93%) 0.0000 0.0008 0.0262 -0.0081 -0.5562 -0.0016 -0.3988 0.0094 0.7286
245.	(0.00219)	RY	(2)	C	14	s(1.37%)p71.76(98.63%) 0.0000 -0.0022 0.1172 0.0001 -0.7254 0.0106 0.6466 0.0107 -0.2042
246.	(0.00105)	RY	(3)	C	14	s(39.85%)p 1.51(60.15%) 0.0000 0.0160 0.6310 0.0173 -0.2388 0.0065 -0.5410 0.0184 -0.5012
247.	(0.00009)	RY	(4)	C	14	s(58.75%)p 0.70(41.25%)
248.	(0.00560)	RY	(1)	C	15	s(3.05%)p31.74(96.95%) 0.0000 -0.0218 0.1734 -0.0218 0.7944 0.0166 -0.1260 -0.0200 0.5669
249.	(0.00351)	RY	(2)	C	15	s(1.78%)p55.17(98.22%) 0.0000 0.0165 0.1324 0.0004 0.0438 -0.0032 -0.9400 -0.0143 -0.3105

250.	(0.00247)	RY	(3)	C 15	s(0.88%)p99.99(99.12%) 0.0000 -0.0268 0.0897 -0.0142 -0.5983 0.0099 -0.2638 0.0033 0.7506
251.	(0.00101)	RY	(4)	C 15	s(94.38%)p 0.06(5.62%) 0.0000 0.0009 0.9715 -0.0051 -0.0930 -0.0029 0.1753 -0.0156 -0.1286
252.	(0.00582)	RY	(1)	C 16	s(1.80%)p54.64(98.20%) 0.0000 -0.0240 0.1319 -0.0112 -0.1722 0.0211 -0.6775 0.0230 -0.7016
253.	(0.00339)	RY	(2)	C 16	s(5.61%)p16.84(94.39%) 0.0000 -0.0040 0.2368 0.0028 0.9525 -0.0003 0.0018 0.0204 -0.1902
254.	(0.00249)	RY	(3)	C 16	s(0.10%)p99.99(99.90%) 0.0000 0.0320 -0.0037 0.0161 0.1359 -0.0121 -0.7296 0.0069 0.6691
255.	(0.00085)	RY	(4)	C 16	s(92.61%)p 0.08(7.39%) 0.0000 0.0020 0.9623 -0.0007 -0.2105 -0.0008 0.0900 0.0134 0.1460
256.	(0.00301)	RY	(1)	C 17	s(1.51%)p65.09(98.49%) 0.0000 0.0214 0.1211 -0.0039 0.1857 0.0034 0.9187 0.0084 0.3261
257.	(0.00240)	RY	(2)	C 17	s(1.31%)p75.19(98.69%) 0.0000 0.0193 0.1129 0.0003 -0.0188 -0.0012 0.3221 -0.0114 -0.9395
258.	(0.00152)	RY	(3)	C 17	s(6.97%)p13.35(93.03%) 0.0000 0.0282 0.2625 -0.0133 0.9406 -0.0064 -0.2052 0.0010 -0.0570
259.	(0.00043)	RY	(4)	C 17	s(90.38%)p 0.11(9.62%) 0.0000 -0.0132 0.9506 0.0049 -0.2811 0.0014 -0.0987 -0.0042 0.0859
260.	(0.00230)	RY	(1)	C 18	s(1.07%)p92.05(98.93%) 0.0000 0.0016 0.1037 -0.0046 -0.8275 -0.0045 -0.3927 0.0049 0.3875
261.	(0.00179)	RY	(2)	C 18	s(7.95%)p11.57(92.05%) 0.0000 0.0179 0.2815 0.0018 -0.4788 -0.0023 0.3305 -0.0087 -0.7628
262.	(0.00082)	RY	(3)	C 18	s(24.21%)p 3.13(75.79%) 0.0000 0.0270 0.4913 -0.0021 0.2734 0.0058 -0.7621 0.0008 -0.3200
263.	(0.00006)	RY	(4)	C 18	s(66.92%)p 0.49(33.08%)
264.	(0.00231)	RY	(1)	C 19	s(1.69%)p58.04(98.31%) 0.0000 0.0044 0.1301 0.0059 0.3693 0.0051 0.9136 -0.0071 -0.1095
265.	(0.00183)	RY	(2)	C 19	s(4.78%)p19.90(95.22%) 0.0000 0.0160 0.2182 0.0024 -0.2684 -0.0084 0.1876 0.0085 0.9191
266.	(0.00084)	RY	(3)	C 19	s(27.51%)p 2.64(72.49%) 0.0000 0.0279 0.5237 -0.0081 0.7534 0.0051 -0.3590 0.0017 0.1685
267.	(0.00005)	RY	(4)	C 19	s(66.17%)p 0.51(33.83%)
268.	(0.00252)	RY	(1)	C 20	s(0.82%)p99.99(99.18%) 0.0000 0.0075 0.0904 -0.0008 0.4398 -0.0011 -0.3452 0.0091 0.8241
269.	(0.00195)	RY	(2)	C 20	s(10.64%)p 8.40(89.36%) 0.0000 0.0239 0.3254 -0.0032 -0.8113 -0.0039 0.1519 0.0054 0.4606
270.	(0.00114)	RY	(3)	C 20	s(21.05%)p 3.75(78.95%) 0.0000 0.0223 0.4583 0.0016 -0.1472 0.0055 -0.8178 0.0000 -0.3145
271.	(0.00010)	RY	(4)	C 20	s(67.64%)p 0.48(32.36%)
272.	(0.00151)	RY	(1)	O 21	s(2.06%)p47.45(97.94%) 0.0000 0.0004 0.1437 0.0079 -0.6120 -0.0061 -0.7172 0.0023 0.3005
273.	(0.00121)	RY	(2)	O 21	s(14.92%)p 5.70(85.08%) 0.0000 -0.0065 0.3863 0.0052 0.1730 -0.0124 0.2896 0.0032 0.8584
274.	(0.00076)	RY	(3)	O 21	s(23.15%)p 3.32(76.85%) 0.0000 0.0049 0.4811 -0.0008 -0.6428 0.0044 0.5331 -0.0092 -0.2666
275.	(0.00016)	RY	(4)	O 21	s(59.87%)p 0.67(40.13%) 0.0000 -0.0012 0.7738 -0.0069 0.4269 0.0033 -0.3428 0.0052 -0.3185
276.	(0.00155)	RY	(1)	O 22	s(0.82%)p99.99(99.18%) 0.0000 -0.0005 0.0907 0.0015 0.7991 -0.0040 0.5236 -0.0022 -0.2811
277.	(0.00128)	RY	(2)	O 22	s(11.58%)p 7.63(88.42%) 0.0000 -0.0079 0.3402 0.0045 -0.3790

278.	(0.00064)	RY	(3)	O	22	-0.0061	0.0585	-0.0064	-0.8585
						s(28.95%)	p 2.45(71.05%)		
						0.0000	0.0072	0.5380	-0.0015 -0.3439
						-0.0015	0.6516	0.0056	0.4094
279.	(0.00016)	RY	(4)	O	22	s(58.65%)	p 0.70(41.35%)		
						0.0000	-0.0026	0.7658	-0.0042 0.3154
						0.0061	-0.5457	-0.0012	0.1270
280.	(0.01567)	RY	(1)	B	23	s(0.07%)	p99.99(99.93%)		
						0.0000	-0.0090	0.0254	0.0106 -0.0915
						0.0012	0.0444	0.0791	-0.9912
281.	(0.00257)	RY	(2)	B	23	s(38.18%)	p 1.62(61.82%)		
						0.0000	0.0054	0.6178	-0.0050 -0.4779
						0.0099	0.6181	0.0018	0.0877
282.	(0.00194)	RY	(3)	B	23	s(31.11%)	p 2.21(68.89%)		
						0.0000	-0.0072	0.5577	0.0050 -0.2858
						-0.0169	-0.7790	0.0057	0.0063
283.	(0.00135)	RY	(4)	B	23	s(30.63%)	p 2.26(69.37%)		
						0.0000	-0.0034	0.5534	0.0300 0.8250
						-0.0002	0.0932	-0.0124	-0.0584
284.	(0.00184)	RY	(1)	N	24	s(0.05%)	p99.99(99.95%)		
						0.0000	0.0193	-0.0096	-0.0075 0.0860
						0.0056	-0.4979	-0.0013	0.8626
285.	(0.00038)	RY	(2)	N	24	s(4.56%)	p20.94(95.44%)		
						0.0000	-0.0199	0.2125	-0.0036 -0.5742
						-0.0043	0.6569	0.0132	0.4393
286.	(0.00035)	RY	(3)	N	24	s(3.66%)	p26.33(96.34%)		
						0.0000	-0.0001	0.1913	-0.0024 -0.7640
						-0.0023	-0.5644	0.0033	-0.2475
287.	(0.00019)	RY	(4)	N	24	s(91.81%)	p 0.09(8.19%)		
						0.0000	0.0046	0.9582	0.0024 0.2808
						-0.0046	-0.0381	0.0007	-0.0394
288.	(0.00150)	RY	(1)	H	25	s(100.00%)			
						0.0002	1.0000		
289.	(0.00160)	RY	(1)	H	26	s(100.00%)			
						-0.0003	1.0000		
290.	(0.00168)	RY	(1)	H	27	s(100.00%)			
						-0.0001	1.0000		
291.	(0.00147)	RY	(1)	H	28	s(100.00%)			
						0.0000	1.0000		
292.	(0.00122)	RY	(1)	H	29	s(100.00%)			
						0.0010	1.0000		
293.	(0.00117)	RY	(1)	H	30	s(100.00%)			
						0.0002	1.0000		
294.	(0.00216)	RY	(1)	H	31	s(100.00%)			
						0.0024	1.0000		
295.	(0.00119)	RY	(1)	H	32	s(100.00%)			
						0.0008	1.0000		
296.	(0.00135)	RY	(1)	H	33	s(100.00%)			
						-0.0002	1.0000		
297.	(0.00401)	RY	(1)	H	34	s(100.00%)			
						-0.0053	1.0000		
298.	(0.00098)	RY	(1)	H	35	s(100.00%)			
						0.0007	1.0000		
299.	(0.00156)	RY	(1)	H	36	s(100.00%)			
						0.0001	1.0000		
300.	(0.00116)	RY	(1)	H	37	s(100.00%)			
						-0.0004	1.0000		
301.	(0.00108)	RY	(1)	H	38	s(100.00%)			
						-0.0006	1.0000		
302.	(0.00201)	RY	(1)	H	39	s(100.00%)			
						0.0009	1.0000		
303.	(0.00129)	RY	(1)	H	40	s(100.00%)			
						0.0013	1.0000		
304.	(0.00351)	RY	(1)	H	41	s(100.00%)			
						-0.0022	1.0000		
305.	(0.00181)	RY	(1)	H	42	s(100.00%)			
						-0.0007	1.0000		
306.	(0.00125)	RY	(1)	H	43	s(100.00%)			
						-0.0016	1.0000		
307.	(0.00187)	RY	(1)	H	44	s(100.00%)			
						0.0008	1.0000		
308.	(0.00162)	RY	(1)	H	45	s(100.00%)			
						0.0007	1.0000		
309.	(0.00136)	RY	(1)	H	46	s(100.00%)			
						0.0018	1.0000		
310.	(0.00151)	RY	(1)	H	47	s(100.00%)			
						0.0006	1.0000		

311.	(0.00192)	RY	(1)	H	48	s(100.00%)				
						-0.0007	1.0000			
312.	(0.00140)	RY	(1)	H	49	s(100.00%)				
						0.0011	1.0000			
313.	(0.00153)	RY	(1)	H	50	s(100.00%)				
						0.0005	1.0000			
314.	(0.00670)	RY	(1)	H	51	s(100.00%)				
						0.0119	0.9999			
315.	(0.03071)	RY	(1)	C	52	s(2.70%)p36.05(97.30%)				
						0.0000	-0.0207	0.1630	0.0862	-0.8265
						-0.0221	0.2902	0.0428	-0.4427	
316.	(0.02116)	RY	(2)	C	52	s(29.63%)p 2.38(70.37%)				
						0.0000	-0.0603	0.5410	0.0419	-0.3680
						0.0577	-0.4785	-0.0415	0.5767	
317.	(0.01255)	RY	(3)	C	52	s(28.45%)p 2.51(71.55%)				
						0.0000	-0.0506	0.5310	-0.0015	0.3104
						0.0431	-0.4251	0.0285	-0.6601	
318.	(0.00319)	RY	(4)	C	52	s(38.73%)p 1.58(61.27%)				
						0.0000	0.0167	0.6221	0.0195	0.2774
						0.0482	0.7081	0.0145	0.1774	
319.	(0.00219)	RY	(1)	F	53	s(52.33%)p 0.91(47.67%)				
						0.0000	0.0009	0.7234	-0.0001	0.1103
						-0.0010	-0.4746	-0.0036	-0.4892	
320.	(0.00049)	RY	(2)	F	53	s(10.27%)p 8.74(89.73%)				
						0.0000	0.0006	0.3204	0.0006	0.5679
						-0.0016	0.7480	-0.0025	-0.1238	
321.	(0.00020)	RY	(3)	F	53	s(0.11%)p99.99(99.89%)				
						0.0000	-0.0002	0.0333	-0.0024	-0.7166
						0.0006	0.4405	-0.0015	-0.5397	
322.	(0.00003)	RY	(4)	F	53	s(37.29%)p 1.68(62.71%)				
323.	(0.00279)	RY	(1)	F	54	s(34.88%)p 1.87(65.12%)				
						0.0000	-0.0021	0.5906	-0.0074	-0.2524
						0.0048	-0.7367	-0.0032	-0.2113	
324.	(0.00093)	RY	(2)	F	54	s(46.24%)p 1.16(53.76%)				
						0.0000	-0.0022	0.6800	-0.0049	-0.3555
						-0.0042	0.6207	-0.0050	0.1609	
325.	(0.00065)	RY	(3)	F	54	s(2.59%)p37.68(97.41%)				
						0.0000	-0.0003	0.1608	-0.0021	0.3599
						-0.0015	0.2585	0.0010	-0.8819	
326.	(0.00007)	RY	(4)	F	54	s(16.30%)p 5.14(83.70%)				
327.	(0.00255)	RY	(1)	F	55	s(40.38%)p 1.48(59.62%)				
						0.0000	-0.0012	0.6354	0.0044	-0.1952
						-0.0025	-0.7373	0.0036	-0.1201	
328.	(0.00087)	RY	(2)	F	55	s(37.45%)p 1.67(62.55%)				
						0.0000	-0.0011	0.6120	0.0005	0.4702
						-0.0048	0.3128	-0.0003	0.5537	
329.	(0.00043)	RY	(3)	F	55	s(0.22%)p99.99(99.78%)				
						0.0000	0.0000	0.0472	0.0000	0.7485
						-0.0006	-0.0500	-0.0002	-0.6596	
330.	(0.00005)	RY	(4)	F	55	s(21.95%)p 3.56(78.05%)				

339. (0.00537) RY (1) O 58	-0.0108 0.5987 0.0141 -0.5857 s(77.93%)p 0.28(22.07%) 0.0000 -0.0124 0.8827 -0.0079 0.0502 0.0013 -0.1670 0.0353 -0.4348
340. (0.00122) RY (2) O 58	s(0.22%)p99.99(99.78%) 0.0000 -0.0022 0.0463 0.0085 0.8570 0.0104 0.5130 0.0092 -0.0033
341. (0.00097) RY (3) O 58	s(0.42%)p99.99(99.58%) 0.0000 -0.0015 0.0645 -0.0041 -0.5002 0.0107 0.8280 0.0011 -0.2445
342. (0.00012) RY (4) O 58	s(21.41%)p 3.67(78.59%) 0.0000 0.0076 0.4626 0.0082 -0.1124 -0.0014 0.1519 -0.0209 0.8659
343. (0.00560) RY (1) O 59	s(72.69%)p 0.38(27.31%) 0.0000 -0.0077 0.8525 0.0231 -0.5200 -0.0011 -0.0457 0.0024 -0.0091
344. (0.00084) RY (2) O 59	s(0.13%)p99.99(99.87%) 0.0000 0.0002 0.0360 0.0087 -0.0205 0.0063 0.7847 0.0030 0.6184
345. (0.00064) RY (3) O 59	s(0.25%)p99.99(99.75%) 0.0000 -0.0004 0.0499 0.0012 0.0413 0.0045 0.6169 -0.0019 -0.7843
346. (0.00008) RY (4) O 59	s(26.92%)p 2.71(73.08%)

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
1. CR (1) C 1	149. BD*(1) C 8- C 11	0.89	10.65	0.087
1. CR (1) C 1	232. RY (1) C 11	1.27	11.21	0.106
1. CR (1) C 1	288. RY (1) H 25	0.76	10.58	0.080
1. CR (1) C 1	289. RY (1) H 26	0.81	10.60	0.083
2. CR (1) C 2	132. BD*(1) C 2- H 27	0.54	10.69	0.068
2. CR (1) C 2	135. BD*(1) C 3- C 9	0.94	10.65	0.089
2. CR (1) C 2	224. RY (1) C 9	1.14	11.24	0.101
2. CR (1) C 2	290. RY (1) H 27	0.79	10.59	0.082
2. CR (1) C 2	291. RY (1) H 28	0.77	10.59	0.081
3. CR (1) C 3	131. BD*(1) C 2- C 9	1.39	10.43	0.108
3. CR (1) C 3	135. BD*(1) C 3- C 9	0.71	10.65	0.077
3. CR (1) C 3	138. BD*(1) C 4- C 5	0.79	10.59	0.082
3. CR (1) C 3	140. BD*(1) C 4- H 30	0.53	10.74	0.068
3. CR (1) C 3	152. BD*(1) C 9- C 12	0.80	10.57	0.082
3. CR (1) C 3	205. RY (2) C 4	0.84	10.78	0.085
3. CR (1) C 3	207. RY (4) C 4	0.61	11.04	0.073
3. CR (1) C 3	224. RY (1) C 9	1.54	11.25	0.117
3. CR (1) C 3	225. RY (2) C 9	0.93	10.95	0.090
3. CR (1) C 3	227. RY (4) C 9	1.00	11.07	0.094
3. CR (1) C 3	292. RY (1) H 29	0.79	10.48	0.081
4. CR (1) C 4	135. BD*(1) C 3- C 9	0.67	10.68	0.075
4. CR (1) C 4	137. BD*(1) C 3- H 29	0.51	10.78	0.066
4. CR (1) C 4	141. BD*(1) C 5- C 10	1.23	10.57	0.102
4. CR (1) C 4	142. BD*(1) C 5- N 24	0.55	10.30	0.067
4. CR (1) C 4	201. RY (2) C 3	1.50	10.75	0.114
4. CR (1) C 4	208. RY (1) C 5	1.88	11.02	0.129
4. CR (1) C 4	209. RY (2) C 5	1.23	11.19	0.105
4. CR (1) C 4	293. RY (1) H 30	0.80	10.56	0.082
5. CR (1) C 5	134. BD*(1) C 3- C 4	0.71	10.67	0.077
5. CR (1) C 5	138. BD*(1) C 4- C 5	0.84	10.68	0.084
5. CR (1) C 5	140. BD*(1) C 4- H 30	0.55	10.83	0.069
5. CR (1) C 5	141. BD*(1) C 5- C 10	0.58	10.64	0.070
5. CR (1) C 5	142. BD*(1) C 5- N 24	0.78	10.37	0.080
5. CR (1) C 5	145. BD*(1) C 6- C 10	1.25	10.63	0.103
5. CR (1) C 5	205. RY (2) C 4	1.47	10.87	0.113
5. CR (1) C 5	228. RY (1) C 10	1.33	11.26	0.109
5. CR (1) C 5	229. RY (2) C 10	0.57	11.38	0.072
5. CR (1) C 5	231. RY (4) C 10	0.70	11.21	0.079
6. CR (1) C 6	141. BD*(1) C 5- C 10	1.20	10.55	0.101
6. CR (1) C 6	146. BD*(1) C 6- B 23	0.68	10.52	0.076
6. CR (1) C 6	147. BD*(1) C 7- C 8	0.90	10.59	0.087
6. CR (1) C 6	182. BD*(1) O 21- B 23	0.63	10.46	0.072
6. CR (1) C 6	217. RY (2) C 7	1.41	10.86	0.111
6. CR (1) C 6	229. RY (2) C 10	1.63	11.29	0.121

6. CR (1) C 6	281. RY (2) B 23	0.77	10.83	0.081
6. CR (1) C 6	282. RY (3) B 23	0.92	10.62	0.088
6. CR (1) C 6	283. RY (4) B 23	0.79	10.59	0.081
7. CR (1) C 7	145. BD* (1) C 6- C 10	0.93	10.53	0.088
7. CR (1) C 7	146. BD* (1) C 6- B 23	0.98	10.52	0.091
7. CR (1) C 7	149. BD* (1) C 8- C 11	0.63	10.65	0.073
7. CR (1) C 7	151. BD* (1) C 8- H 32	0.52	10.78	0.067
7. CR (1) C 7	212. RY (1) C 6	1.20	11.27	0.104
7. CR (1) C 7	213. RY (2) C 6	0.88	11.20	0.088
7. CR (1) C 7	221. RY (2) C 8	1.24	10.72	0.103
7. CR (1) C 7	294. RY (1) H 31	0.90	10.57	0.087
8. CR (1) C 8	128. BD* (1) C 1- C 11	1.37	10.42	0.107
8. CR (1) C 8	143. BD* (1) C 6- C 7	0.82	10.60	0.083
8. CR (1) C 8	149. BD* (1) C 8- C 11	0.61	10.64	0.072
8. CR (1) C 8	154. BD* (1) C 11- C 12	0.82	10.57	0.083
8. CR (1) C 8	217. RY (2) C 7	1.10	10.85	0.097
8. CR (1) C 8	218. RY (3) C 7	0.55	11.06	0.070
8. CR (1) C 8	233. RY (2) C 11	2.06	10.99	0.134
8. CR (1) C 8	235. RY (4) C 11	0.86	11.07	0.087
8. CR (1) C 8	295. RY (1) H 32	0.79	10.48	0.081
9. CR (1) C 9	134. BD* (1) C 3- C 4	0.64	10.60	0.074
9. CR (1) C 9	137. BD* (1) C 3- H 29	0.73	10.79	0.079
9. CR (1) C 9	152. BD* (1) C 9- C 12	0.72	10.60	0.078
9. CR (1) C 9	153. BD* (1) C 10- C 12	1.10	10.60	0.096
9. CR (1) C 9	154. BD* (1) C 11- C 12	0.53	10.62	0.067
9. CR (1) C 9	198. RY (3) C 2	1.01	10.70	0.093
9. CR (1) C 9	201. RY (2) C 3	1.09	10.76	0.097
9. CR (1) C 9	236. RY (1) C 12	1.27	11.24	0.107
9. CR (1) C 9	237. RY (2) C 12	0.50	11.29	0.067
9. CR (1) C 9	238. RY (3) C 12	0.55	11.15	0.070
10. CR (1) C 10	138. BD* (1) C 4- C 5	0.79	10.63	0.082
10. CR (1) C 10	142. BD* (1) C 5- N 24	0.93	10.32	0.088
10. CR (1) C 10	146. BD* (1) C 6- B 23	0.97	10.56	0.090
10. CR (1) C 10	152. BD* (1) C 9- C 12	0.88	10.61	0.086
10. CR (1) C 10	153. BD* (1) C 10- C 12	0.72	10.61	0.078
10. CR (1) C 10	154. BD* (1) C 11- C 12	0.81	10.63	0.083
10. CR (1) C 10	208. RY (1) C 5	1.83	11.04	0.127
10. CR (1) C 10	213. RY (2) C 6	1.05	11.24	0.097
10. CR (1) C 10	214. RY (3) C 6	0.78	11.27	0.084
10. CR (1) C 10	237. RY (2) C 12	2.00	11.30	0.134
11. CR (1) C 11	147. BD* (1) C 7- C 8	0.56	10.61	0.069
11. CR (1) C 11	151. BD* (1) C 8- H 32	0.72	10.80	0.079
11. CR (1) C 11	152. BD* (1) C 9- C 12	0.55	10.59	0.068
11. CR (1) C 11	153. BD* (1) C 10- C 12	1.13	10.59	0.098
11. CR (1) C 11	154. BD* (1) C 11- C 12	0.75	10.61	0.080
11. CR (1) C 11	194. RY (3) C 1	0.84	10.70	0.084
11. CR (1) C 11	221. RY (2) C 8	1.21	10.75	0.102
11. CR (1) C 11	223. RY (4) C 8	0.55	11.09	0.070
11. CR (1) C 11	236. RY (1) C 12	1.51	11.24	0.116
11. CR (1) C 11	238. RY (3) C 12	0.72	11.14	0.080
12. CR (1) C 12	135. BD* (1) C 3- C 9	0.73	10.66	0.079
12. CR (1) C 12	141. BD* (1) C 5- C 10	0.60	10.56	0.071
12. CR (1) C 12	145. BD* (1) C 6- C 10	0.66	10.54	0.075
12. CR (1) C 12	149. BD* (1) C 8- C 11	0.77	10.66	0.081
12. CR (1) C 12	154. BD* (1) C 11- C 12	0.54	10.60	0.068
12. CR (1) C 12	225. RY (2) C 9	2.37	10.96	0.144
12. CR (1) C 12	228. RY (1) C 10	1.67	11.18	0.122
12. CR (1) C 12	232. RY (1) C 11	0.78	11.23	0.084
12. CR (1) C 12	233. RY (2) C 11	1.65	11.01	0.120
13. CR (1) C 13	155. BD* (1) C 13- N 24	0.71	10.31	0.076
13. CR (1) C 13	296. RY (1) H 33	0.79	10.67	0.082
13. CR (1) C 13	297. RY (1) H 34	1.38	10.78	0.109
13. CR (1) C 13	298. RY (1) H 35	0.77	10.68	0.081
14. CR (1) C 14	159. BD* (1) C 14- N 24	0.70	10.31	0.076
14. CR (1) C 14	160. BD* (1) C 14- H 36	0.53	10.71	0.067
14. CR (1) C 14	299. RY (1) H 36	0.85	10.63	0.085
14. CR (1) C 14	300. RY (1) H 37	0.85	10.63	0.085
14. CR (1) C 14	301. RY (1) H 38	0.84	10.66	0.085
15. CR (1) C 15	166. BD* (1) C 15- O 21	1.07	10.33	0.094
15. CR (1) C 15	182. BD* (1) O 21- B 23	1.53	10.54	0.113
15. CR (1) C 15	254. RY (3) C 16	1.04	10.97	0.095
15. CR (1) C 15	258. RY (3) C 17	0.54	10.82	0.068
15. CR (1) C 15	262. RY (3) C 18	0.71	10.90	0.078
16. CR (1) C 16	169. BD* (1) C 16- O 22	0.97	10.36	0.089
16. CR (1) C 16	183. BD* (1) O 22- B 23	1.63	10.56	0.117
16. CR (1) C 16	250. RY (3) C 15	1.29	10.95	0.106
16. CR (1) C 16	266. RY (3) C 19	0.72	10.95	0.079

16. CR (1) C 16	270. RY (3) C 20	0.61	10.90	0.073
17. CR (1) C 17	250. RY (3) C 15	1.57	10.79	0.116
17. CR (1) C 17	302. RY (1) H 39	0.74	10.66	0.079
17. CR (1) C 17	303. RY (1) H 40	0.72	10.62	0.078
17. CR (1) C 17	304. RY (1) H 41	0.99	10.80	0.092
18. CR (1) C 18	248. RY (1) C 15	0.54	10.81	0.068
18. CR (1) C 18	249. RY (2) C 15	1.79	10.93	0.125
18. CR (1) C 18	305. RY (1) H 42	0.71	10.58	0.078
18. CR (1) C 18	306. RY (1) H 43	0.74	10.58	0.079
18. CR (1) C 18	307. RY (1) H 44	0.72	10.62	0.078
19. CR (1) C 19	252. RY (1) C 16	0.58	10.81	0.070
19. CR (1) C 19	253. RY (2) C 16	0.77	10.91	0.082
19. CR (1) C 19	254. RY (3) C 16	0.65	10.82	0.075
19. CR (1) C 19	308. RY (1) H 45	0.74	10.58	0.079
19. CR (1) C 19	309. RY (1) H 46	0.69	10.59	0.076
19. CR (1) C 19	310. RY (1) H 47	0.88	10.67	0.086
20. CR (1) C 20	252. RY (1) C 16	0.52	10.82	0.067
20. CR (1) C 20	253. RY (2) C 16	1.22	10.92	0.103
20. CR (1) C 20	254. RY (3) C 16	0.95	10.82	0.090
20. CR (1) C 20	311. RY (1) H 48	0.78	10.58	0.081
20. CR (1) C 20	312. RY (1) H 49	0.70	10.61	0.077
20. CR (1) C 20	313. RY (1) H 50	0.69	10.63	0.077
21. CR (1) O 21	248. RY (1) C 15	1.70	19.76	0.164
21. CR (1) O 21	249. RY (2) C 15	0.65	19.88	0.101
21. CR (1) O 21	280. RY (1) B 23	2.60	19.52	0.201
21. CR (1) O 21	281. RY (2) B 23	0.82	19.71	0.113
22. CR (1) O 22	252. RY (1) C 16	1.68	19.74	0.163
22. CR (1) O 22	253. RY (2) C 16	0.68	19.84	0.104
22. CR (1) O 22	280. RY (1) B 23	2.76	19.50	0.207
22. CR (1) O 22	281. RY (2) B 23	0.87	19.69	0.117
23. CR (1) B 23	145. BD*(1) C 6- C 10	1.21	7.21	0.083
23. CR (1) B 23	166. BD*(1) C 15- O 21	1.47	6.92	0.090
23. CR (1) B 23	169. BD*(1) C 16- O 22	1.63	6.95	0.095
24. CR (1) N 24	184. BD*(1) N 24- H 51	1.98	15.07	0.154
24. CR (1) N 24	209. RY (2) C 5	1.36	15.41	0.129
24. CR (1) N 24	242. RY (3) C 13	0.86	15.10	0.102
24. CR (1) N 24	246. RY (3) C 14	0.71	15.15	0.093
24. CR (1) N 24	314. RY (1) H 51	2.20	15.12	0.163
37. LP (1) C 12	136. BD*(2) C 3- C 9	94.50	0.15	0.105
37. LP (1) C 12	139. BD*(2) C 4- C 5	0.79	0.11	0.008
37. LP (1) C 12	144. BD*(2) C 6- C 7	0.90	0.15	0.010
37. LP (1) C 12	150. BD*(2) C 8- C 11	89.59	0.15	0.105
37. LP (1) C 12	226. RY (3) C 9	2.06	0.82	0.037
37. LP (1) C 12	230. RY (3) C 10	2.22	0.85	0.039
37. LP (1) C 12	234. RY (3) C 11	2.34	0.81	0.039
37. LP (1) C 12	239. RY (4) C 12	5.67	0.82	0.061
38. LP (1) O 21	146. BD*(1) C 6- B 23	0.89	1.00	0.027
38. LP (1) O 21	163. BD*(1) C 15- C 16	2.52	0.84	0.041
38. LP (1) O 21	165. BD*(1) C 15- C 18	0.84	0.93	0.025
38. LP (1) O 21	183. BD*(1) O 22- B 23	4.07	0.95	0.056
38. LP (1) O 21	184. BD*(1) N 24- H 51	9.47	1.30	0.099
38. LP (1) O 21	248. RY (1) C 15	2.15	1.36	0.048
38. LP (1) O 21	249. RY (2) C 15	1.01	1.48	0.035
38. LP (1) O 21	280. RY (1) B 23	4.00	1.11	0.060
38. LP (1) O 21	281. RY (2) B 23	1.23	1.31	0.036
39. LP (2) O 21	126. LV (1) B 23	57.24	0.31	0.119
39. LP (2) O 21	163. BD*(1) C 15- C 16	0.61	0.64	0.018
39. LP (2) O 21	164. BD*(1) C 15- C 17	4.69	0.71	0.052
39. LP (2) O 21	165. BD*(1) C 15- C 18	1.87	0.73	0.033
39. LP (2) O 21	171. BD*(1) C 17- H 40	0.76	1.00	0.025
39. LP (2) O 21	184. BD*(1) N 24- H 51	2.17	1.11	0.044
40. LP (1) O 22	146. BD*(1) C 6- B 23	1.02	0.97	0.028
40. LP (1) O 22	163. BD*(1) C 15- C 16	3.37	0.80	0.046
40. LP (1) O 22	167. BD*(1) C 16- C 19	0.87	0.87	0.025
40. LP (1) O 22	182. BD*(1) O 21- B 23	5.66	0.90	0.064
40. LP (1) O 22	252. RY (1) C 16	2.03	1.33	0.046
40. LP (1) O 22	253. RY (2) C 16	1.05	1.43	0.035
40. LP (1) O 22	280. RY (1) B 23	4.25	1.08	0.061
40. LP (1) O 22	281. RY (2) B 23	1.21	1.27	0.035
41. LP (2) O 22	126. LV (1) B 23	68.34	0.29	0.125
41. LP (2) O 22	163. BD*(1) C 15- C 16	0.66	0.62	0.018
41. LP (2) O 22	167. BD*(1) C 16- C 19	2.40	0.69	0.036
41. LP (2) O 22	168. BD*(1) C 16- C 20	5.75	0.71	0.057
41. LP (2) O 22	180. BD*(1) C 20- H 49	0.78	0.95	0.024
60. BD (1) C 1- C 2	128. BD*(1) C 1- C 11	0.92	0.97	0.027
60. BD (1) C 1- C 2	129. BD*(1) C 1- H 25	1.42	1.23	0.037
60. BD (1) C 1- C 2	130. BD*(1) C 1- H 26	1.43	1.23	0.037

60. BD (1) C 1- C 2	131. BD* (1) C 2- C 9	0.97	0.97	0.027
60. BD (1) C 1- C 2	132. BD* (1) C 2- H 27	1.50	1.23	0.038
60. BD (1) C 1- C 2	133. BD* (1) C 2- H 28	1.45	1.21	0.037
60. BD (1) C 1- C 2	135. BD* (1) C 3- C 9	4.18	1.19	0.063
60. BD (1) C 1- C 2	149. BD* (1) C 8- C 11	4.03	1.19	0.062
60. BD (1) C 1- C 2	152. BD* (1) C 9- C 12	0.60	1.11	0.023
60. BD (1) C 1- C 2	154. BD* (1) C 11- C 12	0.55	1.12	0.022
60. BD (1) C 1- C 2	225. RY (2) C 9	0.58	1.49	0.026
61. BD (1) C 1- C 11	127. BD* (1) C 1- C 2	0.60	0.96	0.022
61. BD (1) C 1- C 11	129. BD* (1) C 1- H 25	1.94	1.27	0.044
61. BD (1) C 1- C 11	130. BD* (1) C 1- H 26	1.84	1.27	0.043
61. BD (1) C 1- C 11	131. BD* (1) C 2- C 9	0.82	1.01	0.026
61. BD (1) C 1- C 11	133. BD* (1) C 2- H 28	0.85	1.25	0.029
61. BD (1) C 1- C 11	147. BD* (1) C 7- C 8	2.01	1.16	0.043
61. BD (1) C 1- C 11	149. BD* (1) C 8- C 11	2.59	1.23	0.050
61. BD (1) C 1- C 11	153. BD* (1) C 10- C 12	4.58	1.15	0.065
61. BD (1) C 1- C 11	154. BD* (1) C 11- C 12	1.84	1.16	0.041
61. BD (1) C 1- C 11	198. RY (3) C 2	0.53	1.25	0.023
61. BD (1) C 1- C 11	220. RY (1) C 8	0.71	1.73	0.031
62. BD (1) C 1- H 25	127. BD* (1) C 1- C 2	0.54	0.91	0.020
62. BD (1) C 1- H 25	128. BD* (1) C 1- C 11	0.89	0.96	0.026
62. BD (1) C 1- H 25	130. BD* (1) C 1- H 26	1.50	1.22	0.038
62. BD (1) C 1- H 25	131. BD* (1) C 2- C 9	1.07	0.95	0.028
62. BD (1) C 1- H 25	150. BD* (2) C 8- C 11	2.34	0.59	0.033
62. BD (1) C 1- H 25	154. BD* (1) C 11- C 12	1.53	1.11	0.037
62. BD (1) C 1- H 25	234. RY (3) C 11	0.65	1.25	0.025
63. BD (1) C 1- H 26	127. BD* (1) C 1- C 2	0.52	0.91	0.019
63. BD (1) C 1- H 26	128. BD* (1) C 1- C 11	1.05	0.95	0.028
63. BD (1) C 1- H 26	129. BD* (1) C 1- H 25	1.38	1.21	0.036
63. BD (1) C 1- H 26	132. BD* (1) C 2- H 27	1.07	1.21	0.032
63. BD (1) C 1- H 26	150. BD* (2) C 8- C 11	4.37	0.59	0.045
63. BD (1) C 1- H 26	154. BD* (1) C 11- C 12	0.70	1.10	0.025
63. BD (1) C 1- H 26	196. RY (1) C 2	0.50	1.28	0.023
63. BD (1) C 1- H 26	234. RY (3) C 11	0.74	1.24	0.027
64. BD (1) C 2- C 9	127. BD* (1) C 1- C 2	0.63	0.97	0.022
64. BD (1) C 2- C 9	128. BD* (1) C 1- C 11	0.78	1.02	0.025
64. BD (1) C 2- C 9	129. BD* (1) C 1- H 25	0.80	1.27	0.028
64. BD (1) C 2- C 9	132. BD* (1) C 2- H 27	1.75	1.28	0.042
64. BD (1) C 2- C 9	133. BD* (1) C 2- H 28	1.88	1.26	0.043
64. BD (1) C 2- C 9	134. BD* (1) C 3- C 4	2.30	1.15	0.046
64. BD (1) C 2- C 9	135. BD* (1) C 3- C 9	2.94	1.24	0.054
64. BD (1) C 2- C 9	152. BD* (1) C 9- C 12	1.69	1.15	0.039
64. BD (1) C 2- C 9	153. BD* (1) C 10- C 12	4.50	1.15	0.064
64. BD (1) C 2- C 9	200. RY (1) C 3	0.59	1.71	0.028
64. BD (1) C 2- C 9	236. RY (1) C 12	0.79	1.79	0.034
65. BD (1) C 2- H 27	127. BD* (1) C 1- C 2	0.55	0.91	0.020
65. BD (1) C 2- H 27	130. BD* (1) C 1- H 26	1.02	1.22	0.032
65. BD (1) C 2- H 27	131. BD* (1) C 2- C 9	0.94	0.95	0.027
65. BD (1) C 2- H 27	133. BD* (1) C 2- H 28	1.35	1.20	0.036
65. BD (1) C 2- H 27	136. BD* (2) C 3- C 9	4.29	0.59	0.045
65. BD (1) C 2- H 27	152. BD* (1) C 9- C 12	0.75	1.10	0.026
65. BD (1) C 2- H 27	192. RY (1) C 1	0.54	1.29	0.024
65. BD (1) C 2- H 27	226. RY (3) C 9	0.60	1.26	0.025
66. BD (1) C 2- H 28	127. BD* (1) C 1- C 2	0.58	0.91	0.020
66. BD (1) C 2- H 28	128. BD* (1) C 1- C 11	1.03	0.96	0.028
66. BD (1) C 2- H 28	131. BD* (1) C 2- C 9	0.85	0.95	0.025
66. BD (1) C 2- H 28	132. BD* (1) C 2- H 27	1.52	1.22	0.038
66. BD (1) C 2- H 28	136. BD* (2) C 3- C 9	2.60	0.58	0.035
66. BD (1) C 2- H 28	152. BD* (1) C 9- C 12	1.42	1.09	0.035
66. BD (1) C 2- H 28	226. RY (3) C 9	0.70	1.25	0.026
67. BD (1) C 3- C 4	131. BD* (1) C 2- C 9	5.47	1.09	0.069
67. BD (1) C 3- C 4	135. BD* (1) C 3- C 9	4.10	1.32	0.066
67. BD (1) C 3- C 4	137. BD* (1) C 3- H 29	2.81	1.42	0.056
67. BD (1) C 3- C 4	138. BD* (1) C 4- C 5	3.62	1.25	0.060
67. BD (1) C 3- C 4	140. BD* (1) C 4- H 30	3.44	1.40	0.062
67. BD (1) C 3- C 4	142. BD* (1) C 5- N 24	4.43	0.94	0.058
67. BD (1) C 3- C 4	208. RY (1) C 5	2.37	1.66	0.056
67. BD (1) C 3- C 4	225. RY (2) C 9	2.52	1.61	0.057
68. BD (1) C 3- C 9	131. BD* (1) C 2- C 9	2.47	1.13	0.047
68. BD (1) C 3- C 9	134. BD* (1) C 3- C 4	3.08	1.28	0.056
68. BD (1) C 3- C 9	137. BD* (1) C 3- H 29	4.76	1.47	0.075
68. BD (1) C 3- C 9	140. BD* (1) C 4- H 30	1.74	1.45	0.045
68. BD (1) C 3- C 9	152. BD* (1) C 9- C 12	4.30	1.28	0.066
68. BD (1) C 3- C 9	154. BD* (1) C 11- C 12	1.89	1.29	0.044
68. BD (1) C 3- C 9	204. RY (1) C 4	0.86	1.86	0.036
68. BD (1) C 3- C 9	205. RY (2) C 4	1.00	1.49	0.034
68. BD (1) C 3- C 9	237. RY (2) C 12	0.65	1.97	0.032

69. BD (2) C 3- C 9	132. BD* (1) C 2- H 27	1.79	0.94	0.037
69. BD (2) C 3- C 9	133. BD* (1) C 2- H 28	1.28	0.92	0.031
69. BD (2) C 3- C 9	139. BD* (2) C 4- C 5	24.37	0.27	0.072
69. BD (2) C 3- C 9	206. RY (3) C 4	1.33	0.90	0.031
69. BD (2) C 3- C 9	239. RY (4) C 12	0.82	0.98	0.025
70. BD (1) C 3- H 29	134. BD* (1) C 3- C 4	1.35	1.14	0.035
70. BD (1) C 3- H 29	135. BD* (1) C 3- C 9	2.80	1.22	0.052
70. BD (1) C 3- H 29	138. BD* (1) C 4- C 5	3.41	1.15	0.056
70. BD (1) C 3- H 29	152. BD* (1) C 9- C 12	4.36	1.13	0.063
70. BD (1) C 3- H 29	204. RY (1) C 4	0.57	1.72	0.028
70. BD (1) C 3- H 29	224. RY (1) C 9	1.00	1.81	0.038
71. BD (1) C 4- C 5	134. BD* (1) C 3- C 4	3.10	1.28	0.056
71. BD (1) C 4- C 5	137. BD* (1) C 3- H 29	1.53	1.47	0.042
71. BD (1) C 4- C 5	140. BD* (1) C 4- H 30	3.81	1.45	0.066
71. BD (1) C 4- C 5	141. BD* (1) C 5- C 10	5.53	1.26	0.075
71. BD (1) C 4- C 5	145. BD* (1) C 6- C 10	3.52	1.24	0.059
71. BD (1) C 4- C 5	184. BD* (1) N 24- H 51	0.62	1.54	0.028
71. BD (1) C 4- C 5	200. RY (1) C 3	1.04	1.84	0.039
71. BD (1) C 4- C 5	201. RY (2) C 3	0.92	1.44	0.032
71. BD (1) C 4- C 5	228. RY (1) C 10	0.69	1.88	0.032
71. BD (1) C 4- C 5	229. RY (2) C 10	0.65	2.00	0.032
71. BD (1) C 4- C 5	284. RY (1) N 24	0.72	1.78	0.032
72. BD (2) C 4- C 5	125. LV (1) C 10	58.09	0.18	0.090
72. BD (2) C 4- C 5	136. BD* (2) C 3- C 9	13.37	0.33	0.059
72. BD (2) C 4- C 5	155. BD* (1) C 13- N 24	1.51	0.53	0.025
72. BD (2) C 4- C 5	156. BD* (1) C 13- H 33	0.55	0.92	0.020
72. BD (2) C 4- C 5	159. BD* (1) C 14- N 24	1.76	0.52	0.027
72. BD (2) C 4- C 5	160. BD* (1) C 14- H 36	0.68	0.92	0.022
72. BD (2) C 4- C 5	202. RY (3) C 3	1.41	0.91	0.032
72. BD (2) C 4- C 5	230. RY (3) C 10	1.27	1.03	0.032
73. BD (1) C 4- H 30	134. BD* (1) C 3- C 4	1.53	1.16	0.038
73. BD (1) C 4- H 30	135. BD* (1) C 3- C 9	2.85	1.24	0.053
73. BD (1) C 4- H 30	138. BD* (1) C 4- C 5	1.97	1.17	0.043
73. BD (1) C 4- H 30	141. BD* (1) C 5- C 10	5.29	1.14	0.069
73. BD (1) C 4- H 30	142. BD* (1) C 5- N 24	0.82	0.86	0.024
73. BD (1) C 4- H 30	200. RY (1) C 3	0.70	1.71	0.031
73. BD (1) C 4- H 30	209. RY (2) C 5	1.07	1.75	0.039
74. BD (1) C 5- C 10	138. BD* (1) C 4- C 5	5.00	1.28	0.072
74. BD (1) C 5- C 10	140. BD* (1) C 4- H 30	1.40	1.44	0.040
74. BD (1) C 5- C 10	143. BD* (1) C 6- C 7	0.89	1.31	0.030
74. BD (1) C 5- C 10	145. BD* (1) C 6- C 10	4.70	1.23	0.068
74. BD (1) C 5- C 10	153. BD* (1) C 10- C 12	3.45	1.27	0.059
74. BD (1) C 5- C 10	154. BD* (1) C 11- C 12	3.02	1.28	0.056
74. BD (1) C 5- C 10	155. BD* (1) C 13- N 24	0.97	0.96	0.027
74. BD (1) C 5- C 10	159. BD* (1) C 14- N 24	0.88	0.95	0.026
74. BD (1) C 5- C 10	212. RY (1) C 6	0.58	1.97	0.030
74. BD (1) C 5- C 10	236. RY (1) C 12	1.21	1.91	0.043
75. BD (1) C 5- N 24	134. BD* (1) C 3- C 4	1.89	1.32	0.045
75. BD (1) C 5- N 24	138. BD* (1) C 4- C 5	0.68	1.33	0.027
75. BD (1) C 5- N 24	141. BD* (1) C 5- C 10	0.81	1.29	0.029
75. BD (1) C 5- N 24	153. BD* (1) C 10- C 12	1.37	1.31	0.038
75. BD (1) C 5- N 24	155. BD* (1) C 13- N 24	0.96	1.01	0.028
75. BD (1) C 5- N 24	156. BD* (1) C 13- H 33	0.83	1.40	0.030
75. BD (1) C 5- N 24	159. BD* (1) C 14- N 24	0.82	1.00	0.025
75. BD (1) C 5- N 24	160. BD* (1) C 14- H 36	0.95	1.40	0.032
75. BD (1) C 5- N 24	184. BD* (1) N 24- H 51	2.96	1.57	0.061
75. BD (1) C 5- N 24	204. RY (1) C 4	0.53	1.90	0.028
75. BD (1) C 5- N 24	229. RY (2) C 10	0.83	2.03	0.037
75. BD (1) C 5- N 24	241. RY (2) C 13	0.93	1.43	0.032
75. BD (1) C 5- N 24	245. RY (2) C 14	0.69	1.37	0.027
76. BD (1) C 6- C 7	141. BD* (1) C 5- C 10	4.43	1.22	0.066
76. BD (1) C 6- C 7	145. BD* (1) C 6- C 10	3.72	1.20	0.060
76. BD (1) C 6- C 7	146. BD* (1) C 6- B 23	4.33	1.18	0.064
76. BD (1) C 6- C 7	147. BD* (1) C 7- C 8	2.91	1.25	0.054
76. BD (1) C 6- C 7	148. BD* (1) C 7- H 31	3.59	1.45	0.064
76. BD (1) C 6- C 7	151. BD* (1) C 8- H 32	1.46	1.44	0.041
76. BD (1) C 6- C 7	182. BD* (1) O 21- B 23	2.40	1.12	0.046
76. BD (1) C 6- C 7	220. RY (1) C 8	0.64	1.82	0.031
76. BD (1) C 6- C 7	221. RY (2) C 8	1.06	1.39	0.034
76. BD (1) C 6- C 7	228. RY (1) C 10	1.33	1.83	0.044
77. BD (2) C 6- C 7	125. LV (1) C 10	73.47	0.13	0.088
77. BD (2) C 6- C 7	126. LV (1) B 23	29.41	0.24	0.075
77. BD (2) C 6- C 7	144. BD* (2) C 6- C 7	0.79	0.28	0.013
77. BD (2) C 6- C 7	150. BD* (2) C 8- C 11	14.62	0.29	0.058
77. BD (2) C 6- C 7	182. BD* (1) O 21- B 23	0.51	0.68	0.017
77. BD (2) C 6- C 7	222. RY (3) C 8	1.20	0.88	0.029
77. BD (2) C 6- C 7	230. RY (3) C 10	0.82	0.98	0.025

78. BD (1) C 6- C 10	138. BD* (1) C 4- C 5	1.82	1.23	0.042
78. BD (1) C 6- C 10	141. BD* (1) C 5- C 10	4.24	1.20	0.064
78. BD (1) C 6- C 10	143. BD* (1) C 6- C 7	3.12	1.26	0.056
78. BD (1) C 6- C 10	146. BD* (1) C 6- B 23	4.00	1.17	0.061
78. BD (1) C 6- C 10	148. BD* (1) C 7- H 31	1.65	1.43	0.043
78. BD (1) C 6- C 10	152. BD* (1) C 9- C 12	3.10	1.22	0.055
78. BD (1) C 6- C 10	153. BD* (1) C 10- C 12	3.65	1.22	0.060
78. BD (1) C 6- C 10	183. BD* (1) O 22- B 23	0.82	1.12	0.027
78. BD (1) C 6- C 10	209. RY (2) C 5	0.94	1.81	0.037
78. BD (1) C 6- C 10	236. RY (1) C 12	1.18	1.86	0.042
79. BD (1) C 6- B 23	143. BD* (1) C 6- C 7	3.16	1.13	0.053
79. BD (1) C 6- B 23	145. BD* (1) C 6- C 10	2.66	1.05	0.047
79. BD (1) C 6- B 23	147. BD* (1) C 7- C 8	5.39	1.10	0.069
79. BD (1) C 6- B 23	153. BD* (1) C 10- C 12	2.84	1.09	0.050
79. BD (1) C 6- B 23	166. BD* (1) C 15- O 21	2.33	0.76	0.038
79. BD (1) C 6- B 23	169. BD* (1) C 16- O 22	2.16	0.79	0.037
79. BD (1) C 6- B 23	216. RY (1) C 7	1.23	1.68	0.040
79. BD (1) C 6- B 23	228. RY (1) C 10	1.94	1.68	0.051
80. BD (1) C 7- C 8	128. BD* (1) C 1- C 11	5.92	1.07	0.071
80. BD (1) C 7- C 8	143. BD* (1) C 6- C 7	3.06	1.25	0.055
80. BD (1) C 7- C 8	146. BD* (1) C 6- B 23	2.31	1.16	0.046
80. BD (1) C 7- C 8	148. BD* (1) C 7- H 31	2.45	1.42	0.053
80. BD (1) C 7- C 8	149. BD* (1) C 8- C 11	3.60	1.29	0.061
80. BD (1) C 7- C 8	151. BD* (1) C 8- H 32	2.91	1.41	0.057
80. BD (1) C 7- C 8	213. RY (2) C 6	1.87	1.84	0.052
80. BD (1) C 7- C 8	232. RY (1) C 11	1.41	1.85	0.046
80. BD (1) C 7- C 8	233. RY (2) C 11	1.30	1.64	0.041
81. BD (1) C 7- H 31	143. BD* (1) C 6- C 7	2.02	1.15	0.043
81. BD (1) C 7- H 31	145. BD* (1) C 6- C 10	4.92	1.07	0.065
81. BD (1) C 7- H 31	147. BD* (1) C 7- C 8	1.03	1.12	0.030
81. BD (1) C 7- H 31	149. BD* (1) C 8- C 11	3.13	1.19	0.055
81. BD (1) C 7- H 31	182. BD* (1) O 21- B 23	0.51	0.99	0.020
81. BD (1) C 7- H 31	212. RY (1) C 6	0.50	1.81	0.027
81. BD (1) C 7- H 31	220. RY (1) C 8	0.56	1.69	0.027
82. BD (1) C 8- C 11	128. BD* (1) C 1- C 11	2.31	1.12	0.045
82. BD (1) C 8- C 11	147. BD* (1) C 7- C 8	2.63	1.27	0.052
82. BD (1) C 8- C 11	148. BD* (1) C 7- H 31	1.38	1.48	0.040
82. BD (1) C 8- C 11	151. BD* (1) C 8- H 32	4.47	1.47	0.072
82. BD (1) C 8- C 11	152. BD* (1) C 9- C 12	1.98	1.26	0.045
82. BD (1) C 8- C 11	154. BD* (1) C 11- C 12	4.37	1.27	0.067
82. BD (1) C 8- C 11	216. RY (1) C 7	1.15	1.85	0.041
82. BD (1) C 8- C 11	217. RY (2) C 7	1.14	1.55	0.038
82. BD (1) C 8- C 11	237. RY (2) C 12	0.98	1.95	0.039
83. BD (2) C 8- C 11	129. BD* (1) C 1- H 25	1.20	0.92	0.030
83. BD (2) C 8- C 11	130. BD* (1) C 1- H 26	2.04	0.92	0.039
83. BD (2) C 8- C 11	144. BD* (2) C 6- C 7	21.54	0.29	0.071
83. BD (2) C 8- C 11	219. RY (4) C 7	1.11	0.93	0.029
83. BD (2) C 8- C 11	239. RY (4) C 12	0.86	0.96	0.026
84. BD (1) C 8- H 32	143. BD* (1) C 6- C 7	3.29	1.17	0.055
84. BD (1) C 8- H 32	147. BD* (1) C 7- C 8	1.45	1.14	0.036
84. BD (1) C 8- H 32	149. BD* (1) C 8- C 11	2.59	1.21	0.050
84. BD (1) C 8- H 32	154. BD* (1) C 11- C 12	4.24	1.14	0.062
84. BD (1) C 8- H 32	216. RY (1) C 7	0.56	1.71	0.028
84. BD (1) C 8- H 32	232. RY (1) C 11	1.16	1.77	0.041
85. BD (1) C 9- C 12	131. BD* (1) C 2- C 9	1.09	1.08	0.031
85. BD (1) C 9- C 12	133. BD* (1) C 2- H 28	0.58	1.33	0.025
85. BD (1) C 9- C 12	135. BD* (1) C 3- C 9	4.15	1.30	0.066
85. BD (1) C 9- C 12	137. BD* (1) C 3- H 29	2.69	1.41	0.055
85. BD (1) C 9- C 12	145. BD* (1) C 6- C 10	2.18	1.18	0.045
85. BD (1) C 9- C 12	149. BD* (1) C 8- C 11	2.77	1.31	0.054
85. BD (1) C 9- C 12	153. BD* (1) C 10- C 12	3.89	1.22	0.062
85. BD (1) C 9- C 12	154. BD* (1) C 11- C 12	3.94	1.24	0.062
85. BD (1) C 9- C 12	201. RY (2) C 3	0.76	1.38	0.029
85. BD (1) C 9- C 12	228. RY (1) C 10	0.89	1.82	0.036
85. BD (1) C 9- C 12	229. RY (2) C 10	0.71	1.94	0.033
85. BD (1) C 9- C 12	232. RY (1) C 11	1.02	1.87	0.039
86. BD (1) C 10- C 12	128. BD* (1) C 1- C 11	1.48	1.09	0.036
86. BD (1) C 10- C 12	131. BD* (1) C 2- C 9	1.36	1.09	0.034
86. BD (1) C 10- C 12	141. BD* (1) C 5- C 10	3.71	1.21	0.060
86. BD (1) C 10- C 12	142. BD* (1) C 5- N 24	6.21	0.94	0.068
86. BD (1) C 10- C 12	145. BD* (1) C 6- C 10	3.29	1.19	0.056
86. BD (1) C 10- C 12	146. BD* (1) C 6- B 23	2.73	1.18	0.051
86. BD (1) C 10- C 12	152. BD* (1) C 9- C 12	4.13	1.23	0.064
86. BD (1) C 10- C 12	154. BD* (1) C 11- C 12	4.46	1.24	0.067
86. BD (1) C 10- C 12	209. RY (2) C 5	1.01	1.83	0.038
86. BD (1) C 10- C 12	212. RY (1) C 6	1.15	1.93	0.042
86. BD (1) C 10- C 12	224. RY (1) C 9	0.83	1.91	0.035

86. BD (1) C 10- C 12	233. RY (2) C 11	0.88	1.66	0.034
87. BD (1) C 11- C 12	128. BD* (1) C 1- C 11	1.16	1.09	0.032
87. BD (1) C 11- C 12	129. BD* (1) C 1- H 25	0.60	1.34	0.025
87. BD (1) C 11- C 12	135. BD* (1) C 3- C 9	2.70	1.31	0.053
87. BD (1) C 11- C 12	141. BD* (1) C 5- C 10	2.07	1.21	0.045
87. BD (1) C 11- C 12	149. BD* (1) C 8- C 11	4.28	1.31	0.067
87. BD (1) C 11- C 12	151. BD* (1) C 8- H 32	2.47	1.43	0.053
87. BD (1) C 11- C 12	152. BD* (1) C 9- C 12	3.77	1.22	0.061
87. BD (1) C 11- C 12	153. BD* (1) C 10- C 12	4.65	1.23	0.067
87. BD (1) C 11- C 12	220. RY (1) C 8	0.58	1.81	0.029
87. BD (1) C 11- C 12	221. RY (2) C 8	0.60	1.38	0.026
87. BD (1) C 11- C 12	224. RY (1) C 9	1.12	1.90	0.041
87. BD (1) C 11- C 12	229. RY (2) C 10	1.17	1.94	0.043
88. BD (1) C 13- N 24	139. BD* (2) C 4- C 5	1.77	0.74	0.032
88. BD (1) C 13- N 24	141. BD* (1) C 5- C 10	1.21	1.27	0.035
88. BD (1) C 13- N 24	142. BD* (1) C 5- N 24	1.30	0.99	0.032
88. BD (1) C 13- N 24	159. BD* (1) C 14- N 24	0.51	0.97	0.020
88. BD (1) C 13- N 24	161. BD* (1) C 14- H 37	1.15	1.35	0.035
88. BD (1) C 13- N 24	184. BD* (1) N 24- H 51	3.11	1.54	0.062
88. BD (1) C 13- N 24	210. RY (3) C 5	0.94	1.46	0.033
88. BD (1) C 13- N 24	244. RY (1) C 14	1.18	1.36	0.036
89. BD (1) C 13- H 33	142. BD* (1) C 5- N 24	3.11	0.84	0.046
89. BD (1) C 13- H 33	157. BD* (1) C 13- H 34	1.96	1.28	0.045
89. BD (1) C 13- H 33	158. BD* (1) C 13- H 35	1.49	1.19	0.038
90. BD (1) C 13- H 34	156. BD* (1) C 13- H 33	2.11	1.20	0.045
90. BD (1) C 13- H 34	158. BD* (1) C 13- H 35	1.91	1.17	0.042
90. BD (1) C 13- H 34	159. BD* (1) C 14- N 24	3.13	0.80	0.045
91. BD (1) C 13- H 35	156. BD* (1) C 13- H 33	1.55	1.22	0.039
91. BD (1) C 13- H 35	157. BD* (1) C 13- H 34	1.84	1.28	0.043
91. BD (1) C 13- H 35	184. BD* (1) N 24- H 51	1.65	1.39	0.043
92. BD (1) C 14- N 24	139. BD* (2) C 4- C 5	2.07	0.75	0.035
92. BD (1) C 14- N 24	141. BD* (1) C 5- C 10	1.03	1.28	0.032
92. BD (1) C 14- N 24	142. BD* (1) C 5- N 24	1.20	1.01	0.031
92. BD (1) C 14- N 24	155. BD* (1) C 13- N 24	0.52	0.99	0.020
92. BD (1) C 14- N 24	157. BD* (1) C 13- H 34	0.92	1.44	0.033
92. BD (1) C 14- N 24	184. BD* (1) N 24- H 51	2.84	1.55	0.059
92. BD (1) C 14- N 24	210. RY (3) C 5	0.99	1.47	0.034
92. BD (1) C 14- N 24	240. RY (1) C 13	1.17	1.41	0.036
93. BD (1) C 14- H 36	142. BD* (1) C 5- N 24	2.86	0.87	0.045
93. BD (1) C 14- H 36	161. BD* (1) C 14- H 37	1.79	1.23	0.042
93. BD (1) C 14- H 36	162. BD* (1) C 14- H 38	1.74	1.22	0.041
94. BD (1) C 14- H 37	155. BD* (1) C 13- N 24	2.76	0.85	0.043
94. BD (1) C 14- H 37	160. BD* (1) C 14- H 36	1.93	1.24	0.044
94. BD (1) C 14- H 37	162. BD* (1) C 14- H 38	1.76	1.22	0.041
95. BD (1) C 14- H 38	160. BD* (1) C 14- H 36	1.78	1.24	0.042
95. BD (1) C 14- H 38	161. BD* (1) C 14- H 37	1.74	1.23	0.041
95. BD (1) C 14- H 38	184. BD* (1) N 24- H 51	1.57	1.42	0.042
96. BD (1) C 15- C 16	146. BD* (1) C 6- B 23	1.21	1.11	0.033
96. BD (1) C 15- C 16	164. BD* (1) C 15- C 17	0.87	1.01	0.026
96. BD (1) C 15- C 16	165. BD* (1) C 15- C 18	1.13	1.03	0.031
96. BD (1) C 15- C 16	167. BD* (1) C 16- C 19	0.97	1.01	0.028
96. BD (1) C 15- C 16	168. BD* (1) C 16- C 20	0.83	1.03	0.026
96. BD (1) C 15- C 16	170. BD* (1) C 17- H 39	1.01	1.29	0.032
96. BD (1) C 15- C 16	173. BD* (1) C 18- H 42	1.33	1.31	0.037
96. BD (1) C 15- C 16	176. BD* (1) C 19- H 45	1.16	1.30	0.035
96. BD (1) C 15- C 16	179. BD* (1) C 20- H 48	1.23	1.30	0.036
96. BD (1) C 15- C 16	182. BD* (1) O 21- B 23	0.75	1.04	0.025
96. BD (1) C 15- C 16	183. BD* (1) O 22- B 23	0.72	1.06	0.025
96. BD (1) C 15- C 16	257. RY (2) C 17	0.81	1.42	0.030
96. BD (1) C 15- C 16	265. RY (2) C 19	0.62	1.40	0.026
96. BD (1) C 15- C 16	268. RY (1) C 20	0.66	1.33	0.026
97. BD (1) C 15- C 17	163. BD* (1) C 15- C 16	0.97	0.92	0.027
97. BD (1) C 15- C 17	165. BD* (1) C 15- C 18	0.98	1.01	0.028
97. BD (1) C 15- C 17	168. BD* (1) C 16- C 20	1.63	1.01	0.036
97. BD (1) C 15- C 17	170. BD* (1) C 17- H 39	1.90	1.27	0.044
97. BD (1) C 15- C 17	171. BD* (1) C 17- H 40	1.90	1.28	0.044
97. BD (1) C 15- C 17	172. BD* (1) C 17- H 41	1.93	1.31	0.045
97. BD (1) C 15- C 17	175. BD* (1) C 18- H 44	1.91	1.26	0.044
97. BD (1) C 15- C 17	182. BD* (1) O 21- B 23	1.17	1.02	0.031
97. BD (1) C 15- C 17	252. RY (1) C 16	0.84	1.44	0.031
97. BD (1) C 15- C 17	260. RY (1) C 18	0.78	1.29	0.028
97. BD (1) C 15- C 17	272. RY (1) O 21	0.62	1.88	0.031
98. BD (1) C 15- C 18	163. BD* (1) C 15- C 16	1.06	0.95	0.028
98. BD (1) C 15- C 18	164. BD* (1) C 15- C 17	0.98	1.02	0.028
98. BD (1) C 15- C 18	169. BD* (1) C 16- O 22	1.08	0.87	0.027
98. BD (1) C 15- C 18	172. BD* (1) C 17- H 41	1.35	1.34	0.038
98. BD (1) C 15- C 18	173. BD* (1) C 18- H 42	2.81	1.32	0.054

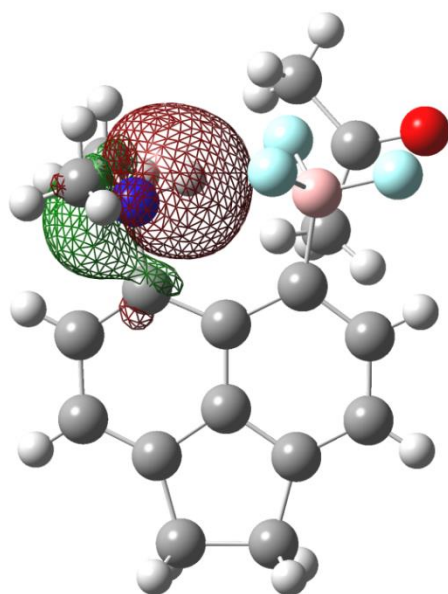
98. BD (1) C 15- C 18	174. BD* (1) C 18- H 43	2.41	1.30	0.050
98. BD (1) C 15- C 18	175. BD* (1) C 18- H 44	2.79	1.30	0.054
98. BD (1) C 15- C 18	182. BD* (1) O 21- B 23	1.64	1.05	0.037
98. BD (1) C 15- C 18	254. RY (3) C 16	0.63	1.48	0.027
98. BD (1) C 15- C 18	256. RY (1) C 17	0.86	1.33	0.030
98. BD (1) C 15- C 18	273. RY (2) O 21	0.61	1.93	0.031
98. BD (1) C 15- C 18	307. RY (1) H 44	0.51	1.28	0.023
99. BD (1) C 15- O 21	146. BD* (1) C 6- B 23	3.41	1.27	0.059
99. BD (1) C 15- O 21	167. BD* (1) C 16- C 19	1.11	1.18	0.032
99. BD (1) C 15- O 21	169. BD* (1) C 16- O 22	1.31	1.02	0.033
99. BD (1) C 15- O 21	171. BD* (1) C 17- H 40	1.15	1.46	0.037
99. BD (1) C 15- O 21	174. BD* (1) C 18- H 43	1.24	1.46	0.038
99. BD (1) C 15- O 21	182. BD* (1) O 21- B 23	1.20	1.20	0.034
99. BD (1) C 15- O 21	183. BD* (1) O 22- B 23	1.37	1.22	0.037
99. BD (1) C 15- O 21	280. RY (1) B 23	2.04	1.38	0.047
100. BD (1) C 16- C 19	163. BD* (1) C 15- C 16	0.97	0.92	0.027
100. BD (1) C 16- C 19	166. BD* (1) C 15- O 21	1.44	0.81	0.030
100. BD (1) C 16- C 19	168. BD* (1) C 16- C 20	1.03	1.01	0.029
100. BD (1) C 16- C 19	176. BD* (1) C 19- H 45	2.14	1.28	0.047
100. BD (1) C 16- C 19	177. BD* (1) C 19- H 46	1.87	1.27	0.044
100. BD (1) C 16- C 19	178. BD* (1) C 19- H 47	2.11	1.28	0.046
100. BD (1) C 16- C 19	181. BD* (1) C 20- H 50	1.70	1.25	0.041
100. BD (1) C 16- C 19	183. BD* (1) O 22- B 23	1.83	1.04	0.039
100. BD (1) C 16- C 19	250. RY (3) C 15	0.79	1.43	0.030
100. BD (1) C 16- C 19	277. RY (2) O 22	0.65	1.82	0.031
101. BD (1) C 16- C 20	163. BD* (1) C 15- C 16	0.92	0.95	0.026
101. BD (1) C 16- C 20	164. BD* (1) C 15- C 17	1.73	1.02	0.037
101. BD (1) C 16- C 20	167. BD* (1) C 16- C 19	0.98	1.02	0.028
101. BD (1) C 16- C 20	178. BD* (1) C 19- H 47	1.22	1.31	0.036
101. BD (1) C 16- C 20	179. BD* (1) C 20- H 48	2.67	1.31	0.053
101. BD (1) C 16- C 20	180. BD* (1) C 20- H 49	2.28	1.27	0.048
101. BD (1) C 16- C 20	181. BD* (1) C 20- H 50	2.30	1.28	0.048
101. BD (1) C 16- C 20	183. BD* (1) O 22- B 23	1.18	1.06	0.032
101. BD (1) C 16- C 20	248. RY (1) C 15	0.70	1.47	0.029
101. BD (1) C 16- C 20	249. RY (2) C 15	0.61	1.59	0.028
101. BD (1) C 16- C 20	264. RY (1) C 19	0.82	1.32	0.029
101. BD (1) C 16- C 20	276. RY (1) O 22	0.68	1.78	0.031
102. BD (1) C 16- O 22	146. BD* (1) C 6- B 23	3.67	1.28	0.061
102. BD (1) C 16- O 22	165. BD* (1) C 15- C 18	1.19	1.20	0.034
102. BD (1) C 16- O 22	166. BD* (1) C 15- O 21	1.35	1.00	0.033
102. BD (1) C 16- O 22	177. BD* (1) C 19- H 46	1.03	1.47	0.035
102. BD (1) C 16- O 22	180. BD* (1) C 20- H 49	1.27	1.44	0.038
102. BD (1) C 16- O 22	182. BD* (1) O 21- B 23	1.41	1.21	0.037
102. BD (1) C 16- O 22	183. BD* (1) O 22- B 23	0.90	1.23	0.030
102. BD (1) C 16- O 22	280. RY (1) B 23	2.43	1.39	0.052
103. BD (1) C 17- H 39	163. BD* (1) C 15- C 16	4.00	0.85	0.052
103. BD (1) C 17- H 39	164. BD* (1) C 15- C 17	0.98	0.92	0.027
103. BD (1) C 17- H 39	166. BD* (1) C 15- O 21	0.93	0.74	0.023
103. BD (1) C 17- H 39	171. BD* (1) C 17- H 40	1.95	1.21	0.043
103. BD (1) C 17- H 39	172. BD* (1) C 17- H 41	2.14	1.24	0.046
104. BD (1) C 17- H 40	164. BD* (1) C 15- C 17	0.71	0.92	0.023
104. BD (1) C 17- H 40	166. BD* (1) C 15- O 21	5.07	0.74	0.055
104. BD (1) C 17- H 40	170. BD* (1) C 17- H 39	1.79	1.20	0.041
104. BD (1) C 17- H 40	172. BD* (1) C 17- H 41	2.01	1.24	0.045
105. BD (1) C 17- H 41	164. BD* (1) C 15- C 17	0.89	0.91	0.025
105. BD (1) C 17- H 41	165. BD* (1) C 15- C 18	3.06	0.93	0.048
105. BD (1) C 17- H 41	170. BD* (1) C 17- H 39	2.06	1.19	0.044
105. BD (1) C 17- H 41	171. BD* (1) C 17- H 40	2.06	1.20	0.044
105. BD (1) C 17- H 41	250. RY (3) C 15	0.79	1.35	0.029
106. BD (1) C 18- H 42	163. BD* (1) C 15- C 16	4.22	0.88	0.055
106. BD (1) C 18- H 42	165. BD* (1) C 15- C 18	1.57	0.97	0.035
106. BD (1) C 18- H 42	174. BD* (1) C 18- H 43	2.05	1.23	0.045
106. BD (1) C 18- H 42	175. BD* (1) C 18- H 44	2.13	1.23	0.046
106. BD (1) C 18- H 42	249. RY (2) C 15	0.56	1.52	0.026
107. BD (1) C 18- H 43	165. BD* (1) C 15- C 18	1.22	0.97	0.031
107. BD (1) C 18- H 43	166. BD* (1) C 15- O 21	6.24	0.77	0.062
107. BD (1) C 18- H 43	173. BD* (1) C 18- H 42	2.03	1.25	0.045
107. BD (1) C 18- H 43	175. BD* (1) C 18- H 44	1.81	1.22	0.042
107. BD (1) C 18- H 43	248. RY (1) C 15	0.85	1.40	0.031
108. BD (1) C 18- H 44	164. BD* (1) C 15- C 17	3.12	0.94	0.048
108. BD (1) C 18- H 44	165. BD* (1) C 15- C 18	1.26	0.97	0.031
108. BD (1) C 18- H 44	166. BD* (1) C 15- O 21	0.98	0.76	0.024
108. BD (1) C 18- H 44	173. BD* (1) C 18- H 42	1.98	1.24	0.044
108. BD (1) C 18- H 44	174. BD* (1) C 18- H 43	1.93	1.22	0.043
108. BD (1) C 18- H 44	249. RY (2) C 15	0.57	1.52	0.026
109. BD (1) C 19- H 45	163. BD* (1) C 15- C 16	3.85	0.86	0.051
109. BD (1) C 19- H 45	167. BD* (1) C 16- C 19	1.12	0.92	0.029

109. BD (1) C 19- H 45	169. BD* (1) C 16- O 22	0.58	0.77	0.019
109. BD (1) C 19- H 45	177. BD* (1) C 19- H 46	1.82	1.21	0.042
109. BD (1) C 19- H 45	178. BD* (1) C 19- H 47	1.93	1.22	0.043
110. BD (1) C 19- H 46	167. BD* (1) C 16- C 19	0.76	0.93	0.024
110. BD (1) C 19- H 46	169. BD* (1) C 16- O 22	5.27	0.78	0.057
110. BD (1) C 19- H 46	176. BD* (1) C 19- H 45	1.68	1.22	0.040
110. BD (1) C 19- H 46	178. BD* (1) C 19- H 47	1.61	1.22	0.040
110. BD (1) C 19- H 46	252. RY (1) C 16	0.76	1.39	0.029
111. BD (1) C 19- H 47	167. BD* (1) C 16- C 19	1.06	0.92	0.028
111. BD (1) C 19- H 47	168. BD* (1) C 16- C 20	3.38	0.93	0.050
111. BD (1) C 19- H 47	169. BD* (1) C 16- O 22	0.71	0.77	0.021
111. BD (1) C 19- H 47	176. BD* (1) C 19- H 45	1.93	1.21	0.043
111. BD (1) C 19- H 47	177. BD* (1) C 19- H 46	1.80	1.20	0.041
111. BD (1) C 19- H 47	254. RY (3) C 16	0.55	1.38	0.025
112. BD (1) C 20- H 48	163. BD* (1) C 15- C 16	4.37	0.87	0.055
112. BD (1) C 20- H 48	168. BD* (1) C 16- C 20	1.55	0.95	0.034
112. BD (1) C 20- H 48	169. BD* (1) C 16- O 22	1.07	0.79	0.026
112. BD (1) C 20- H 48	180. BD* (1) C 20- H 49	1.91	1.19	0.043
112. BD (1) C 20- H 48	181. BD* (1) C 20- H 50	1.92	1.20	0.043
113. BD (1) C 20- H 49	168. BD* (1) C 16- C 20	1.10	0.96	0.029
113. BD (1) C 20- H 49	169. BD* (1) C 16- O 22	5.31	0.79	0.058
113. BD (1) C 20- H 49	179. BD* (1) C 20- H 48	1.82	1.23	0.042
113. BD (1) C 20- H 49	181. BD* (1) C 20- H 50	1.65	1.20	0.040
113. BD (1) C 20- H 49	253. RY (2) C 16	0.98	1.50	0.034
114. BD (1) C 20- H 50	167. BD* (1) C 16- C 19	3.52	0.94	0.051
114. BD (1) C 20- H 50	168. BD* (1) C 16- C 20	1.24	0.96	0.031
114. BD (1) C 20- H 50	179. BD* (1) C 20- H 48	1.95	1.23	0.044
114. BD (1) C 20- H 50	180. BD* (1) C 20- H 49	1.58	1.20	0.039
114. BD (1) C 20- H 50	254. RY (3) C 16	0.93	1.40	0.032
115. BD (1) O 21- B 23	143. BD* (1) C 6- C 7	0.91	1.50	0.033
115. BD (1) O 21- B 23	165. BD* (1) C 15- C 18	1.10	1.34	0.034
115. BD (1) O 21- B 23	166. BD* (1) C 15- O 21	0.75	1.13	0.026
115. BD (1) O 21- B 23	184. BD* (1) N 24- H 51	1.34	1.71	0.043
115. BD (1) O 21- B 23	213. RY (2) C 6	0.86	2.09	0.038
115. BD (1) O 21- B 23	248. RY (1) C 15	3.37	1.77	0.069
115. BD (1) O 21- B 23	280. RY (1) B 23	0.71	1.53	0.029
116. BD (1) O 22- B 23	145. BD* (1) C 6- C 10	1.70	1.41	0.044
116. BD (1) O 22- B 23	146. BD* (1) C 6- B 23	0.65	1.40	0.027
116. BD (1) O 22- B 23	167. BD* (1) C 16- C 19	1.14	1.30	0.034
116. BD (1) O 22- B 23	169. BD* (1) C 16- O 22	0.62	1.15	0.024
116. BD (1) O 22- B 23	212. RY (1) C 6	0.90	2.15	0.039
116. BD (1) O 22- B 23	252. RY (1) C 16	3.40	1.76	0.069
116. BD (1) O 22- B 23	280. RY (1) B 23	0.83	1.51	0.032
117. BD (1) N 24- H 51	138. BD* (1) C 4- C 5	2.36	1.37	0.051
117. BD (1) N 24- H 51	142. BD* (1) C 5- N 24	1.82	1.06	0.039
117. BD (1) N 24- H 51	155. BD* (1) C 13- N 24	1.28	1.05	0.033
117. BD (1) N 24- H 51	158. BD* (1) C 13- H 35	1.03	1.41	0.034
117. BD (1) N 24- H 51	159. BD* (1) C 14- N 24	1.08	1.03	0.030
117. BD (1) N 24- H 51	162. BD* (1) C 14- H 38	1.15	1.41	0.036
117. BD (1) N 24- H 51	208. RY (1) C 5	1.33	1.78	0.043
117. BD (1) N 24- H 51	240. RY (1) C 13	0.53	1.46	0.025
from unit 1 to unit 2				
103. BD (1) C 17- H 39	333. RY (3) S 56	0.06	1.03	0.007
105. BD (1) C 17- H 41	188. BD* (1) C 52- S 56	0.07	0.60	0.006
105. BD (1) C 17- H 41	333. RY (3) S 56	0.21	1.01	0.013
from unit 2 to unit 1				
53. LP (3) O 57	172. BD* (1) C 17- H 41	0.15	0.94	0.011
53. LP (3) O 57	304. RY (1) H 41	0.05	1.07	0.007
56. LP (3) O 58	256. RY (1) C 17	0.05	0.93	0.006
57. LP (1) O 59	157. BD* (1) C 13- H 34	0.39	1.41	0.021
57. LP (1) O 59	297. RY (1) H 34	0.13	1.44	0.012
58. LP (2) O 59	157. BD* (1) C 13- H 34	1.12	0.89	0.028
59. LP (3) O 59	126. LV (1) B 23	0.12	0.19	0.004
59. LP (3) O 59	157. BD* (1) C 13- H 34	0.33	0.89	0.015
59. LP (3) O 59	172. BD* (1) C 17- H 41	0.14	0.91	0.010
59. LP (3) O 59	240. RY (1) C 13	0.05	0.85	0.006
59. LP (3) O 59	282. RY (3) B 23	0.07	0.79	0.007
59. LP (3) O 59	304. RY (1) H 41	0.09	1.05	0.009
121. BD (1) C 52- S 56	256. RY (1) C 17	0.10	1.39	0.011
121. BD (1) C 52- S 56	304. RY (1) H 41	0.11	1.53	0.012
124. BD (1) S 56- O 59	157. BD* (1) C 13- H 34	0.06	1.53	0.009
within unit 2				
25. CR (1) C 52	333. RY (3) S 56	0.59	10.81	0.071
26. CR (1) F 53	317. RY (3) C 52	2.09	25.08	0.204

27. CR (1) F 54	315. RY (1) C 52	5.72	25.06	0.338
27. CR (1) F 54	316. RY (2) C 52	1.00	25.02	0.141
28. CR (1) F 55	315. RY (1) C 52	2.18	25.07	0.209
28. CR (1) F 55	316. RY (2) C 52	2.74	25.02	0.234
30. CR (2) S 56	188. BD*(1) C 52- S 56	1.13	9.65	0.093
30. CR (2) S 56	189. BD*(1) S 56- O 57	0.81	9.90	0.080
30. CR (2) S 56	191. BD*(1) S 56- O 59	1.91	9.81	0.122
30. CR (2) S 56	318. RY (4) C 52	1.07	10.47	0.095
32. CR (4) S 56	188. BD*(1) C 52- S 56	0.69	6.18	0.058
34. CR (1) O 57	332. RY (2) S 56	2.51	19.31	0.197
35. CR (1) O 58	331. RY (1) S 56	3.20	19.28	0.222
36. CR (1) O 59	332. RY (2) S 56	0.74	19.32	0.106
36. CR (1) O 59	333. RY (3) S 56	0.69	19.34	0.103
42. LP (1) F 53	316. RY (2) C 52	0.71	1.66	0.031
42. LP (1) F 53	317. RY (3) C 52	6.78	1.77	0.098
43. LP (2) F 53	186. BD*(1) C 52- F 54	9.12	0.71	0.072
43. LP (2) F 53	187. BD*(1) C 52- F 55	1.55	0.62	0.028
43. LP (2) F 53	188. BD*(1) C 52- S 56	1.49	0.42	0.022
43. LP (2) F 53	315. RY (1) C 52	1.27	1.01	0.032
44. LP (3) F 53	187. BD*(1) C 52- F 55	8.14	0.61	0.063
44. LP (3) F 53	188. BD*(1) C 52- S 56	5.13	0.41	0.041
44. LP (3) F 53	190. BD*(1) S 56- O 58	0.69	0.69	0.019
44. LP (3) F 53	316. RY (2) C 52	0.53	0.95	0.020
45. LP (1) F 54	188. BD*(1) C 52- S 56	0.67	1.06	0.024
45. LP (1) F 54	315. RY (1) C 52	14.24	1.65	0.137
45. LP (1) F 54	316. RY (2) C 52	2.62	1.60	0.058
45. LP (1) F 54	317. RY (3) C 52	0.63	1.71	0.029
46. LP (2) F 54	185. BD*(1) C 52- F 53	4.66	0.56	0.045
46. LP (2) F 54	187. BD*(1) C 52- F 55	15.12	0.71	0.092
46. LP (2) F 54	188. BD*(1) C 52- S 56	19.60	0.51	0.089
47. LP (3) F 54	185. BD*(1) C 52- F 53	28.73	0.56	0.113
47. LP (3) F 54	187. BD*(1) C 52- F 55	12.31	0.71	0.083
48. LP (1) F 55	188. BD*(1) C 52- S 56	0.55	1.10	0.022
48. LP (1) F 55	315. RY (1) C 52	5.68	1.68	0.087
48. LP (1) F 55	316. RY (2) C 52	7.55	1.64	0.099
48. LP (1) F 55	317. RY (3) C 52	0.96	1.75	0.036
49. LP (2) F 55	185. BD*(1) C 52- F 53	2.03	0.54	0.029
49. LP (2) F 55	186. BD*(1) C 52- F 54	13.15	0.78	0.090
49. LP (2) F 55	188. BD*(1) C 52- S 56	14.79	0.49	0.076
49. LP (2) F 55	189. BD*(1) S 56- O 57	0.58	0.74	0.019
50. LP (3) F 55	185. BD*(1) C 52- F 53	24.91	0.54	0.103
50. LP (3) F 55	186. BD*(1) C 52- F 54	6.77	0.78	0.065
51. LP (1) O 57	188. BD*(1) C 52- S 56	0.56	0.81	0.019
51. LP (1) O 57	190. BD*(1) S 56- O 58	1.80	1.09	0.039
51. LP (1) O 57	191. BD*(1) S 56- O 59	0.91	0.97	0.027
51. LP (1) O 57	331. RY (1) S 56	0.71	1.20	0.026
51. LP (1) O 57	332. RY (2) S 56	4.66	1.21	0.067
52. LP (2) O 57	190. BD*(1) S 56- O 58	23.99	0.59	0.106
52. LP (2) O 57	191. BD*(1) S 56- O 59	28.51	0.47	0.104
53. LP (3) O 57	187. BD*(1) C 52- F 55	1.70	0.51	0.026
53. LP (3) O 57	188. BD*(1) C 52- S 56	43.71	0.32	0.105
53. LP (3) O 57	189. BD*(1) S 56- O 57	0.52	0.57	0.015
53. LP (3) O 57	190. BD*(1) S 56- O 58	7.67	0.59	0.060
53. LP (3) O 57	191. BD*(1) S 56- O 59	5.86	0.48	0.047
53. LP (3) O 57	315. RY (1) C 52	0.64	0.90	0.021
54. LP (1) O 58	189. BD*(1) S 56- O 57	1.89	1.04	0.040
54. LP (1) O 58	331. RY (1) S 56	5.81	1.18	0.074
55. LP (2) O 58	189. BD*(1) S 56- O 57	26.84	0.56	0.110
55. LP (2) O 58	191. BD*(1) S 56- O 59	29.14	0.48	0.105
55. LP (2) O 58	332. RY (2) S 56	0.64	0.71	0.019
56. LP (3) O 58	185. BD*(1) C 52- F 53	2.56	0.36	0.027
56. LP (3) O 58	188. BD*(1) C 52- S 56	43.88	0.32	0.105
56. LP (3) O 58	189. BD*(1) S 56- O 57	7.91	0.57	0.060
56. LP (3) O 58	191. BD*(1) S 56- O 59	5.91	0.48	0.048
56. LP (3) O 58	317. RY (3) C 52	0.52	0.97	0.020
57. LP (1) O 59	189. BD*(1) S 56- O 57	0.76	1.07	0.025
57. LP (1) O 59	332. RY (2) S 56	1.46	1.21	0.038
57. LP (1) O 59	333. RY (3) S 56	0.92	1.23	0.030
57. LP (1) O 59	334. RY (4) S 56	0.71	1.21	0.026
58. LP (2) O 59	189. BD*(1) S 56- O 57	18.46	0.54	0.089
58. LP (2) O 59	190. BD*(1) S 56- O 58	17.15	0.57	0.088
58. LP (2) O 59	331. RY (1) S 56	0.52	0.68	0.017
59. LP (3) O 59	186. BD*(1) C 52- F 54	1.40	0.58	0.025
59. LP (3) O 59	188. BD*(1) C 52- S 56	31.94	0.29	0.086
59. LP (3) O 59	189. BD*(1) S 56- O 57	4.87	0.54	0.046
59. LP (3) O 59	190. BD*(1) S 56- O 58	4.11	0.57	0.043
59. LP (3) O 59	191. BD*(1) S 56- O 59	0.92	0.45	0.018

59. LP (3) O 59	315. RY (1) C 52	0.68	0.88	0.022
59. LP (3) O 59	333. RY (3) S 56	0.55	0.70	0.018
118. BD (1) C 52- F 53	185. BD* (1) C 52- F 53	1.78	0.91	0.036
118. BD (1) C 52- F 53	186. BD* (1) C 52- F 54	0.57	1.16	0.023
118. BD (1) C 52- F 53	187. BD* (1) C 52- F 55	0.66	1.07	0.024
118. BD (1) C 52- F 53	190. BD* (1) S 56- O 58	1.03	1.15	0.031
118. BD (1) C 52- F 53	317. RY (3) C 52	0.72	1.52	0.030
119. BD (1) C 52- F 54	185. BD* (1) C 52- F 53	1.74	1.39	0.044
119. BD (1) C 52- F 54	315. RY (1) C 52	1.79	1.93	0.052
120. BD (1) C 52- F 55	185. BD* (1) C 52- F 53	1.81	1.25	0.042
120. BD (1) C 52- F 55	315. RY (1) C 52	0.75	1.79	0.033
120. BD (1) C 52- F 55	316. RY (2) C 52	0.91	1.75	0.036
121. BD (1) C 52- S 56	185. BD* (1) C 52- F 53	0.57	0.82	0.019
121. BD (1) C 52- S 56	188. BD* (1) C 52- S 56	1.90	0.78	0.034
121. BD (1) C 52- S 56	189. BD* (1) S 56- O 57	1.35	1.03	0.033
121. BD (1) C 52- S 56	190. BD* (1) S 56- O 58	1.25	1.06	0.032
121. BD (1) C 52- S 56	191. BD* (1) S 56- O 59	1.89	0.94	0.038
121. BD (1) C 52- S 56	323. RY (1) F 54	0.91	2.41	0.042
121. BD (1) C 52- S 56	327. RY (1) F 55	0.62	2.49	0.035
121. BD (1) C 52- S 56	333. RY (3) S 56	0.66	1.19	0.025
121. BD (1) C 52- S 56	336. RY (2) O 57	0.75	1.86	0.033
121. BD (1) C 52- S 56	340. RY (2) O 58	0.67	1.87	0.032
122. BD (1) S 56- O 57	187. BD* (1) C 52- F 55	1.16	1.30	0.035
122. BD (1) S 56- O 57	188. BD* (1) C 52- S 56	1.44	1.10	0.036
122. BD (1) S 56- O 57	189. BD* (1) S 56- O 57	0.85	1.35	0.030
122. BD (1) S 56- O 57	190. BD* (1) S 56- O 58	1.03	1.38	0.034
122. BD (1) S 56- O 57	191. BD* (1) S 56- O 59	1.83	1.27	0.043
122. BD (1) S 56- O 57	332. RY (2) S 56	1.13	1.50	0.037
123. BD (1) S 56- O 58	185. BD* (1) C 52- F 53	0.71	1.18	0.026
123. BD (1) S 56- O 58	188. BD* (1) C 52- S 56	1.41	1.13	0.036
123. BD (1) S 56- O 58	189. BD* (1) S 56- O 57	0.69	1.38	0.028
123. BD (1) S 56- O 58	190. BD* (1) S 56- O 58	0.82	1.41	0.030
123. BD (1) S 56- O 58	191. BD* (1) S 56- O 59	1.50	1.30	0.039
123. BD (1) S 56- O 58	316. RY (2) C 52	0.66	1.68	0.030
123. BD (1) S 56- O 58	331. RY (1) S 56	1.51	1.52	0.043
124. BD (1) S 56- O 59	186. BD* (1) C 52- F 54	1.47	1.22	0.038
124. BD (1) S 56- O 59	188. BD* (1) C 52- S 56	1.24	0.94	0.030
124. BD (1) S 56- O 59	189. BD* (1) S 56- O 57	1.00	1.19	0.031
124. BD (1) S 56- O 59	190. BD* (1) S 56- O 58	0.90	1.21	0.029
124. BD (1) S 56- O 59	191. BD* (1) S 56- O 59	2.37	1.10	0.046
124. BD (1) S 56- O 59	332. RY (2) S 56	0.50	1.33	0.023
124. BD (1) S 56- O 59	333. RY (3) S 56	0.65	1.35	0.026

6



Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. N	0.0000	0.6483	0.0016	0.0117	0.0003	0.0153	0.0004	0.0000	0.0000
2. H	0.6483	0.0000	0.0078	0.0307	0.0024	0.0437	0.0000	0.0000	0.0000
3. B	0.0016	0.0078	0.0000	0.6427	0.7212	0.6111	0.0004	0.0001	0.0001
4. F	0.0117	0.0307	0.6427	0.0000	0.0259	0.0270	0.0000	0.0001	0.0001
5. F	0.0003	0.0024	0.7212	0.0259	0.0000	0.0243	0.0000	0.0000	0.0000
6. F	0.0153	0.0437	0.6111	0.0270	0.0243	0.0000	0.0000	0.0001	0.0001
7. C	0.0004	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.9140	0.9146
8. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0001	0.9140	0.0000	0.0019
9. H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0001	0.9146	0.0019	0.0000
10. C	0.0005	0.0000	0.0003	0.0000	0.0000	0.0000	0.9991	0.0024	0.0024
11. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0017	0.0016
12. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0016	0.0016
13. C	0.0090	0.0001	0.0002	0.0001	0.0002	0.0001	0.0064	0.0010	0.0010
14. H	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
15. C	0.0073	0.0044	0.0004	0.0004	0.0002	0.0004	0.0003	0.0002	0.0002
16. H	0.0024	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
17. C	0.9012	0.0035	0.0009	0.0008	0.0005	0.0007	0.0006	0.0002	0.0002
18. C	0.0018	0.0015	0.7554	0.0193	0.0178	0.0172	0.0014	0.0035	0.0034
19. C	0.0002	0.0001	0.0146	0.0094	0.0069	0.0077	0.0107	0.0001	0.0001
20. H	0.0001	0.0000	0.0013	0.0007	0.0049	0.0007	0.0003	0.0000	0.0000
21. C	0.0001	0.0001	0.0078	0.0006	0.0011	0.0006	0.0112	0.0070	0.0068
22. H	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0016	0.0001	0.0001
23. C	0.0006	0.0000	0.0002	0.0001	0.0002	0.0000	0.0062	0.0026	0.0027
24. C	0.0062	0.0006	0.0081	0.0039	0.0056	0.0031	0.0079	0.0001	0.0001
25. C	0.0002	0.0000	0.0022	0.0025	0.0007	0.0019	1.0068	0.0034	0.0034
26. C	0.0080	0.0004	0.0059	0.0004	0.0006	0.0003	0.0084	0.0062	0.0063
27. C	0.9108	0.0039	0.0002	0.0035	0.0002	0.0010	0.0000	0.0000	0.0000
28. H	0.0018	0.0054	0.0001	0.0007	0.0001	0.0005	0.0000	0.0000	0.0000
29. H	0.0012	0.0003	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
30. H	0.0012	0.0002	0.0000	0.0022	0.0001	0.0001	0.0000	0.0000	0.0000
31. C	0.9112	0.0037	0.0002	0.0010	0.0002	0.0040	0.0000	0.0000	0.0000
32. H	0.0011	0.0002	0.0000	0.0000	0.0000	0.0012	0.0000	0.0000	0.0000
33. H	0.0013	0.0004	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000
34. H	0.0018	0.0055	0.0001	0.0004	0.0001	0.0009	0.0000	0.0000	0.0000
35. O	0.0000	0.0000	0.0004	0.0001	0.0001	0.0016	0.0000	0.0000	0.0000
36. C	0.0000	0.0000	0.0002	0.0003	0.0002	0.0060	0.0000	0.0000	0.0000
37. C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0015	0.0000	0.0000	0.0000
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000
40. H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0020	0.0000	0.0000	0.0000
41. C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0019	0.0000	0.0000	0.0000
42. H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0037	0.0000	0.0000	0.0000
43. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000

44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
	Atom	10	11	12	13	14	15	16	17	18
1.	N	0.0005	0.0000	0.0000	0.0090	0.0002	0.0073	0.0024	0.9012	0.0018
2.	H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0044	0.0002	0.0035	0.0015
3.	B	0.0003	0.0000	0.0000	0.0002	0.0000	0.0004	0.0000	0.0009	0.7554
4.	F	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0008	0.0193
5.	F	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0005	0.0178
6.	F	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0007	0.0172
7.	C	0.9991	0.0026	0.0026	0.0064	0.0001	0.0003	0.0002	0.0006	0.0014
8.	H	0.0024	0.0017	0.0016	0.0010	0.0000	0.0002	0.0000	0.0002	0.0035
9.	H	0.0024	0.0016	0.0016	0.0010	0.0000	0.0002	0.0000	0.0002	0.0034
10.	C	0.0000	0.9141	0.9135	0.0107	0.0018	0.0105	0.0003	0.0018	0.0005
11.	H	0.9141	0.0000	0.0021	0.0064	0.0001	0.0001	0.0000	0.0028	0.0001
12.	H	0.9135	0.0021	0.0000	0.0064	0.0001	0.0001	0.0000	0.0028	0.0001
13.	C	0.0107	0.0064	0.0064	0.0000	0.9260	1.3067	0.0057	0.0231	0.0052
14.	H	0.0018	0.0001	0.0001	0.9260	0.0000	0.0043	0.0013	0.0059	0.0003
15.	C	0.0105	0.0001	0.0001	1.3067	0.0043	0.0000	0.9282	1.5154	0.0315
16.	H	0.0003	0.0000	0.0000	0.0057	0.0013	0.9282	0.0000	0.0054	0.0002
17.	C	0.0018	0.0028	0.0028	0.0231	0.0059	1.5154	0.0054	0.0000	0.0136
18.	C	0.0005	0.0001	0.0001	0.0052	0.0003	0.0315	0.0002	0.0136	0.0000
19.	C	0.0004	0.0005	0.0005	0.0295	0.0000	0.0008	0.0002	0.0336	1.5134
20.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0085
21.	C	0.0065	0.0009	0.0009	0.0012	0.0002	0.0305	0.0000	0.0005	0.0127
22.	H	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0004	0.0065
23.	C	1.0083	0.0034	0.0035	1.5008	0.0065	0.0123	0.0060	0.0985	0.0083
24.	C	0.0084	0.0003	0.0002	0.0565	0.0002	0.0193	0.0075	1.2500	1.2515
25.	C	0.0057	0.0025	0.0027	0.0357	0.0002	0.0009	0.0002	0.0089	0.1062
26.	C	0.0092	0.0066	0.0067	0.0107	0.0091	0.0608	0.0004	0.0149	0.0153
27.	C	0.0001	0.0001	0.0001	0.0008	0.0000	0.0054	0.0003	0.0100	0.0002
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	0.0005	0.0000
29.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0013	0.0000	0.0071	0.0001
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000
31.	C	0.0001	0.0001	0.0001	0.0008	0.0000	0.0061	0.0002	0.0101	0.0002
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000
33.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0014	0.0000	0.0070	0.0001
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0004	0.0000
35.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
37.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0004
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0004
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Atom	19	20	21	22	23	24	25	26	27
1.	N	0.0002	0.0001	0.0001	0.0000	0.0006	0.0062	0.0002	0.0080	0.9108
2.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0006	0.0000	0.0004	0.0039
3.	B	0.0146	0.0013	0.0078	0.0001	0.0002	0.0081	0.0022	0.0059	0.0002
4.	F	0.0094	0.0007	0.0006	0.0001	0.0001	0.0039	0.0025	0.0004	0.0035
5.	F	0.0069	0.0049	0.0011	0.0001	0.0002	0.0056	0.0007	0.0006	0.0002
6.	F	0.0077	0.0007	0.0006	0.0001	0.0000	0.0031	0.0019	0.0003	0.0010
7.	C	0.0107	0.0003	0.0112	0.0016	0.0062	0.0079	1.0068	0.0084	0.0000
8.	H	0.0001	0.0000	0.0070	0.0001	0.0026	0.0001	0.0034	0.0062	0.0000
9.	H	0.0001	0.0000	0.0068	0.0001	0.0027	0.0001	0.0034	0.0063	0.0000
10.	C	0.0004	0.0002	0.0065	0.0001	1.0083	0.0084	0.0057	0.0092	0.0001
11.	H	0.0005	0.0000	0.0009	0.0000	0.0034	0.0003	0.0025	0.0066	0.0001
12.	H	0.0005	0.0000	0.0009	0.0000	0.0035	0.0002	0.0027	0.0067	0.0001
13.	C	0.0295	0.0000	0.0012	0.0002	1.5008	0.0565	0.0357	0.0107	0.0008
14.	H	0.0000	0.0000	0.0002	0.0000	0.0065	0.0002	0.0002	0.0091	0.0000
15.	C	0.0008	0.0002	0.0305	0.0000	0.0123	0.0193	0.0009	0.0608	0.0054
16.	H	0.0002	0.0000	0.0000	0.0000	0.0060	0.0075	0.0002	0.0004	0.0003
17.	C	0.0336	0.0001	0.0005	0.0004	0.0985	1.2500	0.0089	0.0149	0.0100
18.	C	1.5134	0.0085	0.0127	0.0065	0.0083	1.2515	0.1062	0.0153	0.0002
19.	C	0.0000	0.9181	1.3070	0.0049	0.0037	0.0154	0.0133	0.0547	0.0005
20.	H	0.9181	0.0000	0.0034	0.0014	0.0003	0.0081	0.0059	0.0004	0.0000
21.	C	1.3070	0.0034	0.0000	0.9271	0.0344	0.0604	1.5146	0.0117	0.0001
22.	H	0.0049	0.0014	0.9271	0.0000	0.0002	0.0002	0.0055	0.0092	0.0000
23.	C	0.0037	0.0003	0.0344	0.0002	0.0000	0.0123	0.0153	1.2621	0.0022
24.	C	0.0154	0.0081	0.0604	0.0002	0.0123	0.0000	0.0153	1.2316	0.0067
25.	C	0.0133	0.0059	1.5146	0.0055	0.0153	0.0153	0.0000	1.2419	0.0002
26.	C	0.0547	0.0004	0.0117	0.0092	1.2621	1.2316	1.2419	0.0000	0.0004

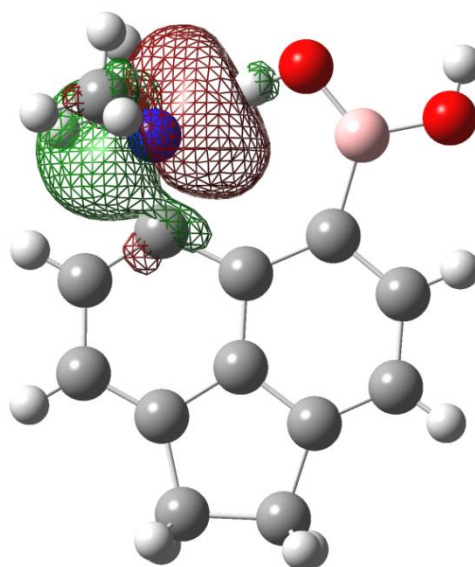
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	Atom	28	29	30	31	32	33	34	35	36
1.	N	0.0018	0.0012	0.0012	0.9112	0.0011	0.0013	0.0018	0.0000	0.0000
2.	H	0.0054	0.0003	0.0002	0.0037	0.0002	0.0004	0.0055	0.0000	0.0000
3.	B	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0004	0.0002
4.	F	0.0007	0.0001	0.0022	0.0010	0.0000	0.0001	0.0004	0.0001	0.0003
5.	F	0.0001	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001	0.0001	0.0002
6.	F	0.0005	0.0001	0.0001	0.0040	0.0012	0.0003	0.0009	0.0016	0.0060
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0001	0.0000	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000
14.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0003	0.0013	0.0001	0.0061	0.0001	0.0014	0.0003	0.0000	0.0000
16.	H	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000
17.	C	0.0005	0.0071	0.0003	0.0101	0.0004	0.0070	0.0004	0.0000	0.0000
18.	C	0.0000	0.0001	0.0000	0.0002	0.0000	0.0001	0.0000	0.0000	0.0001
19.	C	0.0000	0.0001	0.0000	0.0006	0.0000	0.0001	0.0000	0.0001	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0000	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0000	0.0005	0.0000	0.0025	0.0000	0.0006	0.0000	0.0000	0.0000
24.	C	0.0001	0.0003	0.0001	0.0064	0.0001	0.0004	0.0001	0.0000	0.0001
25.	C	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0000	0.0002	0.0000	0.0004	0.0000	0.0002	0.0000	0.0000	0.0000
27.	C	0.9401	0.9324	0.9240	0.0098	0.0072	0.0002	0.0005	0.0000	0.0000
28.	H	0.0000	0.0017	0.0019	0.0004	0.0000	0.0001	0.0003	0.0000	0.0000
29.	H	0.0017	0.0000	0.0022	0.0003	0.0001	0.0001	0.0001	0.0000	0.0000
30.	H	0.0019	0.0022	0.0000	0.0073	0.0005	0.0001	0.0001	0.0000	0.0000
31.	C	0.0004	0.0003	0.0073	0.0000	0.9270	0.9320	0.9393	0.0001	0.0000
32.	H	0.0000	0.0001	0.0005	0.9270	0.0000	0.0022	0.0020	0.0001	0.0001
33.	H	0.0001	0.0001	0.0001	0.9320	0.0022	0.0000	0.0017	0.0000	0.0000
34.	H	0.0003	0.0001	0.0001	0.9393	0.0020	0.0017	0.0000	0.0000	0.0000
35.	O	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	1.8393

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10.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
18.	C	0.0004	0.0002	0.0001	0.0004	0.0000	0.0001	0.0000	0.0000
19.	C	0.0002	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0002	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
25.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0003	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000
32.	H	0.0002	0.0000	0.0000	0.0003	0.0001	0.0001	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	O	0.0582	0.0039	0.0172	0.0165	0.0589	0.0180	0.0136	0.0048
36.	C	1.0011	0.0032	0.0069	0.0066	0.9993	0.0077	0.0057	0.0038
37.	C	0.0000	0.9229	0.9199	0.9200	0.0083	0.0008	0.0003	0.0076
38.	H	0.9229	0.0000	0.0023	0.0023	0.0081	0.0000	0.0003	0.0004
39.	H	0.9199	0.0023	0.0000	0.0026	0.0004	0.0002	0.0000	0.0000
40.	H	0.9200	0.0023	0.0026	0.0000	0.0002	0.0000	0.0000	0.0003
41.	C	0.0083	0.0081	0.0004	0.0002	0.0000	0.9078	0.9310	0.9236
42.	H	0.0008	0.0000	0.0002	0.0000	0.9078	0.0000	0.0025	0.0028
43.	H	0.0003	0.0003	0.0000	0.0000	0.9310	0.0025	0.0000	0.0019
44.	H	0.0076	0.0004	0.0000	0.0003	0.9236	0.0028	0.0019	0.0000

11



Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4	5	6	7	8	9
1. C	0.0000	0.9156	0.9138	1.0005	0.0026	0.0027	0.0062	0.0001	0.0003
2. H	0.9156	0.0000	0.0020	0.0025	0.0015	0.0017	0.0008	0.0000	0.0003
3. H	0.9138	0.0020	0.0000	0.0026	0.0017	0.0020	0.0009	0.0000	0.0003
4. C	1.0005	0.0025	0.0026	0.0000	0.9154	0.9150	0.0106	0.0018	0.0111
5. H	0.0026	0.0015	0.0017	0.9154	0.0000	0.0019	0.0064	0.0001	0.0001
6. H	0.0027	0.0017	0.0020	0.9150	0.0019	0.0000	0.0066	0.0001	0.0001
7. C	0.0062	0.0008	0.0009	0.0106	0.0064	0.0066	0.0000	0.9262	1.3056
8. H	0.0001	0.0000	0.0000	0.0018	0.0001	0.0001	0.9262	0.0000	0.0046
9. C	0.0003	0.0003	0.0003	0.0111	0.0001	0.0001	1.3056	0.0046	0.0000
10. H	0.0002	0.0000	0.0000	0.0003	0.0000	0.0000	0.0048	0.0013	0.9273
11. C	0.0004	0.0001	0.0001	0.0015	0.0030	0.0031	0.0143	0.0059	1.5125
12. C	0.0015	0.0029	0.0034	0.0004	0.0001	0.0002	0.0021	0.0003	0.0322
13. C	0.0112	0.0001	0.0001	0.0004	0.0003	0.0003	0.0269	0.0001	0.0008
14. H	0.0003	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002
15. C	0.0108	0.0060	0.0072	0.0062	0.0009	0.0011	0.0008	0.0002	0.0300
16. H	0.0017	0.0001	0.0001	0.0001	0.0000	0.0000	0.0002	0.0000	0.0000
17. C	0.0061	0.0030	0.0024	1.0046	0.0033	0.0033	1.5113	0.0065	0.0128
18. C	0.0083	0.0001	0.0001	0.0083	0.0001	0.0001	0.0650	0.0002	0.0103
19. C	1.0053	0.0034	0.0034	0.0061	0.0030	0.0024	0.0321	0.0002	0.0013
20. C	0.0083	0.0065	0.0061	0.0086	0.0065	0.0065	0.0116	0.0095	0.0600
21. C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0004	0.0000	0.0071
22. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
23. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0013
24. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0007
25. C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0004	0.0000	0.0064
26. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0005
27. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0013
28. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
29. B	0.0006	0.0002	0.0003	0.0003	0.0000	0.0000	0.0006	0.0000	0.0014
30. N	0.0004	0.0000	0.0000	0.0005	0.0000	0.0000	0.0095	0.0007	0.0188
31. O	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0002	0.0000	0.0012
32. O	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0004	0.0000	0.0008
33. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009
Atom	10	11	12	13	14	15	16	17	18
1. C	0.0002	0.0004	0.0015	0.0112	0.0003	0.0108	0.0017	0.0061	0.0083
2. H	0.0000	0.0001	0.0029	0.0001	0.0000	0.0060	0.0001	0.0030	0.0001
3. H	0.0000	0.0001	0.0034	0.0001	0.0000	0.0072	0.0001	0.0024	0.0001
4. C	0.0003	0.0015	0.0004	0.0004	0.0002	0.0062	0.0001	1.0046	0.0083
5. H	0.0000	0.0030	0.0001	0.0003	0.0000	0.0009	0.0000	0.0033	0.0001

6.	H	0.0000	0.0031	0.0002	0.0003	0.0000	0.0011	0.0000	0.0033	0.0001
7.	C	0.0048	0.0143	0.0021	0.0269	0.0000	0.0008	0.0002	1.5113	0.0650
8.	H	0.0013	0.0059	0.0003	0.0001	0.0000	0.0002	0.0000	0.0065	0.0002
9.	C	0.9273	1.5125	0.0322	0.0008	0.0002	0.0300	0.0000	0.0128	0.0103
10.	H	0.0000	0.0055	0.0001	0.0002	0.0000	0.0000	0.0000	0.0060	0.0072
11.	C	0.0055	0.0000	0.0123	0.0300	0.0001	0.0006	0.0004	0.1022	1.2559
12.	C	0.0001	0.0123	0.0000	1.5109	0.0076	0.0118	0.0065	0.0091	1.2329
13.	C	0.0002	0.0300	1.5109	0.0000	0.9209	1.3055	0.0048	0.0020	0.0104
14.	H	0.0000	0.0001	0.0076	0.9209	0.0000	0.0037	0.0013	0.0003	0.0081
15.	C	0.0000	0.0006	0.0118	1.3055	0.0037	0.0000	0.9267	0.0348	0.0604
16.	H	0.0000	0.0004	0.0065	0.0048	0.0013	0.9267	0.0000	0.0002	0.0002
17.	C	0.0060	0.1022	0.0091	0.0020	0.0003	0.0348	0.0002	0.0000	0.0104
18.	C	0.0072	1.2559	1.2329	0.0104	0.0081	0.0604	0.0002	0.0104	0.0000
19.	C	0.0002	0.0079	0.1033	0.0147	0.0058	1.5152	0.0059	0.0154	0.0109
20.	C	0.0005	0.0115	0.0109	0.0548	0.0004	0.0116	0.0094	1.2523	1.2484
21.	C	0.0002	0.0089	0.0002	0.0006	0.0000	0.0001	0.0000	0.0027	0.0067
22.	H	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
23.	H	0.0001	0.0077	0.0001	0.0001	0.0000	0.0001	0.0000	0.0006	0.0005
24.	H	0.0004	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
25.	C	0.0003	0.0086	0.0002	0.0005	0.0000	0.0000	0.0000	0.0024	0.0072
26.	H	0.0005	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
27.	H	0.0001	0.0074	0.0001	0.0001	0.0000	0.0001	0.0000	0.0005	0.0004
28.	H	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
29.	B	0.0000	0.0017	0.8661	0.0252	0.0018	0.0100	0.0001	0.0005	0.0109
30.	N	0.0041	0.9671	0.0016	0.0003	0.0001	0.0000	0.0000	0.0009	0.0141
31.	O	0.0001	0.0006	0.0132	0.0158	0.0013	0.0008	0.0002	0.0002	0.0044
32.	O	0.0000	0.0005	0.0098	0.0086	0.0028	0.0007	0.0001	0.0002	0.0071
33.	H	0.0000	0.0000	0.0106	0.0003	0.0000	0.0001	0.0000	0.0000	0.0003
34.	H	0.0000	0.0004	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0003

Atom	19	20	21	22	23	24	25	26	27
1.	C	1.0053	0.0083	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0034	0.0065	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0034	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0061	0.0086	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5.	H	0.0030	0.0065	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
6.	H	0.0024	0.0065	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
7.	C	0.0321	0.0116	0.0004	0.0000	0.0001	0.0001	0.0004	0.0001
8.	H	0.0002	0.0095	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0013	0.0600	0.0071	0.0001	0.0013	0.0007	0.0064	0.0005
10.	H	0.0002	0.0005	0.0002	0.0000	0.0001	0.0004	0.0003	0.0005
11.	C	0.0079	0.0115	0.0089	0.0005	0.0077	0.0004	0.0086	0.0004
12.	C	0.1033	0.0109	0.0002	0.0000	0.0001	0.0000	0.0002	0.0000
13.	C	0.0147	0.0548	0.0006	0.0000	0.0001	0.0000	0.0005	0.0000
14.	H	0.0058	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	1.5152	0.0116	0.0001	0.0000	0.0001	0.0000	0.0000	0.0001
16.	H	0.0059	0.0094	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0154	1.2523	0.0027	0.0000	0.0006	0.0000	0.0024	0.0005
18.	C	0.0109	1.2484	0.0067	0.0002	0.0005	0.0002	0.0072	0.0002
19.	C	0.0000	1.2419	0.0002	0.0000	0.0000	0.0000	0.0002	0.0000
20.	C	1.2419	0.0000	0.0003	0.0000	0.0001	0.0000	0.0003	0.0000
21.	C	0.0002	0.0003	0.0000	0.9354	0.9363	0.9406	0.0094	0.0004
22.	H	0.0000	0.0000	0.9354	0.0000	0.0022	0.0014	0.0082	0.0000
23.	H	0.0000	0.0001	0.9363	0.0022	0.0000	0.0012	0.0005	0.0002
24.	H	0.0000	0.0000	0.9406	0.0014	0.0012	0.0000	0.0003	0.0013
25.	C	0.0002	0.0003	0.0094	0.0082	0.0005	0.0003	0.0000	0.9412
26.	H	0.0000	0.0000	0.0004	0.0000	0.0002	0.0013	0.9412	0.0000
27.	H	0.0000	0.0001	0.0004	0.0001	0.0002	0.0002	0.9355	0.0012
28.	H	0.0000	0.0000	0.0082	0.0004	0.0002	0.0000	0.9354	0.0014
29.	B	0.0073	0.0069	0.0001	0.0000	0.0000	0.0001	0.0001	0.0001
30.	N	0.0002	0.0076	0.9575	0.0034	0.0044	0.0192	0.9586	0.0190
31.	O	0.0042	0.0002	0.0011	0.0002	0.0003	0.0012	0.0011	0.0002
32.	O	0.0034	0.0004	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000
33.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	H	0.0000	0.0001	0.0010	0.0001	0.0002	0.0014	0.0010	0.0002

Atom	28	29	30	31	32	33	34
1.	C	0.0000	0.0006	0.0004	0.0001	0.0001	0.0000
2.	H	0.0000	0.0002	0.0000	0.0001	0.0001	0.0000
3.	H	0.0000	0.0003	0.0000	0.0001	0.0001	0.0000
4.	C	0.0000	0.0003	0.0005	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0006	0.0095	0.0002	0.0004	0.0000
8.	H	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000

13. (1.99938) CR (1) C 21	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
14. (1.99938) CR (1) C 25	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
15. (1.99922) CR (1) B 29	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
16. (1.99952) CR (1) N 30	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
17. (1.99979) CR (1) O 31	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
18. (1.99979) CR (1) O 32	s(100.00%)	1.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
19. (1.00025) LP (1) C 20	s(0.00%)p 1.00(100.00%)d 0.00(0.00%)	0.0000	0.0017	0.0004	0.0002	-0.0156
		-0.0009	0.0059	0.0001	-0.9998	-0.0105
		-0.0001	0.0046	0.0007	0.0006	0.0005
20. (1.88481) LP (1) N 30	s(15.07%)p 5.64(84.91%)d 0.00(0.02%)	0.0000	0.3880	-0.0115	-0.0008	0.3431
		-0.0121	0.8544	-0.0353	-0.0098	-0.0004
		-0.0079	0.0004	0.0005	0.0089	0.0073
21. (1.95973) LP (1) O 31	s(25.12%)p 2.98(74.75%)d 0.01(0.13%)	0.0000	0.5012	-0.0031	-0.0004	0.8476
		0.0148	0.1700	-0.0004	-0.0020	0.0002
		-0.0122	0.0013	0.0003	-0.0285	0.0172
22. (1.80182) LP (2) O 31	s(0.05%)p99.99(99.79%)d 3.06(0.16%)	0.0000	0.0226	-0.0006	0.0002	-0.0082
		-0.0003	-0.0376	0.0000	-0.9981	-0.0132
		0.0012	0.0392	0.0049	-0.0002	-0.0022
23. (1.96749) LP (1) O 32	s(26.41%)p 2.78(73.47%)d 0.00(0.12%)	0.0000	0.5139	-0.0082	0.0000	-0.5328
		-0.0071	0.6711	0.0119	-0.0140	-0.0002
		0.0299	-0.0013	0.0025	0.0049	0.0155
24. (1.83494) LP (2) O 32	s(0.06%)p99.99(99.80%)d 2.50(0.14%)	0.0000	0.0237	0.0003	0.0001	0.1023
		0.0012	0.0425	0.0001	-0.9928	-0.0140
		-0.0015	-0.0236	0.0285	0.0039	-0.0042
25. (1.97743) BD (1) C 1- H 2	(61.68%) 0.7854* C 1 s(24.99%)p 3.00(74.94%)d 0.00(0.07%)	0.0000	0.4999	0.0022	-0.0007	-0.4507
		-0.0137	0.2980	0.0061	-0.6761	0.0032
		-0.0093	0.0173	-0.0130	0.0034	0.0117
	(38.32%) 0.6190* H 2 s(99.94%)p 0.00(0.06%)	0.9997	0.0008	0.0126	-0.0085	0.0186
26. (1.97607) BD (1) C 1- H 3	(61.70%) 0.7855* C 1 s(25.08%)p 2.99(74.85%)d 0.00(0.07%)	0.0000	0.5008	0.0021	-0.0006	-0.3798
		-0.0145	0.2528	0.0075	0.7349	-0.0010
		-0.0069	-0.0156	0.0120	0.0025	0.0159
	(38.30%) 0.6189* H 3 s(99.94%)p 0.00(0.06%)	0.9997	0.0009	0.0109	-0.0074	-0.0206
27. (1.98166) BD (1) C 1- C 4	(49.97%) 0.7069* C 1 s(24.57%)p 3.07(75.39%)d 0.00(0.04%)	0.0000	0.4957	0.0001	0.0013	0.0204
		-0.0207	-0.8673	0.0072	-0.0292	0.0004
		-0.0039	-0.0002	0.0012	-0.0160	-0.0096
	(50.03%) 0.7073* C 4 s(24.43%)p 3.09(75.54%)d 0.00(0.04%)	0.0000	0.4942	0.0001	0.0013	-0.0772
		-0.0191	0.8649	-0.0097	0.0304	0.0003
		0.0008	0.0000	0.0012	-0.0165	-0.0096
28. (1.97807) BD (1) C 1- C 19	(49.47%) 0.7034* C 1 s(25.22%)p 2.96(74.73%)d 0.00(0.05%)	0.0000	0.5022	-0.0050	0.0006	0.8071
		-0.0190	0.3074	0.0104	-0.0311	0.0012
		0.0122	-0.0013	-0.0006	0.0146	-0.0098
	(50.53%) 0.7108* C 19 s(30.75%)p 2.25(69.21%)d 0.00(0.04%)					

					0.0000	0.5545	-0.0036	-0.0023	-0.8112
					0.0030	-0.1805	0.0304	0.0253	0.0002
					0.0108	-0.0011	-0.0005	0.0112	-0.0114
29.	(1.97726)	BD (1) C	4- H 5						
	(61.66%)		0.7852* C	4 s(25.13%)p 2.98(74.80%)d 0.00(0.07%)					
				0.0000	0.5013	0.0023	-0.0006	-0.3762	
				-0.0135	-0.3448	-0.0080	0.6981	-0.0024	
				0.0088	-0.0145	-0.0153	0.0004	0.0132	
	(38.34%)		0.6192* H	5 s(99.94%)p 0.00(0.06%)					
				0.9997	0.0008	0.0105	0.0098	-0.0193	
30.	(1.97692)	BD (1) C	4- H 6						
	(61.65%)		0.7852* C	4 s(25.16%)p 2.97(74.77%)d 0.00(0.07%)					
				0.0000	0.5016	0.0022	-0.0006	-0.3860	
				-0.0137	-0.2962	-0.0083	-0.7146	0.0019	
				0.0080	0.0154	0.0135	0.0015	0.0145	
	(38.35%)		0.6193* H	6 s(99.94%)p 0.00(0.06%)					
				0.9997	0.0009	0.0109	0.0085	0.0199	
31.	(1.97757)	BD (1) C	4- C 17						
	(49.39%)		0.7028* C	4 s(25.14%)p 2.98(74.81%)d 0.00(0.05%)					
				0.0000	0.5014	-0.0052	0.0006	0.8383	
				-0.0175	-0.2115	-0.0119	-0.0130	0.0002	
				-0.0081	-0.0005	0.0001	0.0173	-0.0098	
	(50.61%)		0.7114* C	17 s(30.73%)p 2.25(69.24%)d 0.00(0.04%)					
				0.0000	0.5543	-0.0037	-0.0022	-0.8269	
				0.0055	0.0875	-0.0282	0.0096	-0.0006	
				-0.0073	-0.0003	0.0003	0.0133	-0.0115	
32.	(1.98220)	BD (1) C	7- H 8						
	(60.63%)		0.7787* C	7 s(31.78%)p 2.14(68.15%)d 0.00(0.06%)					
				0.0000	0.5638	-0.0028	-0.0033	-0.3970	
				-0.0020	-0.7228	-0.0128	-0.0350	-0.0012	
				0.0184	0.0010	0.0017	-0.0101	-0.0140	
	(39.37%)		0.6274* H	8 s(99.93%)p 0.00(0.07%)					
				0.9997	-0.0013	0.0132	0.0227	0.0012	
33.	(1.97103)	BD (1) C	7- C 9						
	(49.76%)		0.7054* C	7 s(32.92%)p 2.04(67.03%)d 0.00(0.05%)					
				0.0000	0.5738	0.0020	0.0002	0.8181	
				0.0044	-0.0010	-0.0323	-0.0042	-0.0012	
				0.0026	0.0001	0.0004	0.0163	-0.0135	
	(50.24%)		0.7088* C	9 s(33.79%)p 1.96(66.16%)d 0.00(0.05%)					
				0.0000	0.5813	0.0038	0.0025	-0.8127	
				-0.0042	-0.0111	-0.0311	-0.0078	-0.0008	
				0.0003	0.0002	0.0002	0.0163	-0.0140	
34.	(1.97762)	BD (1) C	7- C 17						
	(49.29%)		0.7021* C	7 s(35.11%)p 1.85(64.83%)d 0.00(0.06%)					
				0.0000	0.5926	0.0028	0.0038	-0.4149	
				-0.0263	0.6884	-0.0101	0.0384	-0.0004	
				-0.0165	-0.0009	0.0019	-0.0097	-0.0151	
	(50.71%)		0.7121* C	17 s(37.31%)p 1.68(62.65%)d 0.00(0.05%)					
				0.0000	0.6107	0.0105	0.0012	0.3339	
				-0.0190	-0.7163	-0.0219	-0.0319	-0.0008	
				-0.0158	-0.0010	0.0015	-0.0086	-0.0120	
35.	(1.72510)	BD (2) C	7- C 17						
	(52.17%)		0.7223* C	7 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	0.0006	0.0010	-0.0004	-0.0055	
				-0.0009	0.0519	-0.0001	-0.9983	0.0195	
				-0.0004	0.0034	-0.0188	-0.0009	-0.0018	
	(47.83%)		0.6916* C	17 s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	0.0001	-0.0001	0.0001	-0.0072	
				-0.0008	0.0411	0.0005	-0.9989	0.0066	
				0.0008	-0.0169	0.0125	0.0007	0.0016	
36.	(1.97950)	BD (1) C	9- H 10						
	(60.38%)		0.7770* C	9 s(30.92%)p 2.23(69.01%)d 0.00(0.07%)					
				0.0000	0.5560	0.0015	-0.0040	0.4086	
				-0.0031	-0.7228	-0.0186	-0.0210	-0.0009	
				-0.0189	-0.0006	0.0012	-0.0104	-0.0154	
	(39.62%)		0.6295* H	10 s(99.93%)p 0.00(0.07%)					
				0.9996	-0.0013	-0.0125	0.0239	0.0008	
37.	(1.97904)	BD (1) C	9- C 11						
	(49.98%)		0.7069* C	9 s(35.11%)p 1.85(64.83%)d 0.00(0.06%)					
				0.0000	0.5925	-0.0035	0.0026	0.4144	
				0.0171	0.6893	-0.0099	0.0330	-0.0010	
				0.0173	0.0007	0.0014	-0.0087	-0.0152	
	(50.02%)		0.7073* C	11 s(36.68%)p 1.73(63.27%)d 0.00(0.05%)					
				0.0000	0.6056	0.0017	0.0003	-0.4182	
				0.0023	-0.6763	-0.0163	-0.0160	-0.0013	
				0.0171	0.0004	0.0007	-0.0078	-0.0114	
38.	(1.75405)	BD (2) C	9- C 11						

	(49.10%)	0.7007* C 9	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0033	0.0009	0.0000	0.0115	0.0004	0.0381	-0.0001	-0.9988	0.0193	0.0004	-0.0076	-0.0176	-0.0003	-0.0012
	(50.90%)	0.7134* C 11	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)	0.0000	0.0067	0.0008	0.0000	0.0129	0.0005	0.0217	0.0003	-0.9993	0.0184	-0.0006	0.0146	0.0136	0.0004	0.0009
39. (1.97499)	BD (1) C 11- C 18	(49.16%)	0.7011* C 11	s(36.02%)p 1.77(63.92%)d 0.00(0.05%)	0.0000	0.6002	-0.0049	0.0014	-0.3173	0.0201	0.7334	-0.0026	0.0159	-0.0005	-0.0146	-0.0002	0.0008	-0.0132
	(50.84%)	0.7130* C 18	s(33.75%)p 1.96(66.20%)d 0.00(0.05%)	0.0000	0.5810	0.0027	-0.0002	0.4257	0.0128	-0.6931	0.0117	-0.0028	-0.0003	-0.0139	-0.0002	0.0002	-0.0115	-0.0121
40. (1.98259)	BD (1) C 11- N 30	(39.55%)	0.6288* C 11	s(27.20%)p 2.67(72.70%)d 0.00(0.10%)	0.0000	0.5214	0.0091	-0.0019	0.8500	0.0193	-0.0595	0.0203	0.0132	-0.0001	-0.0038	0.0013	0.0001	0.0261
	(60.45%)	0.7775* N 30	s(30.27%)p 2.30(69.65%)d 0.00(0.08%)	0.0000	0.5502	0.0034	-0.0007	-0.8299	-0.0078	0.0833	0.0113	-0.0260	-0.0015	0.0054	0.0007	0.0004	0.0261	-0.0083
41. (1.97485)	BD (1) C 12- C 13	(50.61%)	0.7114* C 12	s(33.38%)p 1.99(66.57%)d 0.00(0.05%)	0.0000	0.5774	0.0198	-0.0003	-0.5357	-0.0105	0.6146	0.0275	-0.0116	-0.0012	-0.0169	0.0006	-0.0006	0.0007
	(49.39%)	0.7028* C 13	s(35.52%)p 1.81(64.42%)d 0.00(0.05%)	0.0000	0.5960	-0.0007	0.0028	0.4928	0.0146	-0.6327	0.0100	0.0279	-0.0009	-0.0178	0.0006	-0.0011	-0.0052	-0.0143
42. (1.70923)	BD (2) C 12- C 13	(52.78%)	0.7265* C 12	s(0.00%)p 1.00(99.96%)d 0.00(0.03%)	0.0000	0.0034	0.0004	-0.0001	-0.0018	0.0003	-0.0236	-0.0010	-0.9995	-0.0121	0.0005	0.0145	-0.0114	0.0004
	(47.22%)	0.6872* C 13	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000	0.0024	0.0005	0.0000	0.0008	-0.0001	-0.0412	0.0001	-0.9988	0.0172	-0.0002	-0.0080	0.0163	-0.0005	-0.0010
43. (1.97356)	BD (1) C 12- C 18	(48.52%)	0.6966* C 12	s(33.32%)p 2.00(66.62%)d 0.00(0.06%)	0.0000	0.5771	0.0112	0.0008	-0.2643	0.0115	-0.7718	-0.0107	0.0207	0.0005	0.0141	-0.0001	-0.0009	-0.0124
	(51.48%)	0.7175* C 18	s(34.80%)p 1.87(65.16%)d 0.00(0.04%)	0.0000	0.5899	0.0013	-0.0001	0.3659	0.0080	0.7195	-0.0058	-0.0029	-0.0003	0.0106	-0.0002	-0.0003	-0.0115	-0.0114
44. (1.96877)	BD (1) C 12- B 29	(69.49%)	0.8336* C 12	s(33.31%)p 2.00(66.67%)d 0.00(0.02%)	0.0000	0.5768	-0.0202	-0.0002	0.8005	-0.0344	0.1566	-0.0147	-0.0032	0.0002	0.0069	0.0001	-0.0002	0.0098
	(30.51%)	0.5523* B 29	s(39.90%)p 1.50(60.01%)d 0.00(0.09%)	0.0000	0.6311	-0.0256	0.0070	-0.7255	-0.0260	-0.2702	0.0049	-0.0121	0.0004	0.0178	0.0004	-0.0006	0.0224	-0.0078
45. (1.98006)	BD (1) C 13- H 14	(61.07%)	0.7815* C 13	s(31.01%)p 2.22(68.92%)d 0.00(0.07%)	0.0000	0.5569	0.0000	-0.0036	0.3138	0.0009	0.7679	0.0105	-0.0301	-0.0006	0.0151	-0.0008	-0.0018	-0.0156
	(38.93%)	0.6239* H 14	s(99.91%)p 0.00(0.09%)	0.9996	-0.0025	-0.0126	-0.0268	0.0010										
46. (1.97524)	BD (1) C 13- C 15	(49.58%)	0.7041* C 13	s(33.31%)p 2.00(66.64%)d 0.00(0.05%)	0.0000	0.5771	0.0013	0.0021	-0.8110	-0.0079	-0.0874	0.0319	0.0043	-0.0008	0.0027	-0.0003	-0.0002	0.0176
	(50.42%)	0.7101* C 15	s(33.19%)p 2.01(66.76%)d 0.00(0.04%)	0.0000	0.5761	0.0004	0.0006	0.8124	-0.0003	0.0804	0.0303	-0.0161	-0.0008					

				0.0005	-0.0004	-0.0003	0.0165	-0.0132
47.	(1.98233)	BD (1) C 15- H 16						
	(60.61%)	0.7786* C 15	s(31.88%)p 2.13(68.06%)d 0.00(0.07%)					
			0.0000 0.5646 -0.0019 -0.0034 -0.4686					
			-0.0031 0.6784 0.0142 -0.0223 -0.0010					
			-0.0204 0.0008 -0.0011 -0.0059 -0.0141					
	(39.39%)	0.6276* H 16	s(99.93%)p 0.00(0.07%)					
			0.9997 -0.0012 0.0151 -0.0211 0.0008					
48.	(1.97837)	BD (1) C 15- C 19						
	(49.02%)	0.7001* C 15	s(34.75%)p 1.88(65.19%)d 0.00(0.06%)					
			0.0000 0.5895 0.0033 0.0036 -0.3454					
			-0.0262 -0.7281 0.0070 0.0413 -0.0002					
			0.0147 -0.0008 -0.0020 -0.0127 -0.0149					
	(50.98%)	0.7140* C 19	s(37.61%)p 1.66(62.34%)d 0.00(0.05%)					
			0.0000 0.6132 0.0096 0.0013 0.2529					
			-0.0220 0.7469 0.0202 -0.0270 -0.0006					
			0.0134 -0.0007 -0.0014 -0.0115 -0.0117					
49.	(1.71785)	BD (2) C 15- C 19						
	(52.32%)	0.7233* C 15	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
			0.0000 0.0024 0.0009 -0.0002 -0.0169					
			-0.0010 -0.0466 0.0000 -0.9984 0.0186					
			0.0004 0.0011 0.0190 -0.0008 -0.0015					
	(47.68%)	0.6905* C 19	s(0.00%)p 1.00(99.95%)d 0.00(0.04%)					
			0.0000 0.0035 -0.0007 0.0001 -0.0217					
			-0.0007 -0.0317 -0.0002 -0.9990 0.0077					
			-0.0006 -0.0157 -0.0141 0.0005 0.0018					
50.	(1.96937)	BD (1) C 17- C 20						
	(49.14%)	0.7010* C 17	s(31.83%)p 2.14(68.12%)d 0.00(0.05%)					
			0.0000 0.5641 -0.0056 0.0014 0.4517					
			0.0060 0.6903 -0.0049 0.0252 0.0003					
			0.0167 0.0002 0.0009 -0.0065 -0.0150					
	(50.86%)	0.7132* C 20	s(32.67%)p 2.06(67.28%)d 0.00(0.05%)					
			0.0000 0.5716 0.0010 -0.0002 -0.3765					
			0.0011 -0.7287 0.0052 0.0025 0.0004					
			0.0162 0.0003 0.0005 -0.0075 -0.0143					
51.	(1.96424)	BD (1) C 18- C 20						
	(49.43%)	0.7031* C 18	s(31.36%)p 2.19(68.59%)d 0.00(0.05%)					
			0.0000 0.5600 -0.0022 0.0008 -0.8272					
			0.0085 -0.0386 0.0023 0.0090 0.0010					
			0.0037 -0.0005 0.0000 0.0172 -0.0145					
	(50.57%)	0.7111* C 20	s(34.74%)p 1.88(65.21%)d 0.00(0.05%)					
			0.0000 0.5894 -0.0009 0.0011 0.8061					
			-0.0064 0.0459 0.0023 -0.0113 0.0009					
			0.0020 -0.0009 0.0000 0.0176 -0.0134					
52.	(1.96918)	BD (1) C 19- C 20						
	(49.00%)	0.7000* C 19	s(31.49%)p 2.17(68.45%)d 0.00(0.06%)					
			0.0000 0.5612 -0.0048 0.0013 0.5261					
			0.0059 -0.6384 0.0048 0.0108 0.0004					
			-0.0178 -0.0002 -0.0004 -0.0033 -0.0151					
	(51.00%)	0.7141* C 20	s(32.53%)p 2.07(67.42%)d 0.00(0.05%)					
			0.0000 0.5703 0.0012 -0.0004 -0.4558					
			0.0030 0.6828 -0.0046 0.0121 0.0005					
			-0.0174 0.0001 0.0000 -0.0037 -0.0142					
53.	(1.98998)	BD (1) C 21- H 22						
	(61.11%)	0.7817* C 21	s(26.00%)p 2.84(73.92%)d 0.00(0.08%)					
			0.0000 0.5099 0.0004 -0.0003 -0.3112					
			0.0117 0.4428 -0.0080 0.6679 0.0049					
			-0.0078 -0.0140 0.0203 -0.0023 0.0104					
	(38.89%)	0.6236* H 22	s(99.95%)p 0.00(0.05%)					
			0.9998 0.0003 0.0070 -0.0106 -0.0179					
54.	(1.98924)	BD (1) C 21- H 23						
	(60.75%)	0.7794* C 21	s(25.79%)p 2.87(74.13%)d 0.00(0.08%)					
			0.0000 0.5079 0.0013 -0.0003 0.8606					
			-0.0042 0.0200 -0.0013 0.0002 0.0144					
			0.0008 -0.0008 0.0020 0.0240 -0.0145					
	(39.25%)	0.6265* H 23	s(99.94%)p 0.00(0.06%)					
			0.9997 0.0008 -0.0235 -0.0005 -0.0021					
55.	(1.99513)	BD (1) C 21- H 24						
	(59.94%)	0.7742* C 21	s(25.76%)p 2.88(74.16%)d 0.00(0.08%)					
			0.0000 0.5075 -0.0059 -0.0010 -0.2806					
			0.0084 -0.8136 -0.0035 0.0212 0.0186					
			0.0143 -0.0021 -0.0009 -0.0195 -0.0150					
	(40.06%)	0.6329* H 24	s(99.95%)p 0.00(0.05%)					
			0.9997 0.0042 0.0069 0.0220 -0.0022					
56.	(1.98117)	BD (1) C 21- N 30						
	(38.90%)	0.6237* C 21	s(22.42%)p 3.46(77.48%)d 0.00(0.11%)					
			0.0000 0.4734 0.0092 0.0023 -0.2873					

			0.0079	0.3743	0.0176	-0.7428	-0.0060
			-0.0076	0.0159	-0.0197	-0.0015	0.0191
	(61.10%)	0.7816* N 30	s(27.13%)p 2.68(72.80%)d 0.00(0.06%)				
			0.0000	0.5209	0.0053	0.0010	0.2877
			0.0183	-0.3433	0.0051	0.7255	0.0263
			-0.0083	0.0027	-0.0214	-0.0042	0.0096
57.	(1.99514)	BD (1) C 25- H 26					
	(59.87%)	0.7738* C 25	s(25.68%)p 2.89(74.24%)d 0.00(0.08%)				
			0.0000	0.5067	-0.0061	-0.0010	-0.2233
			0.0098	-0.8310	-0.0047	0.0389	-0.0179
			0.0117	0.0012	-0.0023	-0.0214	-0.0146
	(40.13%)	0.6335* H 26	s(99.95%)p 0.00(0.05%)				
			0.9997	0.0040	0.0052	0.0227	0.0007
58.	(1.98930)	BD (1) C 25- H 27					
	(60.82%)	0.7799* C 25	s(25.87%)p 2.86(74.05%)d 0.00(0.08%)				
			0.0000	0.5086	0.0014	-0.0003	0.8564
			-0.0040	0.0809	-0.0021	0.0204	-0.0143
			0.0041	0.0020	-0.0020	0.0238	-0.0142
	(39.18%)	0.6259* H 27	s(99.94%)p 0.00(0.06%)				
			0.9997	0.0009	-0.0234	-0.0021	0.0015
59.	(1.98999)	BD (1) C 25- H 28					
	(61.14%)	0.7819* C 25	s(25.99%)p 2.84(73.93%)d 0.00(0.08%)				
			0.0000	0.5098	0.0002	-0.0003	-0.3201
			0.0128	0.3636	-0.0074	-0.7102	-0.0039
			-0.0062	0.0154	-0.0176	-0.0001	0.0137
	(38.86%)	0.6234* H 28	s(99.95%)p 0.00(0.05%)				
			0.9998	0.0003	0.0072	-0.0086	0.0191
60.	(1.98252)	BD (1) C 25- N 30					
	(38.89%)	0.6236* C 25	s(22.44%)p 3.45(77.45%)d 0.00(0.11%)				
			0.0000	0.4736	0.0098	0.0023	-0.3362
			0.0071	0.4112	0.0188	0.7014	0.0053
			-0.0099	-0.0177	0.0204	-0.0014	0.0154
	(61.11%)	0.7817* N 30	s(27.50%)p 2.63(72.43%)d 0.00(0.06%)				
			0.0000	0.5244	0.0059	0.0009	0.3308
			0.0201	-0.3784	0.0057	-0.6861	-0.0249
			-0.0099	-0.0035	0.0214	-0.0051	0.0071
61.	(1.99502)	BD (1) B 29- O 31					
	(20.26%)	0.4501* B 29	s(31.71%)p 2.14(67.99%)d 0.01(0.30%)				
			0.0000	0.5628	0.0174	-0.0049	0.6668
			0.0418	-0.4829	-0.0197	-0.0004	-0.0013
			-0.0477	-0.0001	-0.0004	0.0176	-0.0205
	(79.74%)	0.8930* O 31	s(41.96%)p 1.38(57.84%)d 0.00(0.20%)				
			0.0000	0.6478	-0.0037	-0.0005	-0.4978
			0.0004	0.5749	-0.0090	-0.0029	0.0003
			-0.0337	-0.0007	0.0002	0.0179	-0.0237
62.	(1.99348)	BD (1) B 29- O 32					
	(19.74%)	0.4443* B 29	s(28.44%)p 2.50(71.24%)d 0.01(0.32%)				
			0.0000	0.5327	0.0251	-0.0062	0.1521
			0.0168	0.8294	0.0303	0.0112	0.0018
			0.0177	0.0006	0.0020	-0.0491	-0.0211
	(80.26%)	0.8959* O 32	s(47.44%)p 1.10(52.39%)d 0.00(0.17%)				
			0.0000	0.6887	-0.0056	-0.0008	-0.2078
			-0.0023	-0.6925	0.0021	-0.0347	0.0002
			0.0024	0.0010	0.0007	-0.0343	-0.0231
63.	(1.98702)	BD (1) O 31- H 34					
	(77.06%)	0.8778* O 31	s(32.80%)p 2.04(67.02%)d 0.01(0.18%)				
			0.0000	0.5726	0.0091	0.0003	-0.1780
			-0.0072	-0.7971	0.0328	0.0445	-0.0009
			0.0329	-0.0025	-0.0030	-0.0140	-0.0228
	(22.94%)	0.4790* H 34	s(99.85%)p 0.00(0.15%)				
			0.9992	0.0128	0.0167	0.0350	-0.0010
64.	(1.98931)	BD (1) O 32- H 33					
	(74.02%)	0.8604* O 32	s(26.04%)p 2.83(73.77%)d 0.01(0.19%)				
			0.0000	0.5099	0.0205	0.0008	0.8115
			-0.0292	0.2569	-0.0281	0.1068	-0.0047
			-0.0028	0.0092	-0.0007	0.0375	-0.0204
	(25.98%)	0.5097* H 33	s(99.85%)p 0.00(0.15%)				
			0.9993	-0.0022	-0.0373	-0.0064	-0.0043
----- non-Lewis -----							
65.	(0.98248)	LV (1) C 18	s(0.00%)p 1.00(100.00%)d 0.00(0.00%)				
			0.0000	0.0017	0.0006	0.0000	-0.0097
			-0.0003	-0.0005	-0.0004	-0.9999	-0.0076
			-0.0001	0.0041	0.0030	0.0004	0.0000
66.	(0.40746)	LV (1) B 29	s(0.00%)p 1.00(99.95%)d 0.00(0.05%)				
			0.0000	-0.0019	0.0019	-0.0012	0.0103
			-0.0016	0.0126	-0.0005	-0.9981	0.0559
			0.0020	-0.0213	-0.0042	-0.0007	-0.0010

[illegible]

				0.0000	-0.6107	-0.0105	-0.0012	-0.3339
				0.0190	0.7163	0.0219	0.0319	0.0008
				0.0158	0.0010	-0.0015	0.0086	0.0120
77.	(0.27211)	BD*(2) C 7- C 17						
	(47.83%)	0.6916* C 7	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	0.0006	0.0010	-0.0004	-0.0055
				-0.0009	0.0519	-0.0001	-0.9983	0.0195
				-0.0004	0.0034	-0.0188	-0.0009	-0.0018
	(52.17%)	-0.7223* C 17	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	0.0001	-0.0001	0.0001	-0.0072
				-0.0008	0.0411	0.0005	-0.9989	0.0066
				0.0008	-0.0169	0.0125	0.0007	0.0016
78.	(0.01154)	BD*(1) C 9- H 10						
	(39.62%)	0.6295* C 9	s(30.92%)p 2.23(69.01%)d 0.00(0.07%)					
				0.0000	-0.5560	-0.0015	0.0040	-0.4086
				0.0031	0.7228	0.0186	0.0210	0.0009
				0.0189	0.0006	-0.0012	0.0104	0.0154
	(60.38%)	-0.7770* H 10	s(99.93%)p 0.00(0.07%)					
				-0.9996	0.0013	0.0125	-0.0239	-0.0008
79.	(0.02649)	BD*(1) C 9- C 11						
	(50.02%)	0.7073* C 9	s(35.11%)p 1.85(64.83%)d 0.00(0.06%)					
				0.0000	-0.5925	0.0035	-0.0026	-0.4144
				-0.0171	-0.6893	0.0099	-0.0330	0.0010
				-0.0173	-0.0007	-0.0014	0.0087	0.0152
	(49.98%)	-0.7069* C 11	s(36.68%)p 1.73(63.27%)d 0.00(0.05%)					
				0.0000	-0.6056	-0.0017	-0.0003	0.4182
				-0.0023	0.6763	0.0163	0.0160	0.0013
				-0.0171	-0.0004	-0.0007	0.0078	0.0114
80.	(0.29375)	BD*(2) C 9- C 11						
	(50.90%)	0.7134* C 9	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	-0.0033	-0.0009	0.0000	-0.0115
				-0.0004	-0.0381	0.0001	0.9988	-0.0193
				-0.0004	0.0076	0.0176	0.0003	0.0012
	(49.10%)	-0.7007* C 11	s(0.00%)p 1.00(99.96%)d 0.00(0.04%)					
				0.0000	-0.0067	-0.0008	0.0000	-0.0129
				-0.0005	-0.0217	-0.0003	0.9993	-0.0184
				0.0006	-0.0146	-0.0136	-0.0004	-0.0009
81.	(0.03380)	BD*(1) C 11- C 18						
	(50.84%)	0.7130* C 11	s(36.02%)p 1.77(63.92%)d 0.00(0.05%)					
				0.0000	0.6002	-0.0049	0.0014	-0.3173
				0.0201	0.7334	-0.0026	0.0159	-0.0005
				-0.0146	-0.0002	0.0008	-0.0132	-0.0116
	(49.16%)	-0.7011* C 18	s(33.75%)p 1.96(66.20%)d 0.00(0.05%)					
				0.0000	0.5810	0.0027	-0.0002	0.4257
				0.0128	-0.6931	0.0117	-0.0028	-0.0003
				-0.0139	-0.0002	0.0002	-0.0115	-0.0121
82.	(0.03188)	BD*(1) C 11- N 30						
	(60.45%)	0.7775* C 11	s(27.20%)p 2.67(72.70%)d 0.00(0.10%)					
				0.0000	0.5214	0.0091	-0.0019	0.8500
				0.0193	-0.0595	0.0203	0.0132	-0.0001
				-0.0038	0.0013	0.0001	0.0261	-0.0174
	(39.55%)	-0.6288* N 30	s(30.27%)p 2.30(69.65%)d 0.00(0.08%)					
				0.0000	0.5502	0.0034	-0.0007	-0.8299
				-0.0078	0.0833	0.0113	-0.0260	-0.0015
				0.0054	0.0007	0.0004	0.0261	-0.0083
83.	(0.01756)	BD*(1) C 12- C 13						
	(49.39%)	0.7028* C 12	s(33.38%)p 1.99(66.57%)d 0.00(0.05%)					
				0.0000	-0.5774	-0.0198	0.0003	0.5357
				0.0105	-0.6146	-0.0275	0.0116	0.0012
				0.0169	-0.0006	0.0006	-0.0007	0.0153
	(50.61%)	-0.7114* C 13	s(35.52%)p 1.81(64.42%)d 0.00(0.05%)					
				0.0000	-0.5960	0.0007	-0.0028	-0.4928
				-0.0146	0.6327	-0.0100	-0.0279	0.0009
				0.0178	-0.0006	0.0011	0.0052	0.0143
84.	(0.25800)	BD*(2) C 12- C 13						
	(47.22%)	0.6872* C 12	s(0.00%)p 1.00(99.96%)d 0.00(0.03%)					
				0.0000	0.0034	0.0004	-0.0001	-0.0018
				0.0003	-0.0236	-0.0010	-0.9995	-0.0121
				0.0005	0.0145	-0.0114	0.0004	0.0006
	(52.78%)	-0.7265* C 13	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)					
				0.0000	0.0024	0.0005	0.0000	0.0008
				-0.0001	-0.0412	0.0001	-0.9988	0.0172
				-0.0002	-0.0080	0.0163	-0.0005	-0.0010
85.	(0.02785)	BD*(1) C 12- C 18						
	(51.48%)	0.7175* C 12	s(33.32%)p 2.00(66.62%)d 0.00(0.06%)					
				0.0000	0.5771	0.0112	0.0008	-0.2643
				0.0115	-0.7718	-0.0107	0.0207	0.0005

				0.0141	-0.0001	-0.0009	-0.0124	-0.0148
	(48.52%)	-0.6966*	C 18	s(34.80%)	p 1.87(65.16%)	d 0.00(0.04%)		
				0.0000	0.5899	0.0013	-0.0001	0.3659
				0.0080	0.7195	-0.0058	-0.0029	-0.0003
				0.0106	-0.0002	-0.0003	-0.0115	-0.0114
86.	(0.03642)	BD*(1)	C 12- B 29					
	(30.51%)	0.5523*	C 12	s(33.31%)	p 2.00(66.67%)	d 0.00(0.02%)		
				0.0000	-0.5768	0.0202	0.0002	-0.8005
				0.0344	-0.1566	0.0147	0.0032	-0.0002
				-0.0069	-0.0001	0.0002	-0.0098	0.0079
	(69.49%)	-0.8336*	B 29	s(39.90%)	p 1.50(60.01%)	d 0.00(0.09%)		
				0.0000	-0.6311	0.0256	-0.0070	0.7255
				0.0260	0.2702	-0.0049	0.0121	-0.0004
				-0.0178	-0.0004	0.0006	-0.0224	0.0078
87.	(0.01259)	BD*(1)	C 13- H 14					
	(38.93%)	0.6239*	C 13	s(31.01%)	p 2.22(68.92%)	d 0.00(0.07%)		
				0.0000	-0.5569	0.0000	0.0036	-0.3138
				-0.0009	-0.7679	-0.0105	0.0301	0.0006
				-0.0151	0.0008	0.0018	0.0156	0.0149
	(61.07%)	-0.7815*	H 14	s(99.91%)	p 0.00(0.09%)			
				-0.9996	0.0025	0.0126	0.0268	-0.0010
88.	(0.02072)	BD*(1)	C 13- C 15					
	(50.42%)	0.7101*	C 13	s(33.31%)	p 2.00(66.64%)	d 0.00(0.05%)		
				0.0000	0.5771	0.0013	0.0021	-0.8110
				-0.0079	-0.0874	0.0319	0.0043	-0.0008
				0.0027	-0.0003	-0.0002	0.0176	-0.0136
	(49.58%)	-0.7041*	C 15	s(33.19%)	p 2.01(66.76%)	d 0.00(0.04%)		
				0.0000	0.5761	0.0004	0.0006	0.8124
				-0.0003	0.0804	0.0303	-0.0161	-0.0008
				0.0005	-0.0004	-0.0003	0.0165	-0.0132
89.	(0.01292)	BD*(1)	C 15- H 16					
	(39.39%)	0.6276*	C 15	s(31.88%)	p 2.13(68.06%)	d 0.00(0.07%)		
				0.0000	-0.5646	0.0019	0.0034	0.4686
				0.0031	-0.6784	-0.0142	0.0223	0.0010
				0.0204	-0.0008	0.0011	0.0059	0.0141
	(60.61%)	-0.7786*	H 16	s(99.93%)	p 0.00(0.07%)			
				-0.9997	0.0012	-0.0151	0.0211	-0.0008
90.	(0.02234)	BD*(1)	C 15- C 19					
	(50.98%)	0.7140*	C 15	s(34.75%)	p 1.88(65.19%)	d 0.00(0.06%)		
				0.0000	-0.5895	-0.0033	-0.0036	0.3454
				0.0262	0.7281	-0.0070	-0.0413	0.0002
				-0.0147	0.0008	0.0020	0.0127	0.0149
	(49.02%)	-0.7001*	C 19	s(37.61%)	p 1.66(62.34%)	d 0.00(0.05%)		
				0.0000	-0.6132	-0.0096	-0.0013	-0.2529
				0.0220	-0.7469	-0.0202	0.0270	0.0006
				-0.0134	0.0007	0.0014	0.0115	0.0117
91.	(0.26041)	BD*(2)	C 15- C 19					
	(47.68%)	0.6905*	C 15	s(0.00%)	p 1.00(99.96%)	d 0.00(0.04%)		
				0.0000	-0.0024	-0.0009	0.0002	0.0169
				0.0010	0.0466	0.0000	0.9984	-0.0186
				-0.0004	-0.0011	-0.0190	0.0008	0.0015
	(52.32%)	-0.7233*	C 19	s(0.00%)	p 1.00(99.95%)	d 0.00(0.04%)		
				0.0000	-0.0035	0.0007	-0.0001	0.0217
				0.0007	0.0317	0.0002	0.9990	-0.0077
				0.0006	0.0157	0.0141	-0.0005	-0.0018
92.	(0.02836)	BD*(1)	C 17- C 20					
	(50.86%)	0.7132*	C 17	s(31.83%)	p 2.14(68.12%)	d 0.00(0.05%)		
				0.0000	0.5641	-0.0056	0.0014	0.4517
				0.0060	0.6903	-0.0049	0.0252	0.0003
				0.0167	0.0002	0.0009	-0.0065	-0.0150
	(49.14%)	-0.7010*	C 20	s(32.67%)	p 2.06(67.28%)	d 0.00(0.05%)		
				0.0000	0.5716	0.0010	-0.0002	-0.3765
				0.0011	-0.7287	0.0052	0.0025	0.0004
				0.0162	0.0003	0.0005	-0.0075	-0.0143
93.	(0.03129)	BD*(1)	C 18- C 20					
	(50.57%)	0.7111*	C 18	s(31.36%)	p 2.19(68.59%)	d 0.00(0.05%)		
				0.0000	-0.5600	0.0022	-0.0008	0.8272
				-0.0085	0.0386	-0.0023	-0.0090	-0.0010
				-0.0037	0.0005	0.0000	-0.0172	0.0145
	(49.43%)	-0.7031*	C 20	s(34.74%)	p 1.88(65.21%)	d 0.00(0.05%)		
				0.0000	-0.5894	0.0009	-0.0011	-0.8061
				0.0064	-0.0459	-0.0023	0.0113	-0.0009
				-0.0020	0.0009	0.0000	-0.0176	0.0134
94.	(0.02860)	BD*(1)	C 19- C 20					
	(51.00%)	0.7141*	C 19	s(31.49%)	p 2.17(68.45%)	d 0.00(0.06%)		
				0.0000	0.5612	-0.0048	0.0013	0.5261
				0.0059	-0.6384	0.0048	0.0108	0.0004

					-0.0178	-0.0002	-0.0004	-0.0033	-0.0151
(49.00%)	-0.7000*	C 20	s(32.53%)p 2.07(67.42%)d 0.00(0.05%)		0.0000	0.5703	0.0012	-0.0004	-0.4558
					0.0030	0.6828	-0.0046	0.0121	0.0005
					-0.0174	0.0001	0.0000	-0.0037	-0.0142
95. (0.00683)	BD*(1) C 21-	H 22	s(26.00%)p 2.84(73.92%)d 0.00(0.08%)		0.0000	-0.5099	-0.0004	0.0003	0.3112
(38.89%)	0.6236*	C 21	-0.0117 -0.4428 0.0080 -0.6679 -0.0049		0.0078	0.0140	-0.0203	0.0023	-0.0104
(61.11%)	-0.7817*	H 22	s(99.95%)p 0.00(0.05%)		-0.9998	-0.0003	-0.0070	0.0106	0.0179
96. (0.00843)	BD*(1) C 21-	H 23	s(25.79%)p 2.87(74.13%)d 0.00(0.08%)		0.0000	-0.5079	-0.0013	0.0003	-0.8606
(39.25%)	0.6265*	C 21	0.0042 -0.0200 0.0013 -0.0002 -0.0144		-0.0008	0.0008	-0.0020	-0.0240	0.0145
(60.75%)	-0.7794*	H 23	s(99.94%)p 0.00(0.06%)		-0.9997	-0.0008	0.0235	0.0005	0.0021
97. (0.01676)	BD*(1) C 21-	H 24	s(25.76%)p 2.88(74.16%)d 0.00(0.08%)		0.0000	-0.5075	0.0059	0.0010	0.2806
(40.06%)	0.6329*	C 21	-0.0084 0.8136 0.0035 -0.0212 -0.0186		-0.0143	0.0021	0.0009	0.0195	0.0150
(59.94%)	-0.7742*	H 24	s(99.95%)p 0.00(0.05%)		-0.9997	-0.0042	-0.0069	-0.0220	0.0022
98. (0.01369)	BD*(1) C 21-	N 30	s(22.42%)p 3.46(77.48%)d 0.00(0.11%)		0.0000	0.4734	0.0092	0.0023	-0.2873
(61.10%)	0.7816*	C 21	0.0079 0.3743 0.0176 -0.7428 -0.0060		-0.0076	0.0159	-0.0197	-0.0015	0.0191
(38.90%)	-0.6237*	N 30	s(27.13%)p 2.68(72.80%)d 0.00(0.06%)		0.0000	0.5209	0.0053	0.0010	0.2877
			0.0183 -0.3433 0.0051 0.7255 0.0263		-0.0083	0.0027	-0.0214	-0.0042	0.0096
99. (0.01677)	BD*(1) C 25-	H 26	s(25.68%)p 2.89(74.24%)d 0.00(0.08%)		0.0000	-0.5067	0.0061	0.0010	0.2233
(40.13%)	0.6335*	C 25	-0.0098 0.8310 0.0047 -0.0389 0.0179		-0.0117	-0.0012	0.0023	0.0214	0.0146
(59.87%)	-0.7738*	H 26	s(99.95%)p 0.00(0.05%)		-0.9997	-0.0040	-0.0052	-0.0227	-0.0007
100. (0.00868)	BD*(1) C 25-	H 27	s(25.87%)p 2.86(74.05%)d 0.00(0.08%)		0.0000	-0.5086	-0.0014	0.0003	-0.8564
(39.18%)	0.6259*	C 25	0.0040 -0.0809 0.0021 -0.0204 0.0143		-0.0041	-0.0020	0.0020	-0.0238	0.0142
(60.82%)	-0.7799*	H 27	s(99.94%)p 0.00(0.06%)		-0.9997	-0.0009	0.0234	0.0021	-0.0015
101. (0.00648)	BD*(1) C 25-	H 28	s(25.99%)p 2.84(73.93%)d 0.00(0.08%)		0.0000	-0.5098	-0.0002	0.0003	0.3201
(38.86%)	0.6234*	C 25	-0.0128 -0.3636 0.0074 0.7102 0.0039		0.0062	-0.0154	0.0176	0.0001	-0.0137
(61.14%)	-0.7819*	H 28	s(99.95%)p 0.00(0.05%)		-0.9998	-0.0003	-0.0072	0.0086	-0.0191
102. (0.01384)	BD*(1) C 25-	N 30	s(22.44%)p 3.45(77.45%)d 0.00(0.11%)		0.0000	0.4736	0.0098	0.0023	-0.3362
(61.11%)	0.7817*	C 25	0.0071 0.4112 0.0188 0.7014 0.0053		-0.0099	-0.0177	0.0204	-0.0014	0.0154
(38.89%)	-0.6236*	N 30	s(27.50%)p 2.63(72.43%)d 0.00(0.06%)		0.0000	0.5244	0.0059	0.0009	0.3308
			0.0201 -0.3784 0.0057 -0.6861 -0.0249		-0.0099	-0.0035	0.0214	-0.0051	0.0071
103. (0.02598)	BD*(1) B 29-	O 31	s(31.71%)p 2.14(67.99%)d 0.01(0.30%)		0.0000	0.5628	0.0174	-0.0049	0.6668
(79.74%)	0.8930*	B 29	0.0418 -0.4829 -0.0197 -0.0004 -0.0013		-0.0477	-0.0001	-0.0004	0.0176	-0.0205
(20.26%)	-0.4501*	O 31	s(						

			0.0168	0.8294	0.0303	0.0112	0.0018
			0.0177	0.0006	0.0020	-0.0491	-0.0211
	(19.74%)	-0.4443* O 32	s(47.44%)p 1.10(52.39%)d 0.00(0.17%)				
			0.0000	0.6887	-0.0056	-0.0008	-0.2078
			-0.0023	-0.6925	0.0021	-0.0347	0.0002
			0.0024	0.0010	0.0007	-0.0343	-0.0231
105.	(0.05258)	BD*(1) O 31- H 34					
	(22.94%)	0.4790* O 31	s(32.80%)p 2.04(67.02%)d 0.01(0.18%)				
			0.0000	-0.5726	-0.0091	-0.0003	0.1780
			0.0072	0.7971	-0.0328	-0.0445	0.0009
			-0.0329	0.0025	0.0030	0.0140	0.0228
	(77.06%)	-0.8778* H 34	s(99.85%)p 0.00(0.15%)				
			-0.9992	-0.0128	-0.0167	-0.0350	0.0010
106.	(0.00696)	BD*(1) O 32- H 33					
	(25.98%)	0.5097* O 32	s(26.04%)p 2.83(73.77%)d 0.01(0.19%)				
			0.0000	-0.5099	-0.0205	-0.0008	-0.8115
			0.0292	-0.2569	0.0281	-0.1068	0.0047
			0.0028	-0.0092	0.0007	-0.0375	0.0204
	(74.02%)	-0.8604* H 33	s(99.85%)p 0.00(0.15%)				
			-0.9993	0.0022	0.0373	0.0064	0.0043
107.	(0.00209)	RY (1) C 1	s(0.47%)p99.99(88.49%)d23.57(11.04%)				
			0.0000	0.0169	0.0642	0.0164	0.0058
			0.3930	-0.0031	-0.3769	0.0099	0.7670
			-0.2066	0.1440	-0.1992	0.0777	-0.0355
108.	(0.00181)	RY (2) C 1	s(0.68%)p99.99(84.02%)d22.45(15.30%)				
			0.0000	0.0260	0.0755	0.0207	0.0080
			0.5738	-0.0029	-0.4499	-0.0064	-0.5554
			-0.3168	-0.1163	0.1602	0.1149	0.0139
109.	(0.00088)	RY (3) C 1	s(2.03%)p47.05(95.46%)d 1.24(2.51%)				
			0.0000	0.0088	0.1421	-0.0021	0.0033
			0.6075	-0.0001	0.7643	0.0002	0.0363
			-0.0785	0.0083	-0.0229	-0.1343	-0.0184
110.	(0.00036)	RY (4) C 1	s(0.16%)p 1.38(0.22%)d99.99(99.62%)				
			0.0000	0.0005	0.0399	0.0031	0.0008
			0.0047	0.0003	0.0016	0.0120	-0.0452
			0.0218	0.8752	0.4756	0.0273	-0.0533
111.	(0.00018)	RY (5) C 1	s(86.76%)p 0.01(1.25%)d 0.14(11.98%)				
			0.0000	0.0017	0.9314	0.0138	-0.0027
			-0.0536	0.0014	-0.0972	-0.0011	-0.0139
			0.3098	-0.0580	-0.0033	0.0215	-0.1416
112.	(0.00004)	RY (6) C 1	s(4.64%)p 0.83(3.85%)d19.73(91.51%)				
113.	(0.00003)	RY (7) C 1	s(47.82%)p 0.18(8.59%)d 0.91(43.59%)				
114.	(0.00002)	RY (8) C 1	s(13.19%)p 0.63(8.37%)d 5.95(78.44%)				
115.	(0.00002)	RY (9) C 1	s(41.41%)p 0.21(8.89%)d 1.20(49.70%)				
116.	(0.00000)	RY (10) C 1	s(2.97%)p 0.32(0.94%)d32.31(96.08%)				
117.	(0.00115)	RY (1) H 2	s(99.25%)p 0.01(0.75%)				
			-0.0003	0.9963	0.0553	-0.0083	-0.0658
118.	(0.00009)	RY (2) H 2	s(0.08%)p99.99(99.92%)				
119.	(0.00005)	RY (3) H 2	s(0.62%)p99.99(99.38%)				
120.	(0.00000)	RY (4) H 2	s(0.10%)p99.99(99.90%)				
121.	(0.00116)	RY (1) H 3	s(99.25%)p 0.01(0.75%)				
			-0.0003	0.9962	0.0596	-0.0102	0.0620
122.	(0.00009)	RY (2) H 3	s(0.09%)p99.99(99.91%)				
123.	(0.00005)	RY (3) H 3	s(0.60%)p99.99(99.40%)				
124.	(0.00000)	RY (4) H 3	s(0.12%)p99.99(99.88%)				
125.	(0.00200)	RY (1) C 4	s(0.05%)p99.99(89.42%)d99.99(10.53%)				
			0.0000	0.0048	0.0217	0.0039	0.0015
			0.0908	0.0014	0.1099	-0.0120	-0.9347
			0.0547	-0.1663	-0.2724	-0.0051	-0.0199
126.	(0.00185)	RY (2) C 4	s(0.62%)p99.99(83.76%)d25.29(15.62%)				
			0.0000	0.0296	0.0682	0.0256	0.0083
			0.5697	0.0048	0.7010	0.0016	0.1466
			0.3883	0.0396	0.0291	0.0552	-0.0034
127.	(0.00094)	RY (3) C 4	s(1.94%)p49.23(95.55%)d 1.29(2.50%)				
			0.0000	0.0111	0.1388	0.0025	0.0038
			0.7342	0.0002	-0.6454	0.0002	-0.0012
			0.0806	-0.0040	0.0219	-0.1337	-0.0138
128.	(0.00036)	RY (4) C 4	s(0.15%)p 1.90(0.29%)d99.99(99.56%)				
			0.0000	0.0005	0.0389	-0.0008	-0.0003
			0.0122	-0.0005	-0.0025	0.0113	-0.0508
			-0.0650	0.9157	-0.3887	-0.0056	-0.0435
129.	(0.00018)	RY (5) C 4	s(88.01%)p 0.01(1.19%)d 0.12(10.80%)				
			0.0000	0.0023	0.9379	0.0203	-0.0017
			-0.0510	-0.0013	0.0953	-0.0003	0.0131
			-0.2795	-0.0496	0.0338	0.0871	-0.1367
130.	(0.00004)	RY (6) C 4	s(4.16%)p 1.12(4.68%)d21.91(91.16%)				
131.	(0.00003)	RY (7) C 4	s(58.15%)p 0.11(6.14%)d 0.61(35.71%)				

132.	(0.00002)	RY	(8)	C	4	s(9.22%)p 1.04(9.63%)d 8.80(81.15%)
133.	(0.00002)	RY	(9)	C	4	s(35.23%)p 0.24(8.53%)d 1.60(56.24%)
134.	(0.00000)	RY	(10)	C	4	s(2.60%)p 0.35(0.91%)d37.08(96.49%)
135.	(0.00114)	RY	(1)	H	5	s(99.25%)p 0.01(0.75%) -0.0003 0.9962 0.0570 0.0133 0.0638
136.	(0.00009)	RY	(2)	H	5	s(0.10%)p99.99(99.90%)
137.	(0.00005)	RY	(3)	H	5	s(0.60%)p99.99(99.40%)
138.	(0.00000)	RY	(4)	H	5	s(0.11%)p99.99(99.89%)
139.	(0.00117)	RY	(1)	H	6	s(99.28%)p 0.01(0.72%) -0.0004 0.9964 0.0556 0.0150 -0.0620
140.	(0.00009)	RY	(2)	H	6	s(0.10%)p99.99(99.90%)
141.	(0.00005)	RY	(3)	H	6	s(0.56%)p99.99(99.44%)
142.	(0.00000)	RY	(4)	H	6	s(0.11%)p99.99(99.89%)
143.	(0.00413)	RY	(1)	C	7	s(0.25%)p99.99(92.00%)d31.12(7.75%) 0.0000 -0.0324 0.0368 -0.0092 -0.0115 -0.3990 -0.0107 -0.8720 -0.0004 -0.0172 -0.2390 -0.0124 -0.0054 0.1416 0.0100
144.	(0.00230)	RY	(2)	C	7	s(0.01%)p99.99(97.96%)d99.99(2.03%) 0.0000 0.0013 0.0100 -0.0006 0.0180 -0.8918 -0.0158 0.4272 0.0006 0.0344 0.0125 0.0094 -0.0104 0.1410 0.0033
145.	(0.00092)	RY	(3)	C	7	s(0.00%)p 1.00(91.64%)d 0.09(8.35%) 0.0000 0.0007 -0.0025 0.0045 -0.0003 0.0224 -0.0007 -0.0336 0.0180 0.9563 -0.0014 0.2762 0.0851 -0.0019 0.0052
146.	(0.00052)	RY	(4)	C	7	s(0.37%)p10.03(3.68%)d99.99(95.96%) 0.0000 -0.0002 0.0582 -0.0166 0.0000 0.0034 -0.0004 0.0025 0.0091 -0.1915 -0.0438 0.8250 -0.5232 -0.0326 -0.0470
147.	(0.00029)	RY	(5)	C	7	s(96.77%)p 0.00(0.46%)d 0.03(2.77%) 0.0000 0.0003 0.9808 -0.0757 0.0005 0.0281 -0.0067 0.0582 0.0004 0.0188 -0.1380 -0.0597 0.0292 -0.0546 -0.0360
148.	(0.00007)	RY	(6)	C	7	s(16.10%)p 0.10(1.54%)d 5.12(82.36%)
149.	(0.00007)	RY	(7)	C	7	s(79.93%)p 0.00(0.35%)d 0.25(19.72%)
150.	(0.00002)	RY	(8)	C	7	s(3.53%)p 2.17(7.67%)d25.15(88.80%)
151.	(0.00001)	RY	(9)	C	7	s(3.21%)p 0.01(0.04%)d30.18(96.76%)
152.	(0.00000)	RY	(10)	C	7	s(0.01%)p99.99(4.68%)d99.99(95.31%)
153.	(0.00111)	RY	(1)	H	8	s(99.77%)p 0.00(0.23%) 0.0024 0.9989 -0.0158 -0.0438 0.0109
154.	(0.00017)	RY	(2)	H	8	s(0.02%)p99.99(99.98%) 0.0000 0.0132 -0.0037 0.0547 -0.9984
155.	(0.00005)	RY	(3)	H	8	s(0.01%)p 1.00(99.99%)
156.	(0.00001)	RY	(4)	H	8	s(0.27%)p99.99(99.73%)
157.	(0.00375)	RY	(1)	C	9	s(0.54%)p99.99(93.40%)d11.21(6.06%) 0.0000 -0.0305 0.0631 0.0220 0.0092 0.5176 -0.0072 -0.8158 -0.0003 -0.0214 0.2180 0.0080 -0.0039 0.1119 0.0208
158.	(0.00230)	RY	(2)	C	9	s(3.48%)p27.12(94.29%)d 0.64(2.23%) 0.0000 0.0130 0.1842 0.0256 -0.0113 0.8141 -0.0128 0.5262 0.0010 0.0540 -0.0766 -0.0146 -0.0054 0.1272 -0.0083
159.	(0.00082)	RY	(3)	C	9	s(0.25%)p99.99(44.82%)d99.99(54.93%) 0.0000 0.0000 0.0503 -0.0026 0.0014 -0.0449 0.0001 -0.0378 0.0220 0.6665 0.0319 -0.7113 -0.2044 0.0161 -0.0153
160.	(0.00061)	RY	(4)	C	9	s(0.10%)p99.99(50.05%)d99.99(49.85%) 0.0000 -0.0001 0.0311 -0.0004 0.0015 -0.0289 0.0010 -0.0341 0.0016 0.7060 -0.0350 0.5351 0.4565 0.0433 0.0257
161.	(0.00046)	RY	(5)	C	9	s(89.74%)p 0.06(5.35%)d 0.05(4.91%) 0.0000 -0.0029 0.9473 -0.0036 0.0105 -0.2138 0.0080 -0.0503 0.0000 -0.0711 -0.0593 0.0264 -0.0226 0.1993 -0.0683
162.	(0.00007)	RY	(6)	C	9	s(8.09%)p 0.21(1.70%)d11.15(90.21%)
163.	(0.00005)	RY	(7)	C	9	s(94.08%)p 0.00(0.31%)d 0.06(5.61%)
164.	(0.00003)	RY	(8)	C	9	s(1.84%)p 2.61(4.81%)d50.64(93.34%)
165.	(0.00002)	RY	(9)	C	9	s(0.33%)p13.26(4.33%)d99.99(95.34%)
166.	(0.00002)	RY	(10)	C	9	s(1.74%)p 0.56(0.97%)d55.89(97.29%)
167.	(0.00124)	RY	(1)	H	10	s(99.79%)p 0.00(0.21%) 0.0023 0.9989 0.0342 -0.0260 0.0158
168.	(0.00018)	RY	(2)	H	10	s(0.03%)p99.99(99.97%) 0.0002 0.0161 0.0217 0.0393 -0.9989
169.	(0.00005)	RY	(3)	H	10	s(0.04%)p99.99(99.96%)
170.	(0.00001)	RY	(4)	H	10	s(0.21%)p99.99(99.79%)
171.	(0.00490)	RY	(1)	C	11	s(3.54%)p24.97(88.39%)d 2.28(8.07%) 0.0000 -0.0099 0.1879 -0.0037 0.0199

				0.4176	-0.0032	-0.8411	-0.0006	-0.0407
				-0.2168	-0.0173	0.0052	-0.1764	0.0471
172.	(0.00451)	RY (2)	C 11	s(2.44%)	p37.66(91.92%)	d 2.31(5.64%)		
				0.0000	0.0181	0.1550	0.0077	0.0100
				-0.8490	0.0156	-0.4393	0.0019	0.0719
				-0.0102	0.0197	-0.0006	0.2333	-0.0386
173.	(0.00313)	RY (3)	C 11	s(0.11%)	p99.99(91.11%)	d82.24(8.79%)		
				0.0000	-0.0007	0.0325	0.0029	-0.0014
				0.0784	-0.0025	0.0095	0.0217	0.9510
				-0.0275	0.2919	-0.0117	-0.0332	0.0254
174.	(0.00096)	RY (4)	C 11	s(55.18%)	p 0.17(9.18%)	d 0.65(35.64%)		
				0.0000	-0.0024	0.7404	0.0597	-0.0209
				0.0178	-0.0107	0.2985	-0.0014	-0.0427
				-0.5780	-0.0029	-0.0833	0.1238	0.0057
175.	(0.00067)	RY (5)	C 11	s(0.06%)	p 3.37(0.20%)	d99.99(99.74%)		
				0.0000	0.0001	0.0230	0.0089	-0.0013
				-0.0076	-0.0025	0.0307	0.0131	0.0294
				-0.0947	-0.0693	0.9908	0.0165	0.0402
176.	(0.00062)	RY (6)	C 11	s(35.19%)	p 0.07(2.59%)	d 1.77(62.22%)		
				0.0000	-0.0053	0.5879	-0.0788	-0.0068
				0.1578	0.0194	-0.0238	0.0009	0.0037
				0.7665	-0.0240	0.0576	0.1753	0.0001
177.	(0.00016)	RY (7)	C 11	s(4.39%)	p 1.84(8.08%)	d19.92(87.53%)		
				0.0000	0.0099	0.2088	0.0158	0.0273
				-0.2679	0.0005	0.0872	0.0002	-0.0247
				0.1094	0.0205	0.0125	-0.9180	0.1413
178.	(0.00015)	RY (8)	C 11	s(0.00%)	p 1.00(8.54%)	d10.71(91.46%)		
				0.0000	0.0007	-0.0028	0.0053	0.0015
				-0.0096	-0.0009	0.0081	-0.0095	0.2917
				-0.0129	-0.9521	-0.0746	-0.0339	-0.0348
179.	(0.00009)	RY (9)	C 11	s(94.64%)	p 0.00(0.08%)	d 0.06(5.28%)		
180.	(0.00003)	RY (10)	C 11	s(4.54%)	p 0.01(0.06%)	d21.00(95.40%)		
181.	(0.00552)	RY (1)	C 12	s(0.50%)	p99.99(96.00%)	d 7.05(3.50%)		
				0.0000	0.0176	0.0677	-0.0088	0.0184
				0.9040	0.0276	-0.3759	0.0002	-0.0196
				-0.0809	0.0030	-0.0013	-0.1686	0.0046
182.	(0.00351)	RY (2)	C 12	s(0.41%)	p99.99(96.37%)	d 7.88(3.22%)		
				0.0000	-0.0057	0.0541	-0.0336	-0.0301
				-0.3581	0.0102	-0.9134	0.0005	0.0085
				-0.0637	0.0044	0.0121	0.1673	-0.0007
183.	(0.00060)	RY (3)	C 12	s(8.74%)	p 4.81(42.02%)	d 5.64(49.25%)		
				0.0000	-0.0024	0.2956	0.0018	0.0095
				-0.0250	-0.0025	0.0308	0.0007	-0.6469
				-0.0183	0.0526	0.6990	-0.0049	-0.0278
184.	(0.00050)	RY (4)	C 12	s(88.61%)	p 0.03(2.28%)	d 0.10(9.12%)		
				0.0000	-0.0066	0.9408	0.0306	0.0294
				-0.0417	-0.0042	0.0743	0.0022	0.1209
				-0.0720	0.0020	-0.2927	0.0114	0.0137
185.	(0.00036)	RY (5)	C 12	s(1.17%)	p43.07(50.26%)	d41.63(48.58%)		
				0.0000	-0.0002	0.1072	0.0132	0.0031
				0.0072	0.0010	0.0084	-0.0201	0.7086
				0.0160	-0.2912	0.6314	-0.0379	-0.0238
186.	(0.00015)	RY (6)	C 12	s(2.57%)	p 0.90(2.32%)	d37.07(95.12%)		
				0.0000	0.0071	-0.0689	0.1444	0.0044
				0.0968	-0.0229	0.1144	-0.0007	0.0135
				-0.7642	-0.0411	0.0312	0.5933	0.1116
187.	(0.00007)	RY (7)	C 12	s(5.43%)	p 0.96(5.23%)	d16.46(89.35%)		
188.	(0.00006)	RY (8)	C 12	s(6.37%)	p 0.67(4.27%)	d14.04(89.36%)		
189.	(0.00003)	RY (9)	C 12	s(70.48%)	p 0.02(1.40%)	d 0.40(28.12%)		
190.	(0.00002)	RY (10)	C 12	s(15.74%)	p 0.00(0.03%)	d 5.35(84.23%)		
191.	(0.00532)	RY (1)	C 13	s(0.08%)	p99.99(94.24%)	d74.20(5.68%)		
				0.0000	0.0272	-0.0029	0.0041	-0.0112
				-0.4966	-0.0099	-0.8338	0.0007	0.0170
				0.1367	-0.0040	-0.0067	-0.1950	-0.0049
192.	(0.00244)	RY (2)	C 13	s(0.10%)	p99.99(97.98%)	d18.55(1.92%)		
				0.0000	-0.0108	0.0265	-0.0146	0.0186
				-0.8527	-0.0041	0.5011	-0.0004	-0.0344
				-0.1207	0.0110	0.0019	-0.0626	0.0241
193.	(0.00073)	RY (3)	C 13	s(0.10%)	p99.99(23.74%)	d99.99(76.17%)		
				0.0000	0.0002	0.0311	-0.0014	0.0007
				-0.0146	0.0005	0.0171	0.0182	0.4863
				-0.0306	-0.8534	0.1799	-0.0036	-0.0011
194.	(0.00053)	RY (4)	C 13	s(0.12%)	p99.99(70.39%)	d99.99(29.49%)		
				0.0000	-0.0003	0.0348	0.0003	-0.0009
				0.0182	0.0004	-0.0291	-0.0052	-0.8383
				-0.0279	-0.3991	0.3662	-0.0191	-0.0194
195.	(0.00034)	RY (5)	C 13	s(83.46%)	p 0.00(0.41%)	d 0.19(16.13%)		

		0.0000	-0.0007	0.9134	-0.0158	0.0097
		-0.0434	0.0004	-0.0444	0.0003	0.0126
		0.1131	0.0351	0.0011	0.3680	-0.1087
196.	(0.00013) RY (6) C 13	s(15.12%)p 0.12(1.75%)d 5.50(83.13%)				
		0.0000	-0.0031	0.3400	0.1887	-0.0197
		0.1267	0.0093	-0.0262	-0.0005	0.0167
		-0.6325	0.0335	-0.0515	-0.6509	-0.0618
197.	(0.00006) RY (7) C 13	s(91.90%)p 0.00(0.25%)d 0.09(7.85%)				
198.	(0.00004) RY (8) C 13	s(3.45%)p 1.50(5.18%)d26.50(91.38%)				
199.	(0.00002) RY (9) C 13	s(5.78%)p 0.05(0.28%)d16.25(93.94%)				
200.	(0.00001) RY (10) C 13	s(0.05%)p99.99(5.84%)d99.99(94.11%)				
201.	(0.00172) RY (1) H 14	s(99.57%)p 0.00(0.43%)				
		0.0042	0.9978	0.0546	0.0361	0.0053
202.	(0.00013) RY (2) H 14	s(0.01%)p 1.00(99.99%)				
		-0.0005	0.0077	-0.0109	-0.0480	-0.9988
203.	(0.00007) RY (3) H 14	s(0.29%)p99.99(99.71%)				
204.	(0.00001) RY (4) H 14	s(0.22%)p99.99(99.78%)				
205.	(0.00407) RY (1) C 15	s(0.17%)p99.99(91.76%)d47.30(8.07%)				
		0.0000	0.0317	-0.0265	0.0005	0.0094
		0.5734	-0.0105	-0.7672	0.0000	0.0072
		-0.2673	0.0125	-0.0003	-0.0948	-0.0119
206.	(0.00206) RY (2) C 15	s(0.22%)p99.99(97.84%)d 8.99(1.94%)				
		0.0000	-0.0043	0.0391	-0.0247	-0.0146
		0.7875	-0.0161	0.5954	-0.0008	-0.0576
		0.0229	-0.0053	-0.0063	-0.1371	-0.0026
207.	(0.00076) RY (3) C 15	s(0.01%)p99.99(94.74%)d99.99(5.25%)				
		0.0000	-0.0004	0.0111	-0.0021	0.0007
		-0.0411	0.0001	-0.0427	-0.0140	-0.9714
		0.0094	-0.0727	0.2161	-0.0153	-0.0138
208.	(0.00049) RY (4) C 15	s(1.16%)p 0.30(0.35%)d84.88(98.49%)				
		0.0000	0.0002	0.1067	-0.0145	0.0004
		0.0033	0.0013	-0.0026	0.0122	0.0574
		0.0569	0.8370	0.5268	-0.0298	-0.0525
209.	(0.00035) RY (5) C 15	s(93.30%)p 0.01(0.76%)d 0.06(5.93%)				
		0.0000	0.0009	0.9646	-0.0508	0.0034
		-0.0133	0.0091	-0.0850	-0.0006	0.0123
		0.1634	-0.1006	-0.0657	-0.1334	-0.0190
210.	(0.00009) RY (6) C 15	s(95.33%)p 0.00(0.12%)d 0.05(4.56%)				
211.	(0.00007) RY (7) C 15	s(4.95%)p 0.33(1.65%)d18.88(93.40%)				
212.	(0.00002) RY (8) C 15	s(3.89%)p 1.85(7.19%)d22.87(88.92%)				
213.	(0.00002) RY (9) C 15	s(1.13%)p 0.59(0.67%)d86.80(98.20%)				
214.	(0.00000) RY (10) C 15	s(0.02%)p99.99(4.95%)d99.99(95.03%)				
215.	(0.00107) RY (1) H 16	s(99.72%)p 0.00(0.28%)				
		0.0025	0.9986	-0.0264	0.0447	0.0115
216.	(0.00016) RY (2) H 16	s(0.02%)p99.99(99.98%)				
		0.0000	0.0132	-0.0178	-0.0502	-0.9985
217.	(0.00005) RY (3) H 16	s(0.00%)p 1.00(100.00%)				
218.	(0.00001) RY (4) H 16	s(0.33%)p99.99(99.67%)				
219.	(0.00437) RY (1) C 17	s(1.54%)p59.37(91.69%)d 4.38(6.76%)				
		0.0000	0.0116	0.1235	0.0078	0.0087
		0.9285	-0.0160	0.2316	-0.0011	0.0300
		-0.1141	-0.0094	-0.0098	0.2329	-0.0128
220.	(0.00319) RY (2) C 17	s(1.01%)p91.17(92.42%)d 6.48(6.57%)				
		0.0000	0.0265	0.0971	0.0003	-0.0159
		-0.2362	0.0012	0.9312	0.0008	0.0312
		-0.2085	-0.0052	0.0031	-0.1446	-0.0355
221.	(0.00173) RY (3) C 17	s(0.05%)p99.99(85.56%)d99.99(14.40%)				
		0.0000	0.0004	0.0217	-0.0028	0.0000
		0.0199	0.0009	0.0298	-0.0141	-0.9242
		-0.0194	0.3119	-0.2142	-0.0086	-0.0192
222.	(0.00070) RY (4) C 17	s(11.95%)p 0.36(4.35%)d 7.00(83.70%)				
		0.0000	-0.0047	0.3456	-0.0065	-0.0009
		-0.0238	0.0082	-0.0961	-0.0083	0.1831
		-0.1260	-0.0979	-0.8886	-0.1231	-0.0827
223.	(0.00065) RY (5) C 17	s(65.02%)p 0.07(4.58%)d 0.47(30.40%)				
		0.0000	-0.0112	0.8061	-0.0144	-0.0016
		-0.0439	0.0198	-0.1983	0.0045	-0.0644
		-0.3239	0.0196	0.3989	-0.1890	-0.0621
224.	(0.00015) RY (6) C 17	s(18.41%)p 0.14(2.63%)d 4.29(78.96%)				
		0.0000	0.0069	0.3709	-0.2155	-0.0109
		0.0311	-0.0176	0.1579	-0.0002	0.0023
		0.8845	0.0204	0.0128	-0.0409	-0.0704
225.	(0.00014) RY (7) C 17	s(0.00%)p 1.00(10.67%)d 8.38(89.33%)				
		0.0000	-0.0003	-0.0004	0.0047	-0.0002
		0.0024	0.0001	-0.0131	-0.0143	0.3260
		-0.0217	0.9439	-0.0277	-0.0140	-0.0298
226.	(0.00008) RY (8) C 17	s(40.81%)p 0.11(4.30%)d 1.34(54.89%)				

227. (0.00006) RY (9) C 17	s(56.90%)p 0.07(3.78%)d 0.69(39.33%)
228. (0.00001) RY (10) C 17	s(4.44%)p 0.02(0.08%)d21.49(95.48%)
229. (0.00587) RY (1) C 18	s(2.23%)p41.44(92.41%)d 2.40(5.36%) 0.0000 0.0100 0.1489 0.0045 -0.0045 -0.7865 0.0070 0.5524 0.0003 -0.0166 -0.1680 0.0048 0.0011 -0.1590 -0.0021
230. (0.00506) RY (2) C 18	s(0.58%)p99.99(94.84%)d 7.93(4.58%) 0.0000 0.0126 0.0732 -0.0162 -0.0003 -0.5620 -0.0150 -0.7948 0.0007 -0.0251 0.1857 0.0045 -0.0018 -0.1062 -0.0046
231. (0.00071) RY (3) C 18	s(0.01%)p 1.00(20.07%)d 3.98(79.92%) 0.0000 0.0000 0.0074 0.0039 0.0002 -0.0111 -0.0003 -0.0036 -0.0065 0.4478 -0.0004 -0.1215 -0.8857 -0.0068 0.0043
232. (0.00050) RY (4) C 18	s(0.01%)p 1.00(64.03%)d 0.56(35.96%) 0.0000 0.0003 -0.0001 0.0084 0.0011 -0.0271 -0.0001 -0.0088 -0.0063 0.7997 0.0058 -0.3871 0.4579 0.0053 0.0050
233. (0.00039) RY (5) C 18	s(91.62%)p 0.04(3.64%)d 0.05(4.73%) 0.0000 -0.0043 0.9571 0.0142 -0.0035 0.1624 0.0021 -0.0475 0.0008 0.0883 -0.0767 0.1983 0.0235 0.0071 -0.0394
234. (0.00033) RY (6) C 18	s(4.58%)p 3.34(15.29%)d17.51(80.14%) 0.0000 -0.0007 0.2139 0.0016 -0.0012 0.0421 0.0006 -0.0086 -0.0008 -0.3886 -0.0241 -0.8915 -0.0727 0.0009 0.0274
235. (0.00012) RY (7) C 18	s(16.92%)p 0.22(3.69%)d 4.69(79.39%) 0.0000 -0.0031 -0.0600 0.4069 -0.0205 0.1580 0.0047 -0.1072 -0.0002 0.0048 -0.3767 0.0045 0.0084 -0.8013 0.0989
236. (0.00010) RY (8) C 18	s(78.98%)p 0.01(0.86%)d 0.26(20.15%)
237. (0.00008) RY (9) C 18	s(1.20%)p 4.35(5.20%)d78.30(93.61%)
238. (0.00002) RY (10) C 18	s(3.96%)p 0.01(0.02%)d24.25(96.02%)
239. (0.00431) RY (1) C 19	s(1.49%)p61.37(91.64%)d 4.60(6.87%) 0.0000 0.0126 0.1210 0.0119 0.0066 0.9426 0.0178 -0.1622 -0.0009 0.0356 0.1680 -0.0185 0.0007 0.2000 -0.0115
240. (0.00332) RY (2) C 19	s(0.86%)p99.99(92.84%)d 7.28(6.30%) 0.0000 0.0270 0.0889 -0.0038 -0.0175 -0.1635 -0.0029 -0.9492 0.0003 -0.0173 0.1626 0.0073 0.0043 -0.1885 -0.0305
241. (0.00176) RY (3) C 19	s(0.48%)p99.99(82.84%)d35.05(16.68%) 0.0000 -0.0009 0.0690 -0.0018 0.0002 0.0297 -0.0016 0.0259 -0.0157 -0.9092 0.0239 0.2788 0.2949 0.0041 -0.0400
242. (0.00066) RY (4) C 19	s(58.87%)p 0.06(3.35%)d 0.64(37.78%) 0.0000 -0.0097 0.7670 -0.0170 -0.0001 -0.0492 -0.0163 0.1615 0.0047 -0.0687 0.1918 0.1070 -0.5203 -0.2377 -0.0483
243. (0.00064) RY (5) C 19	s(21.22%)p 0.30(6.47%)d 3.41(72.32%) 0.0000 -0.0060 0.4606 -0.0048 -0.0002 -0.0371 -0.0101 0.1099 -0.0060 0.2260 0.1323 -0.2289 0.7825 -0.1921 -0.0631
244. (0.00015) RY (6) C 19	s(14.17%)p 0.22(3.09%)d 5.84(82.73%) 0.0000 0.0087 0.3121 -0.2104 -0.0142 0.0658 0.0179 -0.1596 -0.0009 0.0246 -0.8971 0.0482 0.0291 0.1336 -0.0399
245. (0.00013) RY (7) C 19	s(0.08%)p99.99(11.52%)d99.99(88.40%) 0.0000 -0.0008 -0.0134 0.0253 -0.0001 0.0018 -0.0007 0.0139 -0.0143 0.3388 0.0521 0.9223 0.1603 -0.0137 -0.0686
246. (0.00008) RY (8) C 19	s(31.16%)p 0.17(5.27%)d 2.04(63.57%)
247. (0.00006) RY (9) C 19	s(68.05%)p 0.04(2.93%)d 0.43(29.03%)
248. (0.00001) RY (10) C 19	s(3.77%)p 0.02(0.09%)d25.52(96.14%)
249. (0.00459) RY (1) C 20	s(0.01%)p 1.00(94.52%)d 0.06(5.47%) 0.0000 0.0015 0.0095 0.0016 0.0024 0.0272 -0.0122 -0.9717 -0.0003 0.0110 -0.2316 -0.0015 0.0082 0.0313 -0.0039
250. (0.00355) RY (2) C 20	s(0.47%)p99.99(91.84%)d16.39(7.69%) 0.0000 0.0020 0.0651 -0.0212 0.0120 0.9564 -0.0006 0.0265 -0.0006 -0.0540 -0.0359 0.0046 0.0011 -0.2746 -0.0146
251. (0.00062) RY (3) C 20	s(88.99%)p 0.00(0.38%)d 0.12(10.63%) 0.0000 -0.0057 0.9433 0.0072 -0.0031 0.0111 -0.0002 0.0112 0.0003 0.0596 0.0328 0.1108 0.0128 0.2573 -0.1631
252. (0.00055) RY (4) C 20	s(1.10%)p 1.11(1.22%)d88.53(97.67%)

		0.0000	-0.0010	0.1050	0.0017	-0.0008
		0.0035	0.0000	0.0026	-0.0057	0.1104
		0.0073	-0.9869	0.0490	-0.0010	-0.0183
253.	(0.00050) RY (5) C 20	s(0.02%)p 0.32(0.01%)d99.99(99.97%)	0.0000	-0.0002	0.0140	-0.0005
			0.0028	-0.0005	-0.0073	-0.0009
			-0.0020	-0.0479	-0.9985	0.0088
254.	(0.00029) RY (6) C 20	s(0.70%)p99.99(98.20%)d 1.58(1.11%)	0.0000	0.0011	0.0832	0.0077
			-0.0672	0.0000	-0.0124	0.0100
			-0.0015	-0.1019	0.0064	-0.0236
255.	(0.00013) RY (7) C 20	s(8.45%)p 0.94(7.92%)d 9.90(83.63%)	0.0000	0.0043	0.2548	0.1397
			-0.2743	0.0011	-0.0091	-0.0009
			-0.1037	0.0319	-0.0075	-0.9065
256.	(0.00008) RY (8) C 20	s(2.14%)p 2.53(5.41%)d43.18(92.45%)	0.0000	0.0055	0.2470	-0.0023
257.	(0.00005) RY (9) C 20	s(96.02%)p 0.00(0.46%)d 0.04(3.52%)	0.4142	-0.0154	-0.4789	-0.0086
258.	(0.00002) RY (10) C 20	s(2.16%)p 0.06(0.14%)d45.19(97.70%)	0.0862	-0.0934	0.2047	0.0592
259.	(0.00250) RY (1) C 21	s(6.10%)p13.13(80.12%)d 2.26(13.77%)	s(8.66%)p 8.00(69.27%)d 2.55(22.07%)	0.0000	0.0098	0.2935
				-0.7582	-0.0069	-0.3355
				-0.0553	0.2374	0.2436
260.	(0.00177) RY (2) C 21	s(18.70%)p 4.00(74.79%)d 0.35(6.52%)	0.0000	0.0042	0.4254	0.0773
				0.0137	-0.0186	0.7625
				-0.0935	0.1417	0.0632
261.	(0.00064) RY (3) C 21	s(18.61%)p 0.71(13.24%)d 3.66(68.15%)	0.0000	0.0069	0.3526	-0.2484
				-0.2421	0.0083	-0.1108
				-0.0882	-0.3166	-0.5435
262.	(0.00043) RY (4) C 21	s(33.47%)p 0.92(30.66%)d 1.07(35.86%)	0.0002	0.9988	0.0100	0.0468
				s(0.14%)p99.99(99.86%)		
263.	(0.00007) RY (5) C 21	s(15.78%)p 0.72(11.31%)d 4.62(72.91%)	s(0.05%)p99.99(99.95%)			
264.	(0.00003) RY (6) C 21	s(15.66%)p 0.15(2.41%)d 5.23(81.93%)	s(0.09%)p99.99(99.91%)			
265.	(0.00002) RY (7) C 21	s(18.11%)p 0.37(6.65%)d 4.15(75.23%)	s(99.73%)p 0.00(0.27%)	0.0001	0.9986	0.0405
266.	(0.00001) RY (8) C 21	s(15.31%)p 0.02(0.27%)d 5.51(84.42%)	s(0.02%)p99.99(99.98%)			
267.	(0.00000) RY (9) C 21	s(49.62%)p 0.23(11.58%)d 0.78(38.79%)	s(0.12%)p99.99(99.88%)			
268.	(0.00080) RY (1) H 22	s(99.77%)p 0.00(0.23%)	s(0.20%)p99.99(99.80%)			
			s(99.39%)p 0.01(0.61%)	-0.0040	0.9969	-0.0424
269.	(0.00007) RY (2) H 22	s(0.14%)p99.99(99.86%)	s(0.02%)p99.99(99.98%)			
270.	(0.00004) RY (3) H 22	s(0.05%)p99.99(99.95%)	s(0.59%)p99.99(99.41%)			
271.	(0.00000) RY (4) H 22	s(0.09%)p99.99(99.91%)	s(0.06%)p99.99(99.94%)			
272.	(0.00108) RY (1) H 23	s(99.73%)p 0.00(0.27%)	s(4.67%)p17.67(82.56%)d 2.73(12.77%)	0.0000	0.0051	0.2160
				0.4310	-0.0126	-0.4295
				0.1052	0.0816	-0.1434
273.	(0.00007) RY (2) H 23	s(0.02%)p99.99(99.98%)	s(8.99%)p 7.76(69.76%)d 2.36(21.25%)	0.0000	0.0106	0.2991
274.	(0.00004) RY (3) H 23	s(0.12%)p99.99(99.88%)		-0.7416	-0.0083	-0.3724
275.	(0.00001) RY (4) H 23	s(0.20%)p99.99(99.80%)		-0.0247	-0.1967	-0.2384
276.	(0.00257) RY (1) H 24	s(99.39%)p 0.01(0.61%)				
277.	(0.00006) RY (2) H 24	s(0.02%)p99.99(99.98%)				
278.	(0.00004) RY (3) H 24	s(0.59%)p99.99(99.41%)				
279.	(0.00001) RY (4) H 24	s(0.06%)p99.99(99.94%)				
280.	(0.00257) RY (1) C 25	s(4.67%)p17.67(82.56%)d 2.73(12.77%)				
281.	(0.00182) RY (2) C 25	s(8.99%)p 7.76(69.76%)d 2.36(21.25%)				
282.	(0.00064) RY (3) C 25	s(21.04%)p 3.58(75.22%)d 0.18(3.74%)				
283.	(0.00045) RY (4) C 25	s(15.17%)p 0.88(13.35%)d 4.71(71.48%)				
284.	(0.00007) RY (5) C 25	s(35.33%)p 0.76(26.85%)d 1.07(37.82%)				
285.	(0.00003) RY (6) C 25	s(16.64%)p 0.71(11.76%)d 4.30(71.59%)				
286.	(0.00002) RY (7) C 25	s(20.97%)p 0.10(2.06%)d 3.67(76.97%)				
287.	(0.00001) RY (8) C 25	s(11.90%)p 0.58(6.92%)d 6.82(81.19%)				
288.	(0.00001) RY (9) C 25	s(18.89%)p 0.02(0.37%)d 4.28(80.75%)				
289.	(0.00000) RY (10) C 25	s(46.43%)p 0.25(11.46%)d 0.91(42.11%)				
290.	(0.00000) RY (10) C 25	s(46.43%)p 0.25(11.46%)d 0.91(42.11%)				

291.	(0.00248)	RY	(1)	H	26	s(99.38%)p 0.01(0.62%)
						-0.0038 0.9969 -0.0432 0.0009 0.0658
292.	(0.00006)	RY	(2)	H	26	s(0.02%)p99.99(99.98%)
293.	(0.00004)	RY	(3)	H	26	s(0.60%)p99.99(99.40%)
294.	(0.00001)	RY	(4)	H	26	s(0.06%)p99.99(99.94%)
295.	(0.00109)	RY	(1)	H	27	s(99.71%)p 0.00(0.29%)
						-0.0001 0.9985 0.0349 0.0321 0.0257
296.	(0.00007)	RY	(2)	H	27	s(0.02%)p99.99(99.98%)
297.	(0.00004)	RY	(3)	H	27	s(0.15%)p99.99(99.85%)
298.	(0.00001)	RY	(4)	H	27	s(0.17%)p99.99(99.83%)
299.	(0.00078)	RY	(1)	H	28	s(99.77%)p 0.00(0.23%)
						0.0002 0.9989 0.0115 0.0458 -0.0081
300.	(0.00007)	RY	(2)	H	28	s(0.16%)p99.99(99.84%)
301.	(0.00004)	RY	(3)	H	28	s(0.03%)p99.99(99.97%)
302.	(0.00000)	RY	(4)	H	28	s(0.08%)p99.99(99.92%)
303.	(0.01066)	RY	(1)	B	29	s(0.55%)p99.99(93.62%)d10.65(5.83%)
						0.0000 -0.0121 0.0520 0.0512 -0.0584
						0.8353 0.0116 -0.4847 -0.0015 -0.0002
						-0.1770 -0.0098 0.0058 -0.1615 -0.0283
304.	(0.00449)	RY	(2)	B	29	s(18.15%)p 4.16(75.60%)d 0.34(6.25%)
						0.0000 -0.0162 0.3886 0.1739 -0.0194
						0.3998 -0.0484 0.7702 -0.0002 0.0141
						0.1326 -0.0067 0.0749 -0.1925 -0.0470
305.	(0.00194)	RY	(3)	B	29	s(0.67%)p 1.17(0.78%)d99.99(98.55%)
						0.0000 -0.0010 0.0803 0.0154 -0.0005
						0.0168 -0.0056 0.0129 -0.0081 -0.0854
						0.0764 0.3490 -0.9241 -0.0540 -0.0293
306.	(0.00117)	RY	(4)	B	29	s(6.16%)p 1.82(11.19%)d13.41(82.64%)
						0.0000 -0.0028 0.2474 -0.0201 -0.0222
						-0.3156 -0.0329 -0.0939 0.0050 0.0438
						-0.4114 -0.1066 -0.0144 -0.7979 -0.0945
307.	(0.00081)	RY	(5)	B	29	s(0.02%)p99.99(10.80%)d99.99(89.18%)
						0.0000 -0.0041 0.0134 -0.0012 -0.0176
						-0.0145 0.0198 0.1037 -0.0355 -0.3083
						-0.4892 0.7515 0.2671 0.1280 -0.0067
308.	(0.00077)	RY	(6)	B	29	s(2.47%)p 1.70(4.19%)d37.86(93.34%)
						0.0000 -0.0078 0.1360 -0.0780 -0.0296
						0.0307 0.0386 0.1795 0.0135 0.0789
						-0.6951 -0.4383 -0.2410 0.4431 -0.0608
309.	(0.00044)	RY	(7)	B	29	s(88.02%)p 0.04(3.20%)d 0.10(8.78%)
						0.0000 0.0054 -0.6602 0.6665 0.0205
						0.0343 0.0084 0.1732 -0.0012 -0.0183
						-0.1902 -0.0838 -0.0831 -0.1598 0.1103
310.	(0.00024)	RY	(8)	B	29	s(81.54%)p 0.16(12.65%)d 0.07(5.82%)
						0.0000 0.0043 0.5556 0.7118 -0.0007
						-0.1930 0.0132 -0.2972 -0.0011 -0.0269
						0.0645 0.0038 0.0477 0.2262 0.0231
311.	(0.00005)	RY	(9)	B	29	s(0.15%)p99.99(88.66%)d75.84(11.19%)
312.	(0.00000)	RY	(10)	B	29	s(2.23%)p 0.05(0.11%)d43.85(97.66%)
313.	(0.00362)	RY	(1)	N	30	s(5.44%)p16.95(92.14%)d 0.45(2.43%)
						0.0000 -0.0049 0.2318 -0.0248 0.0127
						0.2890 0.0395 0.9144 0.0006 -0.0066
						-0.1051 -0.0044 0.0070 0.0878 0.0738
314.	(0.00085)	RY	(2)	N	30	s(3.19%)p26.50(84.53%)d 3.85(12.28%)
						0.0000 -0.0088 0.1718 -0.0479 -0.0047
						0.6510 0.0075 -0.2480 0.0197 -0.5997
						0.0279 0.1221 -0.0741 0.1867 -0.2583
315.	(0.00084)	RY	(3)	N	30	s(1.38%)p64.30(88.49%)d 7.36(10.13%)
						0.0000 -0.0061 0.1129 -0.0311 -0.0041
						0.5024 0.0064 -0.1782 -0.0243 0.7747
						-0.0192 -0.0951 0.0882 0.1330 -0.2578
316.	(0.00049)	RY	(4)	N	30	s(0.00%)p 1.00(2.59%)d37.57(97.41%)
						0.0000 0.0002 0.0040 -0.0011 0.0005
						0.0161 0.0006 -0.0073 0.0125 -0.1595
						0.0354 -0.9820 0.0774 0.0229 -0.0442
317.	(0.00033)	RY	(5)	N	30	s(0.14%)p81.86(11.14%)d99.99(88.73%)
						0.0000 -0.0025 0.0048 0.0365 -0.0121
						0.3185 0.0065 -0.0895 -0.0007 0.0414
						0.5536 -0.0096 0.0921 -0.0936 0.7506
318.	(0.00027)	RY	(6)	N	30	s(22.09%)p 0.47(10.37%)d 3.06(67.54%)
						0.0000 -0.0096 0.4698 0.0104 0.0190
						-0.3004 -0.0152 -0.1095 -0.0023 0.0298
						0.0429 0.0024 -0.0320 0.7997 0.1816
319.	(0.00019)	RY	(7)	N	30	s(0.05%)p27.71(1.26%)d99.99(98.70%)
						0.0000 0.0019 0.0159 -0.0140 0.0006
						0.0207 0.0016 0.0129 -0.0332 0.1043
						0.1094 -0.0926 -0.9815 -0.0529 0.0196

320. (0.00016) RY (8) N 30	s(28.45%)p 0.18(5.05%)d 2.34(66.50%) 0.0000 0.0137 0.5239 -0.0990 0.0133 -0.2141 0.0076 0.0665 0.0026 0.0028 0.6246 0.0378 0.0814 -0.3154 -0.4092
321. (0.00005) RY (9) N 30	s(52.04%)p 0.07(3.67%)d 0.85(44.29%)
322. (0.00001) RY (10) N 30	s(87.26%)p 0.01(0.96%)d 0.13(11.78%)
323. (0.00100) RY (1) O 31	s(5.90%)p15.85(93.57%)d 0.09(0.53%) 0.0000 0.0105 0.1792 0.1637 0.0105 -0.6101 -0.0163 -0.7452 0.0023 -0.0883 0.0001 0.0032 -0.0004 0.0304 -0.0658
324. (0.00037) RY (2) O 31	s(69.11%)p 0.12(8.22%)d 0.33(22.67%) 0.0000 -0.0082 0.8183 -0.1462 -0.0090 0.1263 0.0211 0.0245 -0.0052 0.2551 0.1111 -0.0161 -0.0650 -0.4372 -0.1368
325. (0.00028) RY (3) O 31	s(4.66%)p18.78(87.54%)d 1.67(7.80%) 0.0000 -0.0026 0.2055 -0.0660 -0.0045 0.1387 0.0055 0.0272 0.0148 -0.9247 0.0223 0.0412 0.2478 -0.1192 -0.0144
326. (0.00016) RY (4) O 31	s(2.56%)p36.11(92.39%)d 1.97(5.05%) 0.0000 0.0058 0.0278 0.1574 -0.0051 0.7618 -0.0330 -0.5813 0.0002 0.0669 -0.1086 -0.0003 0.0107 0.1964 -0.0038
327. (0.00004) RY (5) O 31	s(29.02%)p 0.21(6.11%)d 2.24(64.87%)
328. (0.00003) RY (6) O 31	s(54.54%)p 0.07(3.84%)d 0.76(41.63%)
329. (0.00003) RY (7) O 31	s(0.16%)p34.32(5.62%)d99.99(94.21%)
330. (0.00002) RY (8) O 31	s(9.45%)p 0.08(0.73%)d 9.50(89.82%)
331. (0.00000) RY (9) O 31	s(24.59%)p 0.05(1.33%)d 3.01(74.08%)
332. (0.00000) RY (10) O 31	s(0.07%)p18.51(1.26%)d99.99(98.67%)
333. (0.00070) RY (1) O 32	s(30.07%)p 2.22(66.84%)d 0.10(3.09%) 0.0000 0.0117 0.5417 -0.0844 -0.0101 0.7908 0.0027 -0.1930 0.0019 -0.0753 -0.0041 0.0176 -0.0055 0.1489 -0.0918
334. (0.00037) RY (2) O 32	s(10.39%)p 8.10(84.17%)d 0.52(5.44%) 0.0000 0.0006 0.3201 -0.0368 -0.0028 -0.1659 -0.0015 0.5595 0.0056 -0.7079 -0.1908 0.0482 -0.1185 0.0382 -0.0143
335. (0.00035) RY (3) O 32	s(18.89%)p 4.02(75.99%)d 0.27(5.12%) 0.0000 0.0045 0.4345 -0.0102 0.0004 -0.1221 0.0002 0.5275 -0.0055 0.6832 -0.1926 -0.0413 0.0774 0.0723 -0.0341
336. (0.00007) RY (4) O 32	s(31.07%)p 1.82(56.60%)d 0.40(12.33%)
337. (0.00005) RY (5) O 32	s(38.99%)p 0.10(3.85%)d 1.47(57.17%)
338. (0.00004) RY (6) O 32	s(2.59%)p 0.44(1.14%)d37.24(96.27%)
339. (0.00002) RY (7) O 32	s(25.98%)p 0.15(3.84%)d 2.70(70.18%)
340. (0.00001) RY (8) O 32	s(30.74%)p 0.06(1.91%)d 2.19(67.34%)
341. (0.00000) RY (9) O 32	s(11.17%)p 0.36(3.97%)d 7.60(84.87%)
342. (0.00000) RY (10) O 32	s(0.18%)p12.66(2.26%)d99.99(97.56%)
343. (0.00160) RY (1) H 33	s(92.29%)p 0.08(7.71%) 0.0062 0.9607 0.0616 0.2707 -0.0060
344. (0.00074) RY (2) H 33	s(0.01%)p 1.00(99.99%) -0.0010 0.0071 -0.1479 0.0304 0.9885
345. (0.00047) RY (3) H 33	s(5.30%)p17.85(94.70%) 0.0087 0.2302 0.3652 -0.8984 0.0807
346. (0.00002) RY (4) H 33	s(2.54%)p38.30(97.46%)
347. (0.00379) RY (1) H 34	s(96.24%)p 0.04(3.76%) -0.0174 0.9809 -0.0815 0.1756 -0.0110
348. (0.00061) RY (2) H 34	s(0.00%)p 1.00(100.00%) 0.0029 -0.0008 -0.0566 -0.0834 -0.9949
349. (0.00049) RY (3) H 34	s(0.11%)p99.99(99.89%) 0.0275 -0.0184 -0.9411 -0.3266 0.0810
350. (0.00023) RY (4) H 34	s(3.80%)p25.32(96.20%) 0.0246 0.1934 0.3228 -0.9243 0.0590

A 3D ball-and-stick model of a complex organic molecule. The molecule features a central core with a red mesh surface and a green mesh surface. A red sphere is visible near the center, and a long chain of atoms extends from the right side. The model is set against a white background.

	Atom	1	2	3	4	5	6	7	8	9
1.	C	0.0000	0.9352	0.9320	0.9216	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.9352	0.0000	0.0019	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.9320	0.0019	0.0000	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000
4.	H	0.9216	0.0019	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.9143	0.9145	0.9997	0.0025
6.	H	0.0000	0.0000	0.0000	0.0000	0.9143	0.0000	0.0020	0.0025	0.0019
7.	H	0.0000	0.0000	0.0000	0.0000	0.9145	0.0020	0.0000	0.0025	0.0017
8.	C	0.0000	0.0000	0.0000	0.0000	0.9997	0.0025	0.0025	0.0000	0.9156
9.	H	0.0000	0.0000	0.0000	0.0000	0.0025	0.0017	0.0017	0.9156	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0025	0.0017	0.0017	0.9154	0.0019
11.	C	0.0000	0.0000	0.0000	0.0000	0.0062	0.0008	0.0008	0.0107	0.0065
12.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0018	0.0001
13.	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	0.0003	0.0108	0.0001
14.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0003	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0001	0.0014	0.0030
16.	C	0.0000	0.0000	0.0000	0.0001	0.0015	0.0031	0.0030	0.0004	0.0002
17.	C	0.0000	0.0000	0.0000	0.0000	0.0113	0.0001	0.0001	0.0004	0.0003
18.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0002	0.0000
19.	C	0.0000	0.0000	0.0000	0.0000	0.0110	0.0068	0.0065	0.0063	0.0010
20.	H	0.0000	0.0000	0.0000	0.0000	0.0018	0.0001	0.0001	0.0001	0.0000
21.	C	0.0000	0.0000	0.0000	0.0000	0.0060	0.0026	0.0027	1.0057	0.0033
22.	C	0.0000	0.0000	0.0000	0.0000	0.0083	0.0001	0.0001	0.0082	0.0001
23.	C	0.0000	0.0000	0.0000	0.0000	1.0061	0.0034	0.0035	0.0060	0.0026
24.	C	0.0000	0.0000	0.0000	0.0000	0.0085	0.0061	0.0063	0.0085	0.0064
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0012	0.0006	0.0014	0.0040	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0087	0.0002	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0091	0.0070	0.0024	0.0073	0.0000	0.0000	0.0000	0.0000	0.0000
36.										

44.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0005	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	B	0.0005	0.0000	0.0000	0.0001	0.0007	0.0004	0.0004	0.0003	0.0000
50.	N	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0004	0.0001
51.	O	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0002	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
5.	C	0.0025	0.0062	0.0001	0.0003	0.0002	0.0004	0.0015	0.0113
6.	H	0.0017	0.0008	0.0000	0.0003	0.0000	0.0001	0.0031	0.0001
7.	H	0.0017	0.0008	0.0000	0.0003	0.0000	0.0001	0.0030	0.0001
8.	C	0.9154	0.0107	0.0018	0.0108	0.0003	0.0014	0.0004	0.0004
9.	H	0.0019	0.0065	0.0001	0.0001	0.0000	0.0030	0.0002	0.0003
10.	H	0.0000	0.0066	0.0001	0.0001	0.0000	0.0030	0.0002	0.0003
11.	C	0.0066	0.0000	0.9257	1.3116	0.0049	0.0137	0.0017	0.0250
12.	H	0.0001	0.9257	0.0000	0.0046	0.0013	0.0062	0.0003	0.0001
13.	C	0.0001	1.3116	0.0046	0.0000	0.9267	1.4963	0.0307	0.0009
14.	H	0.0000	0.0049	0.0013	0.9267	0.0000	0.0054	0.0001	0.0002
15.	C	0.0030	0.0137	0.0062	1.4963	0.0054	0.0000	0.0115	0.0279
16.	C	0.0002	0.0017	0.0003	0.0307	0.0001	0.0115	0.0000	1.4992
17.	C	0.0003	0.0250	0.0001	0.0009	0.0002	0.0279	1.4992	0.0000
18.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001	0.0076	0.9217
19.	C	0.0010	0.0009	0.0002	0.0296	0.0000	0.0006	0.0126	1.3029
20.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0004	0.0065	0.0048
21.	C	0.0033	1.5098	0.0063	0.0127	0.0060	0.1013	0.0093	0.0019
22.	C	0.0000	0.0665	0.0002	0.0107	0.0070	1.2567	1.2166	0.0096
23.	C	0.0026	0.0299	0.0002	0.0016	0.0002	0.0075	0.0998	0.0152
24.	C	0.0064	0.0114	0.0096	0.0597	0.0004	0.0113	0.0108	0.0532
25.	C	0.0001	0.0004	0.0000	0.0103	0.0001	0.0094	0.0004	0.0008
26.	H	0.0000	0.0000	0.0000	0.0005	0.0000	0.0005	0.0002	0.0000
27.	H	0.0000	0.0002	0.0000	0.0011	0.0001	0.0073	0.0001	0.0001
28.	H	0.0000	0.0001	0.0000	0.0012	0.0001	0.0004	0.0001	0.0000
29.	C	0.0000	0.0004	0.0000	0.0039	0.0007	0.0080	0.0002	0.0003
30.	H	0.0000	0.0000	0.0000	0.0012	0.0005	0.0004	0.0000	0.0000
31.	H	0.0000	0.0001	0.0000	0.0013	0.0000	0.0065	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0006	0.0000	0.0007	0.0000	0.0000
33.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003	0.0071	0.0020
34.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0046	0.0019
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
37.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0005
38.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0041	0.0016
41.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0010	0.0005
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0006
45.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0004
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0003
49.	B	0.0000	0.0013	0.0000	0.0026	0.0000	0.0030	0.8904	0.0374
50.	N	0.0002	0.0091	0.0006	0.0256	0.0037	0.9855	0.0017	0.0008
51.	O	0.0000	0.0003	0.0000	0.0019	0.0001	0.0013	0.0154	0.0217
52.	H	0.0000	0.0000	0.0000	0.0012	0.0000	0.0004	0.0006	0.0001

Atom	19	20	21	22	23	24	25	26	27
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0110	0.0018	0.0060	0.0083	1.0061	0.0085	0.0000	0.0000
6.	H	0.0068	0.0001	0.0026	0.0001	0.0034	0.0061	0.0000	0.0000
7.	H	0.0065	0.0001	0.0027	0.0001	0.0035	0.0063	0.0000	0.0000
8.	C	0.0063	0.0001	1.0057	0.0082	0.0060	0.0085	0.0000	0.0000
9.	H	0.0010	0.0000	0.0033	0.0001	0.0026	0.0064	0.0001	0.0000
10.	H	0.0010	0.0000	0.0033	0.0000	0.0026	0.0064	0.0001	0.0000

11.	C	0.0009	0.0002	1.5098	0.0665	0.0299	0.0114	0.0004	0.0000	0.0002
12.	H	0.0002	0.0000	0.0063	0.0002	0.0002	0.0096	0.0000	0.0000	0.0000
13.	C	0.0296	0.0000	0.0127	0.0107	0.0016	0.0597	0.0103	0.0005	0.0011
14.	H	0.0000	0.0000	0.0060	0.0070	0.0002	0.0004	0.0001	0.0000	0.0001
15.	C	0.0006	0.0004	0.1013	1.2567	0.0075	0.0113	0.0094	0.0005	0.0073
16.	C	0.0126	0.0065	0.0093	1.2166	0.0998	0.0108	0.0004	0.0002	0.0001
17.	C	1.3029	0.0048	0.0019	0.0096	0.0152	0.0532	0.0008	0.0000	0.0001
18.	H	0.0037	0.0013	0.0003	0.0081	0.0057	0.0004	0.0000	0.0000	0.0000
19.	C	0.0000	0.9259	0.0354	0.0602	1.5166	0.0117	0.0002	0.0000	0.0000
20.	H	0.9259	0.0000	0.0002	0.0002	0.0059	0.0094	0.0000	0.0000	0.0000
21.	C	0.0354	0.0002	0.0000	0.0107	0.0157	1.2484	0.0037	0.0001	0.0006
22.	C	0.0602	0.0002	0.0107	0.0000	0.0109	1.2567	0.0055	0.0001	0.0006
23.	C	1.5166	0.0059	0.0157	0.0109	0.0000	1.2386	0.0002	0.0000	0.0000
24.	C	0.0117	0.0094	1.2484	1.2567	1.2386	0.0000	0.0004	0.0000	0.0001
25.	C	0.0002	0.0000	0.0037	0.0055	0.0002	0.0004	0.0000	0.9351	0.9364
26.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.9351	0.0000	0.0022
27.	H	0.0000	0.0000	0.0006	0.0006	0.0000	0.0001	0.9364	0.0022	0.0000
28.	H	0.0000	0.0000	0.0002	0.0001	0.0000	0.0001	0.9400	0.0015	0.0012
29.	C	0.0001	0.0000	0.0012	0.0083	0.0002	0.0004	0.0088	0.0078	0.0005
30.	H	0.0000	0.0000	0.0003	0.0003	0.0000	0.0000	0.0006	0.0000	0.0002
31.	H	0.0000	0.0000	0.0004	0.0003	0.0000	0.0001	0.0003	0.0001	0.0002
32.	H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0001	0.0080	0.0005	0.0002
33.	C	0.0004	0.0000	0.0002	0.0040	0.0001	0.0001	0.0002	0.0001	0.0000
34.	C	0.0001	0.0000	0.0001	0.0004	0.0003	0.0002	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
38.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	C	0.0001	0.0000	0.0001	0.0003	0.0003	0.0002	0.0000	0.0000	0.0000
41.	C	0.0001	0.0000	0.0000	0.0002	0.0002	0.0001	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0001	0.0001	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
49.	B	0.0100	0.0001	0.0011	0.0145	0.0118	0.0073	0.0008	0.0004	0.0001
50.	N	0.0001	0.0000	0.0048	0.0168	0.0003	0.0079	0.9500	0.0028	0.0045
51.	O	0.0009	0.0002	0.0005	0.0066	0.0069	0.0002	0.0014	0.0001	0.0004
52.	H	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0007	0.0001	0.0002

	Atom	28	29	30	31	32	33	34	35	36
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0087	0.0091	0.0020
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0002	0.0070	0.0001
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014	0.0002	0.0024	0.0001
4.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0040	0.0001	0.0073	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0001	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0012	0.0039	0.0012	0.0013	0.0006	0.0001	0.0001	0.0000	0.0000
14.	H	0.0001	0.0007	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0004	0.0080	0.0004	0.0065	0.0007	0.0003	0.0001	0.0000	0.0000
16.	C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0071	0.0046	0.0002	0.0001
17.	C	0.0000	0.0003	0.0000	0.0000	0.0000	0.0020	0.0019	0.0002	0.0000
18.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0022	0.0006	0.0000	0.0000
19.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0004	0.0001	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0002	0.0012	0.0003	0.0004	0.0001	0.0002	0.0001	0.0000	0.0000
22.	C	0.0001	0.0083	0.0003	0.0003	0.0002	0.0040	0.0004	0.0001	0.0000
23.	C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000
24.	C	0.0001	0.0004	0.0000	0.0001	0.0001	0.0001	0.0002	0.0000	0.0000
25.	C	0.9400	0.0088	0.0006	0.0003	0.0080	0.0002	0.0000	0.0000	0.0000
26.	H	0.0015	0.0078	0.0000	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000
27.	H	0.0012	0.0005	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0003	0.0013	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0003	0.0000	0.9408	0.9339	0.9360	0.0000	0.0000	0.0000	0.0000
30.	H	0.0013	0.9408	0.0000	0.0012	0.0015	0.0000	0.0000	0.0000	0.0000
31.	H	0.0002	0.9339	0.0012	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.9360	0.0015	0.0023	0.0000	0.0000	0.0000	0.0000	0.0000

33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3858	0.0118	0.0078
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	1.3858	0.0000	1.4035	0.0057
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0118	1.4035	0.0000	0.9292
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0078	0.0057	0.9292	0.0000
37.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.1054	0.0135	1.4082	0.0056
38.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119	0.1029	0.0110	0.0083
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0077	0.0004	0.0081	0.0002
40.	C	0.0000	0.0000	0.0000	0.0000	0.0000	1.3825	0.0139	0.1046	0.0004
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0096	1.0169	0.0084	0.0019
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0079	0.0037	0.0087	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0031	0.0019	0.0001
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0031	0.0077	0.0001
45.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0093	0.0091	0.0012	0.0004
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0061	0.0002	0.0001	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0052	0.0001	0.0034	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0002	0.0028	0.0000
49.	B	0.0002	0.0002	0.0001	0.0001	0.0000	0.8491	0.0134	0.0090	0.0003
50.	N	0.0179	0.9611	0.0183	0.0059	0.0021	0.0005	0.0003	0.0000	0.0000
51.	O	0.0015	0.0008	0.0009	0.0003	0.0001	0.0106	0.0074	0.0005	0.0002
52.	H	0.0012	0.0009	0.0011	0.0003	0.0001	0.0077	0.0004	0.0001	0.0000

	Atom	37	38	39	40	41	42	43	44	45
1.	C	1.0160	0.0086	0.0019	0.0084	0.0005	0.0000	0.0000	0.0002	0.0005
2.	H	0.0030	0.0018	0.0002	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000
3.	H	0.0031	0.0081	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002
4.	H	0.0036	0.0085	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
14.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
16.	C	0.0016	0.0003	0.0000	0.0041	0.0010	0.0001	0.0002	0.0006	0.0006
17.	C	0.0005	0.0001	0.0000	0.0016	0.0005	0.0000	0.0000	0.0006	0.0004
18.	H	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0001	0.0001	0.0000	0.0003	0.0002	0.0000	0.0000	0.0000	0.0002
23.	C	0.0001	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0000	0.0002
24.	C	0.0001	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.1054	0.0119	0.0077	1.3825	0.0096	0.0079	0.0072	0.0026	0.0093
34.	C	0.0135	0.1029	0.0004	0.0139	1.0169	0.0037	0.0031	0.0031	0.0091
35.	C	1.4082	0.0110	0.0081	0.1046	0.0084	0.0087	0.0019	0.0077	0.0012
36.	H	0.0056	0.0083	0.0002	0.0004	0.0019	0.0000	0.0001	0.0001	0.0004
37.	C	0.0000	1.4017	0.0056	0.0135	0.0080	0.0001	0.0003	0.0001	0.0079
38.	C	1.4017	0.0000	0.9295	1.4084	0.0013	0.0042	0.0007	0.0013	0.0078
39.	H	0.0056	0.9295	0.0000	0.0057	0.0004	0.0000	0.0000	0.0000	0.0019
40.	C	0.0135	1.4084	0.0057	0.0000	0.0087	0.0001	0.0002	0.0003	1.0156
41.	C	0.0080	0.0013	0.0004	0.0087	0.0000	0.9177	0.9340	0.9272	0.0005
42.	H	0.0001	0.0042	0.0000	0.0001	0.9177	0.0000	0.0020	0.0020	0.0000
43.	H	0.0003	0.0007	0.0000	0.0002	0.9340	0.0020	0.0000	0.0021	0.0002
44.	H	0.0001	0.0013	0.0000	0.0003	0.9272	0.0020	0.0021	0.0000	0.0000
45.	C	0.0079	0.0078	0.0019	1.0156	0.0005	0.0000	0.0002	0.0000	0.0000
46.	H	0.0003	0.0015	0.0002	0.0031	0.0002	0.0000	0.0000	0.0000	0.9356
47.	H	0.0001	0.0094	0.0000	0.0036	0.0000	0.0000	0.0000	0.0000	0.9218
48.	H	0.0001	0.0091	0.0000	0.0034	0.0000	0.0000	0.0000	0.0000	0.9239
49.	B	0.0021	0.0092	0.0004	0.0134	0.0050	0.0002	0.0002	0.0028	0.0044
50.	N	0.0002	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
51.	O	0.0020	0.0005	0.0001	0.0074	0.0008	0.0003	0.0003	0.0003	0.0010
52.	H	0.0002	0.0001	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0001
	Atom	46	47	48	49	50	51	52		

[illegible]

(comp ₁)	Lewis
1. (1.99939) CR (1) C 1	s(100.00%)
	1.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
2. (1.99929) CR (1) C 5	s(100.00%)
	1.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
3. (1.99929) CR (1) C 8	s(100.00%)
	1.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
4. (1.99907) CR (1) C 11	s(100.00%)
	1.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
5. (1.99910) CR (1) C 13	s(100.00%)
	1.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
	0.0000 0.0000 0.0000 0.0000 0.0000
6. (1.99897) CR (1) C 15	s(100.00%)

	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
7. (1.99886) CR (1) C 16	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
8. (1.99918) CR (1) C 17	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
9. (1.99905) CR (1) C 19	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
10. (1.99902) CR (1) C 21	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
11. (1.99890) CR (1) C 22	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
12. (1.99901) CR (1) C 23	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
13. (1.99891) CR (1) C 24	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
14. (1.99936) CR (1) C 25	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
15. (1.99939) CR (1) C 29	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
16. (1.99881) CR (1) C 33	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
17. (1.99906) CR (1) C 34	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
18. (1.99904) CR (1) C 35	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
19. (1.99911) CR (1) C 37	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
20. (1.99905) CR (1) C 38	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
21. (1.99904) CR (1) C 40	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
22. (1.99938) CR (1) C 41	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
23. (1.99939) CR (1) C 45	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
24. (1.99905) CR (1) B 49	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
25. (1.99950) CR (1) N 50	s(100.00%)				
	1.0000	0.0000	0.0000	0.0000	0.0000

					0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	(1.99977)	CR (1) O 51			s(100.00%)					
					1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	(1.02639)	LP (1) C 15			s(0.01%)p 1.00(99.98%)d 0.00(0.02%)					
					0.0000	0.0070	0.0038	0.0002	-0.0087	
					0.0051	-0.0570	-0.0004	0.9981	-0.0151	
					0.0014	-0.0103	-0.0065	0.0006	-0.0022	
28.	(1.02173)	LP (1) C 16			s(0.00%)p 1.00(99.98%)d 0.00(0.02%)					
					0.0000	0.0025	0.0008	0.0000	0.0468	
					0.0046	0.1505	0.0033	-0.9873	-0.0095	
					-0.0001	0.0018	0.0135	0.0012	0.0027	
29.	(0.99796)	LP (1) C 24			s(0.00%)p 1.00(100.00%)d 0.00(0.00%)					
					0.0000	0.0021	0.0000	0.0001	0.0244	
					0.0019	0.0975	0.0052	-0.9949	-0.0102	
					-0.0003	0.0026	0.0033	0.0005	0.0009	
30.	(1.87329)	LP (1) N 50			s(15.30%)p 5.53(84.68%)d 0.00(0.02%)					
					0.0000	0.3910	-0.0110	-0.0009	0.8239	
					-0.0314	-0.1892	0.0110	0.3619	-0.0115	
					0.0034	-0.0101	0.0007	-0.0093	0.0037	
31.	(1.96365)	LP (1) O 51			s(22.99%)p 3.34(76.87%)d 0.01(0.14%)					
					0.0000	0.4795	-0.0013	0.0007	0.5604	
					0.0036	0.6196	0.0117	0.2657	0.0042	
					-0.0276	-0.0147	-0.0158	0.0000	0.0124	
32.	(1.98821)	BD (1) C 1- H 2								
	(61.10%)	0.7817* C 1			s(24.81%)p 3.03(75.12%)d 0.00(0.07%)					
					0.0000	0.4981	0.0015	0.0000	0.1598	
					0.0126	-0.1067	-0.0065	-0.8450	0.0015	
					-0.0003	-0.0072	0.0050	-0.0005	0.0246	
	(38.90%)	0.6237* H 2			s(99.95%)p 0.00(0.05%)					
					0.9997	-0.0002	-0.0047	0.0032	0.0220	
33.	(1.98615)	BD (1) C 1- H 3								
	(61.17%)	0.7821* C 1			s(24.81%)p 3.03(75.12%)d 0.00(0.07%)					
					0.0000	0.4981	0.0016	0.0000	0.1557	
					0.0119	-0.7436	-0.0048	0.4170	-0.0060	
					-0.0059	0.0040	-0.0188	-0.0167	-0.0032	
	(38.83%)	0.6231* H 3			s(99.95%)p 0.00(0.05%)					
					0.9998	-0.0001	-0.0044	0.0190	-0.0098	
34.	(1.97905)	BD (1) C 1- H 4								
	(61.35%)	0.7833* C 1			s(24.66%)p 3.05(75.27%)d 0.00(0.07%)					
					0.0000	0.4965	0.0011	-0.0003	0.5222	
					0.0149	0.6177	-0.0002	0.3134	-0.0015	
					0.0200	0.0100	0.0116	-0.0045	-0.0072	
	(38.65%)	0.6217* H 4			s(99.95%)p 0.00(0.05%)					
					0.9998	0.0002	-0.0130	-0.0153	-0.0075	
35.	(1.98250)	BD (1) C 1- C 37								
	(49.81%)	0.7058* C 1			s(25.63%)p 2.90(74.33%)d 0.00(0.04%)					
					0.0000	0.5063	-0.0048	0.0006	-0.8227	
					0.0166	0.2308	-0.0072	0.1137	-0.0032	
					-0.0086	-0.0042	0.0015	0.0138	-0.0095	
	(50.19%)	0.7084* C 37			s(30.89%)p 2.24(69.07%)d 0.00(0.03%)					
					0.0000	0.5558	-0.0028	-0.0014	0.7904	
					-0.0073	-0.2310	0.0008	-0.1122	-0.0002	
					-0.0084	-0.0042	-0.0002	0.0139	-0.0070	
36.	(1.97648)	BD (1) C 5- H 6								
	(61.73%)	0.7857* C 5			s(25.17%)p 2.97(74.76%)d 0.00(0.07%)					
					0.0000	0.5016	0.0022	-0.0006	-0.0188	
					-0.0025	-0.5688	-0.0152	0.6508	-0.0039	
					0.0000	0.0007	-0.0224	-0.0109	0.0101	
	(38.27%)	0.6186* H 6			s(99.94%)p 0.00(0.06%)					
					0.9997	0.0008	0.0003	0.0161	-0.0177	
37.	(1.97657)	BD (1) C 5- H 7								
	(61.71%)	0.7856* C 5			s(25.16%)p 2.97(74.76%)d 0.00(0.07%)					
					0.0000	0.5016	0.0023	-0.0006	0.0161	
					-0.0026	-0.4214	-0.0155	-0.7547	0.0007	
					-0.0007	-0.0024	0.0190	-0.0065	0.0175	
	(38.29%)	0.6188* H 7			s(99.94%)p 0.00(0.06%)					
					0.9997	0.0008	-0.0006	0.0122	0.0210	
38.	(1.98165)	BD (1) C 5- C 8								
	(49.99%)	0.7070* C 5			s(24.29%)p 3.12(75.67%)d 0.00(0.04%)					
					0.0000	0.4928	-0.0006	0.0010	-0.7121	
					-0.0048	0.4980	-0.0217	0.0345	-0.0025	
					-0.0163	-0.0012	0.0012	0.0022	-0.0097	
	(50.01%)	0.7072* C 8			s(24.31%)p 3.11(75.65%)d 0.00(0.04%)					
					0.0000	0.4931	-0.0005	0.0011	0.6775	

					-0.0196	-0.5435	-0.0102	-0.0401	-0.0017
					-0.0149	-0.0010	0.0006	0.0069	-0.0096
39.	(1.97802)	BD (1) C	5- C 23		s(25.24%)	p 2.96(74.71%)	d 0.00(0.05%)		
	(49.43%)		0.7031* C	5	0.0000	0.5024	-0.0045	0.0007	0.7012
					0.0003	0.5001	-0.0218	0.0698	-0.0024
					0.0184	0.0025	0.0017	0.0053	-0.0098
	(50.57%)		0.7111* C	23	s(30.76%)	p 2.25(69.21%)	d 0.00(0.04%)		
					0.0000	0.5546	-0.0024	-0.0023	-0.5989
					0.0256	-0.5722	-0.0112	-0.0717	-0.0010
					0.0143	0.0022	0.0019	0.0057	-0.0111
40.	(1.97734)	BD (1) C	8- H 9		s(25.21%)	p 2.96(74.72%)	d 0.00(0.07%)		
	(61.65%)		0.7852* C	8	0.0000	0.5021	0.0026	-0.0005	-0.4595
					-0.0143	-0.0631	-0.0068	-0.7293	0.0009
					0.0020	0.0205	0.0011	0.0072	0.0153
	(38.35%)		0.6193* H	9	s(99.94%)	p 0.00(0.06%)			
					0.9997	0.0009	0.0132	0.0017	0.0203
41.	(1.97738)	BD (1) C	8- H 10		s(25.15%)	p 2.97(74.78%)	d 0.00(0.07%)		
	(61.67%)		0.7853* C	8	0.0000	0.5015	0.0022	-0.0006	-0.4955
					-0.0145	-0.2123	-0.0067	0.6759	-0.0031
					0.0065	-0.0206	-0.0074	0.0074	0.0119
	(38.33%)		0.6191* H	10	s(99.94%)	p 0.00(0.06%)			
					0.9997	0.0009	0.0141	0.0056	-0.0186
42.	(1.97800)	BD (1) C	8- C 21		s(25.19%)	p 2.97(74.77%)	d 0.00(0.05%)		
	(49.36%)		0.7026* C	8	0.0000	0.5018	-0.0050	0.0006	0.2891
					-0.0209	0.8092	-0.0068	0.0935	-0.0016
					0.0127	0.0014	0.0036	-0.0141	-0.0095
	(50.64%)		0.7116* C	21	s(31.01%)	p 2.22(68.96%)	d 0.00(0.04%)		
					0.0000	0.5568	-0.0028	-0.0022	-0.3880
					-0.0181	-0.7291	0.0188	-0.0823	0.0004
					0.0091	0.0013	0.0036	-0.0120	-0.0110
43.	(1.98204)	BD (1) C	11- H 12		s(31.49%)	p 2.17(68.45%)	d 0.00(0.06%)		
	(60.66%)		0.7789* C	11	0.0000	0.5611	-0.0025	-0.0035	-0.8231
					-0.0113	0.0805	0.0054	-0.0198	0.0002
					-0.0028	0.0011	0.0001	0.0205	-0.0138
	(39.34%)		0.6272* H	12	s(99.92%)	p 0.00(0.08%)			
					0.9996	-0.0013	0.0276	-0.0017	0.0006
44.	(1.97124)	BD (1) C	11- C 13		s(33.19%)	p 2.01(66.77%)	d 0.00(0.05%)		
	(49.81%)		0.7058* C	11	0.0000	0.5761	0.0027	0.0002	0.4570
					-0.0241	0.6717	0.0229	0.0808	0.0004
					0.0160	0.0022	0.0029	-0.0039	-0.0132
	(50.19%)		0.7084* C	13	s(33.89%)	p 1.95(66.06%)	d 0.00(0.05%)		
					0.0000	0.5822	0.0039	0.0024	-0.4619
					-0.0283	-0.6660	0.0144	-0.0512	-0.0004
					0.0154	0.0017	0.0024	-0.0061	-0.0138
45.	(1.97786)	BD (1) C	11- C 21		s(35.13%)	p 1.85(64.81%)	d 0.00(0.06%)		
	(49.27%)		0.7019* C	11	0.0000	0.5927	0.0016	0.0041	0.3339
					-0.0251	-0.7306	-0.0150	-	

				0.0000	0.5978	-0.0054	0.0012	0.4208
				0.0054	-0.6805	0.0134	-0.0393	0.0059
				-0.0176	-0.0021	0.0020	-0.0083	-0.0118
(50.73%)	0.7122*	C 22	s(33.64%)p 1.97(66.31%)d 0.00(0.05%)	0.0000	0.5800	0.0028	-0.0002	-0.3360
				0.0173	0.7398	0.0020	0.0515	0.0015
				-0.0160	-0.0007	0.0009	-0.0091	-0.0123
49. (1.98327)	BD (1)	C 15- N 50						
(39.52%)	0.6287*	C 15	s(27.40%)p 2.65(72.50%)d 0.00(0.10%)	0.0000	0.5233	0.0105	-0.0019	0.4382
				0.0188	0.7285	0.0102	0.0417	0.0108
				0.0237	0.0002	0.0012	-0.0122	-0.0176
(60.48%)	0.7777*	N 50	s(30.81%)p 2.24(69.11%)d 0.00(0.08%)	0.0000	0.5551	0.0024	-0.0003	-0.4282
				0.0009	-0.7123	-0.0126	0.0033	0.0101
				0.0255	-0.0003	0.0068	-0.0032	-0.0102
50. (1.97307)	BD (1)	C 16- C 17						
(50.58%)	0.7112*	C 16	s(32.47%)p 2.08(67.47%)d 0.00(0.06%)	0.0000	0.5695	0.0199	-0.0002	0.2046
				0.0144	-0.7875	-0.0270	-0.1088	-0.0046
				-0.0059	0.0005	0.0055	-0.0164	-0.0149
(49.42%)	0.7030*	C 17	s(35.57%)p 1.81(64.37%)d 0.00(0.06%)	0.0000	0.5964	-0.0010	0.0030	-0.2499
				0.0105	0.7579	0.0065	0.0818	-0.0009
				-0.0115	-0.0012	0.0048	-0.0143	-0.0138
51. (1.97270)	BD (1)	C 16- C 22						
(48.81%)	0.6987*	C 16	s(32.54%)p 2.07(67.40%)d 0.00(0.06%)	0.0000	0.5703	0.0110	0.0005	-0.7945
				-0.0100	0.2065	0.0070	-0.0047	-0.0012
				-0.0056	0.0006	0.0011	0.0182	-0.0148
(51.19%)	0.7154*	C 22	s(34.65%)p 1.88(65.31%)d 0.00(0.04%)	0.0000	0.5887	-0.0012	0.0000	0.8018
				-0.0047	-0.0987	0.0106	0.0178	0.0001
				-0.0063	-0.0001	0.0002	0.0141	-0.0115
52. (1.96899)	BD (1)	C 16- B 49						
(69.51%)	0.8337*	C 16	s(34.93%)p 1.86(65.05%)d 0.00(0.02%)	0.0000	0.5907	-0.0196	0.0000	0.5687
				-0.0376	0.5588	-0.0214	0.1135	-0.0043
				0.0106	0.0045	0.0029	0.0032	-0.0077
(30.49%)	0.5522*	B 49	s(37.05%)p 1.70(62.86%)d 0.00(0.09%)	0.0000	0.6086	-0.0059	0.0023	-0.6463
				-0.0145	-0.4218	-0.0285	-0.1788	-0.0050
				0.0257	0.0098	0.0016	0.0094	-0.0090
53. (1.97952)	BD (1)	C 17- H 18						
(60.94%)	0.7806*	C 17	s(31.07%)p 2.22(68.86%)d 0.00(0.07%)	0.0000	0.5574	-0.0009	-0.0036	0.8120
				0.0093	-0.1698	-0.0121	-0.0106	-0.0033
				-0.0092	-0.0004	0.0006	0.0197	-0.0148
(39.06%)	0.6250*	H 18	s(99.91%)p 0.00(0.09%)	0.9995	0.0019	-0.0300	0.0045	0.0006
54. (1.97533)	BD (1)	C 17- C 19						
(49.69%)	0.7049*	C 17	s(33.21%)p 2.01(66.74%)d 0.00(0.05%)	0.0000	0.5762	0.0029	0.0019	-0.5264
				0.0228	-0.6177	-0.0240	-0.0878	-0.0016
				0.0175	0.0024	0.0035	-0.0039	-0.0130
(50.31%)	0.7093*	C 19	s(33.15%)p 2.01(66.80%)d 0.00(0.05%)	0.0000	0.5758	0.0022	0.0003	0.5217
				0.0266	0.6232	-0.0161	0.0799	-0.0019
				0.0156	0.0021	0.0037	-0.0055	-0.0128
55. (1.98224)	BD (1)	C 19- H 20						
(60.69%)	0.7790*	C 19	s(31.78%)p 2.14(68.16%)d 0.00(0.06%)	0.0000	0.5637	-0.0018	-0.0034	0.3021
				0.0098	-0.7622	-0.0099	-0.0955	-0.0017
				-0.0129	-0.0015	0.0049	-0.0161	-0.0134
(39.31%)	0.6270*	H 20	s(99.93%)p 0.00(0.07%)	0.9996	-0.0012	-0.0090	0.0250	0.0031
56. (1.97820)	BD (1)	C 19- C 23						
(48.99%)	0.6999*	C 19	s(34.89%)p 1.86(65.05%)d 0.00(0.06%)	0.0000	0.5907	0.0014	0.0040	-0.7971
				-0.0070	0.1193	-0.0265	0.0150	-0.0030
				-0.0064	-0.0007	0.0009	0.0184	-0.0148
(51.01%)	0.7142*	C 23	s(37.44%)p 1.67(62.52%)d 0.00(0.05%)	0.0000	0.6118	0.0095	0.0013	0.7635
				0.0083	-0.2030	-0.0274	-0.0163	-0.0028
				-0.0054	-0.0006	0.0003	0.0169	-0.0118
57. (1.96876)	BD (1)	C 21- C 24						
(48.93%)	0.6995*	C 21	s(31.46%)p 2.18(68.48%)d 0.00(0.06%)					

				0.0000	0.5608	-0.0069	0.0013	0.8269
				-0.0033	-0.0148	0.0054	0.0284	0.0008
				0.0002	0.0012	0.0008	0.0182	-0.0150
	(51.07%)	0.7147*	C 24	s(32.61%)	p 2.07(67.34%)	d 0.00(0.05%)		
				0.0000	0.5710	0.0012	-0.0002	-0.8150
				0.0035	0.0958	0.0008	-0.0094	0.0007
				-0.0010	0.0010	0.0008	0.0176	-0.0140
58.	(1.96471)	BD (1)	C 22- C 24					
	(49.56%)	0.7040*	C 22	s(31.64%)	p 2.16(68.31%)	d 0.00(0.05%)		
				0.0000	0.5625	0.0010	0.0008	-0.4923
				0.0020	-0.6590	0.0027	-0.0801	0.0012
				0.0170	0.0026	0.0036	-0.0027	-0.0139
	(50.44%)	0.7102*	C 24	s(34.85%)	p 1.87(65.10%)	d 0.00(0.05%)		
				0.0000	0.5903	-0.0020	0.0008	0.4879
				-0.0037	0.6381	-0.0102	0.0757	-0.0003
				0.0171	0.0020	0.0030	-0.0044	-0.0131
59.	(1.96899)	BD (1)	C 23- C 24					
	(48.99%)	0.7000*	C 23	s(31.66%)	p 2.16(68.28%)	d 0.00(0.06%)		
				0.0000	0.5627	-0.0059	0.0013	-0.2402
				0.0039	0.7853	-0.0017	0.0919	-0.0002
				-0.0098	-0.0010	0.0044	-0.0153	-0.0148
	(51.01%)	0.7142*	C 24	s(32.49%)	p 2.08(67.46%)	d 0.00(0.05%)		
				0.0000	0.5700	0.0023	-0.0001	0.3110
				0.0018	-0.7574	0.0039	-0.0654	0.0002
				-0.0102	-0.0008	0.0038	-0.0144	-0.0140
60.	(1.98950)	BD (1)	C 25- H 26					
	(61.09%)	0.7816*	C 25	s(26.22%)	p 2.81(73.70%)	d 0.00(0.08%)		
				0.0000	0.5120	0.0001	-0.0002	0.3809
				0.0011	-0.6275	0.0136	-0.4449	-0.0086
				-0.0149	-0.0107	0.0195	-0.0076	-0.0040
	(38.91%)	0.6237*	H 26	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0003	-0.0099	0.0149	0.0125
61.	(1.98975)	BD (1)	C 25- H 27					
	(60.81%)	0.7798*	C 25	s(25.77%)	p 2.88(74.15%)	d 0.00(0.08%)		
				0.0000	0.5076	0.0015	-0.0003	0.5132
				0.0012	0.6894	-0.0046	0.0511	-0.0138
				0.0224	0.0012	0.0032	-0.0072	-0.0157
	(39.19%)	0.6260*	H 27	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0009	-0.0138	-0.0171	0.0006
62.	(1.99526)	BD (1)	C 25- H 28					
	(60.14%)	0.7755*	C 25	s(25.85%)	p 2.87(74.07%)	d 0.00(0.08%)		
				0.0000	0.5084	-0.0056	-0.0010	-0.7526
				0.0082	0.2125	0.0044	-0.3589	-0.0177
				-0.0111	0.0191	-0.0041	0.0160	-0.0074
	(39.86%)	0.6314*	H 28	s(99.95%)	p 0.00(0.05%)			
				0.9997	0.0042	0.0193	-0.0053	0.0108
63.	(1.97683)	BD (1)	C 25- N 50					
	(38.73%)	0.6223*	C 25	s(22.13%)	p 3.51(77.76%)	d 0.00(0.11%)		
				0.0000	0.4704	0.0092	0.0021	-0.1550
				0.0138	-0.2908	-0.0015	0.8177	0.0126
				0.0036	-0.0100	-0.0171	-0.0019	0.0258
	(61.27%)	0.7828*	N 50	s(25.99%)	p 2.85(73.95%)	d 0.00(0.07%)		
				0.0000	0.5097	0.0049	0.0011	0.1720
				0.0194	0.2893	0.0126	-0.7907	-0.0208
				0.0004	0.0031	-0.0115	-0.0075	0.0213
64.	(1.99491)	BD (1)	C 29- H 30					
	(59.92%)	0.7741*	C 29	s(25.65%)	p 2.89(74.26%)	d 0.00(0.08%)		
				0.0000	0.5064	-0.0069	-0.0010	-0.6741
				-0.0032	0.3305	0.0165	-0.4225	0.0136
				-0.0145	0.0182	-0.0109	0.0120	-0.0046
	(40.08%)	0.6331*	H 30	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0040	0.0174	-0.0096	0.0093
65.	(1.98947)	BD (1)	C 29- H 31					
	(61.05%)	0.7813*	C 29	s(26.13%)	p 2.82(73.79%)	d 0.00(0.08%)		
				0.0000	0.5111	0.0025	-0.0001	0.5997
				-0.0100	0.6018	-0.0004	0.1265	0.0109
				0.0248	0.0056	0.0033	-0.0009	-0.0120
	(38.95%)	0.6241*	H 31	s(99.95%)	p 0.00(0.05%)			
				0.9998	0.0008	-0.0145	-0.0156	-0.0047
66.	(1.99025)	BD (1)	C 29- H 32					
	(61.13%)	0.7819*	C 29	s(25.97%)	p 2.85(73.95%)	d 0.00(0.08%)		
				0.0000	0.5096	-0.0006	-0.0003	-0.2524
				0.0037	-0.3385	0.0161	0.7490	0.0035
				0.0070	-0.0114	-0.0168	-0.0003	0.0174
	(38.87%)	0.6235*	H 32	s(99.95%)	p 0.00(0.05%)			
				0.9997	0.0004	0.0067	0.0075	-0.0203
67.	(1.98568)	BD (1)	C 29- N 50					

	(38.83%)	0.6232*	C 29	s(22.22%)p 3.50(77.68%)d 0.00(0.11%)	0.0000	0.4712	0.0106	0.0021	0.3475
					0.0208	-0.6421	-0.0062	-0.4932	0.0038
					-0.0153	-0.0124	0.0236	-0.0109	0.0001
	(61.17%)	0.7821*	N 50	s(27.87%)p 2.59(72.06%)d 0.00(0.06%)	0.0000	0.5279	0.0068	0.0005	-0.3261
					0.0126	0.6095	0.0146	0.4919	0.0223
					-0.0157	-0.0148	0.0095	-0.0052	-0.0080
68. (1.96778)	BD (1) C 33- C 34								
	(50.52%)	0.7108*	C 33	s(33.66%)p 1.97(66.28%)d 0.00(0.06%)	0.0000	0.5800	0.0143	0.0004	0.4087
					0.0089	-0.3501	-0.0064	0.6105	0.0198
					-0.0112	0.0132	-0.0137	0.0049	0.0074
	(49.48%)	0.7034*	C 34	s(35.02%)p 1.85(64.94%)d 0.00(0.05%)	0.0000	0.5918	0.0011	0.0009	-0.4322
					-0.0088	0.3429	0.0024	-0.5872	0.0067
					-0.0087	0.0124	-0.0123	0.0029	0.0085
69. (1.96750)	BD (1) C 33- C 40								
	(50.51%)	0.7107*	C 33	s(33.69%)p 1.97(66.25%)d 0.00(0.06%)	0.0000	0.5803	0.0143	0.0005	0.3586
					0.0089	0.1246	0.0039	-0.7196	-0.0215
					-0.0005	-0.0162	-0.0066	0.0072	0.0149
	(49.49%)	0.7035*	C 40	s(34.98%)p 1.86(64.97%)d 0.00(0.05%)	0.0000	0.5915	0.0013	0.0011	-0.3852
					-0.0115	-0.1206	0.0052	0.6976	-0.0035
					0.0010	-0.0139	-0.0068	0.0048	0.0144
70. (1.96259)	BD (1) C 33- B 49								
	(68.31%)	0.8265*	C 33	s(32.54%)p 2.07(67.44%)d 0.00(0.03%)	0.0000	0.5700	-0.0204	-0.0005	-0.7824
					0.0445	0.2204	-0.0062	0.1082	-0.0019
					-0.0077	-0.0035	-0.0015	0.0125	-0.0048
	(31.69%)	0.5629*	B 49	s(34.88%)p 1.86(65.04%)d 0.00(0.08%)	0.0000	0.5905	-0.0111	0.0033	0.7546
					0.0049	-0.2702	0.0244	-0.0851	-0.0008
					-0.0159	-0.0070	-0.0014	0.0208	-0.0087
71. (1.97437)	BD (1) C 34- C 35								
	(50.12%)	0.7079*	C 34	s(34.38%)p 1.91(65.57%)d 0.00(0.05%)	0.0000	0.5864	0.0030	0.0008	0.7694
					0.0081	-0.2270	-0.0090	-0.1079	0.0182
					-0.0103	-0.0059	0.0005	0.0163	-0.0083
	(49.88%)	0.7063*	C 35	s(34.63%)p 1.89(65.32%)d 0.00(0.05%)	0.0000	0.5884	0.0014	0.0023	-0.7645
					-0.0008	0.2301	-0.0082	0.1230	0.0240
					-0.0119	-0.0055	-0.0007	0.0171	-0.0081
72. (1.98268)	BD (1) C 34- C 41								
	(50.21%)	0.7086*	C 34	s(30.53%)p 2.27(69.43%)d 0.00(0.04%)	0.0000	0.5525	-0.0026	-0.0012	-0.3542
					0.0074	-0.1264	-0.0016	0.7436	-0.0007
					0.0008	-0.0118	-0.0051	0.0038	0.0137
	(49.79%)	0.7056*	C 41	s(25.67%)p 2.89(74.29%)d 0.00(0.04%)	0.0000	0.5067	-0.0060	0.0016	0.3612
					-0.0047	0.1225	-0.0068	-0.7727	0.0170
					0.0021	-0.0128	-0.0041	0.0023	0.0139
73. (1.98085)	BD (1) C 35- H 36								
	(60.13%)	0.7754*	C 35	s(30.54%)p 2.27(69.39%)d 0.00(0.07%)	0.0000	0.5526	-0.0021	-0.0042	0.4154
					0.0059	-0.3666	-0.0058	0.6219	0.0088
					-0.0108	0.0160	-0.0154	0.0029	0.0092
	(39.87%)	0.6315*	H 36	s(99.93%)p 0.00(0.07%)	0.9997	-0.0015	-0.0129	0.0110	-0.0193
74. (1.97484)	BD (1) C 35- C 37								
	(49.94%)	0.7067*	C 35	s(34.67%)p 1.88(65.27%)d 0.00(0.06%)	0.0000	0.5888	0.0024	0.0028	0.3747
					0.0241	0.1153	-0.0102	-0.7059	0.0062
					0.0004	-0.0156	-0.0067	0.0061	0.0153
	(50.06%)	0.7075*	C 37	s(34.56%)p 1.89(65.39%)d 0.00(0.05%)	0.0000	0.5879	0.0020	0.0009	-0.3501
					0.0122	-0.1319	-0.0083	0.7166	0.0136
					0.0009	-0.0151	-0.0053	0.0058	0.0139
75. (1.97473)	BD (1) C 37- C 38								
	(50.08%)	0.7077*	C 37	s(34.49%)p 1.90(65.46%)d 0.00(0.05%)	0.0000	0.5873	0.0022	0.0008	-0.3955
					0.0120	0.3555	0.0023	-0.6094	-0.0178
					-0.0097	0.0129	-0.0128	0.0033	0.0064
	(49.92%)	0.7065*	C 38	s(34.59%)p 1.89(65.35%)d 0.00(0.06%)	0.0000	0.5881	0.0029	0.0027	0.4207
					0.0230	-0.3552	-0.0030	0.5913	-0.0130

					-0.0102	0.0133	-0.0141	0.0039	0.0080
76.	(1.98106)	BD (1) C 38- H 39							
	(60.12%)	0.7754* C 38	s(30.65%)p 2.26(69.28%)d 0.00(0.07%)		0.0000	0.5536	-0.0026	-0.0042	0.3704
					0.0075	0.1366	0.0025	-0.7326	-0.0114
					0.0021	-0.0176	-0.0073	0.0053	0.0172
	(39.88%)	0.6315* H 39	s(99.93%)p 0.00(0.07%)		0.9996	-0.0014	-0.0117	-0.0045	0.0234
77.	(1.97431)	BD (1) C 38- C 40							
	(49.81%)	0.7057* C 38	s(34.60%)p 1.89(65.35%)d 0.00(0.05%)		0.0000	0.5882	0.0014	0.0023	-0.7686
					-0.0020	0.2289	0.0072	0.0990	-0.0211
					-0.0113	-0.0056	-0.0008	0.0174	-0.0082
	(50.19%)	0.7085* C 40	s(34.64%)p 1.89(65.32%)d 0.00(0.05%)		0.0000	0.5885	0.0019	0.0010	0.7698
					0.0067	-0.2177	0.0056	-0.1116	-0.0238
					-0.0106	-0.0042	-0.0002	0.0161	-0.0089
78.	(1.98258)	BD (1) C 40- C 45							
	(50.02%)	0.7072* C 40	s(30.30%)p 2.30(69.66%)d 0.00(0.04%)		0.0000	0.5505	-0.0019	-0.0014	-0.4105
					0.0112	0.3604	-0.0018	-0.6310	0.0010
					-0.0076	0.0111	-0.0114	0.0022	0.0075
	(49.98%)	0.7070* C 45	s(25.67%)p 2.89(74.29%)d 0.00(0.04%)		0.0000	0.5067	-0.0053	0.0019	0.4240
					-0.0037	-0.3764	0.0083	0.6489	-0.0159
					-0.0071	0.0126	-0.0111	0.0007	0.0066
79.	(1.97768)	BD (1) C 41- H 42							
	(61.58%)	0.7847* C 41	s(24.57%)p 3.07(75.36%)d 0.00(0.07%)		0.0000	0.4956	0.0010	-0.0006	0.0817
					-0.0036	0.7202	0.0006	0.4774	0.0153
					0.0035	0.0034	0.0208	-0.0157	-0.0024
	(38.42%)	0.6198* H 42	s(99.95%)p 0.00(0.05%)		0.9998	0.0004	-0.0017	-0.0184	-0.0119
80.	(1.98754)	BD (1) C 41- H 43							
	(61.08%)	0.7815* C 41	s(24.78%)p 3.03(75.15%)d 0.00(0.07%)		0.0000	0.4977	0.0035	-0.0001	0.3938
					-0.0100	-0.6566	-0.0015	0.4064	0.0106
					-0.0163	0.0103	-0.0157	-0.0086	-0.0057
	(38.92%)	0.6239* H 43	s(99.96%)p 0.00(0.04%)		0.9998	-0.0001	-0.0084	0.0159	-0.0101
81.	(1.98234)	BD (1) C 41- H 44							
	(61.19%)	0.7822* C 41	s(24.88%)p 3.02(75.05%)d 0.00(0.07%)		0.0000	0.4988	0.0009	-0.0005	-0.8408
					-0.0035	-0.1849	-0.0084	-0.0950	0.0162
					0.0090	0.0063	0.0015	0.0200	-0.0130
	(38.81%)	0.6230* H 44	s(99.95%)p 0.00(0.05%)		0.9997	0.0005	0.0222	0.0054	0.0010
82.	(1.98932)	BD (1) C 45- H 46							
	(61.13%)	0.7819* C 45	s(24.86%)p 3.02(75.07%)d 0.00(0.07%)		0.0000	0.4985	0.0040	-0.0001	0.5041
					-0.0117	0.0248	0.0064	-0.7041	-0.0072
					0.0011	-0.0223	-0.0002	0.0076	0.0124
	(38.87%)	0.6234* H 46	s(99.96%)p 0.00(0.04%)		0.9998	-0.0002	-0.0113	-0.0009	0.0173
83.	(1.97998)	BD (1) C 45- H 47							
	(61.43%)	0.7837* C 45	s(24.70%)p 3.05(75.23%)d 0.00(0.07%)		0.0000	0.4970	0.0009	-0.0005	-0.2187
					0.0002	0.8088	0.0109	0.2238	-0.0130
					-0.0101	-0.0040	0.0117	-0.0180	-0.0108
	(38.57%)	0.6211* H 47	s(99.95%)p 0.00(0.05%)		0.9997	0.0007	0.0052	-0.0217	-0.0056
84.	(1.98057)	BD (1) C 45- H 48							
	(61.27%)	0.7828* C 45	s(24.67%)p 3.05(75.25%)d 0.00(0.07%)		0.0000	0.4967	-0.0001	-0.0008	-0.7193
					-0.0045	-0.4502	0.0007	-0.1791	-0.0186
					0.0203	0.0066	0.0054	0.0095	-0.0121
	(38.73%)	0.6223* H 48	s(99.95%)p 0.00(0.05%)		0.9998	0.0006	0.0180	0.0114	0.0052
85.	(1.99077)	BD (1) B 49- O 51							
	(19.48%)	0.4414* B 49	s(28.09%)p 2.55(71.60%)d 0.01(0.31%)		0.0000	0.5289	0.0331	-0.0069	-0.0989
					0.0185	0.7919	0.0384	0.2769	0.0226
					-0.0112	-0.0024	0.0275	-0.0458	-0.0106
	(80.52%)	0.8973* O 51	s(46.09%)p 1.17(53.70%)d 0.00(0.21%)		0.0000	0.6789	-0.0075	-0.0013	0.2483
					-0.0002	-0.6476	0.0025	-0.2366	-0.0001
					-0.0013	0.0015	0.0273	-0.0340	-0.0120

86. (1.98582) BD (2) B 49- O 51
(12.49%) 0.3534* B 49 s(0.02%)p99.99(99.56%)d23.29(0.42%)
0.0000 0.0128 0.0021 -0.0033 -0.0268
0.0055 -0.3387 0.0208 0.9361 -0.0583
-0.0034 -0.0121 0.0470 0.0236 0.0356
(87.51%) 0.9355* O 51 s(0.21%)p99.99(99.62%)d 0.82(0.17%)
0.0000 0.0458 0.0017 -0.0002 -0.1109
-0.0001 -0.3355 -0.0030 0.9334 0.0087
0.0110 -0.0220 -0.0203 -0.0080 -0.0253

87. (1.98514) BD (1) O 51- H 52
(76.72%) 0.8759* O 51 s(30.66%)p 2.25(69.12%)d 0.01(0.22%)
0.0000 0.5536 0.0122 0.0004 -0.7800
0.0195 0.2856 -0.0236 -0.0171 -0.0029
0.0005 0.0161 -0.0008 0.0391 -0.0202
(23.28%) 0.4825* H 52 s(99.86%)p 0.00(0.14%)
0.9992 0.0133 0.0363 -0.0074 0.0075

88. (1.93892) 3C (1) C 11- C 13- C 21
(50.75%) 0.7124* C 11 s(0.01%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0093 -0.0004 0.0002 0.0386
-0.0007 0.0854 0.0003 -0.9953 0.0170
0.0010 -0.0148 0.0055 0.0010 -0.0002
(20.43%) 0.4520* C 13 s(0.01%)p 1.00(99.92%)d 0.00(0.08%)
0.0000 0.0076 -0.0010 0.0001 0.0262
0.0011 0.0651 0.0025 -0.9971 0.0043
-0.0017 0.0120 0.0245 0.0015 0.0037
(28.82%) 0.5368* C 21 s(0.00%)p 1.00(99.92%)d 0.00(0.08%)
0.0000 -0.0009 0.0003 0.0000 0.0364
0.0000 0.0923 0.0039 -0.9947 0.0023
0.0007 0.0052 -0.0266 -0.0026 -0.0035

89. (1.93671) 3C (1) C 17- C 19- C 23
(19.24%) 0.4387* C 17 s(0.01%)p 1.00(99.91%)d 0.00(0.08%)
0.0000 0.0078 -0.0012 0.0001 -0.0173
-0.0020 -0.1189 -0.0035 0.9923 -0.0041
0.0025 -0.0212 -0.0192 -0.0025 -0.0045
(50.72%) 0.7122* C 19 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 -0.0011 -0.0012 0.0001 -0.0009
-0.0004 -0.1254 0.0012 0.9918 -0.0172
0.0012 -0.0102 0.0123 0.0015 0.0028
(30.04%) 0.5481* C 23 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)
0.0000 -0.0019 -0.0002 -0.0001 -0.0085
-0.0006 -0.1174 -0.0003 0.9927 -0.0043
-0.0035 0.0269 0.0026 0.0001 0.0005

90. (1.91803) 3C (1) C 33- C 38- C 40
(24.22%) 0.4922* C 33 s(0.01%)p 1.00(99.92%)d 0.00(0.07%)
0.0000 0.0051 0.0060 -0.0007 0.3008
0.0106 0.9012 0.0128 0.3102 0.0079
0.0151 -0.0012 -0.0180 0.0049 -0.0108
(27.04%) 0.5200* C 38 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)
0.0000 -0.0016 -0.0009 0.0004 0.3069
0.0025 0.8956 -0.0096 0.3210 -0.0029
-0.0185 -0.0051 0.0075 -0.0110 0.0036
(48.74%) 0.6981* C 40 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0014 0.0037 -0.0003 0.2996
0.0015 0.8987 -0.0072 0.3197 0.0026
0.0057 0.0063 0.0076 0.0091 0.0065

91. (1.94121) 3C (1) C 34- C 35- C 37
(23.99%) 0.4898* C 34 s(0.00%)p 1.00(99.91%)d 0.00(0.08%)
0.0000 0.0000 0.0045 -0.0005 0.3081
0.0052 0.9023 -0.0037 0.3001 0.0034
0.0215 0.0061 -0.0104 0.0145 -0.0040
(51.54%) 0.7179* C 35 s(0.00%)p 1.00(99.98%)d 0.00(0.02%)
0.0000 -0.0009 -0.0024 0.0002 0.3189
-0.0026 0.8938 -0.0151 0.3146 -0.0049
-0.0040 -0.0052 -0.0072 -0.0066 -0.0053
(24.48%) 0.4947* C 37 s(0.00%)p 1.00(99.92%)d 0.00(0.08%)
0.0000 -0.0033 0.0013 -0.0002 0.3093
0.0018 0.8955 -0.0067 0.3185 0.0023
-0.0164 0.0020 0.0195 -0.0037 0.0126

92. (1.03812) 3Cn(1) C 33- C 38- C 40
(51.17%) 0.7153* C 33 s(0.01%)p 1.00(99.92%)d 0.00(0.07%)
0.0000 0.0051 0.0060 -0.0007 0.3008
0.0106 0.9012 0.0128 0.3102 0.0079
0.0151 -0.0012 -0.0180 0.0049 -0.0108
(48.81%) 0.6986* C 38 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)
0.0000 0.0016 0.0009 -0.0004 -0.3069
-0.0025 -0.8956 0.0096 -0.3210 0.0029
0.0185 0.0051 -0.0075 0.0110 -0.0036

	(0.03%)	0.0160*	C 40	s (0.00%)p 1.00(99.97%)d 0.00(0.03%)
				0.0000 0.0014 0.0037 -0.0003 0.2996
				0.0015 0.8987 -0.0072 0.3197 0.0026
				0.0057 0.0063 0.0076 0.0091 0.0065
----- non-Lewis -----				
93.	(0.98571) LV (1) C 22			s (0.00%)p 1.00(99.99%)d 0.00(0.00%)
				0.0000 0.0047 0.0016 0.0001 -0.0366
				-0.0008 -0.0897 -0.0012 0.9952 0.0088
				-0.0003 -0.0054 -0.0012 -0.0005 -0.0014
94.	(0.00549) BD*(1) C 1- H 2			
	(38.90%)	0.6237*	C 1	s (24.81%)p 3.03(75.12%)d 0.00(0.07%)
				0.0000 -0.4981 -0.0015 0.0000 -0.1598
				-0.0126 0.1067 0.0065 0.8450 -0.0015
				0.0003 0.0072 -0.0050 0.0005 -0.0246
	(61.10%)	-0.7817*	H 2	s (99.95%)p 0.00(0.05%)
				-0.9997 0.0002 0.0047 -0.0032 -0.0220
95.	(0.00623) BD*(1) C 1- H 3			
	(38.83%)	0.6231*	C 1	s (24.81%)p 3.03(75.12%)d 0.00(0.07%)
				0.0000 -0.4981 -0.0016 0.0000 -0.1557
				-0.0119 0.7436 0.0048 -0.4170 0.0060
				0.0059 -0.0040 0.0188 0.0167 0.0032
	(61.17%)	-0.7821*	H 3	s (99.95%)p 0.00(0.05%)
				-0.9998 0.0001 0.0044 -0.0190 0.0098
96.	(0.00863) BD*(1) C 1- H 4			
	(38.65%)	0.6217*	C 1	s (24.66%)p 3.05(75.27%)d 0.00(0.07%)
				0.0000 -0.4965 -0.0011 0.0003 -0.5222
				-0.0149 -0.6177 0.0002 -0.3134 0.0015
				-0.0200 -0.0100 -0.0116 0.0045 0.0072
	(61.35%)	-0.7833*	H 4	s (99.95%)p 0.00(0.05%)
				-0.9998 -0.0002 0.0130 0.0153 0.0075
97.	(0.01679) BD*(1) C 1- C 37			
	(50.19%)	0.7084*	C 1	s (25.63%)p 2.90(74.33%)d 0.00(0.04%)
				0.0000 -0.5063 0.0048 -0.0006 0.8227
				-0.0166 -0.2308 0.0072 -0.1137 0.0032
				0.0086 0.0042 -0.0015 -0.0138 0.0095
	(49.81%)	-0.7058*	C 37	s (30.89%)p 2.24(69.07%)d 0.00(0.03%)
				0.0000 -0.5558 0.0028 0.0014 -0.7904
				0.0073 0.2310 -0.0008 0.1122 0.0002
				0.0084 0.0042 0.0002 -0.0139 0.0070
98.	(0.01041) BD*(1) C 5- H 6			
	(38.27%)	0.6186*	C 5	s (25.17%)p 2.97(74.76%)d 0.00(0.07%)
				0.0000 -0.5016 -0.0022 0.0006 0.0188
				0.0025 0.5688 0.0152 -0.6508 0.0039
				0.0000 -0.0007 0.0224 0.0109 -0.0101
	(61.73%)	-0.7857*	H 6	s (99.94%)p 0.00(0.06%)
				-0.9997 -0.0008 -0.0003 -0.0161 0.0177
99.	(0.01032) BD*(1) C 5- H 7			
	(38.29%)	0.6188*	C 5	s (25.16%)p 2.97(74.76%)d 0.00(0.07%)
				0.0000 -0.5016 -0.0023 0.0006 -0.0161
				0.0026 0.4214 0.0155 0.7547 -0.0007
				0.0007 0.0024 -0.0190 0.0065 -0.0175
	(61.71%)	-0.7856*	H 7	s (99.94%)p 0.00(0.06%)
				-0.9997 -0.0008 0.0006 -0.0122 -0.0210
100.	(0.00817) BD*(1) C 5- C 8			
	(50.01%)	0.7072*	C 5	s (24.29%)p 3.12(75.67%)d 0.00(0.04%)
				0.0000 -0.4928 0.0006 -0.0010 0.7121
				0.0048 -0.4980 0.0217 -0.0345 0.0025
				0.0163 0.0012 -0.0012 -0.0022 0.0097
	(49.99%)	-0.7070*	C 8	s (24.31%)p 3.11(75.65%)d 0.00(0.04%)
				0.0000 -0.4931 0.0005 -0.0011 -0.6775
				0.0196 0.5435 0.0102 0.0401 0.0017
				0.0149 0.0010 -0.0006 -0.0069 0.0096
101.	(0.02344) BD*(1) C 5- C 23			
	(50.57%)	0.7111*	C 5	s (25.24%)p 2.96(74.71%)d 0.00(0.05%)
				0.0000 -0.5024 0.0045 -0.0007 -0.7012
				-0.0003 -0.5001 0.0218 -0.0698 0.0024
				-0.0184 -0.0025 -0.0017 -0.0053 0.0098
	(49.43%)	-0.7031*	C 23	s (30.76%)p 2.25(69.21%)d 0.00(0.04%)
				0.0000 -0.5546 0.0024 0.0023 0.5989
				-0.0256 0.5722 0.0112 0.0717 0.0010
				-0.0143 -0.0022 -0.0019 -0.0057 0.0111
102.	(0.01059) BD*(1) C 8- H 9			
	(38.35%)	0.6193*	C 8	s (25.21%)p 2.96(74.72%)d 0.00(0.07%)
				0.0000 -0.5021 -0.0026 0.0005 0.4595
				0.0143 0.0631 0.0068 0.7293 -0.0009
				-0.0020 -0.0205 -0.0011 -0.0072 -0.0153
	(61.65%)	-0.7852*	H 9	s (99.94%)p 0.00(0.06%)

					-0.9997	-0.0009	-0.0132	-0.0017	-0.0203
103.	(0.01072)	BD*(1) C 8-	H 10	s(25.15%)p 2.97(74.78%)d 0.00(0.07%)	0.0000	-0.5015	-0.0022	0.0006	0.4955
	(38.33%)	0.6191*	C 8	0.0145 0.2123 0.0067 -0.6759 0.0031	-0.0065	0.0206	0.0074	-0.0074	-0.0119
	(61.67%)	-0.7853*	H 10	s(99.94%)p 0.00(0.06%)	-0.9997	-0.0009	-0.0141	-0.0056	0.0186
104.	(0.02294)	BD*(1) C 8-	C 21	s(25.19%)p 2.97(74.77%)d 0.00(0.05%)	0.0000	-0.5018	0.0050	-0.0006	-0.2891
	(50.64%)	0.7116*	C 8	0.0209 -0.8092 0.0068 -0.0935 0.0016	-0.0127	-0.0014	-0.0036	0.0141	0.0095
	(49.36%)	-0.7026*	C 21	s(31.01%)p 2.22(68.96%)d 0.00(0.04%)	0.0000	-0.5568	0.0028	0.0022	0.3880
				0.0181 0.7291 -0.0188 0.0823 -0.0004	-0.0091	-0.0013	-0.0036	0.0120	0.0110
105.	(0.01318)	BD*(1) C 11-	H 12	s(31.49%)p 2.17(68.45%)d 0.00(0.06%)	0.0000	-0.5611	0.0025	0.0035	0.8231
	(39.34%)	0.6272*	C 11	0.0113 -0.0805 -0.0054 0.0198 -0.0002	0.0028	-0.0011	-0.0001	-0.0205	0.0138
	(60.66%)	-0.7789*	H 12	s(99.92%)p 0.00(0.08%)	-0.9996	0.0013	-0.0276	0.0017	-0.0006
106.	(0.01687)	BD*(1) C 11-	C 13	s(33.19%)p 2.01(66.77%)d 0.00(0.05%)	0.0000	-0.5761	-0.0027	-0.0002	-0.4570
	(50.19%)	0.7084*	C 11	0.0241 -0.6717 -0.0229 -0.0808 -0.0004	-0.0160	-0.0022	-0.0029	0.0039	0.0132
	(49.81%)	-0.7058*	C 13	s(33.89%)p 1.95(66.06%)d 0.00(0.05%)	0.0000	-0.5822	-0.0039	-0.0024	0.4619
				0.0283 0.6660 -0.0144 0.0512 0.0004	-0.0154	-0.0017	-0.0024	0.0061	0.0138
107.	(0.02229)	BD*(1) C 11-	C 21	s(35.13%)p 1.85(64.81%)d 0.00(0.06%)	0.0000	-0.5927	-0.0016	-0.0041	-0.3339
	(50.73%)	0.7123*	C 11	0.0251 0.7306 0.0150 0.0442 0.0013	0.0149	0.0007	-0.0025	0.0118	0.0149
	(49.27%)	-0.7019*	C 21	s(37.40%)p 1.67(62.56%)d 0.00(0.05%)	0.0000	-0.6114	-0.0107	-0.0013	0.4042
				0.0281 -0.6776 0.0002 -0.0475 0.0004	0.0133	0.0007	-0.0022	0.0118	0.0118
108.	(0.01140)	BD*(1) C 13-	H 14	s(31.19%)p 2.20(68.75%)d 0.00(0.07%)	0.0000	-0.5584	-0.0004	0.0040	0.3683
	(39.51%)	0.6285*	C 13	0.0184 -0.7413 -0.0087 -0.0430 0.0004	0.0165	0.0008	-0.0026	0.0134	0.0151
	(60.49%)	-0.7778*	H 14	s(99.93%)p 0.00(0.07%)	-0.9996	-0.0010	-0.0123	0.0241	0.0012
109.	(0.02620)	BD*(1) C 13-	C 15	s(34.73%)p 1.88(65.21%)d 0.00(0.06%)	0.0000	-0.5893	0.0024	-0.0028	-0.8057
	(50.21%)	0.7086*	C 13	-0.0018 0.0451 -0.0179 -0.0228 -0.0024	0.0021	-0.0019	-0.0007	-0.0190	0.0151
	(49.79%)	-0.7056*	C 15	s(36.75%)p 1.72(63.20%)d 0.00(0.05%)	0.0000	-0.6062	-0.0010	-0.0004	0.7936
				0.0083 -0.0425 -0.0147 0.0087 -0.0002	0.0015	-0.0017	-0.0004	-0.0186	0.0111
110.	(0.03252)	BD*(1) C 15-	C 22	s(35.74%)p 1.80(64.20%)d 0.00(0.05%)	0.0000	0.5978	-0.0054	0.0012	0.4208
	(50.73%)	0.7122*	C 15	0.0054 -0.6805 0.0134 -0.0393 0.0059	-0.0176	-0.0021	0.0020	-0.0083	-0.0118
	(49.27%)	-0.7019*	C 22	s(33.64%)p 1.97(66.31%)d 0.00(0.05%)	0.0000	0.5800	0.0028	-0.0002	-0.3360
				0.0173 0.7398 0.0020 0.0515 0.0015	-0.0160	-0.0007	0.0009	-0.0091	-0.0123
111.	(0.03061)	BD*(1) C 15-	N 50	s(27.40%)p 2.65(72.50%)d 0.00(0.10%)	0.0000	0.5233	0.0105	-0.0019	0.4382
	(60.48%)	0.7777*	C 15	0.0188 0.7285 0.0102 0.0417 0.0108	0.0237	0.0002	0.0012	-0.0122	-0.0176
	(39.52%)	-0.6287*	N 50	s(30.81%)p 2.24(69.11%)d 0.00(0.08%)	0.0000	0.5551	0.0024	-0.0003	-0.4282
				0.0009 -0.7123 -0.0126 0.0033 0.0101	0.0255	-0.0003	0.0068	-0.0032	-0.0102
112.	(0.01886)	BD*(1) C 16-	C 17						

	(49.42%)	0.7030*	C 16	s(32.47%)p 2.08(67.47%)d 0.00(0.06%)	0.0000 -0.5695 -0.0199 0.0002 -0.2046	-0.0144 0.7875 0.0270 0.1088 0.0046	0.0059 -0.0005 -0.0055 0.0164 0.0149
	(50.58%)	-0.7112*	C 17	s(35.57%)p 1.81(64.37%)d 0.00(0.06%)	0.0000 -0.5964 0.0010 -0.0030 0.2499	-0.0105 -0.7579 -0.0065 -0.0818 0.0009	0.0115 0.0012 -0.0048 0.0143 0.0138
113. (0.03090)	BD*(1) C 16- C 22						
	(51.19%)	0.7154*	C 16	s(32.54%)p 2.07(67.40%)d 0.00(0.06%)	0.0000 -0.5703 -0.0110 -0.0005 0.7945	0.0100 -0.2065 -0.0070 0.0047 0.0012	0.0056 -0.0006 -0.0011 -0.0182 0.0148
	(48.81%)	-0.6987*	C 22	s(34.65%)p 1.88(65.31%)d 0.00(0.04%)	0.0000 -0.5887 0.0012 0.0000 -0.8018	0.0047 0.0987 -0.0106 -0.0178 -0.0001	0.0063 0.0001 -0.0002 -0.0141 0.0115
114. (0.03427)	BD*(1) C 16- B 49						
	(30.49%)	0.5522*	C 16	s(34.93%)p 1.86(65.05%)d 0.00(0.02%)	0.0000 -0.5907 0.0196 0.0000 -0.5687	0.0376 -0.5588 0.0214 -0.1135 0.0043	-0.0106 -0.0045 -0.0029 -0.0032 0.0077
	(69.51%)	-0.8337*	B 49	s(37.05%)p 1.70(62.86%)d 0.00(0.09%)	0.0000 -0.6086 0.0059 -0.0023 0.6463	0.0145 0.4218 0.0285 0.1788 0.0050	-0.0257 -0.0098 -0.0016 -0.0094 0.0090
115. (0.01240)	BD*(1) C 17- H 18						
	(39.06%)	0.6250*	C 17	s(31.07%)p 2.22(68.86%)d 0.00(0.07%)	0.0000 -0.5574 0.0009 0.0036 -0.8120	-0.0093 0.1698 0.0121 0.0106 0.0033	0.0092 0.0004 -0.0006 -0.0197 0.0148
	(60.94%)	-0.7806*	H 18	s(99.91%)p 0.00(0.09%)	-0.9995 -0.0019 0.0300 -0.0045 -0.0006		
116. (0.02078)	BD*(1) C 17- C 19						
	(50.31%)	0.7093*	C 17	s(33.21%)p 2.01(66.74%)d 0.00(0.05%)	0.0000 0.5762 0.0029 0.0019 -0.5264	0.0228 -0.6177 -0.0240 -0.0878 -0.0016	0.0175 0.0024 0.0035 -0.0039 -0.0130
	(49.69%)	-0.7049*	C 19	s(33.15%)p 2.01(66.80%)d 0.00(0.05%)	0.0000 0.5758 0.0022 0.0003 0.5217	0.0266 0.6232 -0.0161 0.0799 -0.0019	0.0156 0.0021 0.0037 -0.0055 -0.0128
117. (0.01299)	BD*(1) C 19- H 20						
	(39.31%)	0.6270*	C 19	s(31.78%)p 2.14(68.16%)d 0.00(0.06%)	0.0000 -0.5637 0.0018 0.0034 -0.3021	-0.0098 0.7622 0.0099 0.0955 0.0017	0.0129 0.0015 -0.0049 0.0161 0.0134
	(60.69%)	-0.7790*	H 20	s(99.93%)p 0.00(0.07%)	-0.9996 0.0012 0.0090 -0.0250 -0.0031		
118. (0.02262)	BD*(1) C 19- C 23						
	(51.01%)	0.7142*	C 19	s(34.89%)p 1.86(65.05%)d 0.00(0.06%)	0.0000 -0.5907 -0.0014 -0.0040 0.7971	0.0070 -0.1193 0.0265 -0.0150 0.0030	0.0064 0.0007 -0.0009 -0.0184 0.0148
	(48.99%)	-0.6999*	C 23	s(37.44%)p 1.67(62.52%)d 0.00(0.05%)	0.0000 -0.6118 -0.0095 -0.0013 -0.7635	-0.0083 0.2030 0.0274 0.0163 0.0028	0.0054 0.0006 -0.0003 -0.0169 0.0118
119. (0.02848)	BD*(1) C 21- C 24						
	(51.07%)	0.7147*	C 21	s(31.46%)p 2.18(68.48%)d 0.00(0.06%)	0.0000 0.5608 -0.0069 0.0013 0.8269	-0.0033 -0.0148 0.0054 0.0284 0.0008	0.0002 0.0012 0.0008 0.0182 -0.0150
	(48.93%)	-0.6995*	C 24	s(32.61%)p 2.07(67.34%)d 0.00(0.05%)	0.0000 0.5710 0.0012 -0.0002 -0.8150	0.0035 0.0958 0.0008 -0.0094 0.0007	-0.0010 0.0010 0.0008 0.0176 -0.0140
120. (0.03113)	BD*(1) C 22- C 24						
	(50.44%)	0.7102*	C 22	s(31.64%)p 2.16(68.31%)d 0.00(0.05%)	0.0000 -0.5625 -0.0010 -0.0008 0.4923	-0.0020 0.6590 -0.0027 0.0801 -0.0012	-0.0170 -0.0026 -0.0036 0.0027 0.0139
	(49.56%)	-0.7040*	C 24	s(34.85%)p 1.87(65.10%)d 0.00(0.05%)	0.0000 -0.5903 0.0020 -0.0008 -0.4879	0.0037 -0.6381 0.0102 -0.0757 0.0003	-0.0171 -0.0020 -0.0030 0.0044 0.0131
121. (0.02874)	BD*(1) C 23- C 24						

	(51.01%)	0.7142*	C 23	s(31.66%)p 2.16(68.28%)d 0.00(0.06%)	0.0000	0.5627	-0.0059	0.0013	-0.2402
					0.0039	0.7853	-0.0017	0.0919	-0.0002
					-0.0098	-0.0010	0.0044	-0.0153	-0.0148
	(48.99%)	-0.7000*	C 24	s(32.49%)p 2.08(67.46%)d 0.00(0.05%)	0.0000	0.5700	0.0023	-0.0001	0.3110
					0.0018	-0.7574	0.0039	-0.0654	0.0002
					-0.0102	-0.0008	0.0038	-0.0144	-0.0140
122. (0.00682)	BD*(1)	C 25-	H 26						
	(38.91%)	0.6237*	C 25	s(26.22%)p 2.81(73.70%)d 0.00(0.08%)	0.0000	-0.5120	-0.0001	0.0002	-0.3809
					-0.0011	0.6275	-0.0136	0.4449	0.0086
					0.0149	0.0107	-0.0195	0.0076	0.0040
	(61.09%)	-0.7816*	H 26	s(99.95%)p 0.00(0.05%)	-0.9998	-0.0003	0.0099	-0.0149	-0.0125
123. (0.00828)	BD*(1)	C 25-	H 27						
	(39.19%)	0.6260*	C 25	s(25.77%)p 2.88(74.15%)d 0.00(0.08%)	0.0000	-0.5076	-0.0015	0.0003	-0.5132
					-0.0012	-0.6894	0.0046	-0.0511	0.0138
					-0.0224	-0.0012	-0.0032	0.0072	0.0157
	(60.81%)	-0.7798*	H 27	s(99.95%)p 0.00(0.05%)	-0.9998	-0.0009	0.0138	0.0171	-0.0006
124. (0.01599)	BD*(1)	C 25-	H 28						
	(39.86%)	0.6314*	C 25	s(25.85%)p 2.87(74.07%)d 0.00(0.08%)	0.0000	-0.5084	0.0056	0.0010	0.7526
					-0.0082	-0.2125	-0.0044	0.3589	0.0177
					0.0111	-0.0191	0.0041	-0.0160	0.0074
	(60.14%)	-0.7755*	H 28	s(99.95%)p 0.00(0.05%)	-0.9997	-0.0042	-0.0193	0.0053	-0.0108
125. (0.01432)	BD*(1)	C 25-	N 50						
	(61.27%)	0.7828*	C 25	s(22.13%)p 3.51(77.76%)d 0.00(0.11%)	0.0000	0.4704	0.0092	0.0021	-0.1550
					0.0138	-0.2908	-0.0015	0.8177	0.0126
					0.0036	-0.0100	-0.0171	-0.0019	0.0258
	(38.73%)	-0.6223*	N 50	s(25.99%)p 2.85(73.95%)d 0.00(0.07%)	0.0000	0.5097	0.0049	0.0011	0.1720
					0.0194	0.2893	0.0126	-0.7907	-0.0208
					0.0004	0.0031	-0.0115	-0.0075	0.0213
126. (0.01658)	BD*(1)	C 29-	H 30						
	(40.08%)	0.6331*	C 29	s(25.65%)p 2.89(74.26%)d 0.00(0.08%)	0.0000	-0.5064	0.0069	0.0010	0.6741
					0.0032	-0.3305	-0.0165	0.4225	-0.0136
					0.0145	-0.0182	0.0109	-0.0120	0.0046
	(59.92%)	-0.7741*	H 30	s(99.95%)p 0.00(0.05%)	-0.9998	-0.0040	-0.0174	0.0096	-0.0093
127. (0.00851)	BD*(1)	C 29-	H 31						
	(38.95%)	0.6241*	C 29	s(26.13%)p 2.82(73.79%)d 0.00(0.08%)	0.0000	-0.5111	-0.0025	0.0001	-0.5997
					0.0100	-0.6018	0.0004	-0.1265	-0.0109
					-0.0248	-0.0056	-0.0033	0.0009	0.0120
	(61.05%)	-0.7813*	H 31	s(99.95%)p 0.00(0.05%)	-0.9998	-0.0008	0.0145	0.0156	0.0047
128. (0.00627)	BD*(1)	C 29-	H 32						
	(38.87%)	0.6235*	C 29	s(25.97%)p 2.85(73.95%)d 0.00(0.08%)	0.0000	-0.5096	0.0006	0.0003	0.2524
					-0.0037	0.3385	-0.0161	-0.7490	-0.0035
					-0.0070	0.0114	0.0168	0.0003	-0.0174
	(61.13%)	-0.7819*	H 32	s(99.95%)p 0.00(0.05%)	-0.9997	-0.0004	-0.0067	-0.0075	0.0203
129. (0.01322)	BD*(1)	C 29-	N 50						
	(61.17%)	0.7821*	C 29	s(22.22%)p 3.50(77.68%)d 0.00(0.11%)	0.0000	0.4712	0.0106	0.0021	0.3475
					0.0208	-0.6421	-0.0062	-0.4932	0.0038
					-0.0153	-0.0124	0.0236	-0.0109	0.0001
	(38.83%)	-0.6232*	N 50	s(27.87%)p 2.59(72.06%)d 0.00(0.06%)	0.0000	0.5279	0.0068	0.0005	-0.3261
					0.0126	0.6095	0.0146	0.4919	0.0223
					-0.0157	-0.0148	0.0095	-0.0052	-0.0080
130. (0.02808)	BD*(1)	C 33-	C 34						
	(49.48%)	0.7034*	C 33	s(33.66%)p 1.97(66.28%)d 0.00(0.06%)	0.0000	-0.5800	-0.0143	-0.0004	-0.4087
					-0.0089	0.3501	0.0064	-0.6105	-0.0198
					0.0112	-0.0132	0.0137	-0.0049	-0.0074
	(50.52%)	-0.7108*	C 34	s(35.02%)p 1.85(64.94%)d 0.00(0.05%)	0.0000	-0.5918	-0.0011	-0.0009	0.4322
					0.0088	-0.3429	-0.0024	0.5872	-0.0067
					0.0087	-0.0124	0.0123	-0.0029	-0.0085

131. (0.02779) BD*(1) C 33- C 40
 (49.49%) 0.7035* C 33 s(33.69%)p 1.97(66.25%)d 0.00(0.06%)
 0.0000 -0.5803 -0.0143 -0.0005 -0.3586
 -0.0089 -0.1246 -0.0039 0.7196 0.0215
 0.0005 0.0162 0.0066 -0.0072 -0.0149
 (50.51%) -0.7107* C 40 s(34.98%)p 1.86(64.97%)d 0.00(0.05%)
 0.0000 -0.5915 -0.0013 -0.0011 0.3852
 0.0115 0.1206 -0.0052 -0.6976 0.0035
 -0.0010 0.0139 0.0068 -0.0048 -0.0144

132. (0.02841) BD*(1) C 33- B 49
 (31.69%) 0.5629* C 33 s(32.54%)p 2.07(67.44%)d 0.00(0.03%)
 0.0000 -0.5700 0.0204 0.0005 0.7824
 -0.0445 -0.2204 0.0062 -0.1082 0.0019
 0.0077 0.0035 0.0015 -0.0125 0.0048
 (68.31%) -0.8265* B 49 s(34.88%)p 1.86(65.04%)d 0.00(0.08%)
 0.0000 -0.5905 0.0111 -0.0033 -0.7546
 -0.0049 0.2702 -0.0244 0.0851 0.0008
 0.0159 0.0070 0.0014 -0.0208 0.0087

133. (0.02446) BD*(1) C 34- C 35
 (49.88%) 0.7063* C 34 s(34.38%)p 1.91(65.57%)d 0.00(0.05%)
 0.0000 -0.5864 -0.0030 -0.0008 -0.7694
 -0.0081 0.2270 0.0090 0.1079 -0.0182
 0.0103 0.0059 -0.0005 -0.0163 0.0083
 (50.12%) -0.7079* C 35 s(34.63%)p 1.89(65.32%)d 0.00(0.05%)
 0.0000 -0.5884 -0.0014 -0.0023 0.7645
 0.0008 -0.2301 0.0082 -0.1230 -0.0240
 0.0119 0.0055 0.0007 -0.0171 0.0081

134. (0.01710) BD*(1) C 34- C 41
 (49.79%) 0.7056* C 34 s(30.53%)p 2.27(69.43%)d 0.00(0.04%)
 0.0000 0.5525 -0.0026 -0.0012 -0.3542
 0.0074 -0.1264 -0.0016 0.7436 -0.0007
 0.0008 -0.0118 -0.0051 0.0038 0.0137
 (50.21%) -0.7086* C 41 s(25.67%)p 2.89(74.29%)d 0.00(0.04%)
 0.0000 0.5067 -0.0060 0.0016 0.3612
 -0.0047 0.1225 -0.0068 -0.7727 0.0170
 0.0021 -0.0128 -0.0041 0.0023 0.0139

135. (0.01295) BD*(1) C 35- H 36
 (39.87%) 0.6315* C 35 s(30.54%)p 2.27(69.39%)d 0.00(0.07%)
 0.0000 -0.5526 0.0021 0.0042 -0.4154
 -0.0059 0.3666 0.0058 -0.6219 -0.0088
 0.0108 -0.0160 0.0154 -0.0029 -0.0092
 (60.13%) -0.7754* H 36 s(99.93%)p 0.00(0.07%)
 -0.9997 0.0015 0.0129 -0.0110 0.0193

136. (0.02308) BD*(1) C 35- C 37
 (50.06%) 0.7075* C 35 s(34.67%)p 1.88(65.27%)d 0.00(0.06%)
 0.0000 0.5888 0.0024 0.0028 0.3747
 0.0241 0.1153 -0.0102 -0.7059 0.0062
 0.0004 -0.0156 -0.0067 0.0061 0.0153
 (49.94%) -0.7067* C 37 s(34.56%)p 1.89(65.39%)d 0.00(0.05%)
 0.0000 0.5879 0.0020 0.0009 -0.3501
 0.0122 -0.1319 -0.0083 0.7166 0.0136
 0.0009 -0.0151 -0.0053 0.0058 0.0139

137. (0.02279) BD*(1) C 37- C 38
 (49.92%) 0.7065* C 37 s(34.49%)p 1.90(65.46%)d 0.00(0.05%)
 0.0000 -0.5873 -0.0022 -0.0008 0.3955
 -0.0120 -0.3555 -0.0023 0.6094 0.0178
 0.0097 -0.0129 0.0128 -0.0033 -0.0064
 (50.08%) -0.7077* C 38 s(34.59%)p 1.89(65.35%)d 0.00(0.06%)
 0.0000 -0.5881 -0.0029 -0.0027 -0.4207
 -0.0230 0.3552 0.0030 -0.5913 0.0130
 0.0102 -0.0133 0.0141 -0.0039 -0.0080

138. (0.01293) BD*(1) C 38- H 39
 (39.88%) 0.6315* C 38 s(30.65%)p 2.26(69.28%)d 0.00(0.07%)
 0.0000 -0.5536 0.0026 0.0042 -0.3704
 -0.0075 -0.1366 -0.0025 0.7326 0.0114
 -0.0021 0.0176 0.0073 -0.0053 -0.0172
 (60.12%) -0.7754* H 39 s(99.93%)p 0.00(0.07%)
 -0.9996 0.0014 0.0117 0.0045 -0.0234

139. (0.02414) BD*(1) C 38- C 40
 (50.19%) 0.7085* C 38 s(34.60%)p 1.89(65.35%)d 0.00(0.05%)
 0.0000 0.5882 0.0014 0.0023 -0.7686
 -0.0020 0.2289 0.0072 0.0990 -0.0211
 -0.0113 -0.0056 -0.0008 0.0174 -0.0082
 (49.81%) -0.7057* C 40 s(34.64%)p 1.89(65.32%)d 0.00(0.05%)
 0.0000 0.5885 0.0019 0.0010 0.7698
 0.0067 -0.2177 0.0056 -0.1116 -0.0238
 -0.0106 -0.0042 -0.0002 0.0161 -0.0089

140.	(0.01728)	BD*(1) C	40- C 45 (49.98%)		C 40 s(30.30%)p	2.30(69.66%)d	0.00(0.04%) 0.0000 0.5505 -0.0019 -0.0014 -0.4105 0.0112 0.3604 -0.0018 -0.6310 0.0010 -0.0076 0.0111 -0.0114 0.0022 0.0075
	(50.02%)	-0.7072*	C 45 s(25.67%)p	2.89(74.29%)d	0.00(0.04%) 0.0000 0.5067 -0.0053 0.0019 0.4240 -0.0037 -0.3764 0.0083 0.6489 -0.0159 -0.0071 0.0126 -0.0111 0.0007 0.0066		
141.	(0.00917)	BD*(1) C	41- H 42 (38.42%)		C 41 s(24.57%)p	3.07(75.36%)d	0.00(0.07%) 0.0000 -0.4956 -0.0010 0.0006 -0.0817 0.0036 -0.7202 -0.0006 -0.4774 -0.0153 -0.0035 -0.0034 -0.0208 0.0157 0.0024
	(61.58%)	-0.7847*	H 42 s(99.95%)p	0.00(0.05%) -0.9998 -0.0004 0.0017 0.0184 0.0119			
142.	(0.00627)	BD*(1) C	41- H 43 (38.92%)		C 41 s(24.78%)p	3.03(75.15%)d	0.00(0.07%) 0.0000 -0.4977 -0.0035 0.0001 -0.3938 0.0100 0.6566 0.0015 -0.4064 -0.0106 0.0163 -0.0103 0.0157 0.0086 0.0057
	(61.08%)	-0.7815*	H 43 s(99.96%)p	0.00(0.04%) -0.9998 0.0001 0.0084 -0.0159 0.0101			
143.	(0.00726)	BD*(1) C	41- H 44 (38.81%)		C 41 s(24.88%)p	3.02(75.05%)d	0.00(0.07%) 0.0000 -0.4988 -0.0009 0.0005 0.8408 0.0035 0.1849 0.0084 0.0950 -0.0162 -0.0090 -0.0063 -0.0015 -0.0200 0.0130
	(61.19%)	-0.7822*	H 44 s(99.95%)p	0.00(0.05%) -0.9997 -0.0005 -0.0222 -0.0054 -0.0010			
144.	(0.00585)	BD*(1) C	45- H 46 (38.87%)		C 45 s(24.86%)p	3.02(75.07%)d	0.00(0.07%) 0.0000 -0.4985 -0.0040 0.0001 -0.5041 0.0117 -0.0248 -0.0064 0.7041 0.0072 -0.0011 0.0223 0.0002 -0.0076 -0.0124
	(61.13%)	-0.7819*	H 46 s(99.96%)p	0.00(0.04%) -0.9998 0.0002 0.0113 0.0009 -0.0173			
145.	(0.00858)	BD*(1) C	45- H 47 (38.57%)		C 45 s(24.70%)p	3.05(75.23%)d	0.00(0.07%) 0.0000 -0.4970 -0.0009 0.0005 0.2187 -0.0002 -0.8088 -0.0109 -0.2238 0.0130 0.0101 0.0040 -0.0117 0.0180 0.0108
	(61.43%)	-0.7837*	H 47 s(99.95%)p	0.00(0.05%) -0.9997 -0.0007 -0.0052 0.0217 0.0056			
146.	(0.00831)	BD*(1) C	45- H 48 (38.73%)		C 45 s(24.67%)p	3.05(75.25%)d	0.00(0.07%) 0.0000 -0.4967 0.0001 0.0008 0.7193 0.0045 0.4502 -0.0007 0.1791 0.0186 -0.0203 -0.0066 -0.0054 -0.0095 0.0121
	(61.27%)	-0.7828*	H 48 s(99.95%)p	0.00(0.05%) -0.9998 -0.0006 -0.0180 -0.0114 -0.0052			
147.	(0.02042)	BD*(1) B	49- O 51 (80.52%)		B 49 s(28.09%)p	2.55(71.60%)d	0.01(0.31%) 0.0000 0.5289 0.0331 -0.0069 -0.0989 0.0185 0.7919 0.0384 0.2769 0.0226 -0.0112 -0.0024 0.0275 -0.0458 -0.0106
	(19.48%)	-0.4414*	O 51 s(46.09%)p	1.17(53.70%)d	0.00(0.21%) 0.0000 0.6789 -0.0075 -0.0013 0.2483 -0.0002 -0.6476 0.0025 -0.2366 -0.0001 -0.0013 0.0015 0.0273 -0.0340 -0.0120		
148.	(0.09706)	BD*(2) B	49- O 51 (87.51%)		B 49 s(0.02%)p	99.99(99.56%)d	23.29(0.42%) 0.0000 -0.0128 -0.0021 0.0033 0.0268 -0.0055 0.3387 -0.0208 -0.9361 0.0583 0.0034 0.0121 -0.0470 -0.0236 -0.0356
	(12.49%)	-0.3534*	O 51 s(0.21%)p	99.99(99.62%)d	0.82(0.17%) 0.0000 -0.0458 -0.0017 0.0002 0.1109 0.0001 0.3355 0.0030 -0.9334 -0.0087 -0.0110 0.0220 0.0203 0.0080 0.0253		
149.	(0.04977)	BD*(1) O	51- H 52 (23.28%)		O 51 s(30.66%)p	2.25(69.12%)d	0.01(0.22%) 0.0000 -0.5536 -0.0122 -0.0004 0.7800 -0.0195 -0.2856 0.0236 0.0171 0.0029 -0.0005 -0.0161 0.0008 -0.0391 0.0202
	(76.72%)	-0.8759*	H 52 s(99.86%)p	0.00(0.14%) -0.9992 -0.0133 -0.0363 0.0074 -0.0075			
150.	(0.99675)	3Cn(1) C	11- C 13- C 21				

	(0.07%)	0.0255* C 11	s(0.01%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 -0.0093 0.0004 -0.0002 -0.0386	0.0007 -0.0854 -0.0003 0.9953 -0.0170	-0.0010 0.0148 -0.0055 -0.0010 0.0002
	(61.02%)	0.7811* C 13	s(0.01%)p 1.00(99.92%)d 0.00(0.08%)	0.0000 0.0076 -0.0010 0.0001 0.0262	0.0011 0.0651 0.0025 -0.9971 0.0043	-0.0017 0.0120 0.0245 0.0015 0.0037
	(38.92%)	0.6239* C 21	s(0.00%)p 1.00(99.92%)d 0.00(0.08%)	0.0000 0.0009 -0.0003 0.0000 -0.0364	0.0000 -0.0923 -0.0039 0.9947 -0.0023	-0.0007 -0.0052 0.0266 0.0026 0.0035
151. (0.89545)	3Cn(1) C 17- C 19- C 23					
	(62.04%)	0.7876* C 17	s(0.01%)p 1.00(99.91%)d 0.00(0.08%)	0.0000 0.0078 -0.0012 0.0001 -0.0173	-0.0020 -0.1189 -0.0035 0.9923 -0.0041	0.0025 -0.0212 -0.0192 -0.0025 -0.0045
	(0.01%)	0.0111* C 19	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 0.0011 0.0012 -0.0001 0.0009	0.0004 0.1254 -0.0012 -0.9918 0.0172	-0.0012 0.0102 -0.0123 -0.0015 -0.0028
	(37.95%)	0.6160* C 23	s(0.00%)p 1.00(99.93%)d 0.00(0.07%)	0.0000 0.0019 0.0002 0.0001 0.0085	0.0006 0.1174 0.0003 -0.9927 0.0043	0.0035 -0.0269 -0.0026 -0.0001 -0.0005
152. (0.96615)	3Cn(1) C 34- C 35- C 37					
	(50.08%)	0.7077* C 34	s(0.00%)p 1.00(99.91%)d 0.00(0.08%)	0.0000 0.0000 0.0045 -0.0005 0.3081	0.0052 0.9023 -0.0037 0.3001 0.0034	0.0215 0.0061 -0.0104 0.0145 -0.0040
	(0.00%)	0.0041* C 35	s(0.00%)p 1.00(99.98%)d 0.00(0.02%)	0.0000 -0.0009 -0.0024 0.0002 0.3189	-0.0026 0.8938 -0.0151 0.3146 -0.0049	-0.0040 -0.0052 -0.0072 -0.0066 -0.0053
	(49.91%)	0.7065* C 37	s(0.00%)p 1.00(99.92%)d 0.00(0.08%)	0.0000 0.0033 -0.0013 0.0002 -0.3093	-0.0018 -0.8955 0.0067 -0.3185 -0.0023	0.0164 -0.0020 -0.0195 0.0037 -0.0126
153. (0.08207)	3C*(1) C 11- C 13- C 21					
	(49.18%)	0.7013* C 11	s(0.01%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 0.0093 -0.0004 0.0002 0.0386	-0.0007 0.0854 0.0003 -0.9953 0.0170	0.0010 -0.0148 0.0055 0.0010 -0.0002
	(18.55%)	-0.4307* C 13	s(0.01%)p 1.00(99.92%)d 0.00(0.08%)	0.0000 0.0076 -0.0010 0.0001 0.0262	0.0011 0.0651 0.0025 -0.9971 0.0043	-0.0017 0.0120 0.0245 0.0015 0.0037
	(32.26%)	0.5680* C 21	s(0.00%)p 1.00(99.92%)d 0.00(0.08%)	0.0000 0.0009 -0.0003 0.0000 -0.0364	0.0000 -0.0923 -0.0039 0.9947 -0.0023	-0.0007 -0.0052 0.0266 0.0026 0.0035
154. (0.08276)	3C*(1) C 17- C 19- C 23					
	(18.72%)	0.4327* C 17	s(0.01%)p 1.00(99.91%)d 0.00(0.08%)	0.0000 0.0078 -0.0012 0.0001 -0.0173	-0.0020 -0.1189 -0.0035 0.9923 -0.0041	0.0025 -0.0212 -0.0192 -0.0025 -0.0045
	(49.27%)	-0.7019* C 19	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 -0.0011 -0.0012 0.0001 -0.0009	-0.0004 -0.1254 0.0012 0.9918 -0.0172	0.0012 -0.0102 0.0123 0.0015 0.0028
	(32.01%)	0.5658* C 23	s(0.00%)p 1.00(99.93%)d 0.00(0.07%)	0.0000 -0.0019 -0.0002 -0.0001 -0.0085	-0.0006 -0.1174 -0.0003 0.9927 -0.0043	-0.0035 0.0269 0.0026 0.0001 0.0005
155. (0.07465)	3C*(1) C 33- C 38- C 40					
	(24.61%)	0.4961* C 33	s(0.01%)p 1.00(99.92%)d 0.00(0.07%)	0.0000 0.0051 0.0060 -0.0007 0.3008	0.0106 0.9012 0.0128 0.3102 0.0079	0.0151 -0.0012 -0.0180 0.0049 -0.0108
	(24.16%)	-0.4915* C 38	s(0.00%)p 1.00(99.94%)d 0.00(0.06%)	0.0000 0.0016 0.0009 -0.0004 -0.3069	-0.0025 -0.8956 0.0096 -0.3210 0.0029	0.0185 0.0051 -0.0075 0.0110 -0.0036
	(51.24%)	0.7158* C 40	s(0.00%)p 1.00(99.97%)d 0.00(0.03%)	0.0000 -0.0014 -0.0037 0.0003 -0.2996	-0.0015 -0.8987 0.0072 -0.3197 -0.0026	-0.0057 -0.0063 -0.0076 -0.0091 -0.0065

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156. (0.08612) 3C*( 1) C 34- C 35- C 37
      ( 25.93%) 0.5092* C 34 s( 0.00%)p 1.00( 99.91%)d 0.00( 0.08%)
                                0.0000 0.0000 0.0045 -0.0005 0.3081
                                0.0052 0.9023 -0.0037 0.3001 0.0034
                                0.0215 0.0061 -0.0104 0.0145 -0.0040
      ( 48.46%) -0.6962* C 35 s( 0.00%)p 1.00( 99.98%)d 0.00( 0.02%)
                                0.0000 -0.0009 -0.0024 0.0002 0.3189
                                -0.0026 0.8938 -0.0151 0.3146 -0.0049
                                -0.0040 -0.0052 -0.0072 -0.0066 -0.0053
      ( 25.61%) 0.5060* C 37 s( 0.00%)p 1.00( 99.92%)d 0.00( 0.08%)
                                0.0000 -0.0033 0.0013 -0.0002 0.3093
                                0.0018 0.8955 -0.0067 0.3185 0.0023
                                -0.0164 0.0020 0.0195 -0.0037 0.0126
157. (0.00219) RY ( 1) C 1 s( 0.01%)p99.99( 93.14%)d99.99( 6.84%)
                                0.0000 0.0006 0.0094 0.0045 0.0005
                                0.0066 -0.0034 -0.3651 0.0095 0.8933
                                0.0987 -0.2245 0.0576 0.0301 0.0640
158. (0.00057) RY ( 2) C 1 s( 0.90%)p43.96( 39.44%)d66.49( 59.66%)
                                0.0000 0.0019 0.0817 0.0479 -0.0032
                                -0.2798 -0.0107 -0.5194 -0.0048 -0.2151
                                0.6031 0.2481 -0.0916 0.3892 -0.1069
159. (0.00040) RY ( 3) C 1 s( 11.04%)p 7.95( 87.77%)d 0.11( 1.19%)
                                0.0000 0.0284 0.3311 0.0013 -0.0029
                                -0.8541 0.0036 0.3544 0.0020 0.1499
                                -0.0915 -0.0260 -0.0302 0.0317 0.0300
160. (0.00004) RY ( 4) C 1 s( 78.04%)p 0.14( 10.81%)d 0.14( 11.15%)
161. (0.00002) RY ( 5) C 1 s( 16.88%)p 1.63( 27.49%)d 3.29( 55.62%)
162. (0.00002) RY ( 6) C 1 s( 29.36%)p 0.26( 7.78%)d 2.14( 62.87%)
163. (0.00001) RY ( 7) C 1 s( 10.25%)p 1.92( 19.66%)d 6.84( 70.09%)
164. (0.00001) RY ( 8) C 1 s( 0.35%)p11.18( 3.92%)d99.99( 95.73%)
165. (0.00000) RY ( 9) C 1 s( 40.13%)p 0.23( 9.10%)d 1.27( 50.77%)
166. (0.00000) RY (10) C 1 s( 13.12%)p 0.08( 1.05%)d 6.54( 85.83%)
167. (0.00100) RY ( 1) H 2 s( 98.77%)p 0.01( 1.23%)
                                0.0004 0.9938 -0.1047 0.0146 -0.0332
168. (0.00007) RY ( 2) H 2 s( 0.54%)p99.99( 99.46%)
169. (0.00007) RY ( 3) H 2 s( 0.67%)p99.99( 99.33%)
170. (0.00001) RY ( 4) H 2 s( 0.07%)p99.99( 99.93%)
171. (0.00102) RY ( 1) H 3 s( 98.77%)p 0.01( 1.23%)
                                0.0001 0.9938 -0.1075 -0.0177 0.0209
172. (0.00008) RY ( 2) H 3 s( 0.60%)p99.99( 99.40%)
173. (0.00007) RY ( 3) H 3 s( 0.63%)p99.99( 99.37%)
174. (0.00000) RY ( 4) H 3 s( 0.05%)p99.99( 99.95%)
175. (0.00095) RY ( 1) H 4 s( 96.93%)p 0.03( 3.07%)
                                0.0000 0.9845 -0.1335 0.1048 0.0438
176. (0.00007) RY ( 2) H 4 s( 1.40%)p70.45( 98.60%)
177. (0.00007) RY ( 3) H 4 s( 1.66%)p59.07( 98.34%)
178. (0.00000) RY ( 4) H 4 s( 0.05%)p99.99( 99.95%)
179. (0.00200) RY ( 1) C 5 s( 0.02%)p99.99( 89.91%)d99.99( 10.08%)
                                0.0000 -0.0037 0.0117 -0.0009 0.0000
                                0.1005 -0.0002 -0.0148 -0.0123 -0.9427
                                -0.0077 0.1037 -0.2955 0.0177 -0.0484
180. (0.00178) RY ( 2) C 5 s( 0.25%)p99.99( 83.29%)d66.57( 16.47%)
                                0.0000 0.0298 0.0366 0.0158 0.0018
                                -0.2056 0.0109 0.8881 -0.0005 -0.0412
                                -0.0085 0.0074 -0.0020 -0.4055 -0.0098
181. (0.00103) RY ( 3) C 5 s( 4.59%)p20.20( 92.78%)d 0.57( 2.63%)
                                0.0000 0.0117 0.2132 0.0182 0.0008
                                0.9405 0.0024 0.1862 0.0007 0.0920
                                -0.1382 -0.0596 0.0084 -0.0553 -0.0228
182. (0.00035) RY ( 4) C 5 s( 0.17%)p 2.52( 0.44%)d99.99( 99.39%)
                                0.0000 -0.0007 0.0409 0.0076 -0.0001
                                -0.0471 0.0014 -0.0167 -0.0115 0.0417
                                0.1298 -0.8771 -0.4397 -0.0266 -0.1170
183. (0.00018) RY ( 5) C 5 s( 85.44%)p 0.04( 3.50%)d 0.13( 11.06%)
                                0.0000 0.0027 0.9242 0.0172 -0.0007
                                -0.1829 -0.0022 0.0391 0.0003 0.0046
                                0.1261 0.0726 0.0184 0.2640 -0.1391
184. (0.00004) RY ( 6) C 5 s( 3.95%)p 1.48( 5.86%)d22.84( 90.19%)
185. (0.00003) RY ( 7) C 5 s( 55.90%)p 0.11( 6.16%)d 0.68( 37.94%)
186. (0.00002) RY ( 8) C 5 s( 12.36%)p 0.78( 9.59%)d 6.31( 78.05%)
187. (0.00002) RY ( 9) C 5 s( 35.51%)p 0.21( 7.55%)d 1.60( 56.94%)
188. (0.00000) RY (10) C 5 s( 1.96%)p 0.52( 1.02%)d49.58( 97.02%)
189. (0.00113) RY ( 1) H 6 s( 99.31%)p 0.01( 0.69%)
                                -0.0004 0.9966 0.0269 0.0463 0.0631
190. (0.00009) RY ( 2) H 6 s( 0.11%)p99.99( 99.89%)
191. (0.00005) RY ( 3) H 6 s( 0.55%)p99.99( 99.45%)
192. (0.00000) RY ( 4) H 6 s( 0.08%)p99.99( 99.92%)

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193.	(0.00114)	RY	(1)	H	7	s(99.30%)p 0.01(0.70%)
						-0.0004 0.9965 0.0310 0.0570 -0.0526
194.	(0.00009)	RY	(2)	H	7	s(0.12%)p99.99(99.88%)
195.	(0.00005)	RY	(3)	H	7	s(0.55%)p99.99(99.45%)
196.	(0.00000)	RY	(4)	H	7	s(0.09%)p99.99(99.91%)
197.	(0.00198)	RY	(1)	C	8	s(0.04%)p99.99(89.61%)d99.99(10.35%)
						0.0000 0.0000 0.0201 0.0021 0.0002
						0.0087 0.0011 0.1442 -0.0120 -0.9355
						0.0270 -0.3201 0.0090 0.0075 -0.0129
198.	(0.00184)	RY	(2)	C	8	s(0.24%)p99.99(84.18%)d64.53(15.58%)
						0.0000 0.0299 0.0347 0.0178 0.0096
						0.9174 0.0045 0.0001 0.0007 0.0100
						0.2050 0.0224 -0.0318 0.3350 -0.0072
199.	(0.00100)	RY	(3)	C	8	s(4.03%)p23.05(92.95%)d 0.75(3.01%)
						0.0000 0.0131 0.1996 0.0176 0.0026
						-0.0477 0.0027 0.9519 0.0009 0.1456
						-0.0762 0.0110 -0.0534 0.1432 -0.0291
200.	(0.00036)	RY	(4)	C	8	s(0.50%)p 1.17(0.58%)d99.99(98.92%)
						0.0000 -0.0006 0.0694 0.0133 0.0003
						0.0006 0.0011 -0.0564 -0.0114 0.0502
						0.0516 -0.1848 -0.9501 -0.1246 -0.1849
201.	(0.00017)	RY	(5)	C	8	s(86.95%)p 0.03(2.72%)d 0.12(10.33%)
						0.0000 0.0021 0.9324 0.0117 -0.0015
						0.0695 -0.0010 -0.1493 0.0014 -0.0105
						-0.0223 0.0243 0.1293 -0.2655 -0.1224
202.	(0.00004)	RY	(6)	C	8	s(3.81%)p 1.58(6.01%)d23.70(90.19%)
203.	(0.00003)	RY	(7)	C	8	s(58.10%)p 0.10(5.58%)d 0.63(36.33%)
204.	(0.00002)	RY	(8)	C	8	s(13.77%)p 0.68(9.37%)d 5.58(76.86%)
205.	(0.00002)	RY	(9)	C	8	s(30.51%)p 0.27(8.18%)d 2.01(61.31%)
206.	(0.00000)	RY	(10)	C	8	s(2.20%)p 0.41(0.90%)d43.97(96.90%)
207.	(0.00119)	RY	(1)	H	9	s(99.28%)p 0.01(0.72%)
						-0.0005 0.9964 0.0411 0.0519 -0.0528
208.	(0.00009)	RY	(2)	H	9	s(0.15%)p99.99(99.85%)
209.	(0.00005)	RY	(3)	H	9	s(0.53%)p99.99(99.47%)
210.	(0.00000)	RY	(4)	H	9	s(0.09%)p99.99(99.91%)
211.	(0.00116)	RY	(1)	H	10	s(99.27%)p 0.01(0.73%)
						-0.0005 0.9963 0.0386 0.0415 0.0642
212.	(0.00009)	RY	(2)	H	10	s(0.16%)p99.99(99.84%)
213.	(0.00005)	RY	(3)	H	10	s(0.55%)p99.99(99.45%)
214.	(0.00000)	RY	(4)	H	10	s(0.08%)p99.99(99.92%)
215.	(0.00429)	RY	(1)	C	11	s(0.32%)p99.99(92.04%)d23.78(7.64%)
						0.0000 -0.0332 0.0447 -0.0104 -0.0163
						-0.9575 0.0008 0.0479 -0.0008 -0.0313
						0.0505 -0.0044 0.0308 -0.2696 0.0136
216.	(0.00242)	RY	(2)	C	11	s(0.00%)p 1.00(98.41%)d 0.02(1.58%)
						0.0000 0.0060 -0.0027 0.0012 0.0000
						-0.0406 0.0241 -0.9893 0.0009 -0.0556
						0.1250 0.0134 0.0050 -0.0022 0.0037
217.	(0.00087)	RY	(3)	C	11	s(0.02%)p99.99(88.26%)d99.99(11.73%)
						0.0000 0.0003 0.0103 -0.0085 0.0007
						0.0285 0.0005 0.0523 -0.0139 -0.9375
						0.0421 -0.2299 -0.2450 -0.0002 -0.0510
218.	(0.00047)	RY	(4)	C	11	s(0.01%)p99.99(6.76%)d99.99(93.22%)
						0.0000 -0.0004 0.0045 0.0100 -0.0001
						-0.0157 0.0001 -0.0133 -0.0007 0.2593
						0.0465 -0.0100 -0.9508 -0.0831 -0.1377
219.	(0.00027)	RY	(5)	C	11	s(98.28%)p 0.01(0.50%)d 0.01(1.21%)
						0.0000 0.0006 0.9895 -0.0618 -0.0047
						0.0693 0.0013 -0.0116 -0.0004 0.0087
						-0.0446 -0.0002 0.0170 -0.0909 -0.0397
220.	(0.00008)	RY	(6)	C	11	s(24.74%)p 0.05(1.27%)d 2.99(73.99%)
221.	(0.00007)	RY	(7)	C	11	s(69.42%)p 0.01(0.55%)d 0.43(30.04%)
222.	(0.00002)	RY	(8)	C	11	s(4.07%)p 1.76(7.17%)d21.82(88.76%)
223.	(0.00001)	RY	(9)	C	11	s(3.29%)p 0.02(0.06%)d29.39(96.66%)
224.	(0.00000)	RY	(10)	C	11	s(0.03%)p99.99(5.00%)d99.99(94.97%)
225.	(0.00111)	RY	(1)	H	12	s(99.80%)p 0.00(0.20%)
						0.0024 0.9990 -0.0416 0.0141 0.0052
226.	(0.00016)	RY	(2)	H	12	s(0.00%)p 1.00(100.00%)
						0.0000 0.0051 0.0305 0.0963 -0.9949
227.	(0.00005)	RY	(3)	H	12	s(0.01%)p99.99(99.99%)
228.	(0.00001)	RY	(4)	H	12	s(0.26%)p99.99(99.74%)
229.	(0.00371)	RY	(1)	C	13	s(0.36%)p99.99(93.43%)d17.29(6.21%)
						0.0000 -0.0317 0.0476 0.0180 0.0030
						-0.4791 0.0110 0.8393 0.0028 -0.0117
						0.1752 0.0392 0.0104 0.1711 0.0228
230.	(0.00229)	RY	(2)	C	13	s(2.73%)p31.53(85.98%)d 4.14(11.29%)
						0.0000 0.0100 0.1644 0.0122 -0.0155

		0.7895	-0.0010	0.4257	0.0081	-0.2345
		0.0787	0.2338	0.2075	-0.0893	0.0324
231.	(0.00195) RY (3) C 13	s(0.08%)p99.99(53.78%)d99.99(46.14%)	0.0000	0.0027	0.0237	0.0160
			0.3205	0.0007	0.2159	-0.0137
			0.0672	-0.5225	-0.4185	-0.0392
232.	(0.00069) RY (4) C 13	s(11.25%)p 3.94(44.27%)d 3.96(44.49%)	0.0000	0.0001	0.3349	-0.0176
			-0.0311	0.0037	-0.0350	-0.0159
			0.1562	-0.6065	-0.2063	-0.0492
233.	(0.00039) RY (5) C 13	s(80.52%)p 0.14(11.04%)d 0.10(8.44%)	0.0000	-0.0029	0.8973	0.0072
			-0.1290	0.0043	-0.1362	0.0032
			0.1114	0.2473	0.0171	-0.0909
234.	(0.00008) RY (6) C 13	s(6.61%)p 0.25(1.64%)d13.89(91.75%)				
235.	(0.00005) RY (7) C 13	s(93.56%)p 0.00(0.25%)d 0.07(6.19%)				
236.	(0.00003) RY (8) C 13	s(1.63%)p 2.64(4.29%)d57.85(94.09%)				
237.	(0.00002) RY (9) C 13	s(2.85%)p 0.08(0.22%)d34.02(96.93%)				
238.	(0.00001) RY (10) C 13	s(0.60%)p 8.64(5.18%)d99.99(94.22%)				
239.	(0.00117) RY (1) H 14	s(99.48%)p 0.01(0.52%)	-0.0017	0.9974	0.0078	-0.0290
240.	(0.00017) RY (2) H 14	s(0.45%)p99.99(99.55%)	-0.0004	0.0669	0.0299	0.0508
241.	(0.00005) RY (3) H 14	s(0.00%)p 1.00(100.00%)				
242.	(0.00001) RY (4) H 14	s(0.14%)p99.99(99.86%)				
243.	(0.00497) RY (1) C 15	s(1.24%)p72.22(89.85%)d 7.16(8.91%)	0.0000	-0.0168	0.1100	-0.0075
			-0.3509	0.0101	0.8760	0.0040
			-0.2640	-0.0364	0.0105	-0.1289
244.	(0.00405) RY (2) C 15	s(2.60%)p35.33(92.02%)d 2.06(5.38%)	0.0000	0.0129	0.1609	-0.0005
			-0.8951	0.0001	-0.3413	0.0054
			0.1827	0.0478	0.0821	-0.1021
245.	(0.00300) RY (3) C 15	s(5.02%)p16.96(85.16%)d 1.95(9.82%)	0.0000	0.0085	0.2238	0.0070
			-0.0514	0.0025	0.0375	-0.0179
			0.0130	-0.1963	-0.2400	-0.0315
246.	(0.00107) RY (4) C 15	s(49.88%)p 0.24(11.92%)d 0.77(38.20%)	0.0000	-0.0037	0.7034	0.0634
			0.2229	-0.0109	-0.1244	-0.0026
			-0.0575	-0.0661	-0.1738	-0.5855
247.	(0.00061) RY (5) C 15	s(33.37%)p 0.09(2.93%)d 1.91(63.70%)	0.0000	-0.0061	0.5721	-0.0797
			0.1051	-0.0155	0.1340	-0.0011
			0.3296	-0.0447	0.5172	0.5076
248.	(0.00059) RY (6) C 15	s(3.77%)p 0.18(0.70%)d25.36(95.54%)	0.0000	-0.0013	0.1883	-0.0469
			-0.0001	-0.0062	0.0805	0.0042
			0.0964	0.8337	-0.4471	0.2259
249.	(0.00016) RY (7) C 15	s(4.35%)p 1.80(7.81%)d20.22(87.85%)	0.0000	0.0102	0.2048	0.0375
			-0.0671	0.0248	-0.2697	0.0032
			-0.8618	0.0460	0.0927	0.3198
250.	(0.00015) RY (8) C 15	s(3.57%)p 2.57(9.17%)d24.42(87.26%)	0.0000	-0.0012	0.1058	0.1566
			-0.0851	-0.0024	0.0115	-0.0053
			0.1084	-0.4900	-0.6411	0.4580
251.	(0.00009) RY (9) C 15	s(92.95%)p 0.00(0.35%)d 0.07(6.70%)				
252.	(0.00002) RY (10) C 15	s(3.36%)p 0.06(0.21%)d28.74(96.43%)				
253.	(0.00492) RY (1) C 16	s(0.12%)p99.99(96.85%)d26.04(3.04%)	0.0000	0.0284	-0.0188	0.0019
			0.2441	-0.0010	0.9432	0.0039
			-0.1719	-0.0261	-0.0064	-0.0088
254.	(0.00375) RY (2) C 16	s(0.10%)p99.99(96.85%)d30.72(3.05%)	0.0000	0.0119	-0.0109	0.0271
			0.9459	0.0338	-0.2583	0.0096
			-0.1337	-0.0068	-0.0220	0.1099
255.	(0.00075) RY (3) C 16	s(0.53%)p99.99(74.30%)d47.20(25.17%)	0.0000	0.0029	0.0713	0.0156
			0.0445	0.0055	-0.1301	-0.0060
			0.0813	-0.4644	0.1714	0.0059
256.	(0.00041) RY (4) C 16	s(97.71%)p 0.00(0.18%)d 0.02(2.11%)	0.0000	-0.0070	0.9883	0.0211
			0.0056	0.0231	0.0217	0.0044
			-0.0067	0.0809	-0.0787	0.0577
257.	(0.00036) RY (5) C 16	s(0.89%)p21.92(19.59%)d89.00(79.52%)	0.0000	-0.0020	0.0888	-0.0322

		-0.0251	-0.0010	0.0598	0.0128	-0.4376
		-0.0133	-0.5652	0.6638	0.1485	0.1135
258.	(0.00016) RY (6) C 16	s(2.44%)p 0.66(1.62%)d39.24(95.93%)				
		0.0000	0.0048	0.0709	0.1393	-0.0150
		0.1230	0.0213	-0.0091	0.0064	-0.0175
		0.1218	0.1072	0.2730	-0.9206	0.1044
259.	(0.00008) RY (7) C 16	s(4.35%)p 0.88(3.84%)d21.10(91.81%)				
260.	(0.00006) RY (8) C 16	s(0.10%)p62.58(6.10%)d99.99(93.81%)				
261.	(0.00003) RY (9) C 16	s(74.07%)p 0.01(0.74%)d 0.34(25.19%)				
262.	(0.00002) RY (10) C 16	s(19.74%)p 0.00(0.02%)d 4.06(80.23%)				
263.	(0.00474) RY (1) C 17	s(0.10%)p99.99(93.48%)d67.30(6.42%)				
		0.0000	0.0274	-0.0062	0.0128	-0.0133
		-0.9050	-0.0138	0.3394	-0.0028	-0.0143
		-0.1176	-0.0126	-0.0284	0.2217	-0.0158
264.	(0.00189) RY (2) C 17	s(0.09%)p99.99(97.85%)d24.06(2.07%)				
		0.0000	-0.0078	0.0267	-0.0092	-0.0033
		-0.3243	0.0158	-0.9178	-0.0034	-0.1751
		-0.1379	-0.0259	-0.0286	-0.0044	0.0124
265.	(0.00183) RY (3) C 17	s(0.16%)p99.99(32.09%)d99.99(67.76%)				
		0.0000	0.0013	0.0388	0.0068	0.0015
		-0.0373	0.0035	-0.0720	-0.0197	0.5603
		0.0625	-0.3225	-0.7286	-0.0959	-0.1720
266.	(0.00051) RY (4) C 17	s(3.97%)p15.16(60.11%)d 9.06(35.92%)				
		0.0000	0.0018	0.1962	-0.0342	0.0008
		-0.0656	0.0029	-0.1440	0.0150	0.7589
		0.0756	0.0102	0.5677	0.1312	0.1179
267.	(0.00032) RY (5) C 17	s(75.45%)p 0.05(3.84%)d 0.27(20.71%)				
		0.0000	-0.0020	0.8683	-0.0253	0.0063
		-0.0477	0.0094	0.0143	0.0006	-0.1891
		0.4110	0.1098	-0.0785	0.0021	-0.1412
268.	(0.00012) RY (6) C 17	s(17.65%)p 0.08(1.49%)d 4.58(80.86%)				
		0.0000	-0.0037	0.3927	0.1494	-0.0007
		0.0459	-0.0207	0.1079	-0.0017	0.0269
		-0.7887	-0.1165	0.0883	-0.3950	-0.0953
269.	(0.00006) RY (7) C 17	s(90.01%)p 0.00(0.33%)d 0.11(9.67%)				
270.	(0.00003) RY (8) C 17	s(6.60%)p 0.90(5.95%)d13.24(87.45%)				
271.	(0.00002) RY (9) C 17	s(0.50%)p 6.81(3.43%)d99.99(96.07%)				
272.	(0.00001) RY (10) C 17	s(5.63%)p 0.28(1.55%)d16.50(92.82%)				
273.	(0.00136) RY (1) H 18	s(99.78%)p 0.00(0.22%)				
		-0.0031	0.9989	-0.0439	-0.0137	-0.0098
274.	(0.00014) RY (2) H 18	s(0.00%)p 1.00(100.00%)				
		-0.0003	0.0065	-0.0161	-0.1795	0.9836
275.	(0.00006) RY (3) H 18	s(0.13%)p99.99(99.87%)				
276.	(0.00001) RY (4) H 18	s(0.18%)p99.99(99.82%)				
277.	(0.00441) RY (1) C 19	s(0.20%)p99.99(92.33%)d36.85(7.47%)				
		0.0000	-0.0316	0.0320	0.0017	0.0069
		0.2236	-0.0129	-0.9290	-0.0021	-0.1003
		0.1844	0.0293	-0.0228	0.1981	0.0086
278.	(0.00221) RY (2) C 19	s(0.40%)p99.99(97.78%)d 4.56(1.82%)				
		0.0000	-0.0090	0.0595	-0.0189	-0.0208
		0.9602	-0.0062	0.2352	-0.0006	0.0059
		-0.0880	-0.0279	-0.0232	0.0952	-0.0066
279.	(0.00083) RY (3) C 19	s(0.27%)p99.99(93.86%)d21.59(5.87%)				
		0.0000	0.0000	0.0509	-0.0112	0.0005
		-0.0255	0.0020	0.1014	-0.0138	-0.9631
		0.0128	-0.0278	-0.2341	-0.0244	-0.0485
280.	(0.00042) RY (4) C 19	s(0.07%)p17.35(1.25%)d99.99(98.68%)				
		0.0000	-0.0002	0.0267	0.0026	-0.0003
		0.0134	-0.0001	0.0174	0.0034	-0.1094
		-0.1421	0.9242	0.3243	0.0363	0.0779
281.	(0.00030) RY (5) C 19	s(96.44%)p 0.01(1.24%)d 0.02(2.32%)				
		0.0000	0.0009	0.9814	-0.0355	0.0052
		-0.0860	-0.0037	0.0374	0.0014	0.0594
		0.0038	-0.0196	-0.0071	0.1445	-0.0435
282.	(0.00009) RY (6) C 19	s(80.35%)p 0.00(0.23%)d 0.24(19.42%)				
283.	(0.00008) RY (7) C 19	s(17.48%)p 0.09(1.52%)d 4.63(81.00%)				
284.	(0.00002) RY (8) C 19	s(3.24%)p 2.17(7.03%)d27.73(89.73%)				
285.	(0.00001) RY (9) C 19	s(1.73%)p 0.07(0.13%)d56.88(98.15%)				
286.	(0.00000) RY (10) C 19	s(0.00%)p 1.00(4.65%)d20.50(95.35%)				
287.	(0.00107) RY (1) H 20	s(99.74%)p 0.00(0.26%)				
		0.0025	0.9987	0.0217	-0.0438	0.0132
288.	(0.00016) RY (2) H 20	s(0.03%)p99.99(99.97%)				
		0.0000	0.0185	0.0112	0.1289	-0.9914
289.	(0.00005) RY (3) H 20	s(0.00%)p 1.00(100.00%)				
290.	(0.00001) RY (4) H 20	s(0.29%)p99.99(99.71%)				
291.	(0.00425) RY (1) C 21	s(0.42%)p99.99(92.44%)d17.18(7.14%)				
		0.0000	0.0034	0.0640	0.0071	-0.0019

		0.4967	0.0170	0.8205	0.0049	0.0649
		0.2189	0.0268	0.0240	-0.1490	0.0015
292.	(0.00333) RY (2) C 21	s(1.88%)p	49.08(92.26%)d	3.12(5.86%)		
		0.0000	0.0285	0.1339	0.0067	-0.0081
		0.8193	-0.0055	-0.5009	-0.0032	-0.0172
		-0.1425	-0.0342	0.0276	-0.1877	-0.0332
293.	(0.00174) RY (3) C 21	s(0.01%)p	1.00(85.90%)d	0.16(14.09%)		
		0.0000	-0.0001	0.0080	-0.0006	0.0009
		0.0153	0.0015	0.0676	-0.0119	-0.9242
		-0.0278	-0.0046	0.3671	0.0422	0.0600
294.	(0.00085) RY (4) C 21	s(0.06%)p	81.49(5.22%)d	99.99(94.71%)		
		0.0000	0.0002	0.0252	-0.0027	0.0000
		0.0126	-0.0027	0.0076	0.0185	-0.2273
		-0.0865	0.7898	-0.5547	-0.0794	-0.0422
295.	(0.00065) RY (5) C 21	s(78.66%)p	0.06(5.02%)d	0.21(16.32%)		
		0.0000	-0.0120	0.8867	-0.0141	0.0176
		-0.2021	-0.0129	0.0928	-0.0004	0.0178
		-0.3081	-0.0590	0.0344	-0.2357	-0.0897
296.	(0.00017) RY (6) C 21	s(0.65%)p	13.34(8.70%)d	99.99(90.65%)		
		0.0000	0.0017	0.0689	-0.0421	-0.0037
		0.0304	-0.0008	0.0069	0.0158	-0.2929
		0.1771	-0.5735	-0.7196	0.0796	-0.1486
297.	(0.00015) RY (7) C 21	s(16.59%)p	0.18(2.97%)d	4.85(80.44%)		
		0.0000	0.0071	0.3569	-0.1962	-0.0201
		0.1529	0.0018	-0.0529	-0.0034	0.0554
		0.2763	0.1627	0.0704	0.8330	-0.0526
298.	(0.00007) RY (8) C 21	s(27.27%)p	0.19(5.27%)d	2.47(67.45%)		
299.	(0.00007) RY (9) C 21	s(69.74%)p	0.03(2.23%)d	0.40(28.02%)		
300.	(0.00001) RY (10) C 21	s(4.85%)p	0.01(0.05%)d	19.60(95.10%)		
301.	(0.00653) RY (1) C 22	s(2.02%)p	46.59(94.08%)d	1.93(3.91%)		
		0.0000	0.0103	0.1416	0.0044	0.0006
		-0.3828	-0.0013	-0.8837	-0.0009	-0.1149
		-0.1953	-0.0263	-0.0032	-0.0134	-0.0053
302.	(0.00475) RY (2) C 22	s(0.03%)p	99.99(93.86%)d	99.99(6.11%)		
		0.0000	-0.0040	0.0004	0.0176	0.0150
		0.8959	-0.0141	-0.3609	0.0001	-0.0717
		-0.0624	-0.0132	0.0216	-0.2378	0.0035
303.	(0.00063) RY (3) C 22	s(1.52%)p	1.81(2.74%)d	63.16(95.74%)		
		0.0000	-0.0007	0.1227	0.0106	-0.0005
		0.0052	-0.0029	0.0457	0.0047	-0.1589
		-0.1316	0.8211	-0.5118	-0.0590	-0.0233
304.	(0.00052) RY (4) C 22	s(1.68%)p	49.90(84.03%)d	8.48(14.28%)		
		0.0000	0.0003	0.1208	0.0474	-0.0028
		-0.0145	-0.0016	0.1614	0.0083	-0.9022
		-0.0940	0.0095	0.3564	0.0337	0.0759
305.	(0.00044) RY (5) C 22	s(85.58%)p	0.02(1.99%)d	0.15(12.44%)		
		0.0000	-0.0037	0.9250	-0.0144	0.0027
		0.0414	-0.0018	0.1258	-0.0036	0.0479
		0.0372	-0.2648	-0.2052	-0.0637	-0.0818
306.	(0.00034) RY (6) C 22	s(9.01%)p	1.31(11.83%)d	8.79(79.16%)		
		0.0000	-0.0015	0.2975	-0.0395	0.0024
		0.0165	0.0010	-0.0171	0.0003	0.3432
		-0.0244	0.4848	0.7387	0.0304	0.0968
307.	(0.00011) RY (7) C 22	s(6.84%)p	0.89(6.12%)d	12.72(87.04%)		
		0.0000	-0.0036	-0.0347	0.2593	-0.0055
		-0.0366	-0.0207	0.1982	-0.0041	0.1418
		-0.8978	-0.1251	0.0239	-0.2162	0.0370
308.	(0.00010) RY (8) C 22	s(90.38%)p	0.00(0.34%)d	0.10(9.28%)		
309.	(0.00008) RY (9) C 22	s(0.43%)p	11.74(5.00%)d	99.99(94.57%)		
310.	(0.00002) RY (10) C 22	s(2.58%)p	0.04(0.09%)d	37.74(97.33%)		
311.	(0.00424) RY (1) C 23	s(0.25%)p	99.99(92.34%)d	29.36(7.40%)		
		0.0000	-0.0018	0.0490	0.0107	0.0184
		0.7576	0.0075	0.5860	0.0020	0.0756
		0.2690	0.0325	0.0086	-0.0231	0.0013
312.	(0.00353) RY (2) C 23	s(2.39%)p	38.46(91.84%)d	2.41(5.77%)		
		0.0000	0.0289	0.1517	0.0066	0.0002
		-0.5964	-0.0105	0.7473	-0.0018	0.0648
		0.0228	0.0361	-0.0368	0.2306	-0.0363
313.	(0.00174) RY (3) C 23	s(0.07%)p	99.99(80.01%)d	99.99(19.92%)		
		0.0000	-0.0008	0.0258	0.0002	0.0000
		0.0286	0.0021	0.0811	-0.0158	-0.8902
		-0.0669	0.4379	0.0517	-0.0067	0.0177
314.	(0.00080) RY (4) C 23	s(1.16%)p	7.72(8.95%)d	77.52(89.89%)		
		0.0000	-0.0017	0.1076	-0.0023	-0.0012
		0.0249	0.0028	-0.0706	-0.0148	0.2893
		-0.0822	0.6617	-0.6582	-0.0782	-0.1223
315.	(0.00067) RY (5) C 23	s(78.87%)p	0.06(4.80%)d	0.21(16.33%)		

		0.0000	-0.0117	0.8879	-0.0125	-0.0160
		0.1412	0.0118	-0.1642	0.0035	-0.0258
		-0.1520	-0.1035	0.0441	0.3494	-0.0741
316.	(0.00016) RY (6) C 23	s(13.85%)p 0.23(3.22%)d 5.99(82.93%)	0.0000	0.0080	0.3172	-0.1945
			0.0074	-0.0750	-0.0211	0.1591
			0.0007	-0.0273	-0.2342	-0.1472
			0.0137	-0.8662	-0.0485	
317.	(0.00015) RY (7) C 23	s(0.32%)p34.71(11.25%)d99.99(88.42%)	0.0000	-0.0009	-0.0389	0.0416
			-0.0011	0.0064	0.0013	0.0101
			0.0165	-0.3348	0.1550	-0.5651
			-0.7210	0.0388	-0.1396	
318.	(0.00008) RY (8) C 23	s(43.18%)p 0.09(4.06%)d 1.22(52.76%)				
319.	(0.00007) RY (9) C 23	s(56.13%)p 0.06(3.54%)d 0.72(40.33%)				
320.	(0.00001) RY (10) C 23	s(3.92%)p 0.01(0.05%)d24.49(96.03%)				
321.	(0.00513) RY (1) C 24	s(0.00%)p 1.00(95.05%)d 0.05(4.95%)	0.0000	0.0024	-0.0014	0.0000
			-0.0050	-0.7943	0.0056	0.5651
			0.0018	0.0106	-0.0544	-0.0081
			0.0248	-0.2142	-0.0020	
322.	(0.00296) RY (2) C 24	s(1.02%)p88.73(90.16%)d 8.69(8.83%)	0.0000	0.0028	0.0994	-0.0164
			0.0090	0.5498	0.0136	0.7711
			0.0059	0.0664	-0.2836	-0.0444
			-0.0210	0.0699	-0.0230	
323.	(0.00058) RY (3) C 24	s(74.30%)p 0.00(0.05%)d 0.35(25.65%)	0.0000	-0.0057	0.8619	0.0089
			-0.0020	-0.0127	-0.0014	-0.0171
			-0.0021	0.0083	0.2832	-0.2388
			-0.2499	-0.0931	-0.2193	
324.	(0.00056) RY (4) C 24	s(15.25%)p 0.05(0.76%)d 5.51(83.99%)	0.0000	-0.0021	0.3905	-0.0030
			-0.0002	0.0071	-0.0003	0.0046
			0.0048	-0.0866	-0.0071	0.6699
			0.6205	0.0268	0.0734	
325.	(0.00051) RY (5) C 24	s(0.06%)p21.00(1.19%)d99.99(98.76%)	0.0000	-0.0001	0.0237	-0.0006
			0.0001	-0.0009	-0.0005	0.0071
			0.0017	-0.1086	0.0747	-0.6887
			0.6985	0.1039	0.0949	
326.	(0.00030) RY (6) C 24	s(0.02%)p99.99(97.44%)d99.99(2.54%)	0.0000	-0.0011	0.0078	0.0135
			0.0004	-0.0239	-0.0008	-0.0393
			-0.0100	0.9860	0.0768	-0.0037
			0.0299	0.0085		
327.	(0.00015) RY (7) C 24	s(9.06%)p 1.08(9.78%)d 8.95(81.15%)	0.0000	0.0035	0.2584	0.1544
			0.0089	-0.1851	0.0115	-0.2472
			-0.0009	0.0477	-0.8562	-0.1098
			0.2500	0.0251		
328.	(0.00008) RY (8) C 24	s(6.74%)p 0.70(4.74%)d13.14(88.52%)				
329.	(0.00005) RY (9) C 24	s(90.81%)p 0.01(0.86%)d 0.09(8.33%)				
330.	(0.00001) RY (10) C 24	s(2.81%)p 0.02(0.06%)d34.61(97.13%)				
331.	(0.00229) RY (1) C 25	s(10.15%)p 7.21(73.11%)d 1.65(16.74%)	0.0000	0.0070	0.3185	0.0014
			-0.0132	-0.5478	0.0147	0.5595
			0.0018	0.3430	0.0281	-0.3010
			0.2654	0.0742	0.0073	
332.	(0.00185) RY (2) C 25	s(2.36%)p32.55(76.66%)d 8.91(20.98%)	0.0000	0.0054	0.1527	0.0143
			-0.0133	-0.5936	-0.0169	-0.5619
			0.0021	-0.3131	0.2406	-0.2559
			-0.1160	-0.0415	-0.2670	
333.	(0.00074) RY (3) C 25	s(24.77%)p 2.73(67.51%)d 0.31(7.72%)	0.0000	0.0061	0.4945	0.0564
			-0.0065	0.3548	0.0029	-0.3802
			-0.0269	0.6356	0.1635	-0.1669
			-0.0590	-0.0948	-0.1006	
334.	(0.00034) RY (4) C 25	s(22.28%)p 0.52(11.58%)d 2.97(66.15%)	0.0000	0.0053	0.3477	-0.3192
			0.0117	-0.3183	-0.0036	-0.0410
			-0.0025	0.1125	-0.1898	0.7050
			-0.2062	0.1405		
335.	(0.00006) RY (5) C 25	s(36.31%)p 1.25(45.51%)d 0.50(18.19%)				
336.	(0.00004) RY (6) C 25	s(6.99%)p 2.13(14.89%)d11.18(78.13%)				
337.	(0.00002) RY (7) C 25	s(20.07%)p 0.06(1.15%)d 3.92(78.77%)				
338.	(0.00001) RY (8) C 25	s(3.03%)p 1.22(3.71%)d30.78(93.26%)				
339.	(0.00001) RY (9) C 25	s(32.58%)p 0.03(0.96%)d 2.04(66.45%)				
340.	(0.00001) RY (10) C 25	s(41.50%)p 0.13(5.24%)d 1.28(53.27%)				
341.	(0.00073) RY (1) H 26	s(99.99%)p 0.00(0.01%)	-0.0002	0.9999	0.0079	0.0028
			-0.0062			
342.	(0.00007) RY (2) H 26	s(0.00%)p 1.00(100.00%)				
343.	(0.00004) RY (3) H 26	s(0.01%)p 1.00(99.99%)				
344.	(0.00000) RY (4) H 26	s(0.05%)p99.99(99.95%)				
345.	(0.00118) RY (1) H 27	s(99.84%)p 0.00(0.16%)	-0.0003	0.9992	0.0246	0.0157
			0.0270			
346.	(0.00007) RY (2) H 27	s(0.01%)p99.99(99.99%)				
347.	(0.00004) RY (3) H 27	s(0.09%)p99.99(99.91%)				
348.	(0.00000) RY (4) H 27	s(0.11%)p99.99(99.89%)				

349.	(0.00272)	RY	(1)	H	28	s(99.56%)p 0.00(0.44%) -0.0040 0.9978 -0.0428 -0.0163 0.0479
350.	(0.00006)	RY	(2)	H	28	s(0.00%)p 1.00(100.00%)
351.	(0.00004)	RY	(3)	H	28	s(0.43%)p99.99(99.57%)
352.	(0.00001)	RY	(4)	H	28	s(0.06%)p99.99(99.94%)
353.	(0.00254)	RY	(1)	C	29	s(2.70%)p31.55(85.24%)d 4.47(12.06%) 0.0000 0.0025 0.1641 -0.0085 0.0073 0.2806 0.0154 0.5173 -0.0104 -0.7110 0.0443 -0.1399 -0.0046 0.1452 0.2792
354.	(0.00180)	RY	(2)	C	29	s(12.72%)p 5.15(65.48%)d 1.72(21.81%) 0.0000 0.0134 0.3560 0.0154 -0.0193 -0.5755 -0.0075 -0.4008 -0.0082 -0.4030 0.3547 0.0946 0.1404 -0.1819 0.1746
355.	(0.00057)	RY	(3)	C	29	s(24.35%)p 2.20(53.55%)d 0.91(22.09%) 0.0000 0.0074 0.4889 -0.0665 -0.0097 0.4593 0.0189 -0.5342 0.0153 -0.1963 -0.3306 -0.1026 -0.1531 0.0276 -0.2774
356.	(0.00043)	RY	(4)	C	29	s(5.93%)p 7.04(41.74%)d 8.82(52.33%) 0.0000 -0.0035 -0.0227 0.2425 -0.0178 0.5933 0.0124 -0.1955 -0.0020 0.1633 0.4741 0.1434 0.2658 -0.2876 0.3531
357.	(0.00006)	RY	(5)	C	29	s(39.60%)p 0.63(24.78%)d 0.90(35.62%)
358.	(0.00003)	RY	(6)	C	29	s(18.51%)p 0.39(7.16%)d 4.02(74.33%)
359.	(0.00002)	RY	(7)	C	29	s(29.54%)p 0.07(1.96%)d 2.32(68.50%)
360.	(0.00001)	RY	(8)	C	29	s(26.00%)p 0.25(6.40%)d 2.60(67.60%)
361.	(0.00001)	RY	(9)	C	29	s(15.14%)p 0.44(6.67%)d 5.17(78.20%)
362.	(0.00000)	RY	(10)	C	29	s(25.54%)p 0.29(7.34%)d 2.63(67.12%)
363.	(0.00253)	RY	(1)	H	30	s(99.55%)p 0.00(0.45%) -0.0040 0.9978 0.0103 -0.0369 -0.0546
364.	(0.00007)	RY	(2)	H	30	s(0.01%)p 1.00(99.99%)
365.	(0.00005)	RY	(3)	H	30	s(0.43%)p99.99(99.57%)
366.	(0.00001)	RY	(4)	H	30	s(0.05%)p99.99(99.95%)
367.	(0.00093)	RY	(1)	H	31	s(99.71%)p 0.00(0.29%) -0.0004 0.9986 0.0498 -0.0185 -0.0080
368.	(0.00007)	RY	(2)	H	31	s(0.04%)p99.99(99.96%)
369.	(0.00004)	RY	(3)	H	31	s(0.23%)p99.99(99.77%)
370.	(0.00000)	RY	(4)	H	31	s(0.07%)p99.99(99.93%)
371.	(0.00088)	RY	(1)	H	32	s(99.74%)p 0.00(0.26%) -0.0001 0.9987 0.0393 0.0086 0.0313
372.	(0.00007)	RY	(2)	H	32	s(0.23%)p99.99(99.77%)
373.	(0.00004)	RY	(3)	H	32	s(0.01%)p99.99(99.99%)
374.	(0.00000)	RY	(4)	H	32	s(0.07%)p99.99(99.93%)
375.	(0.00504)	RY	(1)	C	33	s(0.15%)p99.99(94.56%)d36.15(5.30%) 0.0000 0.0350 0.0013 0.0154 -0.0289 -0.9388 0.0147 0.2136 0.0039 0.1324 0.0616 0.0322 -0.0873 -0.1346 0.1496
376.	(0.00195)	RY	(2)	C	33	s(0.18%)p99.99(96.19%)d20.69(3.63%) 0.0000 -0.0021 0.0417 0.0032 -0.0006 0.0790 0.0058 -0.2164 -0.0261 0.9530 0.0221 -0.0703 0.1383 0.0521 0.0951
377.	(0.00172)	RY	(3)	C	33	s(1.20%)p78.62(94.30%)d 3.75(4.50%) 0.0000 0.0040 0.1085 -0.0146 -0.0003 -0.2410 0.0187 -0.9133 0.0068 -0.2243 0.0206 0.0676 0.1656 0.0460 0.1024
378.	(0.00076)	RY	(4)	C	33	s(2.94%)p 2.39(7.05%)d30.58(90.01%) 0.0000 -0.0013 0.1712 -0.0110 -0.0005 0.0265 0.0149 0.2470 0.0094 -0.0919 -0.1804 0.2817 0.6891 0.2262 0.5121
379.	(0.00046)	RY	(5)	C	33	s(94.66%)p 0.01(0.62%)d 0.05(4.71%) 0.0000 -0.0045 0.9728 -0.0160 -0.0285 -0.0001 -0.0035 0.0736 0.0012 -0.0019 0.0382 -0.0852 -0.1137 0.0226 -0.1581
380.	(0.00019)	RY	(6)	C	33	s(0.08%)p21.04(1.66%)d99.99(98.26%) 0.0000 0.0002 0.0281 -0.0005 -0.0014 0.0068 0.0079 -0.0388 -0.0258 0.1198 -0.3008 0.8838 -0.2145 -0.0541 -0.2490
381.	(0.00010)	RY	(7)	C	33	s(0.72%)p 0.24(0.17%)d99.99(99.11%) 0.0000 -0.0025 -0.0345 0.0774 -0.0040 -0.0061 -0.0150 0.0378 -0.0043 -0.0026 0.6966 0.2513 -0.1672 0.6425 0.0437
382.	(0.00007)	RY	(8)	C	33	s(6.39%)p 0.74(4.74%)d13.92(88.87%)
383.	(0.00004)	RY	(9)	C	33	s(72.16%)p 0.00(0.34%)d 0.38(27.50%)
384.	(0.00003)	RY	(10)	C	33	s(21.64%)p 0.02(0.47%)d 3.60(77.89%)
385.	(0.00568)	RY	(1)	C	34	s(0.89%)p99.99(93.11%)d 6.70(5.99%) 0.0000 0.0111 0.0938 0.0037 0.0097 0.4333 0.0013 0.1279 -0.0131 -0.8525 0.1144 -0.1419 -0.0044 -0.0322 0.1602

386. (0.00355) RY (2) C 34	s(0.01%)p99.99(96.50%)d99.99(3.49%) 0.0000 0.0102 -0.0012 -0.0005 0.0117 -0.8307 0.0012 0.3661 0.0073 -0.3752 -0.0087 -0.1063 0.0672 0.0799 -0.1123
387. (0.00157) RY (3) C 34	s(2.39%)p35.23(84.12%)d 5.65(13.49%) 0.0000 -0.0006 0.1540 -0.0127 -0.0029 -0.2591 -0.0033 -0.8434 -0.0007 -0.2505 0.0100 -0.0868 -0.3120 -0.0744 -0.1562
388. (0.00111) RY (4) C 34	s(1.07%)p 0.71(0.75%)d92.10(98.18%) 0.0000 -0.0008 0.1025 -0.0128 -0.0098 -0.0278 -0.0231 -0.0779 -0.0067 0.0036 0.6752 0.3369 0.0362 0.6397 0.0425
389. (0.00036) RY (5) C 34	s(89.91%)p 0.04(3.21%)d 0.08(6.88%) 0.0000 -0.0024 0.9479 -0.0260 -0.0053 0.0385 -0.0024 0.1575 0.0065 0.0759 -0.1855 0.1197 -0.0218 0.0112 -0.1394
390. (0.00028) RY (6) C 34	s(0.03%)p99.99(3.54%)d99.99(96.43%) 0.0000 -0.0010 0.0072 0.0147 -0.0205 0.1545 0.0101 -0.0896 -0.0088 0.0542 -0.0396 -0.6300 0.4097 0.3786 -0.5046
391. (0.00015) RY (7) C 34	s(0.95%)p12.63(12.01%)d91.52(87.04%) 0.0000 0.0010 0.0635 0.0740 0.0033 -0.1105 0.0116 -0.3140 0.0043 -0.0956 -0.2791 0.2143 0.7505 0.0604 0.4238
392. (0.00010) RY (8) C 34	s(45.98%)p 0.09(4.01%)d 1.09(50.01%)
393. (0.00005) RY (9) C 34	s(53.67%)p 0.05(2.78%)d 0.81(43.55%)
394. (0.00002) RY (10) C 34	s(5.17%)p 0.02(0.09%)d18.33(94.74%)
395. (0.00438) RY (1) C 35	s(1.00%)p92.54(92.30%)d 6.72(6.71%) 0.0000 -0.0299 0.0946 0.0112 0.0057 0.5158 -0.0066 -0.3882 0.0101 0.7114 0.0416 -0.2162 0.1047 0.0688 -0.0538
396. (0.00217) RY (2) C 35	s(0.14%)p99.99(96.46%)d25.11(3.40%) 0.0000 0.0007 0.0368 0.0014 0.0145 -0.7754 0.0006 0.0728 -0.0100 0.5981 0.1093 -0.0515 -0.0662 -0.0489 0.1126
397. (0.00074) RY (3) C 35	s(0.11%)p99.99(93.22%)d60.38(6.67%) 0.0000 -0.0011 -0.0042 0.0330 -0.0032 -0.2975 -0.0111 -0.8776 -0.0040 -0.2707 0.0350 0.0776 0.1781 0.1196 0.1158
398. (0.00048) RY (4) C 35	s(0.88%)p 0.80(0.71%)d99.99(98.41%) 0.0000 0.0002 0.0933 -0.0106 0.0000 0.0141 -0.0013 -0.0618 -0.0003 -0.0552 0.6686 0.0811 -0.5228 0.3495 -0.3675
399. (0.00027) RY (5) C 35	s(95.39%)p 0.02(1.45%)d 0.03(3.15%) 0.0000 -0.0005 0.9729 -0.0855 0.0009 -0.0297 0.0010 0.0499 0.0050 -0.1055 -0.0911 -0.0936 0.0255 0.0669 0.0967
400. (0.00009) RY (6) C 35	s(0.52%)p 6.15(3.18%)d99.99(96.30%)
401. (0.00006) RY (7) C 35	s(89.72%)p 0.01(0.85%)d 0.11(9.43%)
402. (0.00002) RY (8) C 35	s(9.67%)p 0.54(5.26%)d 8.80(85.07%)
403. (0.00001) RY (9) C 35	s(1.34%)p 1.24(1.66%)d72.38(97.00%)
404. (0.00001) RY (10) C 35	s(1.40%)p 3.54(4.95%)d66.95(93.65%)
405. (0.00155) RY (1) H 36	s(99.67%)p 0.00(0.33%) 0.0026 0.9983 0.0332 0.0182 0.0431
406. (0.00018) RY (2) H 36	s(0.17%)p99.99(99.83%) -0.0006 0.0410 -0.3337 -0.8864 -0.3181
407. (0.00004) RY (3) H 36	s(0.00%)p 1.00(100.00%)
408. (0.00001) RY (4) H 36	s(0.23%)p99.99(99.77%)
409. (0.00497) RY (1) C 37	s(1.68%)p55.09(92.57%)d 3.42(5.75%) 0.0000 0.0103 0.1289 -0.0088 -0.0175 -0.9231 0.0078 0.2252 0.0020 0.1500 -0.0743 -0.0318 0.0943 0.1202 -0.1663
410. (0.00397) RY (2) C 37	s(0.07%)p99.99(96.96%)d41.77(2.97%) 0.0000 -0.0009 0.0266 -0.0022 0.0012 -0.0655 -0.0029 0.3280 0.0193 -0.9259 0.0477 -0.1477 0.0553 0.0208 0.0462
411. (0.00160) RY (3) C 37	s(1.71%)p50.90(87.00%)d 6.60(11.29%) 0.0000 -0.0019 0.1295 -0.0177 -0.0021 -0.2448 -0.0077 -0.8542 -0.0026 -0.2836 -0.2451 -0.1116 -0.0545 -0.1932 0.0074
412. (0.00106) RY (4) C 37	s(0.54%)p 0.83(0.45%)d99.99(99.02%) 0.0000 -0.0005 0.0728 -0.0093 -0.0064 0.0070 -0.0220 -0.0615 -0.0093 0.0055 -0.1920 0.2542 0.7349 0.2160 0.5495
413. (0.00036) RY (5) C 37	s(90.56%)p 0.03(2.41%)d 0.08(7.03%) 0.0000 -0.0023 0.9516 -0.0072 0.0086 0.1112 0.0006 0.0801 -0.0046 0.0721

414.	(0.00027)	RY	(6)	C 37	0.1458 -0.1074 -0.1124 -0.0476 0.1504 s(2.22%)p 1.29(2.87%)d42.85(94.92%) 0.0000 0.0004 0.1488 0.0039 0.0024 0.0090 -0.0092 0.0770 0.0241 -0.1483 -0.3027 0.8741 -0.2145 -0.1025 -0.1925
415.	(0.00017)	RY	(7)	C 37	s(0.02%)p99.99(11.01%)d99.99(88.97%) 0.0000 -0.0006 0.0153 0.0005 -0.0033 0.1009 -0.0122 0.2983 -0.0046 0.1035 -0.7292 -0.3033 0.0790 -0.5096 0.0087
416.	(0.00010)	RY	(8)	C 37	s(51.92%)p 0.06(3.09%)d 0.87(44.99%) 0.0000 0.0012 0.1348 0.7079 -0.0072 0.1599 0.0012 -0.0667 0.0008 -0.0285 -0.1054 -0.0755 0.3168 0.2273 -0.5301
417.	(0.00004)	RY	(9)	C 37	s(42.29%)p 0.09(3.71%)d 1.28(54.01%)
418.	(0.00001)	RY	(10)	C 37	s(9.05%)p 0.01(0.11%)d10.04(90.84%)
419.	(0.00438)	RY	(1)	C 38	s(0.42%)p99.99(92.87%)d16.16(6.72%) 0.0000 -0.0297 0.0566 0.0084 0.0014 0.4897 0.0003 0.1398 -0.0115 -0.8180 -0.1257 0.1598 0.0034 0.0210 -0.1593
420.	(0.00182)	RY	(2)	C 38	s(0.00%)p 1.00(97.04%)d 0.03(2.96%) 0.0000 -0.0009 0.0023 0.0001 -0.0144 0.8198 0.0029 -0.3339 -0.0065 0.4319 -0.0010 -0.0992 0.0830 0.0854 -0.0746
421.	(0.00111)	RY	(3)	C 38	s(0.47%)p99.99(51.61%)d99.99(47.92%) 0.0000 -0.0007 0.0682 0.0067 0.0029 -0.1633 0.0081 -0.6633 0.0004 -0.2223 0.4801 0.2588 -0.0070 0.4259 0.0187
422.	(0.00067)	RY	(4)	C 38	s(4.23%)p 9.89(41.84%)d12.75(53.93%) 0.0000 -0.0004 0.2040 -0.0266 0.0058 0.1387 0.0152 0.6053 0.0047 0.1804 0.3546 0.3243 0.2363 0.4552 0.2129
423.	(0.00024)	RY	(5)	C 38	s(91.15%)p 0.02(1.52%)d 0.08(7.33%) 0.0000 -0.0014 0.9483 -0.1107 0.0004 -0.0598 -0.0011 -0.0918 -0.0063 0.0559 -0.2207 -0.0117 -0.1393 -0.0304 -0.0645
424.	(0.00010)	RY	(6)	C 38	s(0.29%)p10.36(2.98%)d99.99(96.74%) 0.0000 -0.0005 -0.0266 0.0465 -0.0208 0.1358 0.0094 -0.0750 -0.0106 0.0710 0.0006 0.6014 -0.3990 -0.4199 0.5198
425.	(0.00006)	RY	(7)	C 38	s(91.24%)p 0.01(0.52%)d 0.09(8.24%)
426.	(0.00002)	RY	(8)	C 38	s(7.80%)p 0.70(5.42%)d11.13(86.78%)
427.	(0.00001)	RY	(9)	C 38	s(1.76%)p 1.39(2.44%)d54.47(95.80%)
428.	(0.00001)	RY	(10)	C 38	s(2.81%)p 1.37(3.84%)d33.27(93.35%)
429.	(0.00150)	RY	(1)	H 39	s(99.83%)p 0.00(0.17%) 0.0025 0.9992 0.0170 0.0012 -0.0370
430.	(0.00018)	RY	(2)	H 39	s(0.00%)p 1.00(100.00%) 0.0000 0.0056 0.3375 0.8791 0.3364
431.	(0.00003)	RY	(3)	H 39	s(0.00%)p 1.00(100.00%)
432.	(0.00001)	RY	(4)	H 39	s(0.23%)p99.99(99.77%)
433.	(0.00539)	RY	(1)	C 40	s(0.58%)p99.99(93.25%)d10.70(6.18%) 0.0000 0.0126 0.0745 0.0075 0.0131 0.4413 -0.0142 -0.3753 0.0105 0.7723 -0.0438 0.2016 -0.1033 -0.0783 0.0492
434.	(0.00383)	RY	(2)	C 40	s(0.17%)p99.99(96.06%)d22.27(3.77%) 0.0000 -0.0107 0.0397 -0.0006 -0.0096 0.8207 -0.0015 -0.0891 0.0111 -0.5281 0.0831 -0.0331 -0.0727 -0.0671 0.1410
435.	(0.00160)	RY	(3)	C 40	s(0.07%)p99.99(87.85%)d99.99(12.08%) 0.0000 0.0011 0.0256 0.0011 -0.0037 -0.2688 -0.0092 -0.8573 -0.0040 -0.2670 0.1449 0.1524 0.1327 0.2042 0.1315
436.	(0.00061)	RY	(4)	C 40	s(0.32%)p 1.67(0.53%)d99.99(99.16%) 0.0000 -0.0003 0.0562 -0.0029 0.0017 -0.0145 0.0007 -0.0653 -0.0009 -0.0283 -0.6763 -0.1197 0.5019 -0.3433 0.3873
437.	(0.00040)	RY	(5)	C 40	s(88.15%)p 0.01(0.88%)d 0.12(10.97%) 0.0000 -0.0022 0.9382 -0.0344 -0.0007 -0.0510 -0.0012 0.0656 -0.0100 0.0429 0.1533 -0.2301 0.0139 0.1056 0.1480
438.	(0.00025)	RY	(6)	C 40	s(4.55%)p 0.72(3.29%)d20.28(92.17%) 0.0000 -0.0003 0.2132 0.0030 -0.0207 0.1557 0.0012 -0.0118 0.0124 -0.0889 -0.3717 0.2772 0.3101 0.3250 -0.7106
439.	(0.00014)	RY	(7)	C 40	s(0.59%)p19.02(11.31%)d99.99(88.10%) 0.0000 0.0003 0.0753 0.0165 0.0020 -0.0874 0.0127 -0.3135 0.0019 -0.0837 -0.2511 -0.4600 -0.4701 -0.4418 -0.4361

440.	(0.00009)	RY	(8)	C 40	s(54.04%)p 0.07(3.56%)d 0.78(42.40%)
441.	(0.00006)	RY	(9)	C 40	s(46.77%)p 0.07(3.28%)d 1.07(49.95%)
442.	(0.00001)	RY	(10)	C 40	s(4.84%)p 0.02(0.07%)d19.65(95.09%)
443.	(0.00181)	RY	(1)	C 41	s(0.12%)p99.99(91.43%)d69.67(8.44%) 0.0000 -0.0017 0.0344 0.0052 0.0089 0.8163 -0.0059 -0.4339 0.0062 0.2439 -0.0144 -0.1755 0.1492 0.1210 -0.1286
444.	(0.00054)	RY	(2)	C 41	s(0.15%)p99.99(38.10%)d99.99(61.76%) 0.0000 -0.0035 0.0219 0.0310 -0.0042 -0.2604 -0.0111 -0.5430 -0.0027 -0.1348 -0.2724 0.1475 0.6099 -0.0995 0.3738
445.	(0.00047)	RY	(3)	C 41	s(18.25%)p 4.43(80.92%)d 0.05(0.82%) 0.0000 0.0294 0.4260 -0.0124 -0.0009 0.3105 0.0026 0.1499 -0.0052 -0.8308 -0.0586 0.0203 0.0173 0.0462 0.0443
446.	(0.00005)	RY	(4)	C 41	s(84.83%)p 0.09(7.48%)d 0.09(7.69%)
447.	(0.00004)	RY	(5)	C 41	s(3.23%)p18.45(59.63%)d11.49(37.14%)
448.	(0.00003)	RY	(6)	C 41	s(56.16%)p 0.12(6.97%)d 0.66(36.87%)
449.	(0.00001)	RY	(7)	C 41	s(7.57%)p 0.62(4.69%)d11.59(87.73%)
450.	(0.00001)	RY	(8)	C 41	s(27.07%)p 0.17(4.71%)d 2.52(68.22%)
451.	(0.00001)	RY	(9)	C 41	s(1.17%)p 4.64(5.45%)d79.58(93.38%)
452.	(0.00000)	RY	(10)	C 41	s(1.56%)p 0.48(0.75%)d62.78(97.69%)
453.	(0.00097)	RY	(1)	H 42	s(97.44%)p 0.03(2.56%) -0.0001 0.9871 0.0728 0.0833 -0.1154
454.	(0.00007)	RY	(2)	H 42	s(2.53%)p38.54(97.47%)
455.	(0.00007)	RY	(3)	H 42	s(0.01%)p99.99(99.99%)
456.	(0.00000)	RY	(4)	H 42	s(0.06%)p99.99(99.94%)
457.	(0.00099)	RY	(1)	H 43	s(98.91%)p 0.01(1.09%) -0.0001 0.9945 0.0424 -0.0216 -0.0929
458.	(0.00008)	RY	(2)	H 43	s(0.44%)p99.99(99.56%)
459.	(0.00007)	RY	(3)	H 43	s(0.64%)p99.99(99.36%)
460.	(0.00000)	RY	(4)	H 43	s(0.05%)p99.99(99.95%)
461.	(0.00110)	RY	(1)	H 44	s(99.65%)p 0.00(0.35%) -0.0009 0.9983 0.0231 -0.0181 -0.0510
462.	(0.00009)	RY	(2)	H 44	s(0.16%)p99.99(99.84%)
463.	(0.00007)	RY	(3)	H 44	s(0.16%)p99.99(99.84%)
464.	(0.00001)	RY	(4)	H 44	s(0.08%)p99.99(99.92%)
465.	(0.00160)	RY	(1)	C 45	s(0.21%)p99.99(89.90%)d46.12(9.89%) 0.0000 -0.0041 0.0460 0.0034 0.0115 0.8161 -0.0006 -0.0700 -0.0106 -0.4773 -0.1084 0.1242 0.0746 0.1195 -0.2277
466.	(0.00059)	RY	(2)	C 45	s(4.67%)p10.73(50.07%)d 9.70(45.27%) 0.0000 0.0160 0.2154 0.0029 0.0002 0.3377 0.0069 0.2394 0.0059 0.5738 0.2462 0.2354 0.3010 0.3982 0.2958
467.	(0.00042)	RY	(3)	C 45	s(9.49%)p 7.55(71.67%)d 1.98(18.84%) 0.0000 0.0247 0.3039 -0.0446 -0.0033 0.2424 -0.0066 -0.6351 0.0029 0.5046 -0.1695 -0.1931 -0.2436 -0.2046 -0.1455
468.	(0.00006)	RY	(4)	C 45	s(72.89%)p 0.22(16.26%)d 0.15(10.86%)
469.	(0.00005)	RY	(5)	C 45	s(22.30%)p 1.95(43.49%)d 1.53(34.21%)
470.	(0.00003)	RY	(6)	C 45	s(45.54%)p 0.18(8.04%)d 1.02(46.41%)
471.	(0.00001)	RY	(7)	C 45	s(21.85%)p 0.43(9.48%)d 3.14(68.67%)
472.	(0.00001)	RY	(8)	C 45	s(19.65%)p 0.20(3.90%)d 3.89(76.44%)
473.	(0.00001)	RY	(9)	C 45	s(1.95%)p 2.87(5.58%)d47.50(92.47%)
474.	(0.00000)	RY	(10)	C 45	s(1.55%)p 1.13(1.76%)d62.22(96.69%)
475.	(0.00097)	RY	(1)	H 46	s(98.72%)p 0.01(1.28%) -0.0001 0.9936 0.0784 -0.0507 0.0642
476.	(0.00008)	RY	(2)	H 46	s(0.01%)p 1.00(99.99%)
477.	(0.00007)	RY	(3)	H 46	s(1.26%)p78.11(98.74%)
478.	(0.00000)	RY	(4)	H 46	s(0.05%)p99.99(99.95%)
479.	(0.00126)	RY	(1)	H 47	s(98.87%)p 0.01(1.13%) -0.0004 0.9943 0.0683 0.0103 0.0807
480.	(0.00008)	RY	(2)	H 47	s(0.66%)p99.99(99.34%)
481.	(0.00006)	RY	(3)	H 47	s(0.45%)p99.99(99.55%)
482.	(0.00001)	RY	(4)	H 47	s(0.07%)p99.99(99.93%)
483.	(0.00123)	RY	(1)	H 48	s(99.13%)p 0.01(0.87%) -0.0006 0.9956 0.0389 -0.0763 0.0374
484.	(0.00009)	RY	(2)	H 48	s(0.36%)p99.99(99.64%)
485.	(0.00007)	RY	(3)	H 48	s(0.52%)p99.99(99.48%)
486.	(0.00000)	RY	(4)	H 48	s(0.05%)p99.99(99.95%)
487.	(0.01093)	RY	(1)	B 49	s(9.08%)p 9.68(87.94%)d 0.33(2.98%) 0.0000 -0.0214 0.2957 0.0542 -0.0326 0.3103 -0.0561 0.8171 -0.0226 0.3327 -0.1559 -0.0501 0.0392 -0.0369 -0.0062
488.	(0.00360)	RY	(2)	B 49	s(3.75%)p23.56(88.40%)d 2.09(7.84%) 0.0000 0.0003 0.1904 0.0356 0.0140

				0.8415	-0.0176	-0.3988	0.0112	0.1276	
				0.2285	0.1050	0.0027	-0.1227	-0.0109	
489.	(0.00220)	RY (3)	B 49	s(0.02%)p99.99(69.11%)d99.99(30.87%)	0.0000	-0.0015	0.0136	-0.0032	0.0090
				-0.2572	-0.0346	-0.2067	0.0792	0.7581	
				-0.0079	0.0568	-0.3999	-0.2175	-0.3134	
490.	(0.00113)	RY (4)	B 49	s(66.03%)p 0.24(15.80%)d 0.28(18.18%)	0.0000	-0.0026	0.8069	-0.0960	0.0139
				-0.1994	-0.0224	-0.0847	-0.0076	-0.3321	
				0.0482	-0.2039	-0.1790	-0.2834	-0.1596	
491.	(0.00087)	RY (5)	B 49	s(8.55%)p 2.10(17.92%)d 8.61(73.54%)	0.0000	-0.0061	0.2793	-0.0861	0.0131
				-0.1909	-0.0233	-0.2220	-0.0249	0.3035	
				-0.2629	0.2360	0.6894	-0.1631	0.3298	
492.	(0.00075)	RY (6)	B 49	s(1.06%)p 8.58(9.09%)d84.81(89.85%)	0.0000	-0.0035	0.1027	-0.0061	0.0241
				-0.2111	0.0085	0.1957	0.0020	0.0858	
				0.8713	0.3309	0.0955	0.0610	0.1302	
493.	(0.00043)	RY (7)	B 49	s(13.04%)p 0.22(2.89%)d 6.45(84.07%)	0.0000	0.0072	0.3490	-0.0928	-0.0077
				-0.0084	0.0342	-0.1264	0.0085	0.1075	
				-0.1486	0.2013	-0.1803	0.8627	0.0360	
494.	(0.00021)	RY (8)	B 49	s(96.36%)p 0.01(1.20%)d 0.03(2.44%)	0.0000	0.0039	0.1137	0.9750	0.0013
				-0.0848	0.0088	-0.0627	0.0053	-0.0278	
				-0.0510	0.0750	-0.0532	0.0097	0.1152	
495.	(0.00008)	RY (9)	B 49	s(0.46%)p18.40(8.42%)d99.99(91.12%)					
496.	(0.00002)	RY (10)	B 49	s(1.62%)p 0.11(0.18%)d60.79(98.21%)					
497.	(0.00361)	RY (1)	N 50	s(6.47%)p14.02(90.69%)d 0.44(2.84%)	0.0000	-0.0054	0.2527	-0.0282	0.0364
				0.8509	-0.0126	-0.2704	0.0100	0.3288	
				0.0403	-0.1009	0.0430	-0.1191	0.0236	
498.	(0.00101)	RY (2)	N 50	s(2.89%)p29.50(85.18%)d 4.13(11.93%)	0.0000	-0.0114	0.1640	-0.0429	0.0039
				0.1692	-0.0140	0.8846	-0.0016	0.2012	
				0.2118	0.0630	-0.1414	0.0406	-0.2210	
499.	(0.00081)	RY (3)	N 50	s(0.37%)p99.99(89.42%)d27.35(10.21%)	0.0000	0.0010	0.0610	0.0032	0.0108
				-0.3786	0.0074	-0.1074	-0.0229	0.8594	
				0.1033	-0.0764	-0.0206	0.1788	0.2307	
500.	(0.00049)	RY (4)	N 50	s(1.36%)p 2.14(2.91%)d70.54(95.74%)	0.0000	-0.0016	0.1165	-0.0003	-0.0082
				-0.0493	0.0009	-0.1189	0.0074	-0.1111	
				0.1024	-0.4929	-0.8383	-0.0012	-0.0347	
501.	(0.00031)	RY (5)	N 50	s(0.63%)p16.32(10.21%)d99.99(89.16%)	0.0000	0.0012	0.0561	-0.0557	0.0062
				-0.1602	0.0185	-0.2293	-0.0043	0.1531	
				0.2258	0.4942	-0.2137	-0.5803	-0.4626	
502.	(0.00025)	RY (6)	N 50	s(14.40%)p 0.51(7.30%)d 5.44(78.30%)	0.0000	-0.0107	0.3780	0.0323	-0.0033
				-0.1512	0.0212	-0.0536	0.0033	-0.2163	
				0.7473	-0.2650	0.3391	-0.1353	0.1448	
503.	(0.00018)	RY (7)	N 50	s(7.49%)p 0.53(4.00%)d11.82(88.51%)	0.0000	0.0054	0.2713	-0.0352	0.0164
				-0.1096	0.0051	-0.1602	-0.0246	0.0380	
				-0.1398	-0.2667	0.2325	0.3814	-0.7713	
504.	(0.00013)	RY (8)	N 50	s(21.65%)p 0.22(4.84%)d 3.40(73.51%)	0.0000	0.0127	0.4577	-0.0824	0.0048
				0.0267	0.0053	-0.1442	0.0215	-0.1624	
				0.1010	0.5833	-0.2341	0.5504	0.1641	
505.	(0.00007)	RY (9)	N 50	s(51.75%)p 0.09(4.85%)d 0.84(43.39%)					
506.	(0.00002)	RY (10)	N 50	s(93.03%)p 0.01(0.80%)d 0.07(6.17%)					
507.	(0.00105)	RY (1)	O 51	s(4.36%)p21.32(92.99%)d 0.61(2.65%)	0.0000	0.0064	0.2062	0.0323	0.0013
				-0.8861	0.0012	-0.3784	-0.0015	-0.0404	
				-0.1331	-0.0429	-0.0111	0.0674	-0.0474	
508.	(0.00030)	RY (2)	O 51	s(74.43%)p 0.10(7.30%)d 0.25(18.27%)	0.0000	-0.0085	0.8473	-0.1619	0.0162
				0.1833	-0.0178	0.1824	-0.0069	0.0741	
				-0.2903	-0.0113	-0.0287	0.2301	-0.2109	
509.	(0.00019)	RY (3)	O 51	s(0.78%)p99.99(94.68%)d 5.79(4.53%)	0.0000	0.0066	0.0793	0.0387	-0.0126
				-0.1583	0.0069	0.4584	0.0027	-0.8435	
				0.1355	-0.1021	-0.0371	-0.1128	-0.0495	
510.	(0.00012)	RY (4)	O 51	s(3.84%)p20.99(80.68%)d 4.03(15.47%)	0.0000	0.0067	0.0362	0.1926	-0.0229
				-0.3442	0.0202	0.6727	0.0026	0.4846	

511.	(0.00004)	RY	(5)	O	51	0.2121	0.1220	0.2170	-0.1966	-0.0957
512.	(0.00003)	RY	(6)	O	51	s(55.35%)	p 0.28(15.63%)	d 0.52(29.02%)		
513.	(0.00001)	RY	(7)	O	51	s(21.46%)	p 0.06(1.35%)	d 3.60(77.19%)		
514.	(0.00001)	RY	(8)	O	51	s(17.14%)	p 0.21(3.53%)	d 4.63(79.34%)		
515.	(0.00001)	RY	(9)	O	51	s(0.21%)	p 5.31(1.13%)	d99.99(98.66%)		
516.	(0.00001)	RY	(10)	O	51	s(22.04%)	p 0.02(0.39%)	d 3.52(77.58%)		
517.	(0.00424)	RY	(1)	H	52	s(0.43%)	p 6.93(3.01%)	d99.99(96.56%)		
						s(97.35%)	p 0.03(2.65%)			
						-0.0162	0.9865	0.0732	-0.1273	-0.0707
518.	(0.00061)	RY	(2)	H	52	s(0.03%)	p99.99(99.97%)			
						-0.0091	0.0160	-0.0257	-0.3983	0.9167
519.	(0.00045)	RY	(3)	H	52	s(0.34%)	p99.99(99.66%)			
						-0.0236	0.0529	0.6982	0.6476	0.2998
520.	(0.00025)	RY	(4)	H	52	s(2.43%)	p40.17(97.57%)			
						0.0266	0.1536	-0.7108	0.6370	0.2544

A 3D ball-and-stick model of a complex organic molecule. The molecule features a central core with a large red mesh sphere and several smaller green mesh spheres. The structure is composed of numerous carbon (grey), hydrogen (white), and oxygen (red) atoms. The molecule has a complex, branched architecture with several long, flexible side chains extending from the central core.

[illegible]

46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	C	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
50.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
51.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0002
54.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0003
57.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0001
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	B	0.0007	0.0004	0.0004	0.0003	0.0001	0.0000	0.0018	0.0001	0.0045
70.	N	0.0003	0.0001	0.0000	0.0004	0.0000	0.0000	0.0092	0.0007	0.0218

	Atom	10	11	12	13	14	15	16	17	18
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1.	C	0.0002	0.0004	0.0014	0.0106	0.0003	0.0113	0.0018	0.0060	0.0078
2.	H	0.0000	0.0001	0.0033	0.0001	0.0000	0.0075	0.0001	0.0020	0.0001
3.	H	0.0000	0.0001	0.0028	0.0001	0.0000	0.0062	0.0001	0.0031	0.0001
4.	C	0.0002	0.0013	0.0004	0.0004	0.0002	0.0061	0.0001	1.0037	0.0081
5.	H	0.0000	0.0034	0.0002	0.0003	0.0000	0.0011	0.0000	0.0037	0.0000
6.	H	0.0000	0.0027	0.0001	0.0003	0.0000	0.0008	0.0000	0.0036	0.0001
7.	C	0.0051	0.0137	0.0010	0.0263	0.0000	0.0006	0.0002	1.5060	0.0663
8.	H	0.0014	0.0056	0.0003	0.0000	0.0000	0.0002	0.0000	0.0065	0.0001
9.	C	0.9270	1.5044	0.0308	0.0004	0.0002	0.0290	0.0000	0.0126	0.0102
10.	H	0.0000	0.0057	0.0001	0.0002	0.0000	0.0000	0.0000	0.0058	0.0072
11.	C	0.0057	0.0000	0.0120	0.0292	0.0001	0.0005	0.0004	0.1054	1.2475
12.	C	0.0001	0.0120	0.0000	1.4842	0.0078	0.0125	0.0061	0.0091	1.2132
13.	C	0.0002	0.0292	1.4842	0.0000	0.9254	1.3021	0.0051	0.0013	0.0096
14.	H	0.0000	0.0001	0.0078	0.9254	0.0000	0.0045	0.0014	0.0003	0.0077
15.	C	0.0000	0.0005	0.0125	1.3021	0.0045	0.0000	0.9270	0.0341	0.0595
16.	H	0.0000	0.0004	0.0061	0.0051	0.0014	0.9270	0.0000	0.0002	0.0001
17.	C	0.0058	0.1054	0.0091	0.0013	0.0003	0.0341	0.0002	0.0000	0.0116
18.	C	0.0072	1.2475	1.2132	0.0096	0.0077	0.0595	0.0001	0.0116	0.0000
19.	C	0.0002	0.0079	0.1032	0.0136	0.0056	1.5149	0.0064	0.0154	0.0117
20.	C	0.0003	0.0106	0.0118	0.0544	0.0003	0.0114	0.0088	1.2487	1.2530
21.	C	0.0003	0.0088	0.0002	0.0005	0.0000	0.0000	0.0000	0.0029	0.0067
22.	H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
23.	H	0.0001	0.0071	0.0001	0.0002	0.0000	0.0000	0.0000	0.0006	0.0003
24.	H	0.0003	0.0005	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002
25.	C	0.0004	0.0083	0.0002	0.0006	0.0000	0.0000	0.0000	0.0026	0.0073
26.	H	0.0004	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003
27.	H	0.0001	0.0070	0.0001	0.0000	0.0000	0.0001	0.0000	0.0005	0.0005
28.	H	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
29.	C	0.0000	0.0003	0.0082	0.0069	0.0008	0.0004	0.0000	0.0002	0.0054
30.	C	0.0000	0.0001	0.0065	0.0017	0.0005	0.0001	0.0000	0.0001	0.0007
31.	C	0.0000	0.0000	0.0002	0.0004	0.0000	0.0000	0.0000	0.0000	0.0002
32.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0000	0.0000	0.0019	0.0007	0.0000	0.0001	0.0000	0.0000	0.0003
34.	C	0.0000	0.0000	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0001	0.0046	0.0019	0.0001	0.0002	0.0000	0.0001	0.0004
37.	C	0.0000	0.0001	0.0007	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0000	0.0000	0.0008	0.0012	0.0000	0.0000	0.0000	0.0000	0.0004
46.	H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001
47.	H	0.0000	0.0000	0.0014	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
48.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	C	0.0000	0.0002	0.0063	0.0095	0.0006	0.0002	0.0001	0.0001	0.0036

50.	C	0.0000	0.0002	0.0058	0.0017	0.0001	0.0002	0.0000	0.0001	0.0004
51.	C	0.0000	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0002
52.	H	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
53.	C	0.0000	0.0001	0.0016	0.0006	0.0000	0.0001	0.0000	0.0000	0.0002
54.	C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	C	0.0000	0.0002	0.0040	0.0012	0.0001	0.0002	0.0000	0.0001	0.0005
57.	C	0.0000	0.0000	0.0006	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001
58.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	C	0.0000	0.0003	0.0012	0.0009	0.0000	0.0002	0.0000	0.0000	0.0004
66.	H	0.0000	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0001
67.	H	0.0000	0.0001	0.0008	0.0004	0.0000	0.0000	0.0000	0.0000	0.0006
68.	H	0.0000	0.0000	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000	0.0001
69.	B	0.0000	0.0044	0.8894	0.0463	0.0017	0.0099	0.0003	0.0015	0.0189
70.	N	0.0045	0.9809	0.0033	0.0029	0.0003	0.0002	0.0000	0.0009	0.0184

	Atom	19	20	21	22	23	24	25	26	27
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1.	C	1.0047	0.0085	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0038	0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0037	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0060	0.0089	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
5.	H	0.0019	0.0059	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
6.	H	0.0031	0.0064	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
7.	C	0.0310	0.0115	0.0004	0.0000	0.0001	0.0001	0.0004	0.0001	0.0001
8.	H	0.0002	0.0086	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0010	0.0599	0.0074	0.0001	0.0012	0.0006	0.0070	0.0006	0.0012
10.	H	0.0002	0.0003	0.0003	0.0000	0.0001	0.0003	0.0004	0.0004	0.0001
11.	C	0.0079	0.0106	0.0088	0.0007	0.0071	0.0005	0.0083	0.0004	0.0070
12.	C	0.1032	0.0118	0.0002	0.0000	0.0001	0.0001	0.0002	0.0001	0.0001
13.	C	0.0136	0.0544	0.0005	0.0000	0.0002	0.0002	0.0006	0.0001	0.0000
14.	H	0.0056	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	1.5149	0.0114	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
16.	H	0.0064	0.0088	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0154	1.2487	0.0029	0.0000	0.0006	0.0000	0.0026	0.0000	0.0005
18.	C	0.0117	1.2530	0.0067	0.0001	0.0003	0.0002	0.0073	0.0003	0.0005
19.	C	0.0000	1.2326	0.0001	0.0000	0.0001	0.0001	0.0002	0.0000	0.0000
20.	C	1.2326	0.0000	0.0003	0.0000	0.0001	0.0000	0.0003	0.0000	0.0001
21.	C	0.0001	0.0003	0.0000	0.9291	0.9323	0.9407	0.0089	0.0004	0.0004
22.	H	0.0000	0.0000	0.9291	0.0000	0.0030	0.0020	0.0077	0.0000	0.0001
23.	H	0.0001	0.0001	0.9323	0.0030	0.0000	0.0017	0.0005	0.0003	0.0002
24.	H	0.0001	0.0000	0.9407	0.0020	0.0017	0.0000	0.0003	0.0016	0.0003
25.	C	0.0002	0.0003	0.0089	0.0077	0.0005	0.0003	0.0000	0.9376	0.9338
26.	H	0.0000	0.0000	0.0004	0.0000	0.0003	0.0016	0.9376	0.0000	0.0017
27.	H	0.0000	0.0001	0.0004	0.0001	0.0002	0.0003	0.9338	0.0017	0.0000
28.	H	0.0000	0.0000	0.0080	0.0004	0.0001	0.0000	0.9349	0.0019	0.0027
29.	C	0.0020	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
30.	C	0.0004	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
31.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000
37.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0000
46.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0002	0.0001
49.	C	0.0027	0.0001	0.0018	0.0006	0.0002	0.0007	0.0002	0.0001	0.0000
50.	C	0.0005	0.0002	0.0014	0.0002	0.0010	0.0002	0.0001	0.0001	0.0000
51.	C	0.0002	0.0000	0.0006	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	C	0.0002	0.0001	0.0003	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000

54.	C	0.0000	0.0000	0.0006	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	C	0.0004	0.0002	0.0004	0.0011	0.0001	0.0001	0.0001	0.0002	0.0001
57.	C	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0004	0.0000	0.0001
58.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0003	0.0001	0.0003
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	C	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	B	0.0122	0.0079	0.0009	0.0002	0.0002	0.0023	0.0005	0.0020	0.0005
70.	N	0.0012	0.0070	0.9581	0.0034	0.0056	0.0205	0.9640	0.0235	0.0064

	Atom	28	29	30	31	32	33	34	35	36
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0001	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0007	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
12.	C	0.0000	0.0082	0.0065	0.0002	0.0001	0.0019	0.0003	0.0000	0.0046
13.	C	0.0000	0.0069	0.0017	0.0004	0.0001	0.0007	0.0002	0.0000	0.0019
14.	H	0.0000	0.0008	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
15.	C	0.0000	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
18.	C	0.0002	0.0054	0.0007	0.0002	0.0000	0.0003	0.0001	0.0000	0.0004
19.	C	0.0000	0.0020	0.0004	0.0001	0.0000	0.0001	0.0000	0.0000	0.0003
20.	C	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002
21.	C	0.0080	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.9349	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26.	H	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
27.	H	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	1.3695	0.0114	0.0074	0.1044	0.0112	0.0076	1.3555
30.	C	0.0000	1.3695	0.0000	1.4039	0.0062	0.0142	0.1011	0.0003	0.0122
31.	C	0.0000	0.0114	1.4039	0.0000	0.9285	1.4034	0.0109	0.0079	0.0997
32.	H	0.0000	0.0074	0.0062	0.9285	0.0000	0.0061	0.0078	0.0002	0.0003
33.	C	0.0000	0.1044	0.0142	1.4034	0.0061	0.0000	1.3898	0.0061	0.0142
34.	C	0.0000	0.0112	0.1011	0.0109	0.0078	1.3898	0.0000	0.9283	1.4204
35.	H	0.0000	0.0076	0.0003	0.0079	0.0002	0.0061	0.9283	0.0000	0.0063
36.	C	0.0000	1.3555	0.0122	0.0997	0.0003	0.0142	1.4204	0.0063	0.0000
37.	C	0.0000	0.0102	1.0139	0.0082	0.0021	0.0077	0.0013	0.0004	0.0087
38.	H	0.0000	0.0061	0.0042	0.0091	0.0000	0.0001	0.0035	0.0000	0.0001
39.	H	0.0000	0.0040	0.0035	0.0086	0.0001	0.0001	0.0024	0.0000	0.0001
40.	H	0.0000	0.0061	0.0034	0.0018	0.0002	0.0003	0.0001	0.0000	0.0002
41.	C	0.0000	0.0012	0.0079	0.0087	0.0020	1.0146	0.0096	0.0021	0.0087
42.	H	0.0000	0.0032	0.0001	0.0093	0.0000	0.0040	0.0050	0.0000	0.0001
43.	H	0.0000	0.0001	0.0002	0.0016	0.0002	0.0033	0.0058	0.0001	0.0001
44.	H	0.0000	0.0026	0.0002	0.0092	0.0000	0.0039	0.0039	0.0000	0.0001
45.	C	0.0002	0.0097	0.0085	0.0013	0.0004	0.0078	0.0084	0.0021	1.0141
46.	H	0.0000	0.0060	0.0002	0.0001	0.0000	0.0003	0.0017	0.0002	0.0033
47.	H	0.0000	0.0052	0.0001	0.0031	0.0000	0.0001	0.0093	0.0000	0.0041
48.	H	0.0003	0.0048	0.0001	0.0028	0.0000	0.0001	0.0091	0.0000	0.0039
49.	C	0.0000	0.0073	0.0047	0.0003	0.0000	0.0018	0.0001	0.0001	0.0059
50.	C	0.0000	0.0046	0.0007	0.0002	0.0000	0.0002	0.0002	0.0001	0.0006
51.	C	0.0000	0.0003	0.0002	0.0000	0.0000	0.0001	0.0001	0.0000	0.0001
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	C	0.0000	0.0019	0.0002	0.0001	0.0000	0.0000	0.0001	0.0000	0.0003
54.	C	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001	0.0001	0.0000	0.0002
55.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	C	0.0000	0.0064	0.0007	0.0001	0.0000	0.0003	0.0002	0.0001	0.0011
57.	C	0.0000	0.0012	0.0008	0.0000	0.0000	0.0002	0.0001	0.0000	0.0007

58.	H	0.0000	0.0011	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0002
59.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
60.	H	0.0000	0.0002	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000	0.0002
61.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	C	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	B	0.0001	0.8730	0.0248	0.0097	0.0004	0.0093	0.0091	0.0003	0.0237
70.	N	0.0031	0.0006	0.0010	0.0000	0.0000	0.0005	0.0001	0.0000	0.0000

Atom		37	38	39	40	41	42	43	44	45
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0007	0.0000	0.0001	0.0001	0.0000	0.0001	0.0000	0.0000	0.0008
13.	C	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012
14.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
19.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
20.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
29.	C	0.0102	0.0061	0.0040	0.0061	0.0012	0.0032	0.0001	0.0026	0.0097
30.	C	1.0139	0.0042	0.0035	0.0034	0.0079	0.0001	0.0002	0.0002	0.0085
31.	C	0.0082	0.0091	0.0086	0.0018	0.0087	0.0093	0.0016	0.0092	0.0013
32.	H	0.0021	0.0000	0.0001	0.0002	0.0020	0.0000	0.0002	0.0000	0.0004
33.	C	0.0077	0.0001	0.0001	0.0003	1.0146	0.0040	0.0033	0.0039	0.0078
34.	C	0.0013	0.0035	0.0024	0.0001	0.0096	0.0050	0.0058	0.0039	0.0084
35.	H	0.0004	0.0000	0.0000	0.0000	0.0021	0.0000	0.0001	0.0000	0.0021

62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	C	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0001	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	B	0.0035	0.0006	0.0008	0.0002	0.0006	0.0003	0.0000	0.0003	0.0036
70.	N	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008

Atom	46	47	48	49	50	51	52	53	54
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0006	0.0002	0.0001	0.0000	0.0002
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0001
12.	C	0.0001	0.0014	0.0001	0.0063	0.0058	0.0001	0.0001	0.0016
13.	C	0.0002	0.0001	0.0000	0.0095	0.0017	0.0004	0.0001	0.0006
14.	H	0.0000	0.0000	0.0000	0.0006	0.0001	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0001
16.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000
18.	C	0.0001	0.0001	0.0000	0.0036	0.0004	0.0002	0.0000	0.0002
19.	C	0.0001	0.0000	0.0000	0.0027	0.0005	0.0002	0.0000	0.0002
20.	C	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0001
21.	C	0.0000	0.0000	0.0000	0.0018	0.0014	0.0006	0.0000	0.0003
22.	H	0.0000	0.0000	0.0000	0.0006	0.0002	0.0001	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0002	0.0010	0.0003	0.0000	0.0000
24.	H	0.0000	0.0000	0.0000	0.0007	0.0002	0.0000	0.0000	0.0000
25.	C	0.0000	0.0000	0.0007	0.0002	0.0001	0.0001	0.0000	0.0001
26.	H	0.0000	0.0000	0.0002	0.0001	0.0001	0.0000	0.0002	0.0000
27.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0060	0.0052	0.0048	0.0073	0.0046	0.0003	0.0000	0.0019
30.	C	0.0002	0.0001	0.0001	0.0047	0.0007	0.0002	0.0000	0.0002
31.	C	0.0001	0.0031	0.0028	0.0003	0.0002	0.0000	0.0000	0.0001
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0003	0.0001	0.0001	0.0018	0.0002	0.0001	0.0000	0.0000
34.	C	0.0017	0.0093	0.0091	0.0001	0.0002	0.0001	0.0000	0.0001
35.	H	0.0002	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000
36.	C	0.0033	0.0041	0.0039	0.0059	0.0006	0.0001	0.0000	0.0003
37.	C	0.0002	0.0000	0.0000	0.0012	0.0007	0.0001	0.0000	0.0002
38.	H	0.0000	0.0000	0.0000	0.0008	0.0001	0.0001	0.0000	0.0001
39.	H	0.0000	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0001
40.	H	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0000	0.0002
41.	C	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
45.	C	0.9357	0.9152	0.9223	0.0005	0.0001	0.0000	0.0000	0.0000
46.	H	0.0000	0.0026	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0026	0.0000	0.0024	0.0001	0.0000	0.0000	0.0000	0.0000
48.	H	0.0026	0.0024	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
49.	C	0.0000	0.0001	0.0002	0.0000	1.3483	0.0108	0.0075	0.1014
50.	C	0.0000	0.0000	0.0001	1.3483	0.0000	1.4230	0.0064	0.0141
51.	C	0.0000	0.0000	0.0000	0.0108	1.4230	0.0000	0.9282	1.3859
52.	H	0.0000	0.0000	0.0000	0.0075	0.0064	0.9282	0.0000	0.0061
53.	C	0.0000	0.0000	0.0000	0.1014	0.0141	1.3859	0.0061	0.0000
54.	C	0.0000	0.0000	0.0000	0.0113	0.0999	0.0115	0.0078	1.4080
55.	H	0.0000	0.0000	0.0000	0.0073	0.0003	0.0080	0.0001	0.0062
56.	C	0.0000	0.0000	0.0000	1.3677	0.0116	0.1001	0.0003	0.0142
57.	C	0.0000	0.0000	0.0001	0.0100	1.0144	0.0082	0.0021	0.0078
58.	H	0.0000	0.0000	0.0000	0.0055	0.0042	0.0093	0.0000	0.0001
59.	H	0.0000	0.0000	0.0004	0.0041	0.0037	0.0087	0.0001	0.0001
60.	H	0.0000	0.0000	0.0000	0.0060	0.0033	0.0018	0.0002	0.0003
61.	C	0.0000	0.0000	0.0000	0.0011	0.0088	0.0095	0.0022	1.0122
62.	H	0.0000	0.0000	0.0000	0.0035	0.0001	0.0057	0.0000	0.0040
63.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0059	0.0001	0.0033
64.	H	0.0000	0.0000	0.0000	0.0019	0.0002	0.0030	0.0001	0.0037
65.	C	0.0000	0.0000	0.0000	0.0101	0.0087	0.0013	0.0004	0.0076

66.	H	0.0000	0.0000	0.0000	0.0058	0.0002	0.0000	0.0000	0.0003	0.0018
67.	H	0.0000	0.0000	0.0000	0.0047	0.0001	0.0027	0.0000	0.0001	0.0086
68.	H	0.0000	0.0000	0.0000	0.0055	0.0001	0.0032	0.0000	0.0001	0.0090
69.	B	0.0002	0.0009	0.0006	0.8829	0.0241	0.0098	0.0003	0.0098	0.0094
70.	N	0.0002	0.0001	0.0009	0.0036	0.0031	0.0004	0.0000	0.0035	0.0001

	Atom	55	56	57	58	59	60	61	62	63
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0040	0.0006	0.0001	0.0001	0.0001	0.0000	0.0001	0.0000
13.	C	0.0000	0.0012	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0005	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0000	0.0004	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000
22.	H	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0000	0.0001	0.0004	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
26.	H	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
27.	H	0.0000	0.0001	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0001	0.0064	0.0012	0.0011	0.0001	0.0002	0.0000	0.0001	0.0000
30.	C	0.0000	0.0007	0.0008	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
31.	C	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0000	0.0003	0.0002	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000
34.	C	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0011	0.0007	0.0002	0.0001	0.0002	0.0000	0.0000	0.0000
37.	C	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	C	0.0000	0.0002	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
49.	C	0.0073	1.3677	0.0100	0.0055	0.0041	0.0060	0.0011	0.0035	0.0003
50.	C	0.0003	0.0116	1.0144	0.0042	0.0037	0.0033	0.0088	0.0001	0.0001
51.	C	0.0080	0.1001	0.0082	0.0093	0.0087	0.0018	0.0095	0.0057	0.0059
52.	H	0.0001	0.0003	0.0021	0.0000	0.0001	0.0002	0.0022	0.0000	0.0001
53.	C	0.0062	0.0142	0.0078	0.0001	0.0001	0.0003	1.0122	0.0040	0.0033
54.	C	0.9280	1.3987	0.0013	0.0033	0.0025	0.0001	0.0089	0.0090	0.0016
55.	H	0.0000	0.0063	0.0004	0.0000	0.0000	0.0000	0.0022	0.0000	0.0002
56.	C	0.0063	0.0000	0.0085	0.0001	0.0001	0.0002	0.0084	0.0001	0.0002
57.	C	0.0004	0.0085	0.0000	0.9129	0.9224	0.9357	0.0005	0.0000	0.0002
58.	H	0.0000	0.0001	0.9129	0.0000	0.0025	0.0027	0.0001	0.0000	0.0000
59.	H	0.0000	0.0001	0.9224	0.0025	0.0000	0.0025	0.0001	0.0000	0.0000
60.	H	0.0000	0.0002	0.9357	0.0027	0.0025	0.0000	0.0001	0.0000	0.0000
61.	C	0.0022	0.0084	0.0005	0.0001	0.0001	0.0001	0.0000	0.9218	0.9355
62.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.9218	0.0000	0.0024
63.	H	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.9355	0.0024	0.0000
64.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.9279	0.0023	0.0024
65.	C	0.0021	1.0144	0.0005	0.0000	0.0000	0.0002	0.0005	0.0000	0.0001
66.	H	0.0002	0.0033	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
67.	H	0.0001	0.0040	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
68.	H	0.0000	0.0038	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
69.	B	0.0003	0.0270	0.0031	0.0007	0.0006	0.0002	0.0006	0.0004	0.0000

70. N 0.0000 0.0060 0.0011 0.0001 0.0021 0.0001 0.0000 0.0002 0.0000

	Atom	64	65	66	67	68	69	70
	----	-----	-----	-----	-----	-----	-----	-----
1.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0003
2.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001
3.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0004
5.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
6.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0002	0.0000	0.0001	0.0000	0.0018	0.0092
8.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0007
9.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0045	0.0218
10.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045
11.	C	0.0000	0.0003	0.0000	0.0001	0.0000	0.0044	0.9809
12.	C	0.0000	0.0012	0.0002	0.0008	0.0003	0.8894	0.0033
13.	C	0.0000	0.0009	0.0003	0.0004	0.0004	0.0463	0.0029
14.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0003
15.	C	0.0000	0.0002	0.0000	0.0000	0.0000	0.0099	0.0002
16.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015	0.0009
18.	C	0.0000	0.0004	0.0001	0.0006	0.0001	0.0189	0.0184
19.	C	0.0000	0.0002	0.0002	0.0002	0.0000	0.0122	0.0012
20.	C	0.0000	0.0003	0.0000	0.0002	0.0000	0.0079	0.0070
21.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.9581
22.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0034
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0056
24.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023	0.0205
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.9640
26.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020	0.0235
27.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0064
28.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0031
29.	C	0.0000	0.0004	0.0000	0.0000	0.0002	0.8730	0.0006
30.	C	0.0000	0.0001	0.0000	0.0000	0.0001	0.0248	0.0010
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0097	0.0000
32.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0093	0.0005
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0091	0.0001
35.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
36.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0237	0.0008
37.	C	0.0000	0.0006	0.0000	0.0000	0.0001	0.0035	0.0001
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0001
39.	H	0.0000	0.0001	0.0000	0.0000	0.0005	0.0008	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
41.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
45.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0036	0.0008
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0001
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0009
49.	C	0.0019	0.0101	0.0058	0.0047	0.0055	0.8829	0.0036
50.	C	0.0002	0.0087	0.0002	0.0001	0.0001	0.0241	0.0031
51.	C	0.0030	0.0013	0.0000	0.0027	0.0032	0.0098	0.0004
52.	H	0.0001	0.0004	0.0000	0.0000	0.0000	0.0003	0.0000
53.	C	0.0037	0.0076	0.0003	0.0001	0.0001	0.0098	0.0035
54.	C	0.0084	0.0081	0.0018	0.0086	0.0090	0.0094	0.0001
55.	H	0.0000	0.0021	0.0002	0.0001	0.0000	0.0003	0.0000
56.	C	0.0002	1.0144	0.0033	0.0040	0.0038	0.0270	0.0060
57.	C	0.0000	0.0005	0.0002	0.0000	0.0000	0.0031	0.0011
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0001
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0021
60.	H	0.0000	0.0002	0.0000	0.0000	0.0000	0.0002	0.0001
61.	C	0.9279	0.0005	0.0001	0.0001	0.0001	0.0006	0.0000
62.	H	0.0023	0.0000	0.0000	0.0000	0.0000	0.0004	0.0002
63.	H	0.0024	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	0.0001
65.	C	0.0001	0.0000	0.9358	0.9179	0.9224	0.0021	0.0001
66.	H	0.0000	0.9358	0.0000	0.0026	0.0025	0.0001	0.0000
67.	H	0.0000	0.9179	0.0026	0.0000	0.0025	0.0005	0.0001
68.	H	0.0000	0.9224	0.0025	0.0025	0.0000	0.0002	0.0001
69.	B	0.0002	0.0021	0.0001	0.0005	0.0002	0.0000	0.0594
70.	N	0.0001	0.0001	0.0000	0.0001	0.0001	0.0594	0.0000

(Occupancy) Bond orbital / Coefficients / Hybrids

----- Lewis -----

1. (1.99911) CR (1) C 1	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
2. (1.99912) CR (1) C 4	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
3. (1.99897) CR (1) C 7	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
4. (1.99898) CR (1) C 9	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
5. (1.99886) CR (1) C 11	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
6. (1.99864) CR (1) C 12	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
7. (1.99905) CR (1) C 13	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
8. (1.99894) CR (1) C 15	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
9. (1.99894) CR (1) C 17	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
10. (1.99880) CR (1) C 18	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
11. (1.99895) CR (1) C 19	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
12. (1.99882) CR (1) C 20	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
13. (1.99914) CR (1) C 21	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
14. (1.99915) CR (1) C 25	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
15. (1.99860) CR (1) C 29	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
16. (1.99898) CR (1) C 30	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
17. (1.99891) CR (1) C 31	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
18. (1.99903) CR (1) C 33	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
19. (1.99890) CR (1) C 34	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
20. (1.99899) CR (1) C 36	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
21. (1.99916) CR (1) C 37	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
22. (1.99916) CR (1) C 41	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
23. (1.99915) CR (1) C 45	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
24. (1.99856) CR (1) C 49	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
25. (1.99900) CR (1) C 50	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				
	0.0000 0.0000 0.0000 0.0000				
26. (1.99889) CR (1) C 51	s(100.00%)				
	1.0000 0.0000 0.0000 0.0000 0.0000				

27. (1.99901) CR (1) C 53	0.0000 0.0000 0.0000 0.0000 s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
28. (1.99890) CR (1) C 54	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
29. (1.99898) CR (1) C 56	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
30. (1.99915) CR (1) C 57	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
31. (1.99916) CR (1) C 61	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
32. (1.99916) CR (1) C 65	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
33. (1.99908) CR (1) B 69	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
34. (1.99940) CR (1) N 70	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
35. (1.00210) LP (1) C 20	s(0.00%)p 1.00(100.00%) 0.0000 0.0025 0.0021 0.0288 0.0022 -0.7432 -0.0071 0.6684 0.0072
36. (1.87713) LP (1) N 70	s(15.14%)p 5.60(84.86%) 0.0000 0.3891 -0.0005 0.7489 -0.0204 -0.3731 0.0117 -0.3844 0.0117
37. (1.97567) BD (1) C 1- H 2 (61.75%) 0.7858* C 1	s(25.22%)p 2.97(74.78%) 0.0000 0.5022 0.0016 -0.1452 -0.0082 -0.8289 -0.0093 0.1983 -0.0119 (38.25%) 0.6185* H 2 s(100.00%) 1.0000 0.0004
38. (1.97756) BD (1) C 1- H 3 (61.73%) 0.7857* C 1	s(24.96%)p 3.01(75.04%) 0.0000 0.4996 0.0018 -0.1989 -0.0080 0.1390 -0.0123 -0.8314 -0.0072 (38.27%) 0.6186* H 3 s(100.00%) 1.0000 0.0001
39. (1.98149) BD (1) C 1- C 4 (49.99%) 0.7070* C 1	s(24.34%)p 3.11(75.66%) 0.0000 0.4933 -0.0004 -0.4986 -0.0134 0.5065 -0.0149 0.5009 -0.0152 (50.01%) 0.7072* C 4 s(24.26%)p 3.12(75.74%) 0.0000 0.4926 -0.0007 0.4527 -0.0243 -0.5276 -0.0022 -0.5230 -0.0012
40. (1.97812) BD (1) C 1- C 19 (49.50%) 0.7036* C 1	s(25.32%)p 2.95(74.68%) 0.0000 0.5032 -0.0036 0.8311 -0.0069 0.1922 -0.0157 0.1362 -0.0165 (50.50%) 0.7106* C 19 s(31.01%)p 2.22(68.99%) 0.0000 0.5569 -0.0067 -0.7572 0.0165 -0.2527 -0.0127 -0.2281 -0.0132
41. (1.97610) BD (1) C 4- H 5 (61.71%) 0.7856* C 4	s(25.27%)p 2.96(74.73%) 0.0000 0.5027 0.0006 -0.4641 -0.0175 0.5484 -0.0022 -0.4806 0.0002 (38.29%) 0.6188* H 5 s(100.00%) 1.0000 0.0003
42. (1.97817) BD (1) C 4- H 6 (61.69%) 0.7854* C 4	s(25.16%)p 2.98(74.84%) 0.0000 0.5016 0.0011 -0.5282 -0.0154 -0.4742 0.0013 0.4943 -0.0043 (38.31%) 0.6189* H 6 s(100.00%) 1.0000 0.0001
43. (1.97753) BD (1) C 4- C 17 (49.48%) 0.7035* C 4	s(25.16%)p 2.97(74.84%) 0.0000 0.5016 -0.0009 0.5483 -0.0197 0.4428 0.0014 0.5012 0.0016 (50.52%) 0.7107* C 17 s(31.09%)p 2.22(68.91%) 0.0000 0.5575 -0.0070 -0.6189 -0.0126 -0.3680 0.0196 -0.4118 0.0232
44. (1.98265) BD (1) C 7- H 8	

	(60.61%)	0.7785*	C 7	s(31.91%)p 2.13(68.09%)					
				0.0000 0.5649 -0.0044 -0.7418 -0.0132					
				0.2169 0.0057 0.2888 0.0071					
	(39.39%)	0.6276*	H 8	s(100.00%)					
				1.0000 -0.0007					
45. (1.97048)	BD (1) C	7- C 9							
	(49.73%)	0.7052*	C 7	s(33.18%)p 2.01(66.82%)					
				0.0000 0.5760 0.0029 0.6676 -0.0142					
				0.3154 0.0160 0.3496 0.0201					
	(50.27%)	0.7090*	C 9	s(33.88%)p 1.95(66.12%)					
				0.0000 0.5820 0.0044 -0.6652 -0.0283					
				-0.3052 0.0157 -0.3524 0.0218					
46. (1.97671)	BD (1) C	7- C 17							
	(49.13%)	0.7009*	C 7	s(34.77%)p 1.88(65.23%)					
				0.0000 0.5896 0.0039 0.0578 -0.0295					
				-0.5068 -0.0035 -0.6255 -0.0038					
	(50.87%)	0.7133*	C 17	s(37.10%)p 1.70(62.90%)					
				0.0000 0.6089 0.0141 -0.1454 -0.0319					
				0.5030 0.0042 0.5948 0.0066					
47. (1.72524)	BD (2) C	7- C 17							
	(51.88%)	0.7203*	C 7	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0069 -0.0010 0.0265 -0.0008					
				-0.7721 0.0172 0.6345 -0.0122					
	(48.12%)	0.6937*	C 17	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0044 -0.0004 0.0272 -0.0003					
				-0.7623 0.0068 0.6466 -0.0004					
48. (1.97976)	BD (1) C	9- H 10							
	(60.40%)	0.7771*	C 9	s(30.91%)p 2.23(69.09%)					
				0.0000 0.5560 0.0005 -0.0908 -0.0154					
				0.5147 0.0072 0.6460 0.0080					
	(39.60%)	0.6293*	H 10	s(100.00%)					
				1.0000 -0.0014					
49. (1.97753)	BD (1) C	9- C 11							
	(49.93%)	0.7066*	C 9	s(35.06%)p 1.85(64.94%)					
				0.0000 0.5921 -0.0022 0.7402 0.0115					
				-0.1864 0.0152 -0.2572 0.0164					
	(50.07%)	0.7076*	C 11	s(36.65%)p 1.73(63.35%)					
				0.0000 0.6054 0.0011 -0.7270 -0.0080					
				0.1793 0.0092 0.2695 0.0092					
50. (1.74508)	BD (2) C	9- C 11							
	(49.90%)	0.7064*	C 9	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0026 0.0016 -0.0234 0.0011					
				0.7790 -0.0167 -0.6262 0.0136					
	(50.10%)	0.7078*	C 11	s(0.01%)p 1.00(99.99%)					
				0.0000 0.0099 0.0007 -0.0239 -0.0018					
				0.7900 -0.0148 -0.6124 0.0087					
51. (1.97132)	BD (1) C	11- C 18							
	(49.05%)	0.7004*	C 11	s(35.10%)p 1.85(64.90%)					
				0.0000 0.5924 -0.0002 0.1412 0.0170					
				-0.4877 0.0073 -0.6252 0.0070					
	(50.95%)	0.7138*	C 18	s(33.63%)p 1.97(66.37%)					
				0.0000 0.5799 0.0066 -0.0569 0.0160					
				0.5283 -0.0025 0.6173 -0.0024					
52. (1.98163)	BD (1) C	11- N 70							
	(40.37%)	0.6354*	C 11	s(28.21%)p 2.55(71.79%)					
				0.0000 0.5311 0.0042 0.6710 0.0235					
				0.3251 -0.0066 0.4018 -0.0050					
	(59.63%)	0.7722*	N 70	s(30.05%)p 2.33(69.95%)					
				0.0000 0.5482 -0.0016 -0.6547 0.0003					
				-0.3199 -0.0066 -0.4105 -0.0076					
53. (1.96594)	BD (1) C	12- C 13							
	(50.87%)	0.7132*	C 12	s(31.48%)p 2.18(68.52%)					
				0.0000 0.5607 0.0203 -0.0601 -0.0101					
				-0.6245 -0.0251 -0.5389 -0.0231					
	(49.13%)	0.7009*	C 13	s(35.37%)p 1.83(64.63%)					
				0.0000 0.5947 -0.0027 0.0108 0.0122					
				0.5440 -0.0040 0.5917 0.0004					
54. (1.70123)	BD (2) C	12- C 13							
	(50.57%)	0.7111*	C 12	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0052 -0.0012 -0.0670 -0.0018					
				0.6528 0.0071 -0.7545 -0.0040					
	(49.43%)	0.7031*	C 13	s(0.03%)p 99.99(99.97%)					
				0.0000 0.0182 0.0008 0.0063 -0.0011					
				0.7266 -0.0102 -0.6865 0.0156					
55. (1.96683)	BD (1) C	12- C 18							
	(49.26%)	0.7018*	C 12	s(32.25%)p 2.10(67.75%)					
				0.0000 0.5677 0.0134 -0.6958 -0.0173					

				0.3019	-0.0027	0.3191	0.0096	
	(50.74%)	0.7123*	C 18	s(34.51%)	p 1.90(65.49%)			
				0.0000	0.5874	-0.0044	0.7192	0.0013
				-0.2124	0.0092	-0.3036	0.0177	
56.	(1.95868)	BD (1)	C 12- B 69					
	(69.33%)	0.8326*	C 12	s(36.12%)	p 1.77(63.88%)			
				0.0000	0.6006	-0.0212	0.7118	-0.0451
				0.3032	-0.0142	0.1950	-0.0044	
	(30.67%)	0.5538*	B 69	s(33.26%)	p 2.01(66.74%)			
				0.0000	0.5767	0.0067	-0.7711	-0.0124
				-0.2671	-0.0028	-0.0364	-0.0024	
57.	(1.98022)	BD (1)	C 13- H 14					
	(60.67%)	0.7789*	C 13	s(31.17%)	p 2.21(68.83%)			
				0.0000	0.5583	-0.0027	0.7132	0.0092
				-0.3013	-0.0143	-0.2975	-0.0068	
	(39.33%)	0.6271*	H 14	s(100.00%)				
				1.0000	-0.0019			
58.	(1.97341)	BD (1)	C 13- C 15					
	(49.75%)	0.7053*	C 13	s(33.32%)	p 2.00(66.68%)			
				0.0000	0.5772	0.0066	-0.7008	0.0125
				-0.2914	-0.0177	-0.2999	-0.0195	
	(50.25%)	0.7089*	C 15	s(33.12%)	p 2.02(66.88%)			
				0.0000	0.5755	0.0011	0.6995	0.0270
				0.2926	-0.0209	0.3038	-0.0204	
59.	(1.98202)	BD (1)	C 15- H 16					
	(60.57%)	0.7782*	C 15	s(32.07%)	p 2.12(67.93%)			
				0.0000	0.5663	-0.0005	0.0300	0.0061
				-0.5727	-0.0066	-0.5918	-0.0073	
	(39.43%)	0.6280*	H 16	s(100.00%)				
				1.0000	-0.0013			
60.	(1.97740)	BD (1)	C 15- C 19					
	(49.07%)	0.7005*	C 15	s(34.63%)	p 1.89(65.37%)			
				0.0000	0.5885	0.0009	-0.7130	-0.0227
				0.2753	-0.0207	0.2609	-0.0219	
	(50.93%)	0.7137*	C 19	s(37.53%)	p 1.66(62.47%)			
				0.0000	0.6125	0.0108	0.6511	-0.0007
				-0.3000	-0.0163	-0.3321	-0.0175	
61.	(1.72446)	BD (2)	C 15- C 19					
	(52.17%)	0.7223*	C 15	s(0.01%)	p 1.00(99.99%)			
				0.0000	0.0092	0.0015	-0.0123	-0.0009
				-0.7143	0.0164	0.6993	-0.0145	
	(47.83%)	0.6916*	C 19	s(0.00%)	p 1.00(100.00%)			
				0.0000	-0.0039	0.0015	0.0273	0.0002
				-0.7182	0.0057	0.6952	-0.0063	
62.	(1.96806)	BD (1)	C 17- C 20					
	(48.93%)	0.6995*	C 17	s(31.70%)	p 2.15(68.30%)			
				0.0000	0.5630	-0.0067	0.7712	0.0017
				-0.1736	0.0069	-0.2410	0.0065	
	(51.07%)	0.7146*	C 20	s(32.73%)	p 2.06(67.27%)			
				0.0000	0.5721	0.0000	-0.7353	-0.0025
				0.2278	-0.0037	0.2829	-0.0047	
63.	(1.96364)	BD (1)	C 18- C 20					
	(49.57%)	0.7041*	C 18	s(31.83%)	p 2.14(68.17%)			
				0.0000	0.5642	0.0019	-0.6910	-0.0048
				-0.3132	0.0066	-0.3256	0.0053	
	(50.43%)	0.7101*	C 20	s(34.96%)	p 1.86(65.04%)			
				0.0000	0.5912	-0.0027	0.6761	-0.0028
				0.3091	-0.0081	0.3125	-0.0102	
64.	(1.96749)	BD (1)	C 19- C 20					
	(48.98%)	0.6998*	C 19	s(31.39%)	p 2.19(68.61%)			
				0.0000	0.5603	-0.0029	0.0412	0.0064
				0.5746	-0.0001	0.5951	-0.0020	
	(51.02%)	0.7143*	C 20	s(32.31%)	p 2.10(67.69%)			
				0.0000	0.5684	0.0039	0.0368	0.0016
				-0.5478	0.0046	-0.6128	0.0043	
65.	(1.98846)	BD (1)	C 21- H 22					
	(61.56%)	0.7846*	C 21	s(26.30%)	p 2.80(73.70%)			
				0.0000	0.5128	-0.0002	-0.0289	0.0042
				0.1940	0.0138	-0.8356	0.0100	
	(38.44%)	0.6200*	H 22	s(100.00%)				
				1.0000	0.0002			
66.	(1.98789)	BD (1)	C 21- H 23					
	(60.96%)	0.7808*	C 21	s(25.85%)	p 2.87(74.15%)			
				0.0000	0.5084	0.0018	0.7435	-0.0055
				0.2611	0.0122	0.3469	-0.0082	
	(39.04%)	0.6248*	H 23	s(100.00%)				
				1.0000	0.0006			

67.	(1.99366)	BD (1) C 21- H 24	(59.69%)	0.7726*	C 21	s(25.64%)p 2.90(74.36%)	0.0000	0.5064	-0.0058	-0.6658	0.0053
							0.3551	0.0235	0.4166	-0.0058	
			(40.31%)	0.6349*	H 24	s(100.00%)	1.0000	0.0041			
68.	(1.97934)	BD (1) C 21- N 70	(39.17%)	0.6259*	C 21	s(22.17%)p 3.51(77.83%)	0.0000	0.4708	0.0094	-0.0549	0.0163
							-0.8759	-0.0128	0.0874	-0.0027	
			(60.83%)	0.7799*	N 70	s(27.43%)p 2.65(72.57%)	0.0000	0.5237	0.0006	0.0934	0.0227
							0.8399	0.0146	-0.1041	-0.0105	
69.	(1.99394)	BD (1) C 25- H 26	(59.88%)	0.7738*	C 25	s(25.78%)p 2.88(74.22%)	0.0000	0.5077	-0.0066	-0.6263	0.0044
							0.4426	-0.0086	0.3917	0.0226	
			(40.12%)	0.6334*	H 26	s(100.00%)	1.0000	0.0049			
70.	(1.98847)	BD (1) C 25- H 27	(60.84%)	0.7800*	C 25	s(25.76%)p 2.88(74.24%)	0.0000	0.5075	0.0027	0.7669	-0.0060
							0.2075	-0.0090	0.3333	0.0088	
			(39.16%)	0.6258*	H 27	s(100.00%)	1.0000	0.0006			
71.	(1.98943)	BD (1) C 25- H 28	(61.11%)	0.7817*	C 25	s(25.95%)p 2.85(74.05%)	0.0000	0.5094	-0.0001	-0.1395	0.0053
							-0.8459	0.0053	0.0719	0.0146	
			(38.89%)	0.6236*	H 28	s(100.00%)	1.0000	-0.0003			
72.	(1.98052)	BD (1) C 25- N 70	(39.67%)	0.6298*	C 25	s(22.48%)p 3.45(77.52%)	0.0000	0.4740	0.0086	0.0002	0.0187
							0.2127	-0.0047	-0.8541	-0.0101	
			(60.33%)	0.7767*	N 70	s(27.35%)p 2.66(72.65%)	0.0000	0.5230	0.0024	0.0358	0.0255
							-0.2287	-0.0165	0.8196	0.0135	
73.	(1.96576)	BD (1) C 29- C 30	(50.63%)	0.7116*	C 29	s(32.69%)p 2.06(67.31%)	0.0000	0.5714	0.0178	0.6120	0.0184
							-0.0125	-0.0048	-0.5455	-0.0210	
			(49.37%)	0.7026*	C 30	s(35.17%)p 1.84(64.83%)	0.0000	0.5930	-0.0006	-0.5799	-0.0029
							0.0815	0.0068	0.5526	-0.0075	
74.	(1.63664)	BD (2) C 29- C 30	(52.75%)	0.7263*	C 29	s(0.02%)p99.99(99.98%)	0.0000	0.0149	0.0002	-0.5228	-0.0062
							-0.6457	-0.0084	-0.5562	-0.0026	
			(47.25%)	0.6874*	C 30	s(0.00%)p 1.00(100.00%)	0.0000	0.0021	0.0017	-0.5562	0.0008
							-0.6737	0.0068	-0.4866	0.0001	
75.	(1.96637)	BD (1) C 29- C 36	(50.69%)	0.7120*	C 29	s(32.87%)p 2.04(67.13%)	0.0000	0.5730	0.0184	0.0096	0.0009
							-0.5313	-0.0152	0.6231	0.0210	
			(49.31%)	0.7022*	C 36	s(34.91%)p 1.86(65.09%)	0.0000	0.5909	0.0000	-0.0385	-0.0082
							0.5274	0.0012	-0.6092	0.0049	
76.	(1.95553)	BD (1) C 29- B 69	(68.49%)	0.8276*	C 29	s(34.33%)p 1.91(65.67%)	0.0000	0.5854	-0.0248	-0.5921	0.0391
							0.5472	-0.0330	-0.0630	0.0073	
			(31.51%)	0.5614*	B 69	s(32.39%)p 2.09(67.61%)	0.0000	0.5691	-0.0034	0.6088	0.0049
							-0.5430	-0.0019	0.1028	0.0032	
77.	(1.97313)	BD (1) C 30- C 31	(50.26%)	0.7089*	C 30	s(34.09%)p 1.93(65.91%)	0.0000	0.5838	0.0062	0.5951	0.0178
							-0.5460	0.0002	0.0783	-0.0181	
			(49.74%)	0.7053*	C 31	s(34.60%)p 1.89(65.40%)	0.0000	0.5882	0.0028	-0.6096	0.0098
							0.5225	0.0096	-0.0928	-0.0225	
78.	(1.98141)	BD (1) C 30- C 37	(50.38%)	0.7098*	C 30	s(30.71%)p 2.26(69.29%)	0.0000	0.5542	-0.0043	-0.0048	0.0068
							0.4911	-0.0057	-0.6720	0.0027	

	(49.62%)	0.7044*	C 37	s(25.50%)p 2.92(74.50%)					
				0.0000 0.5050 -0.0026 -0.0034	0.0056				
				-0.4890 0.0044 0.7110 -0.0144					
79.	(1.98077)	BD (1)	C 31- H 32						
	(60.19%)	0.7758*	C 31	s(30.79%)p 2.25(69.21%)					
				0.0000 0.5549 -0.0049 0.5989	0.0105				
				-0.0289 -0.0009 -0.5765 -0.0101					
	(39.81%)	0.6309*	H 32	s(100.00%)					
				1.0000 -0.0011					
80.	(1.97416)	BD (1)	C 31- C 33						
	(49.80%)	0.7057*	C 31	s(34.49%)p 1.90(65.51%)					
				0.0000 0.5873 0.0043 0.0461	0.0233				
				-0.4945 -0.0133 0.6385 -0.0072					
	(50.20%)	0.7086*	C 33	s(34.40%)p 1.91(65.60%)					
				0.0000 0.5865 0.0026 -0.0118	0.0196				
				0.4965 -0.0035 -0.6393 -0.0149					
81.	(1.66318)	BD (2)	C 31- C 33						
	(52.96%)	0.7278*	C 31	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0013 0.0007 -0.5171	0.0098				
				-0.6937 0.0133 -0.5011 0.0080					
	(47.04%)	0.6858*	C 33	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0047 0.0010 -0.5032	0.0032				
				-0.6890 0.0086 -0.5215 0.0046					
82.	(1.97393)	BD (1)	C 33- C 34						
	(50.17%)	0.7083*	C 33	s(34.39%)p 1.91(65.61%)					
				0.0000 0.5864 0.0033 -0.5874	0.0024				
				0.0111 -0.0149 0.5572 0.0169					
	(49.83%)	0.7059*	C 34	s(34.43%)p 1.90(65.57%)					
				0.0000 0.5867 0.0032 0.6080	0.0149				
				-0.0282 -0.0206 -0.5333 0.0127					
83.	(1.98167)	BD (1)	C 33- C 41						
	(50.22%)	0.7087*	C 33	s(31.20%)p 2.21(68.80%)					
				0.0000 0.5585 -0.0050 0.6335	-0.0069				
				-0.5276 0.0063 0.0908 -0.0021					
	(49.78%)	0.7055*	C 41	s(25.64%)p 2.90(74.36%)					
				0.0000 0.5064 -0.0009 -0.6630	0.0120				
				0.5425 -0.0104 -0.0977 0.0005					
84.	(1.98066)	BD (1)	C 34- H 35						
	(60.18%)	0.7758*	C 34	s(30.74%)p 2.25(69.26%)					
				0.0000 0.5544 -0.0041 0.0104	-0.0003				
				-0.5197 -0.0084 0.6498 0.0102					
	(39.82%)	0.6310*	H 35	s(100.00%)					
				1.0000 -0.0013					
85.	(1.97348)	BD (1)	C 34- C 36						
	(49.79%)	0.7056*	C 34	s(34.72%)p 1.88(65.28%)					
				0.0000 0.5892 0.0028 -0.6153	-0.0134				
				0.5167 -0.0091 -0.0801 0.0237					
	(50.21%)	0.7086*	C 36	s(34.48%)p 1.90(65.52%)					
				0.0000 0.5872 0.0062 0.6120	-0.0009				
				-0.5235 -0.0143 0.0777 0.0184					
86.	(1.67167)	BD (2)	C 34- C 36						
	(53.30%)	0.7301*	C 34	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0001 0.0010 -0.5010	0.0076				
				-0.6796 0.0144 -0.5354 0.0095					
	(46.70%)	0.6834*	C 36	s(0.01%)p 1.00(99.99%)					
				0.0000 0.0077 0.0008 -0.5111	0.0003				
				-0.6691 0.0055 -0.5394 0.0000					
87.	(1.98118)	BD (1)	C 36- C 45						
	(50.30%)	0.7093*	C 36	s(30.58%)p 2.27(69.42%)					
				0.0000 0.5529 -0.0049 -0.6020	0.0069				
				0.0019 -0.0065 0.5759 -0.0012					
	(49.70%)	0.7050*	C 45	s(25.52%)p 2.92(74.48%)					
				0.0000 0.5051 -0.0029 0.6171	-0.0070				
				0.0029 -0.0070 -0.6031 0.0148					
88.	(1.97728)	BD (1)	C 37- H 38						
	(62.01%)	0.7874*	C 37	s(24.72%)p 3.05(75.28%)					
				0.0000 0.4972 -0.0006 0.1751	0.0078				
				0.8225 0.0070 0.2130 -0.0148					
	(37.99%)	0.6164*	H 38	s(100.00%)					
				1.0000 -0.0003					
89.	(1.98082)	BD (1)	C 37- H 39						
	(61.07%)	0.7815*	C 37	s(24.73%)p 3.04(75.27%)					
				0.0000 0.4973 0.0003 -0.7776	0.0035				
				-0.0365 0.0028 -0.3825 -0.0212					
	(38.93%)	0.6239*	H 39	s(100.00%)					
				1.0000 -0.0006					
90.	(1.98812)	BD (1)	C 37- H 40						

	(61.11%)	0.7817*	C 37	s(24.93%)p 3.01(75.07%)					
				0.0000 0.4993 0.0029 0.6038 -0.0055					
				-0.2882 0.0118 -0.5502 -0.0118					
	(38.89%)	0.6236*	H 40	s(100.00%)					
				1.0000 -0.0009					
91. (1.97967)	BD (1) C 41-	H 42							
	(61.41%)	0.7837*	C 41	s(24.70%)p 3.05(75.30%)					
				0.0000 0.4970 0.0002 0.4488 0.0143					
				0.2124 -0.0066 0.7115 0.0006					
	(38.59%)	0.6212*	H 42	s(100.00%)					
				1.0000 -0.0008					
92. (1.98939)	BD (1) C 41-	H 43							
	(61.17%)	0.7821*	C 41	s(24.91%)p 3.01(75.09%)					
				0.0000 0.4991 0.0006 0.5206 0.0095					
				0.0455 -0.0115 -0.6910 0.0060					
	(38.83%)	0.6231*	H 43	s(100.00%)					
				1.0000 -0.0011					
93. (1.98174)	BD (1) C 41-	H 44							
	(61.37%)	0.7834*	C 41	s(24.65%)p 3.06(75.35%)					
				0.0000 0.4965 0.0004 -0.2966 0.0116					
				-0.8115 -0.0097 0.0821 -0.0031					
	(38.63%)	0.6216*	H 44	s(100.00%)					
				1.0000 -0.0008					
94. (1.98875)	BD (1) C 45-	H 46							
	(61.02%)	0.7812*	C 45	s(24.80%)p 3.03(75.20%)					
				0.0000 0.4980 0.0035 0.1883 -0.0137					
				-0.5894 0.0030 0.6074 0.0082					
	(38.98%)	0.6243*	H 46	s(100.00%)					
				1.0000 -0.0010					
95. (1.97763)	BD (1) C 45-	H 47							
	(61.85%)	0.7864*	C 45	s(24.76%)p 3.04(75.24%)					
				0.0000 0.4976 -0.0005 -0.7622 -0.0095					
				-0.1974 -0.0093 -0.3636 0.0127					
	(38.15%)	0.6177*	H 47	s(100.00%)					
				1.0000 -0.0002					
96. (1.97920)	BD (1) C 45-	H 48							
	(61.25%)	0.7826*	C 45	s(24.81%)p 3.03(75.19%)					
				0.0000 0.4981 -0.0003 -0.0527 -0.0057					
				0.7833 -0.0026 0.3676 0.0179					
	(38.75%)	0.6225*	H 48	s(100.00%)					
				1.0000 -0.0004					
97. (1.96668)	BD (1) C 49-	C 50							
	(50.66%)	0.7118*	C 49	s(32.63%)p 2.06(67.37%)					
				0.0000 0.5710 0.0155 0.5486 0.0111					
				0.3478 0.0170 0.5012 0.0135					
	(49.34%)	0.7024*	C 50	s(35.20%)p 1.84(64.80%)					
				0.0000 0.5933 -0.0017 -0.5140 0.0037					
				-0.3757 -0.0089 -0.4924 0.0091					
98. (1.96675)	BD (1) C 49-	C 56							
	(50.60%)	0.7113*	C 49	s(32.96%)p 2.03(67.04%)					
				0.0000 0.5739 0.0169 -0.3138 -0.0043					
				0.4388 0.0175 -0.6154 -0.0200					
	(49.40%)	0.7029*	C 56	s(35.42%)p 1.82(64.58%)					
				0.0000 0.5952 -0.0014 0.2518 -0.0099					
				-0.4487 -0.0108 0.6170 -0.0073					
99. (1.63125)	BD (2) C 49-	C 56							
	(52.42%)	0.7240*	C 49	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0043 0.0024 -0.7424 -0.0066					
				0.3019 0.0064 0.5979 0.0078					
	(47.58%)	0.6898*	C 56	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0018 -0.0042 -0.7575 0.0063					
				0.3393 0.0007 0.5577 -0.0033					
100. (1.95629)	BD (1) C 49-	B 69							
	(68.52%)	0.8278*	C 49	s(34.27%)p 1.92(65.73%)					
				0.0000 0.5849 -0.0224 -0.2214 0.0104					
				-0.7706 0.0475 0.1097 -0.0041					
	(31.48%)	0.5611*	B 69	s(34.32%)p 1.91(65.68%)					
				0.0000 0.5858 0.0012 0.1699 -0.0058					
				0.7870 0.0119 -0.0920 0.0010					
101. (1.97323)	BD (1) C 50-	C 51							
	(50.12%)	0.7080*	C 50	s(34.09%)p 1.93(65.91%)					
				0.0000 0.5838 0.0061 0.2271 0.0178					
				0.7696 0.0096 -0.1208 0.0127					
	(49.88%)	0.7062*	C 51	s(34.64%)p 1.89(65.36%)					
				0.0000 0.5885 0.0011 -0.2492 0.0164					
				-0.7567 -0.0033 0.1348 0.0228					
102. (1.67269)	BD (2) C 50-	C 51							

	(46.45%)	0.6815*	C 50	s(0.02%)p99.99(99.98%)					
				0.0000 0.0137 0.0026 0.7738 -0.0063					
				-0.3240 0.0018 -0.5441 0.0006					
	(53.55%)	0.7318*	C 51	s(0.01%)p 1.00(99.99%)					
				0.0000 0.0070 0.0035 0.7627 -0.0179					
				-0.3434 0.0042 -0.5476 0.0118					
103. (1.98107)	BD (1) C 50-	C 57							
	(50.43%)	0.7101*	C 50	s(30.67%)p 2.26(69.33%)					
				0.0000 0.5537 -0.0034 0.2922 0.0019					
				-0.4014 0.0056 0.6684 -0.0038					
	(49.57%)	0.7041*	C 57	s(25.39%)p 2.94(74.61%)					
				0.0000 0.5039 -0.0026 -0.3059 0.0098					
				0.3928 0.0012 -0.7056 0.0139					
104. (1.98074)	BD (1) C 51-	H 52							
	(60.20%)	0.7759*	C 51	s(30.82%)p 2.24(69.18%)					
				0.0000 0.5551 -0.0033 0.5347 0.0094					
				0.3508 0.0068 0.5316 0.0073					
	(39.80%)	0.6309*	H 52	s(100.00%)					
				1.0000 -0.0013					
105. (1.97382)	BD (1) C 51-	C 53							
	(49.85%)	0.7061*	C 51	s(34.40%)p 1.91(65.60%)					
				0.0000 0.5865 0.0040 -0.2646 0.0161					
				0.4312 0.0286 -0.6316 0.0053					
	(50.15%)	0.7081*	C 53	s(34.47%)p 1.90(65.53%)					
				0.0000 0.5871 0.0035 0.2888 0.0124					
				-0.4066 0.0102 0.6374 0.0115					
106. (1.97399)	BD (1) C 53-	C 54							
	(50.15%)	0.7082*	C 53	s(34.70%)p 1.88(65.30%)					
				0.0000 0.5890 0.0041 -0.5345 -0.0068					
				-0.3278 0.0130 -0.5093 -0.0164					
	(49.85%)	0.7060*	C 54	s(34.63%)p 1.89(65.37%)					
				0.0000 0.5884 0.0051 0.5350 0.0027					
				0.3513 0.0294 0.4929 -0.0142					
107. (1.66783)	BD (2) C 53-	C 54							
	(47.01%)	0.6856*	C 53	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0001 0.0012 0.7496 -0.0106					
				-0.3493 -0.0005 -0.5621 0.0045					
	(52.99%)	0.7280*	C 54	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0013 0.0002 0.7477 -0.0160					
				-0.3469 0.0044 -0.5659 0.0099					
108. (1.98139)	BD (1) C 53-	C 61							
	(50.29%)	0.7092*	C 53	s(30.83%)p 2.24(69.17%)					
				0.0000 0.5553 -0.0066 0.2621 -0.0017					
				0.7778 -0.0079 -0.1339 -0.0004					
	(49.71%)	0.7051*	C 61	s(25.52%)p 2.92(74.48%)					
				0.0000 0.5051 -0.0028 -0.2723 0.0070					
				-0.8066 0.0163 0.1402 -0.0046					
109. (1.98077)	BD (1) C 54-	H 55							
	(60.22%)	0.7760*	C 54	s(30.71%)p 2.26(69.29%)					
				0.0000 0.5542 -0.0043 -0.2935 -0.0036					
				0.4293 0.0094 -0.6498 -0.0104					
	(39.78%)	0.6307*	H 55	s(100.00%)					
				1.0000 -0.0012					
110. (1.97293)	BD (1) C 54-	C 56							
	(49.82%)	0.7058*	C 54	s(34.53%)p 1.90(65.47%)					
				0.0000 0.5876 0.0011 -0.2610 -0.0149					
				-0.7560 0.0006 0.1200 -0.0204					
	(50.18%)	0.7084*	C 56	s(33.86%)p 1.95(66.14%)					
				0.0000 0.5819 0.0050 0.2578 -0.0081					
				0.7626 0.0139 -0.1120 -0.0220					
111. (1.98133)	BD (1) C 56-	C 65							
	(50.44%)	0.7102*	C 56	s(30.68%)p 2.26(69.32%)					
				0.0000 0.5539 -0.0022 -0.5442 0.0024					
				-0.3185 0.0064 -0.5437 0.0031					
	(49.56%)	0.7040*	C 65	s(25.33%)p 2.95(74.67%)					
				0.0000 0.5033 -0.0016 0.5661 -0.0099					
				0.3026 0.0021 0.5783 -0.0123					
112. (1.97693)	BD (1) C 57-	H 58							
	(62.02%)	0.7875*	C 57	s(24.73%)p 3.04(75.27%)					
				0.0000 0.4973 -0.0006 0.5391 0.0122					
				-0.6382 -0.0017 -0.2334 0.0143					
	(37.98%)	0.6163*	H 58	s(100.00%)					
				1.0000 -0.0004					
113. (1.98036)	BD (1) C 57-	H 59							
	(61.31%)	0.7830*	C 57	s(24.90%)p 3.02(75.10%)					
				0.0000 0.4990 -0.0003 -0.6570 0.0065					
				-0.3325 -0.0001 0.4565 0.0187					

	(38.69%)	0.6220*	H 59	s(100.00%)	1.0000	0.0001			
114. (1.98818)	BD (1) C 57-	H 60							
	(60.97%)	0.7808*	C 57	s(24.86%)p 3.02(75.14%)	0.0000	0.4986	0.0035	0.4291	0.0039
					0.5726	-0.0121	0.4890	0.0119	
	(39.03%)	0.6248*	H 60	s(100.00%)	1.0000	-0.0010			
115. (1.97911)	BD (1) C 61-	H 62							
	(61.38%)	0.7834*	C 61	s(24.59%)p 3.07(75.41%)	0.0000	0.4959	0.0005	-0.3653	0.0014
					0.5347	0.0160	0.5783	-0.0024	
	(38.62%)	0.6215*	H 62	s(100.00%)	1.0000	-0.0007			
116. (1.98905)	BD (1) C 61-	H 63							
	(61.18%)	0.7822*	C 61	s(24.94%)p 3.01(75.06%)	0.0000	0.4994	0.0010	-0.2221	0.0084
					0.2491	0.0137	-0.7993	0.0007	
	(38.82%)	0.6230*	H 63	s(100.00%)	1.0000	-0.0011			
117. (1.98380)	BD (1) C 61-	H 64							
	(61.34%)	0.7832*	C 61	s(24.85%)p 3.02(75.15%)	0.0000	0.4985	0.0010	0.8620	0.0045
					0.0360	0.0131	0.0834	-0.0074	
	(38.66%)	0.6218*	H 64	s(100.00%)	1.0000	-0.0008			
118. (1.98879)	BD (1) C 65-	H 66							
	(61.03%)	0.7812*	C 65	s(25.01%)p 3.00(74.99%)	0.0000	0.5001	0.0026	-0.1914	-0.0106
					0.6203	-0.0110	-0.5728	-0.0079	
	(38.97%)	0.6242*	H 66	s(100.00%)	1.0000	-0.0009			
119. (1.97912)	BD (1) C 65-	H 67							
	(61.77%)	0.7859*	C 65	s(24.94%)p 3.01(75.06%)	0.0000	0.4994	-0.0007	-0.7230	-0.0123
					-0.2524	0.0023	0.4047	-0.0137	
	(38.23%)	0.6183*	H 67	s(100.00%)	1.0000	-0.0005			
120. (1.97930)	BD (1) C 65-	H 68							
	(61.25%)	0.7826*	C 65	s(24.60%)p 3.07(75.40%)	0.0000	0.4960	-0.0001	0.3466	-0.0085
					-0.6781	-0.0026	-0.4166	-0.0188	
	(38.75%)	0.6225*	H 68	s(100.00%)	1.0000	-0.0003			
----- non-Lewis -----									
121. (0.98609)	LV (1) C 18			s(0.01%)p 1.00(99.99%)	0.0000	0.0062	0.0036	0.0440	0.0036
					-0.7599	-0.0033	0.6485	0.0083	
122. (0.21568)	LV (1) B 69			s(0.03%)p99.99(99.97%)	0.0000	0.0167	-0.0074	-0.0758	0.0060
					0.1197	-0.0009	0.9894	-0.0260	
123. (0.01094)	BD*(1) C 1-	H 2							
	(38.25%)	0.6185*	C 1	s(25.22%)p 2.97(74.78%)	0.0000	-0.5022	-0.0016	0.1452	0.0082
					0.8289	0.0093	-0.1983	0.0119	
	(61.75%)	-0.7858*	H 2	s(100.00%)	-1.0000	-0.0004			
124. (0.01051)	BD*(1) C 1-	H 3							
	(38.27%)	0.6186*	C 1	s(24.96%)p 3.01(75.04%)	0.0000	-0.4996	-0.0018	0.1989	0.0080
					-0.1390	0.0123	0.8314	0.0072	
	(61.73%)	-0.7857*	H 3	s(100.00%)	-1.0000	-0.0001			
125. (0.00915)	BD*(1) C 1-	C 4							
	(50.01%)	0.7072*	C 1	s(24.34%)p 3.11(75.66%)	0.0000	0.4933	-0.0004	-0.4986	-0.0134
					0.5065	-0.0149	0.5009	-0.0152	
	(49.99%)	-0.7070*	C 4	s(24.26%)p 3.12(75.74%)	0.0000	0.4926	-0.0007	0.4527	-0.0243
					-0.5276	-0.0022	-0.5230	-0.0012	
126. (0.02405)	BD*(1) C 1-	C 19							
	(50.50%)	0.7106*	C 1	s(25.32%)p 2.95(74.68%)	0.0000	-0.5032	0.0036	-0.8311	0.0069
					-0.1922	0.0157	-0.1362	0.0165	
	(49.50%)	-0.7036*	C 19	s(31.01%)p 2.22(68.99%)	0.0000	-0.5569	0.0067	0.7572	-0.0165
					0.2527	0.0127	0.2281	0.0132	

127.	(0.01119)	BD*(1) C	4- H 5 (38.29%)	0.6188*	C	4 s(25.27%)p 2.96(74.73%) 0.0000 -0.5027 -0.0006 0.4641 0.0175 -0.5484 0.0022 0.4806 -0.0002
			(61.71%)	-0.7856*	H 5	s(100.00%) -1.0000 -0.0003
128.	(0.01036)	BD*(1) C	4- H 6 (38.31%)	0.6189*	C	4 s(25.16%)p 2.98(74.84%) 0.0000 -0.5016 -0.0011 0.5282 0.0154 0.4742 -0.0013 -0.4943 0.0043
			(61.69%)	-0.7854*	H 6	s(100.00%) -1.0000 -0.0001
129.	(0.02368)	BD*(1) C	4- C 17 (50.52%)	0.7107*	C	4 s(25.16%)p 2.97(74.84%) 0.0000 -0.5016 0.0009 -0.5483 0.0197 -0.4428 -0.0014 -0.5012 -0.0016
			(49.48%)	-0.7035*	C 17	s(31.09%)p 2.22(68.91%) 0.0000 -0.5575 0.0070 0.6189 0.0126 0.3680 -0.0196 0.4118 -0.0232
130.	(0.01288)	BD*(1) C	7- H 8 (39.39%)	0.6276*	C	7 s(31.91%)p 2.13(68.09%) 0.0000 -0.5649 0.0044 0.7418 0.0132 -0.2169 -0.0057 -0.2888 -0.0071
			(60.61%)	-0.7785*	H 8	s(100.00%) -1.0000 0.0007
131.	(0.01786)	BD*(1) C	7- C 9 (50.27%)	0.7090*	C	7 s(33.18%)p 2.01(66.82%) 0.0000 -0.5760 -0.0029 -0.6676 0.0142 -0.3154 -0.0160 -0.3496 -0.0201
			(49.73%)	-0.7052*	C 9	s(33.88%)p 1.95(66.12%) 0.0000 -0.5820 -0.0044 0.6652 0.0283 0.3052 -0.0157 0.3524 -0.0218
132.	(0.02265)	BD*(1) C	7- C 17 (50.87%)	0.7133*	C	7 s(34.77%)p 1.88(65.23%) 0.0000 -0.5896 -0.0039 -0.0578 0.0295 0.5068 0.0035 0.6255 0.0038
			(49.13%)	-0.7009*	C 17	s(37.10%)p 1.70(62.90%) 0.0000 -0.6089 -0.0141 0.1454 0.0319 -0.5030 -0.0042 -0.5948 -0.0066
133.	(0.27549)	BD*(2) C	7- C 17 (48.12%)	0.6937*	C	7 s(0.00%)p 1.00(100.00%) 0.0000 0.0069 -0.0010 0.0265 -0.0008 -0.7721 0.0172 0.6345 -0.0122
			(51.88%)	-0.7203*	C 17	s(0.00%)p 1.00(100.00%) 0.0000 0.0044 -0.0004 0.0272 -0.0003 -0.7623 0.0068 0.6466 -0.0004
134.	(0.01189)	BD*(1) C	9- H 10 (39.60%)	0.6293*	C	9 s(30.91%)p 2.23(69.09%) 0.0000 -0.5560 -0.0005 0.0908 0.0154 -0.5147 -0.0072 -0.6460 -0.0080
			(60.40%)	-0.7771*	H 10	s(100.00%) -1.0000 0.0014
135.	(0.02983)	BD*(1) C	9- C 11 (50.07%)	0.7076*	C	9 s(35.06%)p 1.85(64.94%) 0.0000 -0.5921 0.0022 -0.7402 -0.0115 0.1864 -0.0152 0.2572 -0.0164
			(49.93%)	-0.7066*	C 11	s(36.65%)p 1.73(63.35%) 0.0000 -0.6054 -0.0011 0.7270 0.0080 -0.1793 -0.0092 -0.2695 -0.0092
136.	(0.28839)	BD*(2) C	9- C 11 (50.10%)	0.7078*	C	9 s(0.00%)p 1.00(100.00%) 0.0000 -0.0026 -0.0016 0.0234 -0.0011 -0.7790 0.0167 0.6262 -0.0136
			(49.90%)	-0.7064*	C 11	s(0.01%)p 1.00(99.99%) 0.0000 -0.0099 -0.0007 0.0239 0.0018 -0.7900 0.0148 0.6124 -0.0087
137.	(0.03615)	BD*(1) C	11- C 18 (50.95%)	0.7138*	C 11	s(35.10%)p 1.85(64.90%) 0.0000 0.5924 -0.0002 0.1412 0.0170 -0.4877 0.0073 -0.6252 0.0070
			(49.05%)	-0.7004*	C 18	s(33.63%)p 1.97(66.37%) 0.0000 0.5799 0.0066 -0.0569 0.0160 0.5283 -0.0025 0.6173 -0.0024
138.	(0.02968)	BD*(1) C	11- N 70 (59.63%)	0.7722*	C 11	s(28.21%)p 2.55(71.79%) 0.0000 0.5311 0.0042 0.6710 0.0235 0.3251 -0.0066 0.4018 -0.0050

	(40.37%)	-0.6354*	N 70	s(30.05%)p 2.33(69.95%)					
				0.0000 0.5482 -0.0016 -0.6547 0.0003					
				-0.3199 -0.0066 -0.4105 -0.0076					
139.	(0.02099)	BD*(1)	C 12- C 13						
	(49.13%)	0.7009*	C 12	s(31.48%)p 2.18(68.52%)					
				0.0000 -0.5607 -0.0203 0.0601 0.0101					
				0.6245 0.0251 0.5389 0.0231					
	(50.87%)	-0.7132*	C 13	s(35.37%)p 1.83(64.63%)					
				0.0000 -0.5947 0.0027 -0.0108 -0.0122					
				-0.5440 0.0040 -0.5917 -0.0004					
140.	(0.26749)	BD*(2)	C 12- C 13						
	(49.43%)	0.7031*	C 12	s(0.00%)p 1.00(100.00%)					
				0.0000 0.0052 0.0012 0.0670 0.0018					
				-0.6528 -0.0071 0.7545 0.0040					
	(50.57%)	-0.7111*	C 13	s(0.03%)p 99.99(99.97%)					
				0.0000 -0.0182 -0.0008 -0.0063 0.0011					
				-0.7266 0.0102 0.6865 -0.0156					
141.	(0.03433)	BD*(1)	C 12- C 18						
	(50.74%)	0.7123*	C 12	s(32.25%)p 2.10(67.75%)					
				0.0000 -0.5677 -0.0134 0.6958 0.0173					
				-0.3019 0.0027 -0.3191 -0.0096					
	(49.26%)	-0.7018*	C 18	s(34.51%)p 1.90(65.49%)					
				0.0000 -0.5874 0.0044 -0.7192 -0.0013					
				0.2124 -0.0092 0.3036 -0.0177					
142.	(0.02674)	BD*(1)	C 12- B 69						
	(30.67%)	0.5538*	C 12	s(36.12%)p 1.77(63.88%)					
				0.0000 -0.6006 0.0212 -0.7118 0.0451					
				-0.3032 0.0142 -0.1950 0.0044					
	(69.33%)	-0.8326*	B 69	s(33.26%)p 2.01(66.74%)					
				0.0000 -0.5767 -0.0067 0.7711 0.0124					
				0.2671 0.0028 0.0364 0.0024					
143.	(0.01181)	BD*(1)	C 13- H 14						
	(39.33%)	0.6271*	C 13	s(31.17%)p 2.21(68.83%)					
				0.0000 -0.5583 0.0027 -0.7132 -0.0092					
				0.3013 0.0143 0.2975 0.0068					
	(60.67%)	-0.7789*	H 14	s(100.00%)					
				-1.0000 0.0019					
144.	(0.02088)	BD*(1)	C 13- C 15						
	(50.25%)	0.7089*	C 13	s(33.32%)p 2.00(66.68%)					
				0.0000 0.5772 0.0066 -0.7008 0.0125					
				-0.2914 -0.0177 -0.2999 -0.0195					
	(49.75%)	-0.7053*	C 15	s(33.12%)p 2.02(66.88%)					
				0.0000 0.5755 0.0011 0.6995 0.0270					
				0.2926 -0.0209 0.3038 -0.0204					
145.	(0.01257)	BD*(1)	C 15- H 16						
	(39.43%)	0.6280*	C 15	s(32.07%)p 2.12(67.93%)					
				0.0000 -0.5663 0.0005 -0.0300 -0.0061					
				0.5727 0.0066 0.5918 0.0073					
	(60.57%)	-0.7782*	H 16	s(100.00%)					
				-1.0000 0.0013					
146.	(0.02307)	BD*(1)	C 15- C 19						
	(50.93%)	0.7137*	C 15	s(34.63%)p 1.89(65.37%)					
				0.0000 -0.5885 -0.0009 0.7130 0.0227					
				-0.2753 0.0207 -0.2609 0.0219					
	(49.07%)	-0.7005*	C 19	s(37.53%)p 1.66(62.47%)					
				0.0000 -0.6125 -0.0108 -0.6511 0.0007					
				0.3000 0.0163 0.3321 0.0175					
147.	(0.26328)	BD*(2)	C 15- C 19						
	(47.83%)	0.6916*	C 15	s(0.01%)p 1.00(99.99%)					
				0.0000 0.0092 0.0015 -0.0123 -0.0009					
				-0.7143 0.0164 0.6993 -0.0145					
	(52.17%)	-0.7223*	C 19	s(0.00%)p 1.00(100.00%)					
				0.0000 -0.0039 0.0015 0.0273 0.0002					
				-0.7182 0.0057 0.6952 -0.0063					
148.	(0.02975)	BD*(1)	C 17- C 20						
	(51.07%)	0.7146*	C 17	s(31.70%)p 2.15(68.30%)					
				0.0000 0.5630 -0.0067 0.7712 0.0017					
				-0.1736 0.0069 -0.2410 0.0065					
	(48.93%)	-0.6995*	C 20	s(32.73%)p 2.06(67.27%)					
				0.0000 0.5721 0.0000 -0.7353 -0.0025					
				0.2278 -0.0037 0.2829 -0.0047					
149.	(0.03321)	BD*(1)	C 18- C 20						
	(50.43%)	0.7101*	C 18	s(31.83%)p 2.14(68.17%)					
				0.0000 -0.5642 -0.0019 0.6910 0.0048					
				0.3132 -0.0066 0.3256 -0.0053					
	(49.57%)	-0.7041*	C 20	s(34.96%)p 1.86(65.04%)					
				0.0000 -0.5912 0.0027 -0.6761 0.0028					

				-0.3091	0.0081	-0.3125	0.0102	
150.	(0.02957)	BD*(1) C 19-	C 20	s(31.39%)	p 2.19(68.61%)			
	(51.02%)	0.7143*	C 19	0.0000	0.5603	-0.0029	0.0412	0.0064
				0.5746	-0.0001	0.5951	-0.0020	
	(48.98%)	-0.6998*	C 20	s(32.31%)	p 2.10(67.69%)			
				0.0000	0.5684	0.0039	0.0368	0.0016
				-0.5478	0.0046	-0.6128	0.0043	
151.	(0.00800)	BD*(1) C 21-	H 22	s(26.30%)	p 2.80(73.70%)			
	(38.44%)	0.6200*	C 21	0.0000	-0.5128	0.0002	0.0289	-0.0042
				-0.1940	-0.0138	0.8356	-0.0100	
	(61.56%)	-0.7846*	H 22	s(100.00%)				
				-1.0000	-0.0002			
152.	(0.00966)	BD*(1) C 21-	H 23	s(25.85%)	p 2.87(74.15%)			
	(39.04%)	0.6248*	C 21	0.0000	-0.5084	-0.0018	-0.7435	0.0055
				-0.2611	-0.0122	-0.3469	0.0082	
	(60.96%)	-0.7808*	H 23	s(100.00%)				
				-1.0000	-0.0006			
153.	(0.01788)	BD*(1) C 21-	H 24	s(25.64%)	p 2.90(74.36%)			
	(40.31%)	0.6349*	C 21	0.0000	-0.5064	0.0058	0.6658	-0.0053
				-0.3551	-0.0235	-0.4166	0.0058	
	(59.69%)	-0.7726*	H 24	s(100.00%)				
				-1.0000	-0.0041			
154.	(0.01352)	BD*(1) C 21-	N 70	s(22.17%)	p 3.51(77.83%)			
	(60.83%)	0.7799*	C 21	0.0000	0.4708	0.0094	-0.0549	0.0163
				-0.8759	-0.0128	0.0874	-0.0027	
	(39.17%)	-0.6259*	N 70	s(27.43%)	p 2.65(72.57%)			
				0.0000	0.5237	0.0006	0.0934	0.0227
				0.8399	0.0146	-0.1041	-0.0105	
155.	(0.01973)	BD*(1) C 25-	H 26	s(25.78%)	p 2.88(74.22%)			
	(40.12%)	0.6334*	C 25	0.0000	-0.5077	0.0066	0.6263	-0.0044
				-0.4426	0.0086	-0.3917	-0.0226	
	(59.88%)	-0.7738*	H 26	s(100.00%)				
				-1.0000	-0.0049			
156.	(0.00980)	BD*(1) C 25-	H 27	s(25.76%)	p 2.88(74.24%)			
	(39.16%)	0.6258*	C 25	0.0000	-0.5075	-0.0027	-0.7669	0.0060
				-0.2075	0.0090	-0.3333	-0.0088	
	(60.84%)	-0.7800*	H 27	s(100.00%)				
				-1.0000	-0.0006			
157.	(0.00701)	BD*(1) C 25-	H 28	s(25.95%)	p 2.85(74.05%)			
	(38.89%)	0.6236*	C 25	0.0000	-0.5094	0.0001	0.1395	-0.0053
				0.8459	-0.0053	-0.0719	-0.0146	
	(61.11%)	-0.7817*	H 28	s(100.00%)				
				-1.0000	0.0003			
158.	(0.01361)	BD*(1) C 25-	N 70	s(22.48%)	p 3.45(77.52%)			
	(60.33%)	0.7767*	C 25	0.0000	0.4740	0.0086	0.0002	0.0187
				0.2127	-0.0047	-0.8541	-0.0101	
	(39.67%)	-0.6298*	N 70	s(27.35%)	p 2.66(72.65%)			
				0.0000	0.5230	0.0024	0.0358	0.0255
				-0.2287	-0.0165	0.8196	0.0135	
159.	(0.03015)	BD*(1) C 29-	C 30	s(32.69%)	p 2.06(67.31%)			
	(49.37%)	0.7026*	C 29	0.0000	-0.5714	-0.0178	-0.6120	-0.0184
				0.0125	0.0048	0.5455	0.0210	
	(50.63%)	-0.7116*	C 30	s(35.17%)	p 1.84(64.83%)			
				0.0000</				

				0.0000	-0.5909	0.0000	0.0385	0.0082
				-0.5274	-0.0012	0.6092	-0.0049	
162.	(0.02418)	BD*(1) C 29- B 69						
	(31.51%)	0.5614* C 29	s(34.33%)p 1.91(65.67%)					
			0.0000	-0.5854	0.0248	0.5921	-0.0391	
			-0.5472	0.0330	0.0630	-0.0073		
	(68.49%)	-0.8276* B 69	s(32.39%)p 2.09(67.61%)					
			0.0000	-0.5691	0.0034	-0.6088	-0.0049	
			0.5430	0.0019	-0.1028	-0.0032		
163.	(0.02393)	BD*(1) C 30- C 31						
	(49.74%)	0.7053* C 30	s(34.09%)p 1.93(65.91%)					
			0.0000	-0.5838	-0.0062	-0.5951	-0.0178	
			0.5460	-0.0002	-0.0783	0.0181		
	(50.26%)	-0.7089* C 31	s(34.60%)p 1.89(65.40%)					
			0.0000	-0.5882	-0.0028	0.6096	-0.0098	
			-0.5225	-0.0096	0.0928	0.0225		
164.	(0.01758)	BD*(1) C 30- C 37						
	(49.62%)	0.7044* C 30	s(30.71%)p 2.26(69.29%)					
			0.0000	0.5542	-0.0043	-0.0048	0.0068	
			0.4911	-0.0057	-0.6720	0.0027		
	(50.38%)	-0.7098* C 37	s(25.50%)p 2.92(74.50%)					
			0.0000	0.5050	-0.0026	-0.0034	0.0056	
			-0.4890	0.0044	0.7110	-0.0144		
165.	(0.01309)	BD*(1) C 31- H 32						
	(39.81%)	0.6309* C 31	s(30.79%)p 2.25(69.21%)					
			0.0000	-0.5549	0.0049	-0.5989	-0.0105	
			0.0289	0.0009	0.5765	0.0101		
	(60.19%)	-0.7758* H 32	s(100.00%)					
			-1.0000	0.0011				
166.	(0.02372)	BD*(1) C 31- C 33						
	(50.20%)	0.7086* C 31	s(34.49%)p 1.90(65.51%)					
			0.0000	0.5873	0.0043	0.0461	0.0233	
			-0.4945	-0.0133	0.6385	-0.0072		
	(49.80%)	-0.7057* C 33	s(34.40%)p 1.91(65.60%)					
			0.0000	0.5865	0.0026	-0.0118	0.0196	
			0.4965	-0.0035	-0.6393	-0.0149		
167.	(0.35139)	BD*(2) C 31- C 33						
	(47.04%)	0.6858* C 31	s(0.00%)p 1.00(100.00%)					
			0.0000	-0.0013	-0.0007	0.5171	-0.0098	
			0.6937	-0.0133	0.5011	-0.0080		
	(52.96%)	-0.7278* C 33	s(0.00%)p 1.00(100.00%)					
			0.0000	-0.0047	-0.0010	0.5032	-0.0032	
			0.6890	-0.0086	0.5215	-0.0046		
168.	(0.02456)	BD*(1) C 33- C 34						
	(49.83%)	0.7059* C 33	s(34.39%)p 1.91(65.61%)					
			0.0000	-0.5864	-0.0033	0.5874	-0.0024	
			-0.0111	0.0149	-0.5572	-0.0169		
	(50.17%)	-0.7083* C 34	s(34.43%)p 1.90(65.57%)					
			0.0000	-0.5867	-0.0032	-0.6080	-0.0149	
			0.0282	0.0206	0.5333	-0.0127		
169.	(0.01753)	BD*(1) C 33- C 41						
	(49.78%)	0.7055* C 33	s(31.20%)p 2.21(68.80%)					
			0.0000	0.5585	-0.0050	0.6335	-0.0069	
			-0.5276	0.0063	0.0908	-0.0021		
	(50.22%)	-0.7087* C 41	s(25.64%)p 2.90(74.36%)					
			0.0000	0.5064	-0.0009	-0.6630	0.0120	
			0.5425	-0.0104	-0.0977	0.0005		
170.	(0.01320)	BD*(1) C 34- H 35						
	(39.82%)	0.6310* C 34	s(30.74%)p 2.25(69.26%)					
			0.0000	-0.5544	0.0041	-0.0104	0.0003	
			0.5197	0.0084	-0.6498	-0.0102		
	(60.18%)	-0.7758* H 35	s(100.00%)					
			-1.0000	0.0013				
171.	(0.02375)	BD*(1) C 34- C 36						
	(50.21%)	0.7086* C 34	s(34.72%)p 1.88(65.28%)					
			0.0000	0.5892	0.0028	-0.6153	-0.0134	
			0.5167	-0.0091	-0.0801	0.0237		
	(49.79%)	-0.7056* C 36	s(34.48%)p 1.90(65.52%)					
			0.0000	0.5872	0.0062	0.6120	-0.0009	
			-0.5235	-0.0143	0.0777	0.0184		
172.	(0.33279)	BD*(2) C 34- C 36						
	(46.70%)	0.6834* C 34	s(0.00%)p 1.00(100.00%)					
			0.0000	0.0001	-0.0010	0.5010	-0.0076	
			0.6796	-0.0144	0.5354	-0.0095		
	(53.30%)	-0.7301* C 36	s(0.01%)p 1.00(99.99%)					
			0.0000	-0.0077	-0.0008	0.5111	-0.0003	
			0.6691	-0.0055	0.5394	0.0000		

173. (0.01774) BD*(1) C 36- C 45
 (49.70%) 0.7050* C 36 s(30.58%)p 2.27(69.42%)
 0.0000 0.5529 -0.0049 -0.6020 0.0069
 0.0019 -0.0065 0.5759 -0.0012
 (50.30%) -0.7093* C 45 s(25.52%)p 2.92(74.48%)
 0.0000 0.5051 -0.0029 0.6171 -0.0070
 0.0029 -0.0070 -0.6031 0.0148

174. (0.00947) BD*(1) C 37- H 38
 (37.99%) 0.6164* C 37 s(24.72%)p 3.05(75.28%)
 0.0000 -0.4972 0.0006 -0.1751 -0.0078
 -0.8225 -0.0070 -0.2130 0.0148
 (62.01%) -0.7874* H 38 s(100.00%)
 -1.0000 0.0003

175. (0.00819) BD*(1) C 37- H 39
 (38.93%) 0.6239* C 37 s(24.73%)p 3.04(75.27%)
 0.0000 -0.4973 -0.0003 0.7776 -0.0035
 0.0365 -0.0028 0.3825 0.0212
 (61.07%) -0.7815* H 39 s(100.00%)
 -1.0000 0.0006

176. (0.00637) BD*(1) C 37- H 40
 (38.89%) 0.6236* C 37 s(24.93%)p 3.01(75.07%)
 0.0000 -0.4993 -0.0029 -0.6038 0.0055
 0.2882 -0.0118 0.5502 0.0118
 (61.11%) -0.7817* H 40 s(100.00%)
 -1.0000 0.0009

177. (0.00826) BD*(1) C 41- H 42
 (38.59%) 0.6212* C 41 s(24.70%)p 3.05(75.30%)
 0.0000 -0.4970 -0.0002 -0.4488 -0.0143
 -0.2124 0.0066 -0.7115 -0.0006
 (61.41%) -0.7837* H 42 s(100.00%)
 -1.0000 0.0008

178. (0.00544) BD*(1) C 41- H 43
 (38.83%) 0.6231* C 41 s(24.91%)p 3.01(75.09%)
 0.0000 -0.4991 -0.0006 -0.5206 -0.0095
 -0.0455 0.0115 0.6910 -0.0060
 (61.17%) -0.7821* H 43 s(100.00%)
 -1.0000 0.0011

179. (0.00782) BD*(1) C 41- H 44
 (38.63%) 0.6216* C 41 s(24.65%)p 3.06(75.35%)
 0.0000 -0.4965 -0.0004 0.2966 -0.0116
 0.8115 0.0097 -0.0821 0.0031
 (61.37%) -0.7834* H 44 s(100.00%)
 -1.0000 0.0008

180. (0.00637) BD*(1) C 45- H 46
 (38.98%) 0.6243* C 45 s(24.80%)p 3.03(75.20%)
 0.0000 -0.4980 -0.0035 -0.1883 0.0137
 0.5894 -0.0030 -0.6074 -0.0082
 (61.02%) -0.7812* H 46 s(100.00%)
 -1.0000 0.0010

181. (0.00943) BD*(1) C 45- H 47
 (38.15%) 0.6177* C 45 s(24.76%)p 3.04(75.24%)
 0.0000 -0.4976 0.0005 0.7622 0.0095
 0.1974 0.0093 0.3636 -0.0127
 (61.85%) -0.7864* H 47 s(100.00%)
 -1.0000 0.0002

182. (0.00920) BD*(1) C 45- H 48
 (38.75%) 0.6225* C 45 s(24.81%)p 3.03(75.19%)
 0.0000 -0.4981 0.0003 0.0527 0.0057
 -0.7833 0.0026 -0.3676 -0.0179
 (61.25%) -0.7826* H 48 s(100.00%)
 -1.0000 0.0004

183. (0.02943) BD*(1) C 49- C 50
 (49.34%) 0.7024* C 49 s(32.63%)p 2.06(67.37%)
 0.0000 -0.5710 -0.0155 -0.5486 -0.0111
 -0.3478 -0.0170 -0.5012 -0.0135
 (50.66%) -0.7118* C 50 s(35.20%)p 1.84(64.80%)
 0.0000 -0.5933 0.0017 0.5140 -0.0037
 0.3757 0.0089 0.4924 -0.0091

184. (0.03010) BD*(1) C 49- C 56
 (49.40%) 0.7029* C 49 s(32.96%)p 2.03(67.04%)
 0.0000 -0.5739 -0.0169 0.3138 0.0043
 -0.4388 -0.0175 0.6154 0.0200
 (50.60%) -0.7113* C 56 s(35.42%)p 1.82(64.58%)
 0.0000 -0.5952 0.0014 -0.2518 0.0099
 0.4487 0.0108 -0.6170 0.0073

185. (0.35530) BD*(2) C 49- C 56
 (47.58%) 0.6898* C 49 s(0.00%)p 1.00(100.00%)

				0.0000	0.0043	0.0024	-0.7424	-0.0066
				0.3019	0.0064	0.5979	0.0078	
	(52.42%)	-0.7240*	C 56	s(0.00%)	p 1.00	(100.00%)		
				0.0000	-0.0018	-0.0042	-0.7575	0.0063
				0.3393	0.0007	0.5577	-0.0033	
186.	(0.02791)	BD*(1)	C 49- B 69					
	(31.48%)	0.5611*	C 49	s(34.27%)	p 1.92	(65.73%)		
				0.0000	-0.5849	0.0224	0.2214	-0.0104
				0.7706	-0.0475	-0.1097	0.0041	
	(68.52%)	-0.8278*	B 69	s(34.32%)	p 1.91	(65.68%)		
				0.0000	-0.5858	-0.0012	-0.1699	0.0058
				-0.7870	-0.0119	0.0920	-0.0010	
187.	(0.02384)	BD*(1)	C 50- C 51					
	(49.88%)	0.7062*	C 50	s(34.09%)	p 1.93	(65.91%)		
				0.0000	-0.5838	-0.0061	-0.2271	-0.0178
				-0.7696	-0.0096	0.1208	-0.0127	
	(50.12%)	-0.7080*	C 51	s(34.64%)	p 1.89	(65.36%)		
				0.0000	-0.5885	-0.0011	0.2492	-0.0164
				0.7567	0.0033	-0.1348	-0.0228	
188.	(0.32808)	BD*(2)	C 50- C 51					
	(53.55%)	0.7318*	C 50	s(0.02%)	p99.99	(99.98%)		
				0.0000	0.0137	0.0026	0.7738	-0.0063
				-0.3240	0.0018	-0.5441	0.0006	
	(46.45%)	-0.6815*	C 51	s(0.01%)	p 1.00	(99.99%)		
				0.0000	0.0070	0.0035	0.7627	-0.0179
				-0.3434	0.0042	-0.5476	0.0118	
189.	(0.01727)	BD*(1)	C 50- C 57					
	(49.57%)	0.7041*	C 50	s(30.67%)	p 2.26	(69.33%)		
				0.0000	0.5537	-0.0034	0.2922	0.0019
				-0.4014	0.0056	0.6684	-0.0038	
	(50.43%)	-0.7101*	C 57	s(25.39%)	p 2.94	(74.61%)		
				0.0000	0.5039	-0.0026	-0.3059	0.0098
				0.3928	0.0012	-0.7056	0.0139	
190.	(0.01319)	BD*(1)	C 51- H 52					
	(39.80%)	0.6309*	C 51	s(30.82%)	p 2.24	(69.18%)		
				0.0000	-0.5551	0.0033	-0.5347	-0.0094
				-0.3508	-0.0068	-0.5316	-0.0073	
	(60.20%)	-0.7759*	H 52	s(100.00%)				
				-1.0000	0.0013			
191.	(0.02465)	BD*(1)	C 51- C 53					
	(50.15%)	0.7081*	C 51	s(34.40%)	p 1.91	(65.60%)		
				0.0000	0.5865	0.0040	-0.2646	0.0161
				0.4312	0.0286	-0.6316	0.0053	
	(49.85%)	-0.7061*	C 53	s(34.47%)	p 1.90	(65.53%)		
				0.0000	0.5871	0.0035	0.2888	0.0124
				-0.4066	0.0102	0.6374	0.0115	
192.	(0.02389)	BD*(1)	C 53- C 54					
	(49.85%)	0.7060*	C 53	s(34.70%)	p 1.88	(65.30%)		
				0.0000	-0.5890	-0.0041	0.5345	0.0068
				0.3278	-0.0130	0.5093	0.0164	
	(50.15%)	-0.7082*	C 54	s(34.63%)	p 1.89	(65.37%)		
				0.0000	-0.5884	-0.0051	-0.5350	-0.0027
				-0.3513	-0.0294	-0.4929	0.0142	
193.	(0.34999)	BD*(2)	C 53- C 54					
	(52.99%)	0.7280*	C 53	s(0.00%)	p 1.00	(100.00%)		
				0.0000	-0.0001	0.0012	0.7496	-0.0106
				-0.3493	-0.0005	-0.5621	0.0045	
	(47.01%)	-0.6856*	C 54	s(0.00%)	p 1.00	(100.00%)		
				0.0000	0.0013	0.0002	0.7477	-0.0160
				-0.3469	0.0044	-0.5659	0.0099	
194.	(0.01822)	BD*(1)	C 53- C 61					
	(49.71%)	0.7051*	C 53	s(30.83%)	p 2.24	(69.17%)		
				0.0000	0.5553	-0.0066	0.2621	-0.0017
				0.7778	-0.0079	-0.1339	-0.0004	
	(50.29%)	-0.7092*	C 61	s(25.52%)	p 2.92	(74.48%)		
				0.0000	0.5051	-0.0028	-0.2723	0.0070
				-0.8066	0.0163	0.1402	-0.0046	
195.	(0.01333)	BD*(1)	C 54- H 55					
	(39.78%)	0.6307*	C 54	s(30.71%)	p 2.26	(69.29%)		
				0.0000	-0.5542	0.0043	0.2935	0.0036
				-0.4293	-0.0094	0.6498	0.0104	
	(60.22%)	-0.7760*	H 55	s(100.00%)				
				-1.0000	0.0012			
196.	(0.02408)	BD*(1)	C 54- C 56					
	(50.18%)	0.7084*	C 54	s(34.53%)	p 1.90	(65.47%)		
				0.0000	0.5876	0.0011	-0.2610	-0.0149
				-0.7560	0.0006	0.1200	-0.0204	

	(49.82%)	-0.7058*	C 56	s(33.86%)p 1.95(66.14%)					
				0.0000	0.5819	0.0050	0.2578	-0.0081	
				0.7626	0.0139	-0.1120	-0.0220		
197.	(0.01731)	BD*(1)	C 56- C 65						
	(49.56%)	0.7040*	C 56	s(30.68%)p 2.26(69.32%)					
				0.0000	0.5539	-0.0022	-0.5442	0.0024	
				-0.3185	0.0064	-0.5437	0.0031		
	(50.44%)	-0.7102*	C 65	s(25.33%)p 2.95(74.67%)					
				0.0000	0.5033	-0.0016	0.5661	-0.0099	
				0.3026	0.0021	0.5783	-0.0123		
198.	(0.00957)	BD*(1)	C 57- H 58						
	(37.98%)	0.6163*	C 57	s(24.73%)p 3.04(75.27%)					
				0.0000	-0.4973	0.0006	-0.5391	-0.0122	
				0.6382	0.0017	0.2334	-0.0143		
	(62.02%)	-0.7875*	H 58	s(100.00%)					
				-1.0000	0.0004				
199.	(0.00959)	BD*(1)	C 57- H 59						
	(38.69%)	0.6220*	C 57	s(24.90%)p 3.02(75.10%)					
				0.0000	-0.4990	0.0003	0.6570	-0.0065	
				0.3325	0.0001	-0.4565	-0.0187		
	(61.31%)	-0.7830*	H 59	s(100.00%)					
				-1.0000	-0.0001				
200.	(0.00638)	BD*(1)	C 57- H 60						
	(39.03%)	0.6248*	C 57	s(24.86%)p 3.02(75.14%)					
				0.0000	-0.4986	-0.0035	-0.4291	-0.0039	
				-0.5726	0.0121	-0.4890	-0.0119		
	(60.97%)	-0.7808*	H 60	s(100.00%)					
				-1.0000	0.0010				
201.	(0.00859)	BD*(1)	C 61- H 62						
	(38.62%)	0.6215*	C 61	s(24.59%)p 3.07(75.41%)					
				0.0000	-0.4959	-0.0005	0.3653	-0.0014	
				-0.5347	-0.0160	-0.5783	0.0024		
	(61.38%)	-0.7834*	H 62	s(100.00%)					
				-1.0000	0.0007				
202.	(0.00546)	BD*(1)	C 61- H 63						
	(38.82%)	0.6230*	C 61	s(24.94%)p 3.01(75.06%)					
				0.0000	-0.4994	-0.0010	0.2221	-0.0084	
				-0.2491	-0.0137	0.7993	-0.0007		
	(61.18%)	-0.7822*	H 63	s(100.00%)					
				-1.0000	0.0011				
203.	(0.00704)	BD*(1)	C 61- H 64						
	(38.66%)	0.6218*	C 61	s(24.85%)p 3.02(75.15%)					
				0.0000	-0.4985	-0.0010	-0.8620	-0.0045	
				-0.0360	-0.0131	-0.0834	0.0074		
	(61.34%)	-0.7832*	H 64	s(100.00%)					
				-1.0000	0.0008				
204.	(0.00624)	BD*(1)	C 65- H 66						
	(38.97%)	0.6242*	C 65	s(25.01%)p 3.00(74.99%)					
				0.0000	-0.5001	-0.0026	0.1914	0.0106	
				-0.6203	0.0110	0.5728	0.0079		
	(61.03%)	-0.7812*	H 66	s(100.00%)					
				-1.0000	0.0009				
205.	(0.00888)	BD*(1)	C 65- H 67						
	(38.23%)	0.6183*	C 65	s(24.94%)p 3.01(75.06%)					
				0.0000	-0.4994	0.0007	0.7230	0.0123	
				0.2524	-0.0023	-0.4047	0.0137		
	(61.77%)	-0.7859*	H 67	s(100.00%)					
				-1.0000	0.0005				
206.	(0.00925)	BD*(1)	C 65- H 68						
	(38.75%)	0.6225*	C 65	s(24.60%)p 3.07(75.40%)					
				0.0000	-0.4960	0.0001	-0.3466	0.0085	
				0.6781	0.0026	0.4166	0.0188		
	(61.25%)	-0.7826*	H 68	s(100.00%)					
				-1.0000	0.0003				
207.	(0.00202)	RY (1)	C 1	s(0.65%)p99.99(99.35%)					
				0.0000	0.0287	0.0755	0.0034	0.0261	
				0.0028	0.1195	0.0065	0.9892		
208.	(0.00167)	RY (2)	C 1	s(0.10%)p99.99(99.90%)					
				0.0000	-0.0195	0.0248	-0.0020	0.1746	
				-0.0038	-0.9777	0.0000	0.1122		
209.	(0.00108)	RY (3)	C 1	s(4.56%)p20.95(95.44%)					
				0.0000	0.0204	0.2125	-0.0028	0.9601	
				0.0034	0.1693	0.0028	-0.0627		
210.	(0.00021)	RY (4)	C 1	s(94.86%)p 0.05(5.14%)					
				0.0000	-0.0058	0.9739	0.0039	-0.2159	
				0.0012	-0.0213	0.0008	-0.0659		
211.	(0.00165)	RY (1)	H 2	s(100.00%)					

212.	(0.00162)	RY	(1)	H	3	-0.0004	1.0000				
						s(100.00%)					
213.	(0.00199)	RY	(1)	C	4	-0.0001	1.0000				
						s(1.22%)p81.01(98.78%)					
						0.0000	0.0258	0.1074	0.0057	0.6970	
						0.0010	0.3014	-0.0041	-0.6412		
214.	(0.00158)	RY	(2)	C	4	s(0.63%)p99.99(99.37%)					
						0.0000	0.0246	0.0756	0.0028	0.6359	
						-0.0026	-0.6577	0.0003	0.3958		
215.	(0.00090)	RY	(3)	C	4	s(1.67%)p58.76(98.33%)					
						0.0000	0.0128	0.1287	0.0001	0.2861	
						-0.0028	0.6865	-0.0029	0.6558		
216.	(0.00020)	RY	(4)	C	4	s(96.62%)p 0.03(3.38%)					
						0.0000	-0.0065	0.9830	0.0008	-0.1625	
						0.0007	-0.0723	0.0006	-0.0463		
217.	(0.00166)	RY	(1)	H	5	s(100.00%)					
218.	(0.00162)	RY	(1)	H	6	-0.0003	1.0000				
						s(100.00%)					
219.	(0.00434)	RY	(1)	C	7	-0.0001	1.0000				
						s(0.15%)p99.99(99.85%)					
						0.0000	0.0370	0.0124	0.0052	0.9231	
						-0.0027	-0.2197	-0.0028	-0.3130		
220.	(0.00191)	RY	(2)	C	7	s(0.05%)p99.99(99.95%)					
						0.0000	0.0030	0.0221	0.0086	-0.3825	
						0.0143	-0.5612	0.0178	-0.7332		
221.	(0.00080)	RY	(3)	C	7	s(0.05%)p99.99(99.95%)					
						0.0000	-0.0009	0.0216	-0.0009	-0.0146	
						0.0159	0.7976	-0.0138	-0.6023		
222.	(0.00029)	RY	(4)	C	7	s(99.89%)p 0.00(0.11%)					
						0.0000	-0.0020	0.9994	-0.0056	-0.0026	
						0.0006	-0.0021	0.0033	0.0331		
223.	(0.00135)	RY	(1)	H	8	s(100.00%)					
224.	(0.00384)	RY	(1)	C	9	0.0007	1.0000				
						s(0.27%)p99.99(99.73%)					
						0.0000	0.0389	0.0347	-0.0120	0.3459	
						-0.0061	-0.5857	-0.0065	-0.7310		
225.	(0.00275)	RY	(2)	C	9	s(6.94%)p13.42(93.06%)					
						0.0000	0.0041	0.2633	-0.0239	0.9013	
						0.0026	0.2108	0.0066	0.2706		
226.	(0.00080)	RY	(3)	C	9	s(92.21%)p 0.08(7.79%)					
						0.0000	-0.0041	0.9602	0.0115	-0.2571	
						0.0004	0.0331	-0.0011	-0.1030		
227.	(0.00070)	RY	(4)	C	9	s(0.74%)p99.99(99.26%)					
						0.0000	0.0001	0.0858	0.0037	-0.0275	
						-0.0165	-0.7814	0.0139	0.6171		
228.	(0.00160)	RY	(1)	H	10	s(100.00%)					
229.	(0.00493)	RY	(1)	C	11	0.0014	1.0000				
						s(0.82%)p99.99(99.18%)					
						0.0000	0.0169	0.0889	0.0242	-0.9923	
						-0.0043	-0.0202	-0.0016	0.0787		
230.	(0.00421)	RY	(2)	C	11	s(1.66%)p59.08(98.34%)					
						0.0000	-0.0108	0.1286	0.0115	0.0599	
						0.0071	0.6231	0.0043	0.7690		
231.	(0.00304)	RY	(3)	C	11	s(0.01%)p99.99(99.99%)					
						0.0000	0.0007	0.0122	0.0033	-0.0643	
						0.0141	0.7766	-0.0093	-0.6264		
232.	(0.00139)	RY	(4)	C	11	s(97.54%)p 0.03(2.46%)					
						0.0000	-0.0029	0.9876	-0.0057	0.0823	
						-0.0030	-0.0889	-0.0020	-0.0994		
233.	(0.00477)	RY	(1)	C	12	s(1.71%)p57.46(98.29%)					
						0.0000	-0.0483	0.1215	-0.0188	-0.8022	
						0.0025	-0.3582	0.0049	-0.4590		
234.	(0.00305)	RY	(2)	C	12	s(2.58%)p37.78(97.42%)					
						0.0000	0.0047	0.1605	0.0070	0.5900	
						0.0267	-0.5823	0.0181	-0.5348		
235.	(0.00116)	RY	(3)	C	12	s(2.71%)p35.89(97.29%)					
						0.0000	-0.0136	0.1641	0.0036	-0.0753	
						0.0024	-0.6820	-0.0084	0.7085		
236.	(0.00056)	RY	(4)	C	12	s(93.15%)p 0.07(6.85%)					
						0.0000	0.0012	0.9651	0.0271	0.0152	
						0.0112	0.2582	0.0080	0.0265		
237.	(0.00464)	RY	(1)	C	13	s(0.25%)p99.99(99.75%)					
						0.0000	-0.0289	0.0411	0.0065	0.8569	
						0.0089	-0.2754	0.0016	-0.4326		
238.	(0.00171)	RY	(2)	C	13	s(4.40%)p21.73(95.60%)					
						0.0000	0.0118	0.2094	-0.0040	0.4807	
						-0.0101	0.6357	-0.0076	0.5663		

239.	(0.00071)	RY	(3)	C 13	s(4.73%)p20.13(95.27%) 0.0000 0.0064 0.2174 0.0060 -0.1498 0.0140 0.6643 -0.0103 -0.6990
240.	(0.00046)	RY	(4)	C 13	s(90.71%)p 0.10(9.29%) 0.0000 -0.0036 0.9524 0.0062 -0.1085 0.0008 -0.2795 0.0074 0.0538
241.	(0.00193)	RY	(1)	H 14	s(100.00%) 0.0019 1.0000
242.	(0.00389)	RY	(1)	C 15	s(1.26%)p78.09(98.74%) 0.0000 -0.0402 0.1050 -0.0008 0.0427 -0.0124 -0.7175 -0.0096 -0.6859
243.	(0.00285)	RY	(2)	C 15	s(0.18%)p99.99(99.82%) 0.0000 -0.0037 0.0423 -0.0352 0.9966 0.0012 0.0076 0.0029 0.0607
244.	(0.00076)	RY	(3)	C 15	s(0.33%)p99.99(99.67%) 0.0000 0.0020 0.0572 0.0003 -0.0413 -0.0155 -0.6860 0.0151 0.7238
245.	(0.00036)	RY	(4)	C 15	s(98.39%)p 0.02(1.61%) 0.0000 0.0034 0.9919 0.0015 -0.0446 0.0024 0.1152 -0.0019 0.0284
246.	(0.00136)	RY	(1)	H 16	s(100.00%) 0.0013 1.0000
247.	(0.00399)	RY	(1)	C 17	s(1.40%)p70.24(98.60%) 0.0000 0.0114 0.1179 -0.0068 0.8982 0.0143 0.3032 0.0146 0.2948
248.	(0.00302)	RY	(2)	C 17	s(0.21%)p99.99(99.79%) 0.0000 0.0351 0.0297 -0.0170 0.4214 -0.0065 -0.6144 -0.0010 -0.6652
249.	(0.00183)	RY	(3)	C 17	s(0.69%)p99.99(99.31%) 0.0000 -0.0012 0.0833 0.0019 0.0107 -0.0051 -0.7268 0.0021 0.6817
250.	(0.00070)	RY	(4)	C 17	s(97.80%)p 0.02(2.20%) 0.0000 -0.0032 0.9889 0.0041 -0.1203 -0.0124 0.0437 -0.0147 -0.0725
251.	(0.00648)	RY	(1)	C 18	s(2.09%)p46.93(97.91%) 0.0000 0.0098 0.1441 0.0056 -0.9599 0.0043 -0.2071 0.0096 -0.1211
252.	(0.00419)	RY	(2)	C 18	s(0.10%)p99.99(99.90%) 0.0000 -0.0117 0.0289 -0.0067 -0.2333 0.0121 0.7201 0.0112 0.6525
253.	(0.00071)	RY	(3)	C 18	s(3.85%)p24.99(96.15%) 0.0000 -0.0049 0.1961 -0.0050 0.0765 0.0070 -0.6471 -0.0057 0.7327
254.	(0.00061)	RY	(4)	C 18	s(93.99%)p 0.06(6.01%) 0.0000 -0.0025 0.9695 0.0052 0.1341 -0.0035 0.1403 -0.0080 -0.1495
255.	(0.00458)	RY	(1)	C 19	s(0.38%)p99.99(99.62%) 0.0000 -0.0035 0.0612 0.0119 0.9450 -0.0031 0.2026 -0.0035 0.2491
256.	(0.00290)	RY	(2)	C 19	s(4.51%)p21.17(95.49%) 0.0000 0.0274 0.2106 -0.0050 -0.3250 -0.0096 0.6503 -0.0093 0.6528
257.	(0.00174)	RY	(3)	C 19	s(0.19%)p99.99(99.81%) 0.0000 -0.0018 0.0431 -0.0007 0.0310 0.0058 0.7082 -0.0062 -0.7040
258.	(0.00066)	RY	(4)	C 19	s(94.99%)p 0.05(5.01%) 0.0000 -0.0070 0.9746 -0.0120 0.0097 0.0064 -0.1845 0.0053 -0.1254
259.	(0.00464)	RY	(1)	C 20	s(0.09%)p99.99(99.91%) 0.0000 -0.0033 0.0293 -0.0027 0.7568 -0.0033 -0.4003 -0.0047 -0.5159
260.	(0.00301)	RY	(2)	C 20	s(0.81%)p99.99(99.19%) 0.0000 0.0071 0.0898 0.0032 0.6486 0.0103 0.4743 0.0076 0.5883
261.	(0.00079)	RY	(3)	C 20	s(98.81%)p 0.01(1.19%) 0.0000 -0.0012 0.9940 0.0013 -0.0801 0.0041 -0.0736 0.0009 -0.0040
262.	(0.00037)	RY	(4)	C 20	s(0.29%)p99.99(99.71%) 0.0000 -0.0006 0.0542 0.0004 -0.0137 -0.0067 0.7805 0.0073 -0.6225
263.	(0.00240)	RY	(1)	C 21	s(9.57%)p 9.44(90.43%) 0.0000 0.0056 0.3094 0.0001 0.0887 0.0096 -0.2188 0.0135 0.9210
264.	(0.00200)	RY	(2)	C 21	s(13.02%)p 6.68(86.98%) 0.0000 0.0120 0.3607 -0.0111 -0.9014 -0.0025 -0.2224 -0.0022 -0.0872
265.	(0.00078)	RY	(3)	C 21	s(23.03%)p 3.34(76.97%)

		0.0000	0.0071	0.4798	-0.0040	0.3979
		0.0276	-0.6915	-0.0031	-0.3640	
266.	(0.00012) RY (4) C 21	s(54.41%)	p 0.84(45.59%)			
		0.0000	-0.0159	0.7375	0.0017	0.1446
		-0.0074	0.6507	-0.0015	-0.1069	
267.	(0.00139) RY (1) H 22	s(100.00%)				
		-0.0002	1.0000			
268.	(0.00168) RY (1) H 23	s(100.00%)				
		-0.0006	1.0000			
269.	(0.00364) RY (1) H 24	s(100.00%)				
		-0.0041	1.0000			
270.	(0.00219) RY (1) C 25	s(3.96%)	p24.24(96.04%)			
		0.0000	0.0031	0.1990	0.0039	0.3752
		0.0102	0.9052	0.0094	0.0069	
271.	(0.00170) RY (2) C 25	s(26.07%)	p 2.84(73.93%)			
		0.0000	0.0157	0.5103	-0.0124	-0.7453
		0.0016	0.1996	0.0013	-0.3794	
272.	(0.00052) RY (3) C 25	s(11.02%)	p 8.07(88.98%)			
		0.0000	0.0049	0.3320	-0.0053	0.5234
		-0.0051	-0.2846	0.0265	-0.7308	
273.	(0.00004) RY (4) C 25	s(58.99%)	p 0.70(41.01%)			
274.	(0.00391) RY (1) H 26	s(100.00%)				
		-0.0049	1.0000			
275.	(0.00147) RY (1) H 27	s(100.00%)				
		-0.0006	1.0000			
276.	(0.00122) RY (1) H 28	s(100.00%)				
		0.0003	1.0000			
277.	(0.00403) RY (1) C 29	s(0.97%)	p99.99(99.03%)			
		0.0000	-0.0462	0.0870	0.0180	0.7933
		-0.0200	-0.5976	0.0050	0.0548	
278.	(0.00257) RY (2) C 29	s(0.75%)	p99.99(99.25%)			
		0.0000	-0.0042	0.0866	0.0161	-0.4058
		0.0142	-0.4537	-0.0239	0.7880	
279.	(0.00132) RY (3) C 29	s(0.61%)	p99.99(99.39%)			
		0.0000	0.0023	0.0784	-0.0025	0.4464
		-0.0030	0.6588	-0.0117	0.6004	
280.	(0.00053) RY (4) C 29	s(97.75%)	p 0.02(2.25%)			
		0.0000	-0.0020	0.9887	-0.0287	-0.0690
		0.0247	0.0397	-0.0007	-0.1213	
281.	(0.00548) RY (1) C 30	s(0.96%)	p99.99(99.04%)			
		0.0000	0.0119	0.0974	0.0011	-0.0473
		-0.0122	-0.5842	0.0081	0.8041	
282.	(0.00330) RY (2) C 30	s(0.45%)	p99.99(99.55%)			
		0.0000	-0.0139	0.0657	-0.0156	0.7996
		0.0061	-0.5007	0.0037	-0.3244	
283.	(0.00144) RY (3) C 30	s(0.01%)	p 1.00(99.99%)			
		0.0000	0.0013	0.0076	-0.0010	-0.5968
		-0.0034	-0.6315	-0.0041	-0.4949	
284.	(0.00042) RY (4) C 30	s(98.61%)	p 0.01(1.39%)			
		0.0000	-0.0012	0.9930	-0.0022	-0.0438
		0.0075	0.0952	-0.0032	-0.0535	
285.	(0.00437) RY (1) C 31	s(0.54%)	p99.99(99.46%)			
		0.0000	-0.0342	0.0653	0.0050	0.7021
		0.0000	-0.0044	-0.0031	-0.7082	
286.	(0.00179) RY (2) C 31	s(0.52%)	p99.99(99.48%)			
		0.0000	0.0030	0.0718	0.0097	-0.5130
		-0.0153	0.6890	0.0116	-0.5064	
287.	(0.00072) RY (3) C 31	s(0.00%)	p 1.00(100.00%)			
		0.0000	-0.0007	0.0043	-0.0103	-0.4929
		-0.0114	-0.7229	-0.0101	-0.4838	
288.	(0.00040) RY (4) C 31	s(99.05%)	p 0.01(0.95%)			
		0.0000	0.0005	0.9952	0.0039	-0.0070
		0.0022	-0.0463	-0.0056	0.0851	
289.	(0.00181) RY (1) H 32	s(100.00%)				
		0.0011	1.0000			
290.	(0.00481) RY (1) C 33	s(1.59%)	p62.04(98.41%)			
		0.0000	0.0114	0.1254	-0.0103	-0.7923
		0.0152	0.5966	-0.0048	0.0087	
291.	(0.00383) RY (2) C 33	s(0.21%)	p99.99(99.79%)			
		0.0000	0.0002	0.0463	-0.0124	0.3081
		-0.0070	0.4121	0.0223	-0.8558	
292.	(0.00155) RY (3) C 33	s(0.18%)	p99.99(99.82%)			
		0.0000	-0.0003	0.0428	-0.0047	-0.5149
		-0.0067	-0.6854	-0.0054	-0.5131	
293.	(0.00038) RY (4) C 33	s(98.03%)	p 0.02(1.97%)			
		0.0000	-0.0021	0.9901	0.0078	0.1081
		-0.0046	-0.0651	0.0006	0.0610	

294. (0.00440) RY (1) C 34	s(0.95%)p99.99(99.05%) 0.0000 -0.0350 0.0910 0.0001 0.0244 -0.0060 -0.6108 0.0055 0.7853
295. (0.00215) RY (2) C 34	s(0.05%)p99.99(99.95%) 0.0000 0.0002 0.0229 0.0202 -0.8991 -0.0081 0.3320 -0.0074 0.2835
296. (0.00066) RY (3) C 34	s(0.01%)p99.99(99.99%) 0.0000 0.0008 0.0102 0.0105 0.4363 0.0121 0.7171 0.0098 0.5431
297. (0.00042) RY (4) C 34	s(99.11%)p 0.01(0.89%) 0.0000 0.0019 0.9955 -0.0003 0.0140 -0.0023 0.0408 0.0047 -0.0839
298. (0.00181) RY (1) H 35	s(100.00%) 0.0013 1.0000
299. (0.00568) RY (1) C 36	s(1.12%)p88.05(98.88%) 0.0000 0.0100 0.1055 0.0107 0.7142 -0.0015 -0.0069 -0.0075 -0.6917
300. (0.00322) RY (2) C 36	s(0.15%)p99.99(99.85%) 0.0000 -0.0140 0.0365 -0.0096 0.4590 0.0087 -0.7421 -0.0092 0.4867
301. (0.00155) RY (3) C 36	s(0.01%)p 1.00(99.99%) 0.0000 0.0014 0.0096 0.0012 0.5192 0.0029 0.6697 0.0024 0.5308
302. (0.00045) RY (4) C 36	s(98.74%)p 0.01(1.26%) 0.0000 -0.0015 0.9937 -0.0071 -0.0977 0.0037 0.0216 0.0039 0.0503
303. (0.00193) RY (1) C 37	s(0.17%)p99.99(99.83%) 0.0000 -0.0045 0.0413 0.0084 0.8367 -0.0044 -0.5072 -0.0072 -0.2022
304. (0.00055) RY (2) C 37	s(18.34%)p 4.45(81.66%) 0.0000 0.0307 0.4271 -0.0039 -0.0795 0.0013 -0.4151 -0.0001 0.7988
305. (0.00023) RY (3) C 37	s(0.57%)p99.99(99.43%) 0.0000 -0.0003 0.0754 -0.0049 0.5398 -0.0025 0.7384 -0.0020 0.3971
306. (0.00010) RY (4) C 37	s(81.04%)p 0.23(18.96%) 0.0000 -0.0144 0.9001 0.0002 -0.0459 -0.0001 0.1584 0.0046 -0.4030
307. (0.00147) RY (1) H 38	s(100.00%) 0.0003 1.0000
308. (0.00135) RY (1) H 39	s(100.00%) 0.0006 1.0000
309. (0.00143) RY (1) H 40	s(100.00%) 0.0009 1.0000
310. (0.00221) RY (1) C 41	s(0.02%)p99.99(99.98%) 0.0000 0.0023 0.0152 -0.0031 -0.4339 -0.0023 -0.3272 0.0060 0.8393
311. (0.00052) RY (2) C 41	s(10.49%)p 8.53(89.51%) 0.0000 0.0287 0.3227 -0.0003 -0.7185 0.0009 0.5983 -0.0002 -0.1442
312. (0.00024) RY (3) C 41	s(0.17%)p99.99(99.83%) 0.0000 -0.0014 0.0407 0.0026 -0.4697 0.0022 -0.7116 0.0020 -0.5210
313. (0.00002) RY (4) C 41	s(89.41%)p 0.12(10.59%)
314. (0.00141) RY (1) H 42	s(100.00%) 0.0008 1.0000
315. (0.00139) RY (1) H 43	s(100.00%) 0.0011 1.0000
316. (0.00149) RY (1) H 44	s(100.00%) 0.0008 1.0000
317. (0.00197) RY (1) C 45	s(0.28%)p99.99(99.72%) 0.0000 -0.0066 0.0523 0.0022 0.5463 -0.0070 -0.7393 0.0083 0.3899
318. (0.00064) RY (2) C 45	s(18.28%)p 4.47(81.72%) 0.0000 0.0297 0.4265 -0.0005 0.6043 0.0023 0.1285 -0.0024 -0.6599
319. (0.00023) RY (3) C 45	s(0.02%)p99.99(99.98%) 0.0000 0.0012 0.0145 0.0026 -0.4902 0.0052 -0.6608 0.0030 -0.5682
320. (0.00012) RY (4) C 45	s(81.53%)p 0.23(18.47%) 0.0000 -0.0136 0.9028 0.0008 -0.3093 0.0017 -0.0073 -0.0038 0.2983
321. (0.00144) RY (1) H 46	s(100.00%) 0.0010 1.0000
322. (0.00135) RY (1) H 47	s(100.00%) 0.0002 1.0000
323. (0.00194) RY (1) H 48	s(100.00%)

324.	(0.00482)	RY	(1)	C	49	0.0004 1.0000 s(2.28%)p42.77(97.72%) 0.0000 -0.0491 0.1429 0.0080 0.2807 0.0179 0.9418 -0.0050 -0.1049
325.	(0.00245)	RY	(2)	C	49	s(1.15%)p85.82(98.85%) 0.0000 0.0019 0.1073 -0.0111 0.2196 -0.0024 0.0263 -0.0236 0.9690
326.	(0.00196)	RY	(3)	C	49	s(5.84%)p16.11(94.16%) 0.0000 -0.0034 0.2417 0.0091 -0.9192 -0.0097 0.2567 0.0000 0.1747
327.	(0.00058)	RY	(4)	C	49	s(90.86%)p 0.10(9.14%) 0.0000 0.0023 0.9532 -0.0090 0.1664 -0.0323 -0.2088 0.0072 -0.1376
328.	(0.00528)	RY	(1)	C	50	s(0.60%)p99.99(99.40%) 0.0000 0.0110 0.0767 -0.0083 -0.3658 0.0060 0.5483 -0.0094 -0.7479
329.	(0.00337)	RY	(2)	C	50	s(0.15%)p99.99(99.85%) 0.0000 0.0133 0.0360 0.0056 -0.5581 0.0158 -0.7757 0.0026 -0.2917
330.	(0.00186)	RY	(3)	C	50	s(3.79%)p25.35(96.21%) 0.0000 0.0021 0.1948 -0.0038 -0.7192 0.0017 0.3032 0.0047 0.5940
331.	(0.00055)	RY	(4)	C	50	s(95.48%)p 0.05(4.52%) 0.0000 -0.0025 0.9772 -0.0022 0.1926 -0.0074 -0.0749 0.0034 -0.0491
332.	(0.00430)	RY	(1)	C	51	s(1.44%)p68.50(98.56%) 0.0000 -0.0367 0.1142 0.0073 0.6339 0.0001 0.4721 0.0062 0.6007
333.	(0.00231)	RY	(2)	C	51	s(0.01%)p 1.00(99.99%) 0.0000 0.0018 0.0094 -0.0023 0.0608 0.0221 -0.8154 -0.0128 0.5751
334.	(0.00069)	RY	(3)	C	51	s(0.07%)p99.99(99.93%) 0.0000 0.0011 0.0269 -0.0162 -0.7686 0.0069 0.3292 0.0127 0.5474
335.	(0.00043)	RY	(4)	C	51	s(98.61%)p 0.01(1.39%) 0.0000 0.0030 0.9930 0.0001 -0.0526 0.0011 -0.0556 0.0051 -0.0894
336.	(0.00180)	RY	(1)	H	52	s(100.00%) 0.0013 1.0000
337.	(0.00501)	RY	(1)	C	53	s(2.04%)p48.01(97.96%) 0.0000 0.0097 0.1425 -0.0085 -0.2402 -0.0123 -0.9470 0.0032 0.1574
338.	(0.00360)	RY	(2)	C	53	s(0.17%)p99.99(99.83%) 0.0000 -0.0014 0.0413 0.0121 -0.5669 -0.0007 0.0133 0.0208 -0.8223
339.	(0.00151)	RY	(3)	C	53	s(0.46%)p99.99(99.54%) 0.0000 -0.0010 0.0675 0.0076 0.7877 -0.0038 -0.2802 -0.0064 -0.5443
340.	(0.00037)	RY	(4)	C	53	s(97.34%)p 0.03(2.66%) 0.0000 -0.0021 0.9866 0.0022 0.0045 0.0105 0.1553 -0.0013 0.0490
341.	(0.00433)	RY	(1)	C	54	s(0.84%)p99.99(99.16%) 0.0000 -0.0357 0.0847 -0.0047 -0.3282 0.0005 0.5488 -0.0064 -0.7633
342.	(0.00196)	RY	(2)	C	54	s(0.01%)p99.99(99.99%) 0.0000 0.0043 0.0113 0.0120 -0.5471 0.0193 -0.7731 0.0079 -0.3197
343.	(0.00075)	RY	(3)	C	54	s(0.11%)p99.99(99.89%) 0.0000 0.0003 0.0335 -0.0140 -0.7673 0.0072 0.3127 0.0110 0.5585
344.	(0.00044)	RY	(4)	C	54	s(99.15%)p 0.01(0.85%) 0.0000 0.0017 0.9958 -0.0031 0.0600 0.0005 -0.0485 -0.0052 0.0498
345.	(0.00181)	RY	(1)	H	55	s(100.00%) 0.0012 1.0000
346.	(0.00497)	RY	(1)	C	56	s(0.62%)p99.99(99.38%) 0.0000 0.0144 0.0772 0.0119 0.6133 0.0057 0.3693 0.0101 0.6936
347.	(0.00352)	RY	(2)	C	56	s(0.01%)p99.99(99.99%) 0.0000 0.0118 0.0015 0.0003 -0.0106 0.0195 -0.8787 -0.0072 0.4767
348.	(0.00151)	RY	(3)	C	56	s(0.04%)p99.99(99.96%) 0.0000 -0.0006 0.0210 -0.0040 -0.7891 0.0039 0.3002 0.0040 0.5355
349.	(0.00046)	RY	(4)	C	56	s(99.35%)p 0.01(0.65%) 0.0000 -0.0020 0.9968 -0.0062 -0.0308 -0.0043 -0.0337 0.0018 -0.0657

350. (0.00187) RY (1) C 57	s(0.98%)p99.99(99.02%) 0.0000 -0.0033 0.0987 0.0051 0.4620 0.0065 0.8801 0.0075 0.0456
351. (0.00065) RY (2) C 57	s(17.77%)p 4.63(82.23%) 0.0000 0.0309 0.4204 -0.0018 -0.4533 -0.0034 0.2298 -0.0014 -0.7510
352. (0.00029) RY (3) C 57	s(8.80%)p10.37(91.20%) 0.0000 -0.0026 0.2966 -0.0056 0.7564 -0.0009 -0.4088 0.0005 -0.4157
353. (0.00013) RY (4) C 57	s(72.58%)p 0.38(27.42%) 0.0000 -0.0139 0.8518 -0.0003 -0.0932 -0.0004 -0.0730 -0.0046 0.5101
354. (0.00139) RY (1) H 58	s(100.00%) 0.0004 1.0000
355. (0.00187) RY (1) H 59	s(100.00%) -0.0001 1.0000
356. (0.00140) RY (1) H 60	s(100.00%) 0.0010 1.0000
357. (0.00225) RY (1) C 61	s(0.01%)p 1.00(99.99%) 0.0000 0.0016 0.0072 0.0036 0.5929 -0.0004 -0.0824 0.0054 0.8010
358. (0.00054) RY (2) C 61	s(11.13%)p 7.98(88.87%) 0.0000 0.0301 0.3323 -0.0019 -0.2658 -0.0025 -0.8987 0.0009 0.1012
359. (0.00024) RY (3) C 61	s(0.26%)p99.99(99.74%) 0.0000 -0.0041 0.0513 -0.0029 0.7586 0.0031 -0.2720 0.0021 -0.5899
360. (0.00002) RY (4) C 61	s(88.70%)p 0.13(11.30%)
361. (0.00138) RY (1) H 62	s(100.00%) 0.0007 1.0000
362. (0.00137) RY (1) H 63	s(100.00%) 0.0011 1.0000
363. (0.00144) RY (1) H 64	s(100.00%) 0.0008 1.0000
364. (0.00198) RY (1) C 65	s(0.79%)p99.99(99.21%) 0.0000 -0.0019 0.0890 -0.0016 0.1418 0.0072 0.9239 -0.0085 -0.3439
365. (0.00059) RY (2) C 65	s(18.82%)p 4.31(81.18%) 0.0000 0.0303 0.4328 0.0003 0.6040 -0.0046 0.1111 0.0010 0.6592
366. (0.00024) RY (3) C 65	s(0.02%)p99.99(99.98%) 0.0000 -0.0028 0.0139 -0.0027 0.7172 0.0034 -0.3382 0.0038 -0.6091
367. (0.00012) RY (4) C 65	s(80.48%)p 0.24(19.52%) 0.0000 -0.0145 0.8970 0.0011 -0.3166 -0.0001 -0.1400 0.0032 -0.2745
368. (0.00143) RY (1) H 66	s(100.00%) 0.0009 1.0000
369. (0.00156) RY (1) H 67	s(100.00%) 0.0005 1.0000
370. (0.00144) RY (1) H 68	s(100.00%) 0.0003 1.0000
371. (0.00506) RY (1) B 69	s(0.81%)p99.99(99.19%) 0.0000 0.0084 0.0896 -0.0071 0.8223 0.0089 -0.5594 -0.0052 0.0517
372. (0.00435) RY (2) B 69	s(0.01%)p99.99(99.99%) 0.0000 -0.0010 0.0119 0.0082 -0.5645 0.0076 -0.8180 0.0054 0.1093
373. (0.00302) RY (3) B 69	s(0.53%)p99.99(99.47%) 0.0000 0.0007 0.0727 0.0070 -0.0239 -0.0022 -0.1148 -0.0246 -0.9901
374. (0.00198) RY (4) B 69	s(98.64%)p 0.01(1.36%) 0.0000 -0.0033 0.9932 0.0065 -0.0655 -0.0008 0.0687 0.0103 0.0663
375. (0.00470) RY (1) N 70	s(4.26%)p22.46(95.74%) 0.0000 -0.0116 0.2061 0.0215 0.7164 -0.0161 -0.4318 -0.0212 -0.5065
376. (0.00083) RY (2) N 70	s(2.21%)p44.23(97.79%) 0.0000 -0.0123 0.1482 -0.0055 0.6246 -0.0068 0.2649 -0.0201 0.7191
377. (0.00077) RY (3) N 70	s(0.05%)p99.99(99.95%) 0.0000 -0.0022 0.0225 -0.0034 0.1767 -0.0221 0.8612 0.0150 -0.4752
378. (0.00016) RY (4) N 70	s(93.50%)p 0.07(6.50%) 0.0000 0.0039 0.9670 -0.0045 -0.2526 0.0043 0.0314 0.0045 0.0088

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
1. CR (1) C 1	146. BD*(1) C 15- C 19	0.94	10.66	0.089
1. CR (1) C 1	211. RY (1) H 2	0.73	10.60	0.078
1. CR (1) C 1	212. RY (1) H 3	0.71	10.60	0.078
1. CR (1) C 1	255. RY (1) C 19	1.35	11.23	0.110
2. CR (1) C 4	132. BD*(1) C 7- C 17	0.95	10.65	0.090
2. CR (1) C 4	217. RY (1) H 5	0.73	10.60	0.078
2. CR (1) C 4	218. RY (1) H 6	0.71	10.60	0.078
2. CR (1) C 4	247. RY (1) C 17	1.16	11.18	0.102
3. CR (1) C 7	129. BD*(1) C 4- C 17	1.43	10.43	0.109
3. CR (1) C 7	132. BD*(1) C 7- C 17	0.65	10.64	0.074
3. CR (1) C 7	135. BD*(1) C 9- C 11	0.79	10.61	0.082
3. CR (1) C 7	148. BD*(1) C 17- C 20	0.77	10.59	0.081
3. CR (1) C 7	223. RY (1) H 8	0.71	10.48	0.077
3. CR (1) C 7	225. RY (2) C 9	1.01	10.81	0.093
3. CR (1) C 7	226. RY (3) C 9	0.80	11.06	0.084
3. CR (1) C 7	248. RY (2) C 17	2.42	11.04	0.146
3. CR (1) C 7	250. RY (4) C 17	0.65	11.08	0.076
4. CR (1) C 9	130. BD*(1) C 7- H 8	0.53	10.74	0.067
4. CR (1) C 9	132. BD*(1) C 7- C 17	0.68	10.65	0.076
4. CR (1) C 9	135. BD*(1) C 9- C 11	0.52	10.62	0.066
4. CR (1) C 9	137. BD*(1) C 11- C 18	1.01	10.58	0.092
4. CR (1) C 9	138. BD*(1) C 11- N 70	0.71	10.40	0.077
4. CR (1) C 9	220. RY (2) C 7	1.07	10.71	0.096
4. CR (1) C 9	228. RY (1) H 10	0.80	10.54	0.082
4. CR (1) C 9	229. RY (1) C 11	2.80	11.10	0.157
5. CR (1) C 11	131. BD*(1) C 7- C 9	0.79	10.63	0.082
5. CR (1) C 11	134. BD*(1) C 9- H 10	0.55	10.79	0.069
5. CR (1) C 11	135. BD*(1) C 9- C 11	0.63	10.67	0.073
5. CR (1) C 11	137. BD*(1) C 11- C 18	0.51	10.63	0.066
5. CR (1) C 11	141. BD*(1) C 12- C 18	1.10	10.61	0.096
5. CR (1) C 11	149. BD*(1) C 18- C 20	0.58	10.65	0.070
5. CR (1) C 11	154. BD*(1) C 21- N 70	0.52	10.42	0.065
5. CR (1) C 11	158. BD*(1) C 25- N 70	0.50	10.42	0.065
5. CR (1) C 11	224. RY (1) C 9	0.63	11.20	0.075
5. CR (1) C 11	225. RY (2) C 9	1.25	10.86	0.104
5. CR (1) C 11	252. RY (2) C 18	1.84	11.35	0.129
5. CR (1) C 11	376. RY (2) N 70	0.68	11.12	0.078
6. CR (1) C 12	137. BD*(1) C 11- C 18	1.04	10.56	0.094
6. CR (1) C 12	142. BD*(1) C 12- B 69	1.38	10.48	0.107
6. CR (1) C 12	144. BD*(1) C 13- C 15	0.87	10.56	0.085
6. CR (1) C 12	149. BD*(1) C 18- C 20	0.61	10.58	0.071
6. CR (1) C 12	238. RY (2) C 13	1.39	10.88	0.110
6. CR (1) C 12	251. RY (1) C 18	0.92	11.17	0.090
6. CR (1) C 12	252. RY (2) C 18	0.61	11.28	0.074
6. CR (1) C 12	371. RY (1) B 69	1.12	10.80	0.098
6. CR (1) C 12	372. RY (2) B 69	2.54	10.77	0.148
7. CR (1) C 13	141. BD*(1) C 12- C 18	0.82	10.56	0.083
7. CR (1) C 13	142. BD*(1) C 12- B 69	1.22	10.50	0.101
7. CR (1) C 13	145. BD*(1) C 15- H 16	0.54	10.74	0.068
7. CR (1) C 13	146. BD*(1) C 15- C 19	0.65	10.65	0.074
7. CR (1) C 13	233. RY (1) C 12	1.15	11.21	0.101
7. CR (1) C 13	234. RY (2) C 12	1.35	11.12	0.109
7. CR (1) C 13	241. RY (1) H 14	0.82	10.61	0.083
7. CR (1) C 13	243. RY (2) C 15	1.38	10.69	0.108
8. CR (1) C 15	126. BD*(1) C 1- C 19	1.45	10.42	0.110
8. CR (1) C 15	139. BD*(1) C 12- C 13	0.82	10.60	0.083
8. CR (1) C 15	146. BD*(1) C 15- C 19	0.65	10.64	0.074
8. CR (1) C 15	150. BD*(1) C 19- C 20	0.78	10.58	0.081
8. CR (1) C 15	238. RY (2) C 13	0.91	10.88	0.089
8. CR (1) C 15	240. RY (4) C 13	0.64	11.05	0.075
8. CR (1) C 15	246. RY (1) H 16	0.76	10.47	0.080
8. CR (1) C 15	255. RY (1) C 19	1.04	11.22	0.096
8. CR (1) C 15	256. RY (2) C 19	1.27	10.97	0.105
8. CR (1) C 15	258. RY (4) C 19	1.00	11.05	0.094
9. CR (1) C 17	130. BD*(1) C 7- H 8	0.72	10.76	0.078
9. CR (1) C 17	131. BD*(1) C 7- C 9	0.61	10.60	0.072
9. CR (1) C 17	148. BD*(1) C 17- C 20	0.83	10.61	0.084
9. CR (1) C 17	149. BD*(1) C 18- C 20	1.11	10.62	0.097
9. CR (1) C 17	150. BD*(1) C 19- C 20	0.58	10.61	0.070

9. CR (1) C 17	215. RY (3) C 4	0.86	10.66	0.085
9. CR (1) C 17	220. RY (2) C 7	1.46	10.73	0.112
9. CR (1) C 17	259. RY (1) C 20	1.79	11.26	0.127
9. CR (1) C 17	261. RY (3) C 20	0.54	11.15	0.069
10. CR (1) C 18	135. BD*(1) C 9- C 11	0.69	10.63	0.076
10. CR (1) C 18	138. BD*(1) C 11- N 70	0.66	10.42	0.074
10. CR (1) C 18	142. BD*(1) C 12- B 69	1.09	10.51	0.095
10. CR (1) C 18	148. BD*(1) C 17- C 20	0.92	10.60	0.088
10. CR (1) C 18	149. BD*(1) C 18- C 20	0.62	10.61	0.072
10. CR (1) C 18	150. BD*(1) C 19- C 20	0.88	10.60	0.086
10. CR (1) C 18	230. RY (2) C 11	1.72	11.11	0.124
10. CR (1) C 18	232. RY (4) C 11	0.68	11.16	0.078
10. CR (1) C 18	234. RY (2) C 12	1.16	11.14	0.101
10. CR (1) C 18	260. RY (2) C 20	1.79	11.26	0.127
11. CR (1) C 19	144. BD*(1) C 13- C 15	0.58	10.60	0.070
11. CR (1) C 19	145. BD*(1) C 15- H 16	0.72	10.77	0.079
11. CR (1) C 19	148. BD*(1) C 17- C 20	0.58	10.61	0.070
11. CR (1) C 19	149. BD*(1) C 18- C 20	1.10	10.62	0.096
11. CR (1) C 19	150. BD*(1) C 19- C 20	0.80	10.61	0.082
11. CR (1) C 19	209. RY (3) C 1	0.98	10.68	0.091
11. CR (1) C 19	243. RY (2) C 15	1.43	10.71	0.110
11. CR (1) C 19	245. RY (4) C 15	0.52	11.12	0.068
11. CR (1) C 19	259. RY (1) C 20	0.83	11.26	0.086
11. CR (1) C 19	260. RY (2) C 20	0.92	11.27	0.091
11. CR (1) C 19	261. RY (3) C 20	0.55	11.15	0.070
12. CR (1) C 20	132. BD*(1) C 7- C 17	0.75	10.65	0.080
12. CR (1) C 20	137. BD*(1) C 11- C 18	0.66	10.57	0.075
12. CR (1) C 20	141. BD*(1) C 12- C 18	0.72	10.56	0.078
12. CR (1) C 20	146. BD*(1) C 15- C 19	0.75	10.65	0.080
12. CR (1) C 20	247. RY (1) C 17	1.21	11.17	0.104
12. CR (1) C 20	248. RY (2) C 17	1.09	11.04	0.098
12. CR (1) C 20	251. RY (1) C 18	2.15	11.18	0.139
12. CR (1) C 20	256. RY (2) C 19	2.09	10.98	0.135
13. CR (1) C 21	138. BD*(1) C 11- N 70	0.50	10.40	0.064
13. CR (1) C 21	267. RY (1) H 22	0.85	10.75	0.085
13. CR (1) C 21	268. RY (1) H 23	0.75	10.69	0.080
13. CR (1) C 21	269. RY (1) H 24	0.63	10.66	0.073
13. CR (1) C 21	377. RY (3) N 70	0.76	11.07	0.082
14. CR (1) C 25	138. BD*(1) C 11- N 70	0.51	10.41	0.065
14. CR (1) C 25	274. RY (1) H 26	0.66	10.66	0.075
14. CR (1) C 25	275. RY (1) H 27	0.71	10.66	0.078
14. CR (1) C 25	276. RY (1) H 28	0.75	10.67	0.080
15. CR (1) C 29	162. BD*(1) C 29- B 69	1.07	10.45	0.094
15. CR (1) C 29	163. BD*(1) C 30- C 31	0.68	10.59	0.076
15. CR (1) C 29	164. BD*(1) C 30- C 37	0.78	10.41	0.081
15. CR (1) C 29	171. BD*(1) C 34- C 36	0.70	10.60	0.077
15. CR (1) C 29	173. BD*(1) C 36- C 45	0.73	10.41	0.078
15. CR (1) C 29	281. RY (1) C 30	0.66	11.20	0.077
15. CR (1) C 29	282. RY (2) C 30	1.57	10.93	0.117
15. CR (1) C 29	299. RY (1) C 36	0.56	11.20	0.071
15. CR (1) C 29	300. RY (2) C 36	1.73	10.92	0.123
15. CR (1) C 29	371. RY (1) B 69	3.56	10.78	0.175
16. CR (1) C 30	159. BD*(1) C 29- C 30	0.60	10.62	0.072
16. CR (1) C 30	161. BD*(1) C 29- C 36	0.67	10.62	0.075
16. CR (1) C 30	162. BD*(1) C 29- B 69	1.22	10.50	0.101
16. CR (1) C 30	165. BD*(1) C 31- H 32	0.58	10.77	0.070
16. CR (1) C 30	166. BD*(1) C 31- C 33	0.83	10.65	0.084
16. CR (1) C 30	277. RY (1) C 29	0.75	11.28	0.082
16. CR (1) C 30	278. RY (2) C 29	1.24	11.08	0.104
16. CR (1) C 30	286. RY (2) C 31	1.40	10.83	0.110
16. CR (1) C 30	304. RY (2) C 37	0.74	10.82	0.080
17. CR (1) C 31	159. BD*(1) C 29- C 30	0.90	10.57	0.087
17. CR (1) C 31	164. BD*(1) C 30- C 37	0.65	10.41	0.073
17. CR (1) C 31	168. BD*(1) C 33- C 34	0.71	10.60	0.077
17. CR (1) C 31	169. BD*(1) C 33- C 41	0.78	10.41	0.080
17. CR (1) C 31	282. RY (2) C 30	2.36	10.93	0.143
17. CR (1) C 31	289. RY (1) H 32	0.70	10.50	0.077
17. CR (1) C 31	291. RY (2) C 33	2.44	10.88	0.146
18. CR (1) C 33	163. BD*(1) C 30- C 31	0.81	10.64	0.083
18. CR (1) C 33	165. BD*(1) C 31- H 32	0.61	10.77	0.073
18. CR (1) C 33	166. BD*(1) C 31- C 33	0.53	10.65	0.067
18. CR (1) C 33	168. BD*(1) C 33- C 34	0.52	10.65	0.066
18. CR (1) C 33	170. BD*(1) C 34- H 35	0.62	10.77	0.073
18. CR (1) C 33	171. BD*(1) C 34- C 36	0.79	10.65	0.082
18. CR (1) C 33	286. RY (2) C 31	1.20	10.83	0.102
18. CR (1) C 33	288. RY (4) C 31	0.60	11.10	0.073
18. CR (1) C 33	295. RY (2) C 34	1.31	10.81	0.106

18. CR (1) C 33	297. RY (4) C 34	0.51	11.11	0.067
18. CR (1) C 33	311. RY (2) C 41	0.80	10.68	0.082
19. CR (1) C 34	161. BD* (1) C 29- C 36	0.92	10.57	0.088
19. CR (1) C 34	166. BD* (1) C 31- C 33	0.69	10.60	0.076
19. CR (1) C 34	169. BD* (1) C 33- C 41	0.79	10.41	0.081
19. CR (1) C 34	173. BD* (1) C 36- C 45	0.68	10.42	0.075
19. CR (1) C 34	290. RY (1) C 33	1.01	11.20	0.095
19. CR (1) C 34	291. RY (2) C 33	1.72	10.88	0.122
19. CR (1) C 34	298. RY (1) H 35	0.70	10.49	0.077
19. CR (1) C 34	299. RY (1) C 36	0.59	11.21	0.073
19. CR (1) C 34	300. RY (2) C 36	2.21	10.93	0.139
20. CR (1) C 36	159. BD* (1) C 29- C 30	0.68	10.62	0.076
20. CR (1) C 36	161. BD* (1) C 29- C 36	0.61	10.62	0.072
20. CR (1) C 36	162. BD* (1) C 29- B 69	1.19	10.50	0.100
20. CR (1) C 36	168. BD* (1) C 33- C 34	0.83	10.65	0.084
20. CR (1) C 36	170. BD* (1) C 34- H 35	0.59	10.77	0.071
20. CR (1) C 36	278. RY (2) C 29	1.76	11.08	0.124
20. CR (1) C 36	295. RY (2) C 34	1.31	10.81	0.106
20. CR (1) C 36	318. RY (2) C 45	0.72	10.85	0.079
21. CR (1) C 37	159. BD* (1) C 29- C 30	0.61	10.56	0.072
21. CR (1) C 37	281. RY (1) C 30	1.37	11.19	0.110
21. CR (1) C 37	307. RY (1) H 38	0.84	10.68	0.084
21. CR (1) C 37	308. RY (1) H 39	0.72	10.74	0.078
21. CR (1) C 37	309. RY (1) H 40	0.67	10.60	0.075
22. CR (1) C 41	166. BD* (1) C 31- C 33	0.52	10.60	0.066
22. CR (1) C 41	168. BD* (1) C 33- C 34	0.53	10.60	0.067
22. CR (1) C 41	290. RY (1) C 33	1.24	11.20	0.105
22. CR (1) C 41	314. RY (1) H 42	0.72	10.58	0.078
22. CR (1) C 41	315. RY (1) H 43	0.70	10.60	0.077
22. CR (1) C 41	316. RY (1) H 44	0.71	10.59	0.077
23. CR (1) C 45	161. BD* (1) C 29- C 36	0.57	10.56	0.069
23. CR (1) C 45	299. RY (1) C 36	1.36	11.19	0.110
23. CR (1) C 45	321. RY (1) H 46	0.66	10.60	0.075
23. CR (1) C 45	322. RY (1) H 47	0.80	10.68	0.083
23. CR (1) C 45	323. RY (1) H 48	0.83	10.84	0.084
24. CR (1) C 49	186. BD* (1) C 49- B 69	1.06	10.46	0.094
24. CR (1) C 49	187. BD* (1) C 50- C 51	0.68	10.59	0.076
24. CR (1) C 49	189. BD* (1) C 50- C 57	0.78	10.41	0.080
24. CR (1) C 49	196. BD* (1) C 54- C 56	0.67	10.59	0.075
24. CR (1) C 49	197. BD* (1) C 56- C 65	0.83	10.41	0.083
24. CR (1) C 49	329. RY (2) C 50	1.91	10.94	0.129
24. CR (1) C 49	346. RY (1) C 56	0.57	11.22	0.071
24. CR (1) C 49	347. RY (2) C 56	1.72	10.92	0.122
24. CR (1) C 49	372. RY (2) B 69	3.13	10.75	0.164
25. CR (1) C 50	183. BD* (1) C 49- C 50	0.57	10.62	0.069
25. CR (1) C 50	184. BD* (1) C 49- C 56	0.69	10.62	0.076
25. CR (1) C 50	186. BD* (1) C 49- B 69	1.19	10.51	0.100
25. CR (1) C 50	190. BD* (1) C 51- H 52	0.59	10.77	0.071
25. CR (1) C 50	191. BD* (1) C 51- C 53	0.82	10.65	0.083
25. CR (1) C 50	324. RY (1) C 49	0.72	11.28	0.081
25. CR (1) C 50	325. RY (2) C 49	1.27	11.08	0.106
25. CR (1) C 50	333. RY (2) C 51	1.23	10.80	0.103
25. CR (1) C 50	351. RY (2) C 57	0.69	10.84	0.077
26. CR (1) C 51	183. BD* (1) C 49- C 50	0.90	10.57	0.087
26. CR (1) C 51	189. BD* (1) C 50- C 57	0.63	10.41	0.072
26. CR (1) C 51	192. BD* (1) C 53- C 54	0.73	10.61	0.078
26. CR (1) C 51	194. BD* (1) C 53- C 61	0.79	10.40	0.081
26. CR (1) C 51	328. RY (1) C 50	0.69	11.21	0.079
26. CR (1) C 51	329. RY (2) C 50	1.98	10.95	0.131
26. CR (1) C 51	336. RY (1) H 52	0.70	10.49	0.077
26. CR (1) C 51	337. RY (1) C 53	0.81	11.19	0.085
26. CR (1) C 51	338. RY (2) C 53	1.90	10.88	0.128
27. CR (1) C 53	187. BD* (1) C 50- C 51	0.79	10.64	0.082
27. CR (1) C 53	190. BD* (1) C 51- H 52	0.63	10.77	0.074
27. CR (1) C 53	191. BD* (1) C 51- C 53	0.52	10.65	0.067
27. CR (1) C 53	192. BD* (1) C 53- C 54	0.58	10.66	0.070
27. CR (1) C 53	195. BD* (1) C 54- H 55	0.64	10.76	0.074
27. CR (1) C 53	196. BD* (1) C 54- C 56	0.84	10.64	0.084
27. CR (1) C 53	333. RY (2) C 51	1.48	10.80	0.113
27. CR (1) C 53	342. RY (2) C 54	1.48	10.82	0.113
27. CR (1) C 53	344. RY (4) C 54	0.51	11.11	0.067
27. CR (1) C 53	358. RY (2) C 61	0.76	10.69	0.080
28. CR (1) C 54	184. BD* (1) C 49- C 56	0.88	10.57	0.086
28. CR (1) C 54	191. BD* (1) C 51- C 53	0.76	10.60	0.080
28. CR (1) C 54	194. BD* (1) C 53- C 61	0.80	10.40	0.081
28. CR (1) C 54	197. BD* (1) C 56- C 65	0.61	10.41	0.071
28. CR (1) C 54	337. RY (1) C 53	0.61	11.19	0.074

28. CR (1) C 54	338. RY (2) C 53	2.27	10.88	0.140
28. CR (1) C 54	345. RY (1) H 55	0.70	10.50	0.076
28. CR (1) C 54	347. RY (2) C 56	2.27	10.92	0.141
29. CR (1) C 56	183. BD* (1) C 49- C 50	0.68	10.62	0.076
29. CR (1) C 56	184. BD* (1) C 49- C 56	0.59	10.62	0.071
29. CR (1) C 56	186. BD* (1) C 49- B 69	1.21	10.51	0.101
29. CR (1) C 56	192. BD* (1) C 53- C 54	0.83	10.66	0.084
29. CR (1) C 56	195. BD* (1) C 54- H 55	0.57	10.77	0.070
29. CR (1) C 56	324. RY (1) C 49	0.64	11.28	0.076
29. CR (1) C 56	325. RY (2) C 49	1.18	11.08	0.102
29. CR (1) C 56	342. RY (2) C 54	1.23	10.82	0.103
29. CR (1) C 56	365. RY (2) C 65	0.72	10.84	0.079
30. CR (1) C 57	183. BD* (1) C 49- C 50	0.62	10.55	0.072
30. CR (1) C 57	328. RY (1) C 50	1.37	11.19	0.110
30. CR (1) C 57	354. RY (1) H 58	0.84	10.69	0.084
30. CR (1) C 57	355. RY (1) H 59	0.83	10.84	0.085
30. CR (1) C 57	356. RY (1) H 60	0.65	10.60	0.074
31. CR (1) C 61	191. BD* (1) C 51- C 53	0.51	10.61	0.066
31. CR (1) C 61	192. BD* (1) C 53- C 54	0.51	10.61	0.065
31. CR (1) C 61	337. RY (1) C 53	1.24	11.19	0.105
31. CR (1) C 61	361. RY (1) H 62	0.72	10.58	0.078
31. CR (1) C 61	362. RY (1) H 63	0.70	10.60	0.077
31. CR (1) C 61	363. RY (1) H 64	0.71	10.59	0.078
32. CR (1) C 65	184. BD* (1) C 49- C 56	0.65	10.56	0.074
32. CR (1) C 65	346. RY (1) C 56	1.35	11.21	0.110
32. CR (1) C 65	368. RY (1) H 66	0.67	10.60	0.075
32. CR (1) C 65	369. RY (1) H 67	0.85	10.74	0.085
32. CR (1) C 65	370. RY (1) H 68	0.74	10.71	0.080
33. CR (1) B 69	139. BD* (1) C 12- C 13	0.51	7.21	0.054
33. CR (1) B 69	141. BD* (1) C 12- C 18	1.16	7.17	0.082
33. CR (1) B 69	159. BD* (1) C 29- C 30	0.69	7.22	0.063
33. CR (1) B 69	161. BD* (1) C 29- C 36	0.76	7.22	0.066
33. CR (1) B 69	183. BD* (1) C 49- C 50	0.66	7.21	0.062
33. CR (1) B 69	184. BD* (1) C 49- C 56	0.77	7.21	0.066
34. CR (1) N 70	135. BD* (1) C 9- C 11	0.55	14.76	0.080
34. CR (1) N 70	229. RY (1) C 11	1.31	15.24	0.126
34. CR (1) N 70	230. RY (2) C 11	0.87	15.24	0.103
34. CR (1) N 70	265. RY (3) C 21	0.70	15.04	0.092
34. CR (1) N 70	272. RY (3) C 25	0.65	14.87	0.088
35. LP (1) C 20	133. BD* (2) C 7- C 17	98.51	0.14	0.106
35. LP (1) C 20	136. BD* (2) C 9- C 11	0.92	0.13	0.010
35. LP (1) C 20	140. BD* (2) C 12- C 13	0.98	0.14	0.011
35. LP (1) C 20	147. BD* (2) C 15- C 19	94.94	0.14	0.105
35. LP (1) C 20	249. RY (3) C 17	2.41	0.80	0.039
35. LP (1) C 20	253. RY (3) C 18	2.31	0.89	0.040
35. LP (1) C 20	257. RY (3) C 19	2.30	0.80	0.038
35. LP (1) C 20	262. RY (4) C 20	5.64	0.82	0.061
36. LP (1) N 70	122. LV (1) B 69	4.63	0.30	0.033
36. LP (1) N 70	135. BD* (1) C 9- C 11	8.00	0.86	0.074
36. LP (1) N 70	137. BD* (1) C 11- C 18	3.23	0.82	0.046
36. LP (1) N 70	151. BD* (1) C 21- H 22	0.64	0.93	0.022
36. LP (1) N 70	152. BD* (1) C 21- H 23	1.18	0.91	0.029
36. LP (1) N 70	153. BD* (1) C 21- H 24	5.64	0.89	0.063
36. LP (1) N 70	155. BD* (1) C 25- H 26	5.79	0.89	0.064
36. LP (1) N 70	156. BD* (1) C 25- H 27	1.55	0.90	0.033
37. BD (1) C 1- H 2	124. BD* (1) C 1- H 3	1.20	1.17	0.033
37. BD (1) C 1- H 2	126. BD* (1) C 1- C 19	0.96	0.95	0.027
37. BD (1) C 1- H 2	127. BD* (1) C 4- H 5	0.85	1.17	0.028
37. BD (1) C 1- H 2	147. BD* (2) C 15- C 19	3.74	0.59	0.042
37. BD (1) C 1- H 2	150. BD* (1) C 19- C 20	0.91	1.11	0.028
37. BD (1) C 1- H 2	257. RY (3) C 19	0.68	1.24	0.026
38. BD (1) C 1- H 3	123. BD* (1) C 1- H 2	1.21	1.17	0.034
38. BD (1) C 1- H 3	126. BD* (1) C 1- C 19	0.89	0.95	0.026
38. BD (1) C 1- H 3	128. BD* (1) C 4- H 6	0.51	1.17	0.022
38. BD (1) C 1- H 3	129. BD* (1) C 4- C 17	0.82	0.95	0.025
38. BD (1) C 1- H 3	147. BD* (2) C 15- C 19	2.97	0.59	0.037
38. BD (1) C 1- H 3	150. BD* (1) C 19- C 20	1.15	1.11	0.032
38. BD (1) C 1- H 3	214. RY (2) C 4	0.53	1.23	0.023
38. BD (1) C 1- H 3	257. RY (3) C 19	0.78	1.24	0.028
39. BD (1) C 1- C 4	123. BD* (1) C 1- H 2	1.31	1.20	0.035
39. BD (1) C 1- C 4	124. BD* (1) C 1- H 3	1.36	1.20	0.036
39. BD (1) C 1- C 4	126. BD* (1) C 1- C 19	1.02	0.98	0.028
39. BD (1) C 1- C 4	127. BD* (1) C 4- H 5	1.33	1.20	0.036
39. BD (1) C 1- C 4	128. BD* (1) C 4- H 6	1.34	1.19	0.036
39. BD (1) C 1- C 4	129. BD* (1) C 4- C 17	1.01	0.98	0.028
39. BD (1) C 1- C 4	132. BD* (1) C 7- C 17	4.19	1.19	0.063
39. BD (1) C 1- C 4	146. BD* (1) C 15- C 19	4.08	1.20	0.062

39. BD (1) C 1- C 4	148. BD* (1) C 17- C 20	0.55	1.14	0.022
39. BD (1) C 1- C 4	150. BD* (1) C 19- C 20	0.56	1.13	0.022
39. BD (1) C 1- C 4	256. RY (2) C 19	0.54	1.53	0.026
40. BD (1) C 1- C 19	123. BD* (1) C 1- H 2	1.68	1.23	0.041
40. BD (1) C 1- C 19	124. BD* (1) C 1- H 3	1.86	1.23	0.043
40. BD (1) C 1- C 19	125. BD* (1) C 1- C 4	0.65	0.96	0.022
40. BD (1) C 1- C 19	128. BD* (1) C 4- H 6	0.63	1.23	0.025
40. BD (1) C 1- C 19	129. BD* (1) C 4- C 17	0.82	1.01	0.026
40. BD (1) C 1- C 19	144. BD* (1) C 13- C 15	2.00	1.16	0.043
40. BD (1) C 1- C 19	146. BD* (1) C 15- C 19	3.11	1.23	0.055
40. BD (1) C 1- C 19	149. BD* (1) C 18- C 20	4.31	1.19	0.064
40. BD (1) C 1- C 19	150. BD* (1) C 19- C 20	1.79	1.17	0.041
40. BD (1) C 1- C 19	259. RY (1) C 20	0.73	1.82	0.032
41. BD (1) C 4- H 5	123. BD* (1) C 1- H 2	0.84	1.17	0.028
41. BD (1) C 4- H 5	128. BD* (1) C 4- H 6	1.18	1.17	0.033
41. BD (1) C 4- H 5	129. BD* (1) C 4- C 17	0.97	0.95	0.027
41. BD (1) C 4- H 5	133. BD* (2) C 7- C 17	3.70	0.59	0.042
41. BD (1) C 4- H 5	148. BD* (1) C 17- C 20	0.84	1.11	0.027
41. BD (1) C 4- H 5	249. RY (3) C 17	0.78	1.24	0.028
42. BD (1) C 4- H 6	125. BD* (1) C 1- C 4	0.51	0.90	0.019
42. BD (1) C 4- H 6	126. BD* (1) C 1- C 19	0.85	0.95	0.025
42. BD (1) C 4- H 6	127. BD* (1) C 4- H 5	1.22	1.17	0.034
42. BD (1) C 4- H 6	129. BD* (1) C 4- C 17	0.90	0.95	0.026
42. BD (1) C 4- H 6	133. BD* (2) C 7- C 17	2.94	0.59	0.037
42. BD (1) C 4- H 6	148. BD* (1) C 17- C 20	1.28	1.11	0.034
42. BD (1) C 4- H 6	249. RY (3) C 17	0.74	1.24	0.027
43. BD (1) C 4- C 17	124. BD* (1) C 1- H 3	0.67	1.23	0.026
43. BD (1) C 4- C 17	125. BD* (1) C 1- C 4	0.63	0.96	0.022
43. BD (1) C 4- C 17	126. BD* (1) C 1- C 19	0.81	1.01	0.026
43. BD (1) C 4- C 17	127. BD* (1) C 4- H 5	1.77	1.23	0.042
43. BD (1) C 4- C 17	128. BD* (1) C 4- H 6	1.81	1.23	0.042
43. BD (1) C 4- C 17	131. BD* (1) C 7- C 9	1.98	1.16	0.043
43. BD (1) C 4- C 17	132. BD* (1) C 7- C 17	2.69	1.23	0.051
43. BD (1) C 4- C 17	148. BD* (1) C 17- C 20	2.07	1.17	0.044
43. BD (1) C 4- C 17	149. BD* (1) C 18- C 20	4.47	1.18	0.065
43. BD (1) C 4- C 17	209. RY (3) C 1	0.55	1.25	0.023
43. BD (1) C 4- C 17	219. RY (1) C 7	0.72	1.74	0.032
43. BD (1) C 4- C 17	260. RY (2) C 20	0.66	1.83	0.031
44. BD (1) C 7- H 8	131. BD* (1) C 7- C 9	1.43	1.13	0.036
44. BD (1) C 7- H 8	132. BD* (1) C 7- C 17	2.33	1.20	0.047
44. BD (1) C 7- H 8	135. BD* (1) C 9- C 11	3.42	1.17	0.057
44. BD (1) C 7- H 8	148. BD* (1) C 17- C 20	4.04	1.15	0.061
44. BD (1) C 7- H 8	224. RY (1) C 9	0.59	1.71	0.028
44. BD (1) C 7- H 8	247. RY (1) C 17	1.20	1.73	0.041
45. BD (1) C 7- C 9	129. BD* (1) C 4- C 17	5.69	1.08	0.070
45. BD (1) C 7- C 9	130. BD* (1) C 7- H 8	2.94	1.38	0.057
45. BD (1) C 7- C 9	132. BD* (1) C 7- C 17	3.77	1.29	0.062
45. BD (1) C 7- C 9	134. BD* (1) C 9- H 10	2.82	1.39	0.056
45. BD (1) C 7- C 9	135. BD* (1) C 9- C 11	4.04	1.26	0.064
45. BD (1) C 7- C 9	138. BD* (1) C 11- N 70	4.06	1.05	0.058
45. BD (1) C 7- C 9	230. RY (2) C 11	2.28	1.75	0.056
45. BD (1) C 7- C 9	247. RY (1) C 17	1.61	1.82	0.048
45. BD (1) C 7- C 9	248. RY (2) C 17	1.00	1.69	0.037
46. BD (1) C 7- C 17	129. BD* (1) C 4- C 17	2.35	1.12	0.046
46. BD (1) C 7- C 17	130. BD* (1) C 7- H 8	4.18	1.43	0.069
46. BD (1) C 7- C 17	131. BD* (1) C 7- C 9	2.85	1.27	0.054
46. BD (1) C 7- C 17	134. BD* (1) C 9- H 10	1.61	1.43	0.043
46. BD (1) C 7- C 17	148. BD* (1) C 17- C 20	4.34	1.28	0.067
46. BD (1) C 7- C 17	150. BD* (1) C 19- C 20	2.15	1.28	0.047
46. BD (1) C 7- C 17	224. RY (1) C 9	1.56	1.84	0.048
46. BD (1) C 7- C 17	225. RY (2) C 9	0.59	1.50	0.027
46. BD (1) C 7- C 17	260. RY (2) C 20	1.35	1.94	0.046
47. BD (2) C 7- C 17	127. BD* (1) C 4- H 5	1.97	0.89	0.037
47. BD (2) C 7- C 17	128. BD* (1) C 4- H 6	1.46	0.88	0.032
47. BD (2) C 7- C 17	136. BD* (2) C 9- C 11	19.91	0.29	0.068
47. BD (2) C 7- C 17	227. RY (4) C 9	1.35	0.91	0.031
47. BD (2) C 7- C 17	262. RY (4) C 20	0.88	0.97	0.026
48. BD (1) C 9- H 10	131. BD* (1) C 7- C 9	1.18	1.13	0.033
48. BD (1) C 9- H 10	132. BD* (1) C 7- C 17	3.09	1.20	0.054
48. BD (1) C 9- H 10	135. BD* (1) C 9- C 11	2.21	1.17	0.045
48. BD (1) C 9- H 10	137. BD* (1) C 11- C 18	5.01	1.13	0.067
48. BD (1) C 9- H 10	219. RY (1) C 7	0.65	1.71	0.030
48. BD (1) C 9- H 10	229. RY (1) C 11	0.91	1.66	0.035
49. BD (1) C 9- C 11	130. BD* (1) C 7- H 8	1.53	1.42	0.042
49. BD (1) C 9- C 11	131. BD* (1) C 7- C 9	3.58	1.26	0.060
49. BD (1) C 9- C 11	134. BD* (1) C 9- H 10	3.56	1.43	0.064
49. BD (1) C 9- C 11	137. BD* (1) C 11- C 18	4.20	1.26	0.065

49. BD (1) C 9- C 11	138. BD* (1) C 11- N 70	0.96	1.09	0.029
49. BD (1) C 9- C 11	141. BD* (1) C 12- C 18	3.35	1.25	0.058
49. BD (1) C 9- C 11	219. RY (1) C 7	0.59	1.84	0.030
49. BD (1) C 9- C 11	220. RY (2) C 7	0.91	1.40	0.032
49. BD (1) C 9- C 11	251. RY (1) C 18	1.59	1.87	0.049
49. BD (1) C 9- C 11	375. RY (1) N 70	0.52	1.81	0.027
50. BD (2) C 9- C 11	121. LV (1) C 18	58.10	0.16	0.087
50. BD (2) C 9- C 11	133. BD* (2) C 7- C 17	16.33	0.30	0.063
50. BD (2) C 9- C 11	152. BD* (1) C 21- H 23	0.68	0.91	0.022
50. BD (2) C 9- C 11	154. BD* (1) C 21- N 70	1.85	0.61	0.030
50. BD (2) C 9- C 11	156. BD* (1) C 25- H 27	0.68	0.89	0.022
50. BD (2) C 9- C 11	158. BD* (1) C 25- N 70	1.58	0.60	0.028
50. BD (2) C 9- C 11	221. RY (3) C 7	1.39	0.89	0.031
50. BD (2) C 9- C 11	253. RY (3) C 18	1.06	1.05	0.030
51. BD (1) C 11- C 18	134. BD* (1) C 9- H 10	1.76	1.39	0.044
51. BD (1) C 11- C 18	135. BD* (1) C 9- C 11	3.62	1.27	0.061
51. BD (1) C 11- C 18	138. BD* (1) C 11- N 70	1.05	1.06	0.030
51. BD (1) C 11- C 18	139. BD* (1) C 12- C 13	1.19	1.26	0.034
51. BD (1) C 11- C 18	141. BD* (1) C 12- C 18	4.65	1.21	0.067
51. BD (1) C 11- C 18	149. BD* (1) C 18- C 20	3.53	1.25	0.059
51. BD (1) C 11- C 18	150. BD* (1) C 19- C 20	3.23	1.24	0.057
51. BD (1) C 11- C 18	154. BD* (1) C 21- N 70	0.89	1.02	0.027
51. BD (1) C 11- C 18	158. BD* (1) C 25- N 70	1.07	1.02	0.029
51. BD (1) C 11- C 18	225. RY (2) C 9	0.73	1.46	0.029
51. BD (1) C 11- C 18	233. RY (1) C 12	1.02	1.86	0.039
51. BD (1) C 11- C 18	259. RY (1) C 20	1.50	1.89	0.048
51. BD (1) C 11- C 18	375. RY (1) N 70	0.82	1.77	0.034
52. BD (1) C 11- N 70	131. BD* (1) C 7- C 9	1.99	1.28	0.045
52. BD (1) C 11- N 70	135. BD* (1) C 9- C 11	1.88	1.32	0.044
52. BD (1) C 11- N 70	137. BD* (1) C 11- C 18	1.65	1.28	0.041
52. BD (1) C 11- N 70	149. BD* (1) C 18- C 20	1.89	1.31	0.044
52. BD (1) C 11- N 70	152. BD* (1) C 21- H 23	1.14	1.37	0.035
52. BD (1) C 11- N 70	156. BD* (1) C 25- H 27	1.13	1.36	0.035
52. BD (1) C 11- N 70	251. RY (1) C 18	1.33	1.89	0.045
52. BD (1) C 11- N 70	264. RY (2) C 21	0.83	1.56	0.032
53. BD (1) C 12- C 13	122. LV (1) B 69	2.21	0.71	0.035
53. BD (1) C 12- C 13	137. BD* (1) C 11- C 18	3.93	1.23	0.062
53. BD (1) C 12- C 13	141. BD* (1) C 12- C 18	3.04	1.22	0.054
53. BD (1) C 12- C 13	142. BD* (1) C 12- B 69	5.46	1.15	0.071
53. BD (1) C 12- C 13	143. BD* (1) C 13- H 14	3.33	1.42	0.061
53. BD (1) C 12- C 13	144. BD* (1) C 13- C 15	3.04	1.23	0.055
53. BD (1) C 12- C 13	145. BD* (1) C 15- H 16	1.55	1.40	0.042
53. BD (1) C 12- C 13	186. BD* (1) C 49- B 69	0.95	1.15	0.030
53. BD (1) C 12- C 13	242. RY (1) C 15	0.72	1.79	0.032
53. BD (1) C 12- C 13	243. RY (2) C 15	1.26	1.34	0.037
53. BD (1) C 12- C 13	251. RY (1) C 18	1.29	1.84	0.043
53. BD (1) C 12- C 13	371. RY (1) B 69	1.14	1.47	0.037
54. BD (2) C 12- C 13	121. LV (1) C 18	63.95	0.14	0.086
54. BD (2) C 12- C 13	122. LV (1) B 69	14.22	0.27	0.055
54. BD (2) C 12- C 13	147. BD* (2) C 15- C 19	16.77	0.29	0.062
54. BD (2) C 12- C 13	162. BD* (1) C 29- B 69	1.40	0.71	0.028
54. BD (2) C 12- C 13	186. BD* (1) C 49- B 69	2.48	0.71	0.038
54. BD (2) C 12- C 13	244. RY (3) C 15	1.36	0.87	0.031
54. BD (2) C 12- C 13	253. RY (3) C 18	0.92	1.03	0.027
55. BD (1) C 12- C 18	135. BD* (1) C 9- C 11	1.57	1.25	0.040
55. BD (1) C 12- C 18	137. BD* (1) C 11- C 18	4.14	1.21	0.063
55. BD (1) C 12- C 18	139. BD* (1) C 12- C 13	2.52	1.24	0.050
55. BD (1) C 12- C 18	142. BD* (1) C 12- B 69	5.97	1.14	0.073
55. BD (1) C 12- C 18	143. BD* (1) C 13- H 14	1.81	1.40	0.045
55. BD (1) C 12- C 18	148. BD* (1) C 17- C 20	3.18	1.23	0.056
55. BD (1) C 12- C 18	149. BD* (1) C 18- C 20	4.62	1.24	0.068
55. BD (1) C 12- C 18	229. RY (1) C 11	0.73	1.74	0.032
55. BD (1) C 12- C 18	259. RY (1) C 20	1.02	1.87	0.039
55. BD (1) C 12- C 18	372. RY (2) B 69	0.71	1.42	0.028
56. BD (1) C 12- B 69	139. BD* (1) C 12- C 13	3.63	1.10	0.057
56. BD (1) C 12- B 69	141. BD* (1) C 12- C 18	4.65	1.06	0.063
56. BD (1) C 12- B 69	144. BD* (1) C 13- C 15	4.72	1.08	0.064
56. BD (1) C 12- B 69	149. BD* (1) C 18- C 20	3.20	1.10	0.053
56. BD (1) C 12- B 69	159. BD* (1) C 29- C 30	1.22	1.11	0.033
56. BD (1) C 12- B 69	160. BD* (2) C 29- C 30	1.09	0.58	0.022
56. BD (1) C 12- B 69	183. BD* (1) C 49- C 50	1.29	1.10	0.034
56. BD (1) C 12- B 69	185. BD* (2) C 49- C 56	0.55	0.58	0.016
56. BD (1) C 12- B 69	237. RY (1) C 13	1.11	1.64	0.038
56. BD (1) C 12- B 69	251. RY (1) C 18	0.53	1.68	0.027
56. BD (1) C 12- B 69	252. RY (2) C 18	1.25	1.80	0.042
57. BD (1) C 13- H 14	122. LV (1) B 69	0.54	0.60	0.016
57. BD (1) C 13- H 14	139. BD* (1) C 12- C 13	1.99	1.15	0.043

57. BD (1) C 13- H 14	141. BD* (1) C 12- C 18	4.21	1.11	0.061
57. BD (1) C 13- H 14	144. BD* (1) C 13- C 15	1.23	1.12	0.033
57. BD (1) C 13- H 14	146. BD* (1) C 15- C 19	3.22	1.19	0.055
57. BD (1) C 13- H 14	233. RY (1) C 12	0.88	1.75	0.035
57. BD (1) C 13- H 14	242. RY (1) C 15	0.54	1.68	0.027
58. BD (1) C 13- C 15	126. BD* (1) C 1- C 19	5.89	1.07	0.071
58. BD (1) C 13- C 15	139. BD* (1) C 12- C 13	3.15	1.24	0.056
58. BD (1) C 13- C 15	142. BD* (1) C 12- B 69	2.36	1.14	0.046
58. BD (1) C 13- C 15	143. BD* (1) C 13- H 14	2.78	1.40	0.056
58. BD (1) C 13- C 15	145. BD* (1) C 15- H 16	2.72	1.39	0.055
58. BD (1) C 13- C 15	146. BD* (1) C 15- C 19	4.26	1.29	0.066
58. BD (1) C 13- C 15	233. RY (1) C 12	0.53	1.85	0.028
58. BD (1) C 13- C 15	234. RY (2) C 12	1.88	1.77	0.051
58. BD (1) C 13- C 15	255. RY (1) C 19	0.80	1.86	0.034
58. BD (1) C 13- C 15	256. RY (2) C 19	1.40	1.62	0.042
59. BD (1) C 15- H 16	139. BD* (1) C 12- C 13	3.36	1.16	0.056
59. BD (1) C 15- H 16	144. BD* (1) C 13- C 15	1.39	1.13	0.035
59. BD (1) C 15- H 16	146. BD* (1) C 15- C 19	2.32	1.20	0.047
59. BD (1) C 15- H 16	150. BD* (1) C 19- C 20	4.15	1.14	0.061
59. BD (1) C 15- H 16	237. RY (1) C 13	0.61	1.70	0.029
59. BD (1) C 15- H 16	255. RY (1) C 19	1.39	1.78	0.044
60. BD (1) C 15- C 19	126. BD* (1) C 1- C 19	2.72	1.12	0.049
60. BD (1) C 15- C 19	143. BD* (1) C 13- H 14	1.43	1.45	0.041
60. BD (1) C 15- C 19	144. BD* (1) C 13- C 15	3.19	1.27	0.057
60. BD (1) C 15- C 19	145. BD* (1) C 15- H 16	4.01	1.44	0.068
60. BD (1) C 15- C 19	148. BD* (1) C 17- C 20	2.05	1.28	0.046
60. BD (1) C 15- C 19	150. BD* (1) C 19- C 20	4.08	1.28	0.064
60. BD (1) C 15- C 19	237. RY (1) C 13	0.96	1.84	0.038
60. BD (1) C 15- C 19	238. RY (2) C 13	0.80	1.58	0.032
60. BD (1) C 15- C 19	259. RY (1) C 20	0.53	1.93	0.028
60. BD (1) C 15- C 19	260. RY (2) C 20	0.78	1.94	0.035
61. BD (2) C 15- C 19	123. BD* (1) C 1- H 2	1.76	0.88	0.035
61. BD (2) C 15- C 19	124. BD* (1) C 1- H 3	1.63	0.88	0.034
61. BD (2) C 15- C 19	140. BD* (2) C 12- C 13	19.40	0.30	0.068
61. BD (2) C 15- C 19	239. RY (3) C 13	1.11	0.97	0.029
61. BD (2) C 15- C 19	262. RY (4) C 20	0.89	0.97	0.026
62. BD (1) C 17- C 20	128. BD* (1) C 4- H 6	0.58	1.30	0.025
62. BD (1) C 17- C 20	129. BD* (1) C 4- C 17	1.38	1.08	0.034
62. BD (1) C 17- C 20	130. BD* (1) C 7- H 8	2.67	1.39	0.054
62. BD (1) C 17- C 20	132. BD* (1) C 7- C 17	4.05	1.30	0.065
62. BD (1) C 17- C 20	141. BD* (1) C 12- C 18	2.35	1.21	0.048
62. BD (1) C 17- C 20	146. BD* (1) C 15- C 19	2.63	1.30	0.052
62. BD (1) C 17- C 20	149. BD* (1) C 18- C 20	5.47	1.25	0.074
62. BD (1) C 17- C 20	150. BD* (1) C 19- C 20	3.60	1.24	0.060
62. BD (1) C 17- C 20	219. RY (1) C 7	0.63	1.81	0.030
62. BD (1) C 17- C 20	220. RY (2) C 7	0.62	1.36	0.026
62. BD (1) C 17- C 20	252. RY (2) C 18	1.06	1.95	0.041
62. BD (1) C 17- C 20	255. RY (1) C 19	1.35	1.87	0.045
63. BD (1) C 18- C 20	126. BD* (1) C 1- C 19	1.55	1.09	0.037
63. BD (1) C 18- C 20	129. BD* (1) C 4- C 17	1.55	1.09	0.037
63. BD (1) C 18- C 20	137. BD* (1) C 11- C 18	3.26	1.23	0.057
63. BD (1) C 18- C 20	138. BD* (1) C 11- N 70	3.78	1.06	0.056
63. BD (1) C 18- C 20	141. BD* (1) C 12- C 18	4.16	1.22	0.064
63. BD (1) C 18- C 20	142. BD* (1) C 12- B 69	2.67	1.16	0.050
63. BD (1) C 18- C 20	148. BD* (1) C 17- C 20	5.45	1.25	0.074
63. BD (1) C 18- C 20	150. BD* (1) C 19- C 20	4.51	1.24	0.067
63. BD (1) C 18- C 20	229. RY (1) C 11	1.44	1.76	0.045
63. BD (1) C 18- C 20	233. RY (1) C 12	1.03	1.87	0.039
63. BD (1) C 18- C 20	248. RY (2) C 17	0.68	1.70	0.030
63. BD (1) C 18- C 20	255. RY (1) C 19	0.53	1.88	0.028
63. BD (1) C 18- C 20	256. RY (2) C 19	0.73	1.64	0.031
64. BD (1) C 19- C 20	123. BD* (1) C 1- H 2	0.52	1.30	0.023
64. BD (1) C 19- C 20	124. BD* (1) C 1- H 3	0.57	1.29	0.024
64. BD (1) C 19- C 20	126. BD* (1) C 1- C 19	1.21	1.07	0.032
64. BD (1) C 19- C 20	132. BD* (1) C 7- C 17	2.77	1.29	0.053
64. BD (1) C 19- C 20	137. BD* (1) C 11- C 18	2.25	1.22	0.047
64. BD (1) C 19- C 20	145. BD* (1) C 15- H 16	2.67	1.39	0.054
64. BD (1) C 19- C 20	146. BD* (1) C 15- C 19	3.98	1.30	0.064
64. BD (1) C 19- C 20	148. BD* (1) C 17- C 20	3.65	1.24	0.060
64. BD (1) C 19- C 20	149. BD* (1) C 18- C 20	4.74	1.25	0.069
64. BD (1) C 19- C 20	242. RY (1) C 15	0.61	1.78	0.029
64. BD (1) C 19- C 20	243. RY (2) C 15	0.92	1.34	0.031
64. BD (1) C 19- C 20	247. RY (1) C 17	1.10	1.82	0.040
64. BD (1) C 19- C 20	251. RY (1) C 18	0.62	1.83	0.030
64. BD (1) C 19- C 20	252. RY (2) C 18	1.10	1.95	0.041
65. BD (1) C 21- H 22	152. BD* (1) C 21- H 23	1.94	1.19	0.043
65. BD (1) C 21- H 22	153. BD* (1) C 21- H 24	1.46	1.17	0.037

65. BD (1) C 21- H 22	158. BD* (1) C 25- N 70	3.00	0.88	0.046
66. BD (1) C 21- H 23	138. BD* (1) C 11- N 70	3.06	0.93	0.048
66. BD (1) C 21- H 23	151. BD* (1) C 21- H 22	1.81	1.20	0.042
66. BD (1) C 21- H 23	153. BD* (1) C 21- H 24	1.32	1.17	0.035
67. BD (1) C 21- H 24	151. BD* (1) C 21- H 22	1.55	1.21	0.039
67. BD (1) C 21- H 24	152. BD* (1) C 21- H 23	1.48	1.20	0.037
68. BD (1) C 21- N 70	136. BD* (2) C 9- C 11	2.67	0.71	0.039
68. BD (1) C 21- N 70	137. BD* (1) C 11- C 18	1.19	1.23	0.034
68. BD (1) C 21- N 70	138. BD* (1) C 11- N 70	0.56	1.06	0.022
68. BD (1) C 21- N 70	151. BD* (1) C 21- H 22	0.94	1.34	0.032
68. BD (1) C 21- N 70	152. BD* (1) C 21- H 23	0.95	1.32	0.032
68. BD (1) C 21- N 70	153. BD* (1) C 21- H 24	0.64	1.31	0.026
68. BD (1) C 21- N 70	157. BD* (1) C 25- H 28	1.46	1.32	0.039
68. BD (1) C 21- N 70	231. RY (3) C 11	1.07	1.43	0.035
68. BD (1) C 21- N 70	270. RY (1) C 25	0.81	1.40	0.030
69. BD (1) C 25- H 26	156. BD* (1) C 25- H 27	1.49	1.19	0.038
69. BD (1) C 25- H 26	157. BD* (1) C 25- H 28	1.53	1.20	0.038
70. BD (1) C 25- H 27	138. BD* (1) C 11- N 70	3.07	0.94	0.048
70. BD (1) C 25- H 27	155. BD* (1) C 25- H 26	1.36	1.18	0.036
70. BD (1) C 25- H 27	157. BD* (1) C 25- H 28	1.62	1.19	0.039
71. BD (1) C 25- H 28	154. BD* (1) C 21- N 70	2.93	0.90	0.046
71. BD (1) C 25- H 28	155. BD* (1) C 25- H 26	1.38	1.18	0.036
71. BD (1) C 25- H 28	156. BD* (1) C 25- H 27	1.77	1.19	0.041
72. BD (1) C 25- N 70	136. BD* (2) C 9- C 11	2.57	0.72	0.038
72. BD (1) C 25- N 70	137. BD* (1) C 11- C 18	1.50	1.24	0.039
72. BD (1) C 25- N 70	138. BD* (1) C 11- N 70	0.58	1.07	0.022
72. BD (1) C 25- N 70	151. BD* (1) C 21- H 22	1.40	1.35	0.039
72. BD (1) C 25- N 70	155. BD* (1) C 25- H 26	0.73	1.31	0.028
72. BD (1) C 25- N 70	156. BD* (1) C 25- H 27	1.04	1.32	0.033
72. BD (1) C 25- N 70	157. BD* (1) C 25- H 28	0.91	1.32	0.031
72. BD (1) C 25- N 70	229. RY (1) C 11	0.54	1.76	0.028
72. BD (1) C 25- N 70	231. RY (3) C 11	0.74	1.44	0.029
72. BD (1) C 25- N 70	263. RY (1) C 21	0.93	1.45	0.033
73. BD (1) C 29- C 30	122. LV (1) B 69	1.02	0.69	0.024
73. BD (1) C 29- C 30	161. BD* (1) C 29- C 36	3.79	1.25	0.061
73. BD (1) C 29- C 30	162. BD* (1) C 29- B 69	5.69	1.13	0.071
73. BD (1) C 29- C 30	163. BD* (1) C 30- C 31	3.61	1.27	0.060
73. BD (1) C 29- C 30	164. BD* (1) C 30- C 37	1.60	1.09	0.037
73. BD (1) C 29- C 30	165. BD* (1) C 31- H 32	1.76	1.39	0.044
73. BD (1) C 29- C 30	173. BD* (1) C 36- C 45	3.12	1.09	0.052
73. BD (1) C 29- C 30	285. RY (1) C 31	0.64	1.80	0.030
73. BD (1) C 29- C 30	286. RY (2) C 31	0.50	1.45	0.024
73. BD (1) C 29- C 30	300. RY (2) C 36	1.04	1.60	0.036
74. BD (2) C 29- C 30	122. LV (1) B 69	8.61	0.25	0.042
74. BD (2) C 29- C 30	142. BD* (1) C 12- B 69	2.73	0.70	0.039
74. BD (2) C 29- C 30	167. BD* (2) C 31- C 33	18.91	0.27	0.064
74. BD (2) C 29- C 30	172. BD* (2) C 34- C 36	23.56	0.27	0.072
74. BD (2) C 29- C 30	174. BD* (1) C 37- H 38	2.20	0.87	0.039
74. BD (2) C 29- C 30	175. BD* (1) C 37- H 39	1.40	0.86	0.031
74. BD (2) C 29- C 30	186. BD* (1) C 49- B 69	2.10	0.69	0.034
74. BD (2) C 29- C 30	287. RY (3) C 31	1.65	0.87	0.034
74. BD (2) C 29- C 30	301. RY (3) C 36	0.93	0.94	0.026
75. BD (1) C 29- C 36	159. BD* (1) C 29- C 30	3.85	1.25	0.062
75. BD (1) C 29- C 36	162. BD* (1) C 29- B 69	5.54	1.13	0.071
75. BD (1) C 29- C 36	164. BD* (1) C 30- C 37	3.31	1.09	0.054
75. BD (1) C 29- C 36	170. BD* (1) C 34- H 35	1.79	1.39	0.045
75. BD (1) C 29- C 36	171. BD* (1) C 34- C 36	3.61	1.27	0.060
75. BD (1) C 29- C 36	173. BD* (1) C 36- C 45	1.53	1.09	0.036
75. BD (1) C 29- C 36	180. BD* (1) C 45- H 46	0.52	1.31	0.023
75. BD (1) C 29- C 36	282. RY (2) C 30	1.11	1.60	0.038
75. BD (1) C 29- C 36	294. RY (1) C 34	0.62	1.80	0.030
75. BD (1) C 29- C 36	295. RY (2) C 34	0.63	1.43	0.027
76. BD (1) C 29- B 69	140. BD* (2) C 12- C 13	0.68	0.55	0.017
76. BD (1) C 29- B 69	141. BD* (1) C 12- C 18	2.42	1.05	0.045
76. BD (1) C 29- B 69	159. BD* (1) C 29- C 30	3.90	1.09	0.058
76. BD (1) C 29- B 69	161. BD* (1) C 29- C 36	3.99	1.09	0.059
76. BD (1) C 29- B 69	163. BD* (1) C 30- C 31	3.71	1.11	0.057
76. BD (1) C 29- B 69	171. BD* (1) C 34- C 36	3.71	1.12	0.057
76. BD (1) C 29- B 69	184. BD* (1) C 49- C 56	1.44	1.09	0.035
76. BD (1) C 29- B 69	185. BD* (2) C 49- C 56	1.20	0.56	0.023
76. BD (1) C 29- B 69	281. RY (1) C 30	2.03	1.72	0.053
76. BD (1) C 29- B 69	299. RY (1) C 36	2.15	1.72	0.054
77. BD (1) C 30- C 31	159. BD* (1) C 29- C 30	3.99	1.25	0.063
77. BD (1) C 30- C 31	162. BD* (1) C 29- B 69	2.90	1.13	0.051
77. BD (1) C 30- C 31	164. BD* (1) C 30- C 37	1.25	1.09	0.033
77. BD (1) C 30- C 31	165. BD* (1) C 31- H 32	3.73	1.40	0.065
77. BD (1) C 30- C 31	166. BD* (1) C 31- C 33	4.12	1.28	0.065

77. BD (1) C 30- C 31	169. BD* (1) C 33- C 41	3.17	1.09	0.052
77. BD (1) C 30- C 31	277. RY (1) C 29	0.85	1.91	0.036
77. BD (1) C 30- C 31	278. RY (2) C 29	0.73	1.71	0.031
77. BD (1) C 30- C 31	290. RY (1) C 33	1.44	1.88	0.046
77. BD (1) C 30- C 31	291. RY (2) C 33	1.68	1.56	0.046
77. BD (1) C 30- C 31	303. RY (1) C 37	0.56	1.42	0.025
78. BD (1) C 30- C 37	159. BD* (1) C 29- C 30	2.24	1.17	0.046
78. BD (1) C 30- C 37	161. BD* (1) C 29- C 36	2.70	1.17	0.050
78. BD (1) C 30- C 37	163. BD* (1) C 30- C 31	1.66	1.19	0.040
78. BD (1) C 30- C 37	166. BD* (1) C 31- C 33	2.86	1.20	0.052
78. BD (1) C 30- C 37	174. BD* (1) C 37- H 38	2.15	1.24	0.046
78. BD (1) C 30- C 37	175. BD* (1) C 37- H 39	1.97	1.23	0.044
78. BD (1) C 30- C 37	176. BD* (1) C 37- H 40	2.02	1.23	0.045
78. BD (1) C 30- C 37	277. RY (1) C 29	0.82	1.83	0.034
78. BD (1) C 30- C 37	285. RY (1) C 31	0.83	1.73	0.034
79. BD (1) C 31- H 32	159. BD* (1) C 29- C 30	4.08	1.14	0.061
79. BD (1) C 31- H 32	163. BD* (1) C 30- C 31	2.03	1.16	0.043
79. BD (1) C 31- H 32	166. BD* (1) C 31- C 33	1.97	1.17	0.043
79. BD (1) C 31- H 32	168. BD* (1) C 33- C 34	3.66	1.17	0.058
79. BD (1) C 31- H 32	281. RY (1) C 30	1.16	1.77	0.040
79. BD (1) C 31- H 32	290. RY (1) C 33	1.17	1.77	0.041
80. BD (1) C 31- C 33	163. BD* (1) C 30- C 31	4.03	1.28	0.064
80. BD (1) C 31- C 33	164. BD* (1) C 30- C 37	2.69	1.10	0.049
80. BD (1) C 31- C 33	165. BD* (1) C 31- H 32	3.74	1.40	0.065
80. BD (1) C 31- C 33	168. BD* (1) C 33- C 34	3.66	1.29	0.061
80. BD (1) C 31- C 33	169. BD* (1) C 33- C 41	1.38	1.09	0.035
80. BD (1) C 31- C 33	170. BD* (1) C 34- H 35	2.28	1.40	0.050
80. BD (1) C 31- C 33	281. RY (1) C 30	1.41	1.89	0.046
80. BD (1) C 31- C 33	282. RY (2) C 30	1.93	1.61	0.050
80. BD (1) C 31- C 33	294. RY (1) C 34	0.53	1.81	0.028
80. BD (1) C 31- C 33	310. RY (1) C 41	0.52	1.31	0.023
81. BD (2) C 31- C 33	160. BD* (2) C 29- C 30	23.51	0.29	0.073
81. BD (2) C 31- C 33	172. BD* (2) C 34- C 36	17.80	0.28	0.064
81. BD (2) C 31- C 33	177. BD* (1) C 41- H 42	2.57	0.87	0.042
81. BD (2) C 31- C 33	179. BD* (1) C 41- H 44	2.23	0.87	0.039
81. BD (2) C 31- C 33	283. RY (3) C 30	0.91	0.96	0.026
81. BD (2) C 31- C 33	296. RY (3) C 34	1.47	0.88	0.032
82. BD (1) C 33- C 34	165. BD* (1) C 31- H 32	2.21	1.40	0.050
82. BD (1) C 33- C 34	166. BD* (1) C 31- C 33	3.58	1.29	0.061
82. BD (1) C 33- C 34	169. BD* (1) C 33- C 41	1.41	1.10	0.035
82. BD (1) C 33- C 34	170. BD* (1) C 34- H 35	3.67	1.41	0.064
82. BD (1) C 33- C 34	171. BD* (1) C 34- C 36	4.15	1.29	0.065
82. BD (1) C 33- C 34	173. BD* (1) C 36- C 45	2.80	1.10	0.050
82. BD (1) C 33- C 34	178. BD* (1) C 41- H 43	0.52	1.31	0.023
82. BD (1) C 33- C 34	299. RY (1) C 36	1.23	1.89	0.043
82. BD (1) C 33- C 34	300. RY (2) C 36	1.98	1.61	0.051
82. BD (1) C 33- C 34	310. RY (1) C 41	0.63	1.31	0.026
83. BD (1) C 33- C 41	163. BD* (1) C 30- C 31	2.69	1.20	0.051
83. BD (1) C 33- C 41	166. BD* (1) C 31- C 33	1.85	1.21	0.042
83. BD (1) C 33- C 41	168. BD* (1) C 33- C 34	1.90	1.21	0.043
83. BD (1) C 33- C 41	171. BD* (1) C 34- C 36	2.71	1.21	0.051
83. BD (1) C 33- C 41	177. BD* (1) C 41- H 42	1.98	1.23	0.044
83. BD (1) C 33- C 41	178. BD* (1) C 41- H 43	1.86	1.23	0.043
83. BD (1) C 33- C 41	179. BD* (1) C 41- H 44	1.96	1.23	0.044
83. BD (1) C 33- C 41	285. RY (1) C 31	0.75	1.73	0.032
83. BD (1) C 33- C 41	294. RY (1) C 34	0.77	1.73	0.033
84. BD (1) C 34- H 35	161. BD* (1) C 29- C 36	4.19	1.14	0.062
84. BD (1) C 34- H 35	166. BD* (1) C 31- C 33	3.69	1.17	0.059
84. BD (1) C 34- H 35	168. BD* (1) C 33- C 34	1.94	1.17	0.043
84. BD (1) C 34- H 35	171. BD* (1) C 34- C 36	2.06	1.17	0.044
84. BD (1) C 34- H 35	290. RY (1) C 33	1.27	1.77	0.042
84. BD (1) C 34- H 35	299. RY (1) C 36	1.23	1.77	0.042
85. BD (1) C 34- C 36	161. BD* (1) C 29- C 36	3.90	1.26	0.062
85. BD (1) C 34- C 36	162. BD* (1) C 29- B 69	2.83	1.14	0.051
85. BD (1) C 34- C 36	168. BD* (1) C 33- C 34	4.35	1.28	0.067
85. BD (1) C 34- C 36	169. BD* (1) C 33- C 41	3.19	1.09	0.053
85. BD (1) C 34- C 36	170. BD* (1) C 34- H 35	3.74	1.40	0.065
85. BD (1) C 34- C 36	173. BD* (1) C 36- C 45	1.34	1.10	0.034
85. BD (1) C 34- C 36	277. RY (1) C 29	1.03	1.91	0.040
85. BD (1) C 34- C 36	278. RY (2) C 29	0.59	1.71	0.028
85. BD (1) C 34- C 36	290. RY (1) C 33	0.73	1.89	0.033
85. BD (1) C 34- C 36	291. RY (2) C 33	2.16	1.56	0.052
85. BD (1) C 34- C 36	317. RY (1) C 45	0.52	1.43	0.024
86. BD (2) C 34- C 36	160. BD* (2) C 29- C 30	16.77	0.29	0.062
86. BD (2) C 34- C 36	167. BD* (2) C 31- C 33	24.77	0.28	0.075
86. BD (2) C 34- C 36	181. BD* (1) C 45- H 47	2.44	0.88	0.041
86. BD (2) C 34- C 36	182. BD* (1) C 45- H 48	2.30	0.89	0.040

86. BD (2) C 34- C 36	279. RY (3) C 29	0.79	1.10	0.026
86. BD (2) C 34- C 36	292. RY (3) C 33	0.88	0.93	0.025
87. BD (1) C 36- C 45	159. BD* (1) C 29- C 30	2.83	1.17	0.051
87. BD (1) C 36- C 45	161. BD* (1) C 29- C 36	2.18	1.17	0.045
87. BD (1) C 36- C 45	168. BD* (1) C 33- C 34	2.85	1.20	0.052
87. BD (1) C 36- C 45	171. BD* (1) C 34- C 36	1.74	1.20	0.041
87. BD (1) C 36- C 45	180. BD* (1) C 45- H 46	2.06	1.23	0.045
87. BD (1) C 36- C 45	181. BD* (1) C 45- H 47	2.10	1.24	0.045
87. BD (1) C 36- C 45	182. BD* (1) C 45- H 48	2.11	1.24	0.046
87. BD (1) C 36- C 45	277. RY (1) C 29	0.88	1.83	0.036
87. BD (1) C 36- C 45	294. RY (1) C 34	0.76	1.73	0.032
88. BD (1) C 37- H 38	160. BD* (2) C 29- C 30	3.93	0.58	0.043
88. BD (1) C 37- H 38	163. BD* (1) C 30- C 31	1.13	1.13	0.032
88. BD (1) C 37- H 38	164. BD* (1) C 30- C 37	1.16	0.95	0.030
88. BD (1) C 37- H 38	175. BD* (1) C 37- H 39	1.38	1.17	0.036
88. BD (1) C 37- H 38	176. BD* (1) C 37- H 40	1.53	1.17	0.038
88. BD (1) C 37- H 38	283. RY (3) C 30	0.77	1.25	0.028
89. BD (1) C 37- H 39	122. LV (1) B 69	0.85	0.56	0.020
89. BD (1) C 37- H 39	160. BD* (2) C 29- C 30	2.89	0.59	0.037
89. BD (1) C 37- H 39	163. BD* (1) C 30- C 31	1.93	1.14	0.042
89. BD (1) C 37- H 39	164. BD* (1) C 30- C 37	1.07	0.96	0.029
89. BD (1) C 37- H 39	174. BD* (1) C 37- H 38	1.48	1.18	0.037
89. BD (1) C 37- H 39	176. BD* (1) C 37- H 40	1.50	1.18	0.038
90. BD (1) C 37- H 40	159. BD* (1) C 29- C 30	4.15	1.11	0.061
90. BD (1) C 37- H 40	164. BD* (1) C 30- C 37	1.11	0.96	0.029
90. BD (1) C 37- H 40	174. BD* (1) C 37- H 38	1.66	1.18	0.040
90. BD (1) C 37- H 40	175. BD* (1) C 37- H 39	1.67	1.17	0.040
91. BD (1) C 41- H 42	166. BD* (1) C 31- C 33	1.48	1.15	0.037
91. BD (1) C 41- H 42	167. BD* (2) C 31- C 33	4.12	0.59	0.044
91. BD (1) C 41- H 42	169. BD* (1) C 33- C 41	1.09	0.96	0.029
91. BD (1) C 41- H 42	178. BD* (1) C 41- H 43	1.42	1.17	0.036
91. BD (1) C 41- H 42	179. BD* (1) C 41- H 44	1.33	1.17	0.035
91. BD (1) C 41- H 42	292. RY (3) C 33	0.71	1.23	0.026
92. BD (1) C 41- H 43	168. BD* (1) C 33- C 34	3.99	1.15	0.060
92. BD (1) C 41- H 43	169. BD* (1) C 33- C 41	1.04	0.96	0.028
92. BD (1) C 41- H 43	177. BD* (1) C 41- H 42	1.51	1.17	0.038
92. BD (1) C 41- H 43	179. BD* (1) C 41- H 44	1.52	1.17	0.038
92. BD (1) C 41- H 43	291. RY (2) C 33	0.57	1.43	0.026
93. BD (1) C 41- H 44	166. BD* (1) C 31- C 33	2.03	1.15	0.043
93. BD (1) C 41- H 44	167. BD* (2) C 31- C 33	3.10	0.59	0.038
93. BD (1) C 41- H 44	169. BD* (1) C 33- C 41	1.06	0.96	0.028
93. BD (1) C 41- H 44	177. BD* (1) C 41- H 42	1.35	1.17	0.035
93. BD (1) C 41- H 44	178. BD* (1) C 41- H 43	1.44	1.17	0.037
93. BD (1) C 41- H 44	292. RY (3) C 33	0.61	1.23	0.024
94. BD (1) C 45- H 46	161. BD* (1) C 29- C 36	4.06	1.12	0.060
94. BD (1) C 45- H 46	173. BD* (1) C 36- C 45	1.12	0.96	0.029
94. BD (1) C 45- H 46	181. BD* (1) C 45- H 47	1.65	1.18	0.039
94. BD (1) C 45- H 46	182. BD* (1) C 45- H 48	1.72	1.19	0.040
95. BD (1) C 45- H 47	171. BD* (1) C 34- C 36	1.51	1.14	0.037
95. BD (1) C 45- H 47	172. BD* (2) C 34- C 36	3.74	0.58	0.042
95. BD (1) C 45- H 47	173. BD* (1) C 36- C 45	1.20	0.95	0.030
95. BD (1) C 45- H 47	180. BD* (1) C 45- H 46	1.55	1.17	0.038
95. BD (1) C 45- H 47	182. BD* (1) C 45- H 48	1.44	1.18	0.037
95. BD (1) C 45- H 47	301. RY (3) C 36	0.68	1.25	0.026
96. BD (1) C 45- H 48	122. LV (1) B 69	0.59	0.56	0.016
96. BD (1) C 45- H 48	171. BD* (1) C 34- C 36	1.60	1.14	0.038
96. BD (1) C 45- H 48	172. BD* (2) C 34- C 36	3.57	0.58	0.041
96. BD (1) C 45- H 48	173. BD* (1) C 36- C 45	1.12	0.96	0.029
96. BD (1) C 45- H 48	180. BD* (1) C 45- H 46	1.55	1.18	0.038
96. BD (1) C 45- H 48	181. BD* (1) C 45- H 47	1.46	1.18	0.037
96. BD (1) C 45- H 48	301. RY (3) C 36	0.62	1.25	0.025
97. BD (1) C 49- C 50	142. BD* (1) C 12- B 69	0.74	1.14	0.026
97. BD (1) C 49- C 50	184. BD* (1) C 49- C 56	3.64	1.24	0.060
97. BD (1) C 49- C 50	186. BD* (1) C 49- B 69	5.77	1.13	0.072
97. BD (1) C 49- C 50	187. BD* (1) C 50- C 51	3.57	1.26	0.060
97. BD (1) C 49- C 50	189. BD* (1) C 50- C 57	1.50	1.08	0.036
97. BD (1) C 49- C 50	190. BD* (1) C 51- H 52	1.78	1.39	0.044
97. BD (1) C 49- C 50	197. BD* (1) C 56- C 65	3.40	1.08	0.054
97. BD (1) C 49- C 50	332. RY (1) C 51	0.52	1.79	0.027
97. BD (1) C 49- C 50	333. RY (2) C 51	0.69	1.43	0.028
97. BD (1) C 49- C 50	347. RY (2) C 56	1.22	1.59	0.039
97. BD (1) C 49- C 50	371. RY (1) B 69	0.71	1.46	0.029
98. BD (1) C 49- C 56	122. LV (1) B 69	0.67	0.69	0.019
98. BD (1) C 49- C 56	183. BD* (1) C 49- C 50	3.64	1.24	0.060
98. BD (1) C 49- C 56	186. BD* (1) C 49- B 69	5.93	1.14	0.073
98. BD (1) C 49- C 56	189. BD* (1) C 50- C 57	3.17	1.09	0.052
98. BD (1) C 49- C 56	195. BD* (1) C 54- H 55	1.74	1.39	0.044

98. BD (1) C 49- C 56	196. BD* (1) C 54- C 56	3.68	1.26	0.061
98. BD (1) C 49- C 56	197. BD* (1) C 56- C 65	1.55	1.09	0.037
98. BD (1) C 49- C 56	329. RY (2) C 50	1.05	1.62	0.037
98. BD (1) C 49- C 56	341. RY (1) C 54	0.54	1.80	0.028
98. BD (1) C 49- C 56	342. RY (2) C 54	0.56	1.45	0.025
98. BD (1) C 49- C 56	372. RY (2) B 69	0.64	1.43	0.027
99. BD (2) C 49- C 56	122. LV (1) B 69	11.55	0.25	0.048
99. BD (2) C 49- C 56	142. BD* (1) C 12- B 69	1.68	0.70	0.031
99. BD (2) C 49- C 56	162. BD* (1) C 29- B 69	2.28	0.69	0.035
99. BD (2) C 49- C 56	185. BD* (2) C 49- C 56	0.55	0.28	0.011
99. BD (2) C 49- C 56	188. BD* (2) C 50- C 51	23.12	0.27	0.071
99. BD (2) C 49- C 56	193. BD* (2) C 53- C 54	18.87	0.27	0.064
99. BD (2) C 49- C 56	205. BD* (1) C 65- H 67	1.62	0.88	0.034
99. BD (2) C 49- C 56	206. BD* (1) C 65- H 68	1.87	0.86	0.036
99. BD (2) C 49- C 56	330. RY (3) C 50	0.78	1.01	0.025
99. BD (2) C 49- C 56	343. RY (3) C 54	1.59	0.87	0.033
100. BD (1) C 49- B 69	139. BD* (1) C 12- C 13	0.99	1.09	0.029
100. BD (1) C 49- B 69	140. BD* (2) C 12- C 13	1.40	0.55	0.025
100. BD (1) C 49- B 69	160. BD* (2) C 29- C 30	0.94	0.56	0.020
100. BD (1) C 49- B 69	161. BD* (1) C 29- C 36	1.33	1.09	0.034
100. BD (1) C 49- B 69	183. BD* (1) C 49- C 50	3.93	1.09	0.058
100. BD (1) C 49- B 69	184. BD* (1) C 49- C 56	4.11	1.09	0.060
100. BD (1) C 49- B 69	187. BD* (1) C 50- C 51	3.66	1.11	0.057
100. BD (1) C 49- B 69	196. BD* (1) C 54- C 56	3.54	1.11	0.056
100. BD (1) C 49- B 69	328. RY (1) C 50	1.84	1.72	0.050
100. BD (1) C 49- B 69	346. RY (1) C 56	1.73	1.74	0.049
101. BD (1) C 50- C 51	183. BD* (1) C 49- C 50	3.81	1.25	0.062
101. BD (1) C 50- C 51	186. BD* (1) C 49- B 69	2.93	1.14	0.052
101. BD (1) C 50- C 51	189. BD* (1) C 50- C 57	1.26	1.09	0.033
101. BD (1) C 50- C 51	190. BD* (1) C 51- H 52	3.79	1.40	0.065
101. BD (1) C 50- C 51	191. BD* (1) C 51- C 53	4.44	1.28	0.067
101. BD (1) C 50- C 51	194. BD* (1) C 53- C 61	3.28	1.08	0.053
101. BD (1) C 50- C 51	324. RY (1) C 49	0.90	1.92	0.037
101. BD (1) C 50- C 51	325. RY (2) C 49	0.63	1.71	0.029
101. BD (1) C 50- C 51	337. RY (1) C 53	0.92	1.87	0.037
101. BD (1) C 50- C 51	338. RY (2) C 53	1.78	1.56	0.047
101. BD (1) C 50- C 51	350. RY (1) C 57	0.52	1.42	0.024
102. BD (2) C 50- C 51	185. BD* (2) C 49- C 56	16.35	0.29	0.061
102. BD (2) C 50- C 51	193. BD* (2) C 53- C 54	25.03	0.28	0.075
102. BD (2) C 50- C 51	198. BD* (1) C 57- H 58	2.53	0.89	0.042
102. BD (2) C 50- C 51	199. BD* (1) C 57- H 59	2.04	0.89	0.038
102. BD (2) C 50- C 51	339. RY (3) C 53	0.87	0.94	0.026
103. BD (1) C 50- C 57	183. BD* (1) C 49- C 50	2.10	1.16	0.044
103. BD (1) C 50- C 57	184. BD* (1) C 49- C 56	2.75	1.17	0.051
103. BD (1) C 50- C 57	187. BD* (1) C 50- C 51	1.70	1.19	0.040
103. BD (1) C 50- C 57	191. BD* (1) C 51- C 53	2.93	1.20	0.053
103. BD (1) C 50- C 57	198. BD* (1) C 57- H 58	2.21	1.24	0.047
103. BD (1) C 50- C 57	199. BD* (1) C 57- H 59	2.05	1.24	0.045
103. BD (1) C 50- C 57	200. BD* (1) C 57- H 60	1.96	1.23	0.044
103. BD (1) C 50- C 57	324. RY (1) C 49	1.02	1.83	0.038
103. BD (1) C 50- C 57	332. RY (1) C 51	0.69	1.71	0.031
104. BD (1) C 51- H 52	183. BD* (1) C 49- C 50	4.09	1.14	0.061
104. BD (1) C 51- H 52	187. BD* (1) C 50- C 51	2.13	1.16	0.044
104. BD (1) C 51- H 52	191. BD* (1) C 51- C 53	1.95	1.17	0.043
104. BD (1) C 51- H 52	192. BD* (1) C 53- C 54	3.70	1.18	0.059
104. BD (1) C 51- H 52	328. RY (1) C 50	1.17	1.78	0.041
104. BD (1) C 51- H 52	337. RY (1) C 53	1.33	1.76	0.043
105. BD (1) C 51- C 53	187. BD* (1) C 50- C 51	4.22	1.28	0.066
105. BD (1) C 51- C 53	189. BD* (1) C 50- C 57	2.63	1.10	0.048
105. BD (1) C 51- C 53	190. BD* (1) C 51- H 52	3.63	1.41	0.064
105. BD (1) C 51- C 53	192. BD* (1) C 53- C 54	3.65	1.30	0.062
105. BD (1) C 51- C 53	194. BD* (1) C 53- C 61	1.46	1.09	0.036
105. BD (1) C 51- C 53	195. BD* (1) C 54- H 55	2.29	1.41	0.051
105. BD (1) C 51- C 53	328. RY (1) C 50	1.09	1.89	0.041
105. BD (1) C 51- C 53	329. RY (2) C 50	2.07	1.63	0.052
105. BD (1) C 51- C 53	341. RY (1) C 54	0.58	1.81	0.029
105. BD (1) C 51- C 53	342. RY (2) C 54	0.54	1.46	0.025
105. BD (1) C 51- C 53	357. RY (1) C 61	0.61	1.30	0.025
106. BD (1) C 53- C 54	190. BD* (1) C 51- H 52	2.27	1.41	0.050
106. BD (1) C 53- C 54	191. BD* (1) C 51- C 53	3.71	1.29	0.062
106. BD (1) C 53- C 54	194. BD* (1) C 53- C 61	1.49	1.09	0.036
106. BD (1) C 53- C 54	195. BD* (1) C 54- H 55	3.76	1.41	0.065
106. BD (1) C 53- C 54	196. BD* (1) C 54- C 56	4.20	1.28	0.065
106. BD (1) C 53- C 54	197. BD* (1) C 56- C 65	2.52	1.10	0.047
106. BD (1) C 53- C 54	332. RY (1) C 51	0.59	1.81	0.029
106. BD (1) C 53- C 54	346. RY (1) C 56	1.39	1.91	0.046
106. BD (1) C 53- C 54	347. RY (2) C 56	1.92	1.61	0.050

106. BD (1) C 53- C 54	357. RY (1) C 61	0.53	1.31	0.023
107. BD (2) C 53- C 54	185. BD* (2) C 49- C 56	22.92	0.29	0.073
107. BD (2) C 53- C 54	188. BD* (2) C 50- C 51	17.60	0.29	0.063
107. BD (2) C 53- C 54	201. BD* (1) C 61- H 62	2.73	0.87	0.043
107. BD (2) C 53- C 54	203. BD* (1) C 61- H 64	1.72	0.87	0.035
107. BD (2) C 53- C 54	334. RY (3) C 51	1.53	0.89	0.033
107. BD (2) C 53- C 54	348. RY (3) C 56	0.88	0.99	0.026
108. BD (1) C 53- C 61	187. BD* (1) C 50- C 51	2.75	1.20	0.051
108. BD (1) C 53- C 61	191. BD* (1) C 51- C 53	1.92	1.21	0.043
108. BD (1) C 53- C 61	192. BD* (1) C 53- C 54	1.96	1.22	0.044
108. BD (1) C 53- C 61	196. BD* (1) C 54- C 56	2.83	1.19	0.052
108. BD (1) C 53- C 61	201. BD* (1) C 61- H 62	1.98	1.23	0.044
108. BD (1) C 53- C 61	202. BD* (1) C 61- H 63	1.82	1.23	0.042
108. BD (1) C 53- C 61	203. BD* (1) C 61- H 64	1.87	1.23	0.043
108. BD (1) C 53- C 61	332. RY (1) C 51	0.74	1.72	0.032
108. BD (1) C 53- C 61	341. RY (1) C 54	0.75	1.73	0.032
109. BD (1) C 54- H 55	184. BD* (1) C 49- C 56	4.05	1.14	0.061
109. BD (1) C 54- H 55	191. BD* (1) C 51- C 53	3.78	1.17	0.059
109. BD (1) C 54- H 55	192. BD* (1) C 53- C 54	2.02	1.18	0.044
109. BD (1) C 54- H 55	196. BD* (1) C 54- C 56	2.09	1.16	0.044
109. BD (1) C 54- H 55	337. RY (1) C 53	1.30	1.76	0.043
109. BD (1) C 54- H 55	346. RY (1) C 56	1.09	1.79	0.039
110. BD (1) C 54- C 56	184. BD* (1) C 49- C 56	4.00	1.25	0.063
110. BD (1) C 54- C 56	186. BD* (1) C 49- B 69	3.02	1.14	0.052
110. BD (1) C 54- C 56	192. BD* (1) C 53- C 54	4.37	1.29	0.067
110. BD (1) C 54- C 56	194. BD* (1) C 53- C 61	3.30	1.08	0.053
110. BD (1) C 54- C 56	195. BD* (1) C 54- H 55	3.80	1.40	0.065
110. BD (1) C 54- C 56	197. BD* (1) C 56- C 65	1.17	1.09	0.032
110. BD (1) C 54- C 56	324. RY (1) C 49	1.07	1.91	0.040
110. BD (1) C 54- C 56	337. RY (1) C 53	1.14	1.87	0.041
110. BD (1) C 54- C 56	338. RY (2) C 53	1.85	1.56	0.048
110. BD (1) C 54- C 56	364. RY (1) C 65	0.53	1.40	0.024
111. BD (1) C 56- C 65	183. BD* (1) C 49- C 50	2.73	1.17	0.050
111. BD (1) C 56- C 65	184. BD* (1) C 49- C 56	2.16	1.17	0.045
111. BD (1) C 56- C 65	192. BD* (1) C 53- C 54	2.95	1.21	0.053
111. BD (1) C 56- C 65	196. BD* (1) C 54- C 56	1.63	1.19	0.039
111. BD (1) C 56- C 65	204. BD* (1) C 65- H 66	1.94	1.23	0.044
111. BD (1) C 56- C 65	205. BD* (1) C 65- H 67	2.11	1.24	0.046
111. BD (1) C 56- C 65	206. BD* (1) C 65- H 68	2.00	1.23	0.044
111. BD (1) C 56- C 65	324. RY (1) C 49	1.06	1.83	0.039
111. BD (1) C 56- C 65	341. RY (1) C 54	0.76	1.72	0.032
112. BD (1) C 57- H 58	187. BD* (1) C 50- C 51	1.17	1.13	0.032
112. BD (1) C 57- H 58	188. BD* (2) C 50- C 51	3.83	0.57	0.042
112. BD (1) C 57- H 58	189. BD* (1) C 50- C 57	1.14	0.95	0.029
112. BD (1) C 57- H 58	199. BD* (1) C 57- H 59	1.47	1.18	0.037
112. BD (1) C 57- H 58	200. BD* (1) C 57- H 60	1.57	1.17	0.038
112. BD (1) C 57- H 58	330. RY (3) C 50	0.78	1.31	0.029
113. BD (1) C 57- H 59	122. LV (1) B 69	0.62	0.56	0.017
113. BD (1) C 57- H 59	187. BD* (1) C 50- C 51	1.79	1.13	0.040
113. BD (1) C 57- H 59	188. BD* (2) C 50- C 51	3.25	0.58	0.039
113. BD (1) C 57- H 59	189. BD* (1) C 50- C 57	1.14	0.95	0.029
113. BD (1) C 57- H 59	198. BD* (1) C 57- H 58	1.52	1.18	0.038
113. BD (1) C 57- H 59	200. BD* (1) C 57- H 60	1.56	1.17	0.038
114. BD (1) C 57- H 60	183. BD* (1) C 49- C 50	4.11	1.11	0.060
114. BD (1) C 57- H 60	189. BD* (1) C 50- C 57	1.08	0.95	0.029
114. BD (1) C 57- H 60	198. BD* (1) C 57- H 58	1.71	1.18	0.040
114. BD (1) C 57- H 60	199. BD* (1) C 57- H 59	1.71	1.19	0.040
115. BD (1) C 61- H 62	192. BD* (1) C 53- C 54	1.05	1.16	0.031
115. BD (1) C 61- H 62	193. BD* (2) C 53- C 54	4.26	0.59	0.045
115. BD (1) C 61- H 62	194. BD* (1) C 53- C 61	1.05	0.95	0.028
115. BD (1) C 61- H 62	202. BD* (1) C 61- H 63	1.38	1.17	0.036
115. BD (1) C 61- H 62	203. BD* (1) C 61- H 64	1.31	1.17	0.035
115. BD (1) C 61- H 62	339. RY (3) C 53	0.87	1.24	0.029
116. BD (1) C 61- H 63	191. BD* (1) C 51- C 53	3.72	1.15	0.058
116. BD (1) C 61- H 63	194. BD* (1) C 53- C 61	1.01	0.95	0.028
116. BD (1) C 61- H 63	201. BD* (1) C 61- H 62	1.49	1.17	0.037
116. BD (1) C 61- H 63	203. BD* (1) C 61- H 64	1.53	1.17	0.038
117. BD (1) C 61- H 64	192. BD* (1) C 53- C 54	2.41	1.16	0.047
117. BD (1) C 61- H 64	193. BD* (2) C 53- C 54	2.50	0.59	0.034
117. BD (1) C 61- H 64	194. BD* (1) C 53- C 61	1.04	0.95	0.028
117. BD (1) C 61- H 64	201. BD* (1) C 61- H 62	1.37	1.17	0.036
117. BD (1) C 61- H 64	202. BD* (1) C 61- H 63	1.48	1.17	0.037
118. BD (1) C 65- H 66	184. BD* (1) C 49- C 56	4.27	1.11	0.062
118. BD (1) C 65- H 66	197. BD* (1) C 56- C 65	1.07	0.95	0.029
118. BD (1) C 65- H 66	205. BD* (1) C 65- H 67	1.69	1.19	0.040
118. BD (1) C 65- H 66	206. BD* (1) C 65- H 68	1.63	1.17	0.039
119. BD (1) C 65- H 67	185. BD* (2) C 49- C 56	3.33	0.58	0.039

119. BD (1) C 65- H 67	196. BD* (1) C 54- C 56	1.57	1.13	0.038
119. BD (1) C 65- H 67	197. BD* (1) C 56- C 65	1.13	0.95	0.029
119. BD (1) C 65- H 67	204. BD* (1) C 65- H 66	1.59	1.17	0.038
119. BD (1) C 65- H 67	206. BD* (1) C 65- H 68	1.47	1.17	0.037
119. BD (1) C 65- H 67	348. RY (3) C 56	0.57	1.28	0.024
120. BD (1) C 65- H 68	185. BD* (2) C 49- C 56	3.50	0.58	0.040
120. BD (1) C 65- H 68	196. BD* (1) C 54- C 56	1.34	1.13	0.035
120. BD (1) C 65- H 68	197. BD* (1) C 56- C 65	1.07	0.95	0.028
120. BD (1) C 65- H 68	204. BD* (1) C 65- H 66	1.48	1.17	0.037
120. BD (1) C 65- H 68	205. BD* (1) C 65- H 67	1.43	1.18	0.037
120. BD (1) C 65- H 68	348. RY (3) C 56	0.68	1.28	0.026

Atom		1	2	3	4	5	6	7	8	9
1.	B	0.0000	0.0178	0.8764	0.0036	0.0078	0.0047	0.0000	0.0413	0.0017
2.	C	0.0178	0.0000	1.2176	1.2580	1.2498	0.0106	0.0071	0.0098	0.0079
3.	C	0.8764	1.2176	0.0000	0.0112	0.0106	0.0325	0.0001	1.4944	0.0080
4.	C	0.0036	1.2580	0.0112	0.0000	0.0098	1.4979	0.0057	0.0307	0.0001
5.	C	0.0078	1.2498	0.0106	0.0098	0.0000	0.0649	0.0003	0.0580	0.0002
6.	C	0.0047	0.0106	0.0325	1.4979	0.0649	0.0000	0.9267	0.0002	0.0002
7.	H	0.0000	0.0071	0.0001	0.0057	0.0003	0.9267	0.0000	0.0002	0.0000
8.	C	0.0413	0.0098	1.4944	0.0307	0.0580	0.0002	0.0002	0.0000	0.9250
9.	H	0.0017	0.0079	0.0080	0.0001	0.0002	0.0002	0.0000	0.9250	0.0000
10.	C	0.0011	0.0073	0.0003	0.0089	0.0003	0.0073	0.0003	0.0005	0.0000
11.	H	0.0033	0.0002	0.0001	0.0005	0.0000	0.0005	0.0004	0.0003	0.0000
12.	H	0.0004	0.0003	0.0001	0.0069	0.0001	0.0013	0.0001	0.0002	0.0000
13.	H	0.0002	0.0001	0.0000	0.0006	0.0000	0.0001	0.0000	0.0000	0.0000
14.	C	0.0093	0.0097	0.1068	0.0077	1.2578	0.0004	0.0002	0.0109	0.0059
15.	H	0.0004	0.0071	0.0002	0.0001	0.0050	0.0000	0.0000	0.0085	0.0002
16.	C	0.0012	0.0091	0.0097	0.1098	1.2677	0.0116	0.0064	0.0005	0.0003
17.	H	0.0002	0.0070	0.0002	0.0002	0.0051	0.0084	0.0001	0.0001	0.0000
18.	C	0.0007	0.0077	0.0002	0.0083	0.0003	0.0073	0.0004	0.0007	0.0000
19.	H	0.0001	0.0002	0.0000	0.0007	0.0000	0.0001	0.0000	0.0000	0.0000
20.	H	0.0006	0.0005	0.0001	0.0066	0.0001	0.0012	0.0001	0.0000	0.0000
21.	H	0.0027	0.0003	0.0001	0.0004	0.0000	0.0006	0.0004	0.0001	0.0000
22.	C	0.0011	0.0637	0.0004	0.0136	0.0115	1.3087	0.0055	0.0266	0.0000
23.	H	0.0001	0.0001	0.0003	0.0060	0.0081	0.0049	0.0014	0.0000	0.0000
24.	C	0.0095	0.0593	0.0123	0.0004	0.0119	0.0304	0.0000	1.2950	0.0043
25.	H	0.0003	0.0001	0.0061	0.0003	0.0080	0.0000	0.0000	0.0046	0.0013
26.	N	0.0909	0.0181	0.0041	0.9795	0.0070	0.0202	0.0045	0.0042	0.0004
27.	C	0.8825	0.0039	0.0066	0.0002	0.0001	0.0008	0.0000	0.0099	0.0005
28.	C	0.0245	0.0004	0.0057	0.0002	0.0002	0.0002	0.0000	0.0015	0.0001
29.	C	0.0276	0.0004	0.0034	0.0002	0.0002	0.0003	0.0000	0.0010	0.0001
30.	C	0.0101	0.0002	0.0001	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000
31.	H	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
32.	C	0.0092	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
33.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0100	0.0002	0.0013	0.0001	0.0001	0.0002	0.0000	0.0005	0.0000
35.	C	0.0018	0.0005	0.0013	0.0004	0.0004	0.0002	0.0000	0.0011	0.0000
36.										

46.	H	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	C	0.8768	0.0053	0.0083	0.0004	0.0001	0.0006	0.0000	0.0073	0.0007
48.	C	0.0263	0.0007	0.0065	0.0001	0.0002	0.0001	0.0000	0.0015	0.0004
49.	C	0.0250	0.0004	0.0046	0.0001	0.0002	0.0001	0.0000	0.0019	0.0001
50.	C	0.0090	0.0001	0.0003	0.0000	0.0001	0.0000	0.0000	0.0002	0.0000
51.	H	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	C	0.0100	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
53.	H	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
54.	C	0.0101	0.0003	0.0018	0.0000	0.0001	0.0000	0.0000	0.0006	0.0000
55.	C	0.0031	0.0007	0.0007	0.0001	0.0000	0.0001	0.0000	0.0019	0.0000
56.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
57.	H	0.0015	0.0003	0.0023	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
58.	H	0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
59.	C	0.0032	0.0001	0.0006	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
60.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
62.	H	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	C	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	Atom	10	11	12	13	14	15	16	17	18
1.	B	0.0011	0.0033	0.0004	0.0002	0.0093	0.0004	0.0012	0.0002	0.0007
2.	C	0.0073	0.0002	0.0003	0.0001	0.0097	0.0071	0.0091	0.0070	0.0077
3.	C	0.0003	0.0001	0.0001	0.0000	0.1068	0.0002	0.0097	0.0002	0.0002
4.	C	0.0089	0.0005	0.0069	0.0006	0.0077	0.0001	0.1098	0.0002	0.0083
5.	C	0.0003	0.0000	0.0001	0.0000	1.2578	0.0050	1.2677	0.0051	0.0003
6.	C	0.0073	0.0005	0.0013	0.0001	0.0004	0.0000	0.0116	0.0084	0.0073
7.	H	0.0003	0.0004	0.0001	0.0000	0.0002	0.0000	0.0064	0.0001	0.0004
8.	C	0.0005	0.0003	0.0002	0.0000	0.0109	0.0085	0.0005	0.0001	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0059	0.0002	0.0003	0.0000	0.0000
10.	C	0.0000	0.9401	0.9318	0.9282	0.0001	0.0000	0.0030	0.0000	0.0087
11.	H	0.9401	0.0000	0.0018	0.0020	0.0001	0.0000	0.0000	0.0000	0.0003
12.	H	0.9318	0.0018	0.0000	0.0031	0.0001	0.0000	0.0006	0.0000	0.0005
13.	H	0.9282	0.0020	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0077
14.	C	0.0001	0.0001	0.0001	0.0000	0.0000	0.9282	0.0096	0.0012	0.0002
15.	H	0.0000	0.0000	0.0000	0.0000	0.9282	0.0000	0.0013	0.0002	0.0000
16.	C	0.0030	0.0000	0.0006	0.0000	0.0096	0.0013	0.0000	0.9285	0.0029
17.	H	0.0000	0.0000	0.0000	0.0000	0.0012	0.0002	0.9285	0.0000	0.0000
18.	C	0.0087	0.0003	0.0005	0.0077	0.0002	0.0000	0.0029	0.0000	0.0000
19.	H	0.0078	0.0000	0.0002	0.0004	0.0000	0.0000	0.0000	0.0000	0.9348
20.	H	0.0004	0.0002	0.0001	0.0001	0.0000	0.0000	0.0005	0.0000	0.9338
21.	H	0.0004	0.0014	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.9377
22.	C	0.0004	0.0001	0.0001	0.0000	0.0313	0.0002	1.5374	0.0062	0.0004
23.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0062	0.0018	0.0000
24.	C	0.0001	0.0000	0.0000	0.0000	1.5487	0.0065	0.0370	0.0002	0.0001
25.	H	0.0000	0.0000	0.0000	0.0000	0.0059	0.0018	0.0001	0.0000	0.0000
26.	N	0.9557	0.0185	0.0051	0.0032	0.0015	0.0003	0.0010	0.0004	0.9598
27.	C	0.0020	0.0008	0.0003	0.0007	0.0031	0.0000	0.0002	0.0000	0.0002
28.	C	0.0017	0.0002	0.0012	0.0003	0.0005	0.0000	0.0001	0.0000	0.0001
29.	C	0.0005	0.0001	0.0001	0.0011	0.0003	0.0000	0.0001	0.0000	0.0002
30.	C	0.0007	0.0000	0.0002	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	C	0.0007	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0003	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001
35.	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000

[illegible]

Atom		19	20	21	22	23	24	25	26	27
1.	B	0.0001	0.0006	0.0027	0.0011	0.0001	0.0095	0.0003	0.0909	0.8825
2.	C	0.0002	0.0005	0.0003	0.0637	0.0001	0.0593	0.0001	0.0181	0.0039
3.	C	0.0000	0.0001	0.0001	0.0004	0.0003	0.0123	0.0061	0.0041	0.0066
4.	C	0.0007	0.0066	0.0004	0.0136	0.0060	0.0004	0.0003	0.9795	0.0002
5.	C	0.0000	0.0001	0.0000	0.0115	0.0081	0.0119	0.0080	0.0070	0.0001
6.	C	0.0001	0.0012	0.0006	1.3087	0.0049	0.0304	0.0000	0.0202	0.0008
7.	H	0.0000	0.0001	0.0004	0.0055	0.0014	0.0000	0.0000	0.0045	0.0000
8.	C	0.0000	0.0000	0.0001	0.0266	0.0000	1.2950	0.0046	0.0042	0.0099
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043	0.0013	0.0004	0.0000
10.	C	0.0078	0.0004	0.0004	0.0004	0.0000	0.0001	0.0000	0.9557	0.0020
11.	H	0.0000	0.0002	0.0014	0.0001	0.0000	0.0000	0.0000	0.0185	0.0008
12.	H	0.0002	0.0001	0.0003	0.0001	0.0000	0.0000	0.0000	0.0051	0.0003
13.	H	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0032	0.0007
14.	C	0.0000	0.0000	0.0000	0.0313	0.0001	1.5487	0.0059	0.0015	0.0031
15.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.0065	0.0018	0.0003	0.0000
16.	C	0.0000	0.0005	0.0000	1.5374	0.0062	0.0370	0.0001	0.0010	0.0002
17.	H	0.0000	0.0000	0.0000	0.0062	0.0018	0.0002	0.0000	0.0004	0.0000
18.	C	0.9348	0.9338	0.9377	0.0004	0.0000	0.0001	0.0000	0.9598	0.0002
19.	H	0.0000	0.0027	0.0020	0.0000	0.0000	0.0000	0.0000	0.0027	0.0000
20.	H	0.0027	0.0000	0.0017	0.0001	0.0000	0.0000	0.0000	0.0060	0.0000
21.	H	0.0020	0.0017	0.0000	0.0001	0.0000	0.0000	0.0000	0.0212	0.0001
22.	C	0.0000	0.0001	0.0001	0.0000	0.9286	0.0001	0.0002	0.0091	0.0000
23.	H	0.0000	0.0000	0.0000	0.9286	0.0000	0.0002	0.0000	0.0007	0.0000
24.	C	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.9301	0.0004	0.0002
25.	H	0.0000	0.0000	0.0000	0.0002	0.0000	0.9301	0.0000	0.0001	0.0001
26.	N	0.0027	0.0060	0.0212	0.0091	0.0007	0.0004	0.0001	0.0000	0.0037
27.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002	0.0001	0.0037	0.0000
28.	C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0002	0.0000	0.0043	1.3480
29.	C	0.0000	0.0001	0.0003	0.0001	0.0000	0.0002	0.0000	0.0074	1.3641
30.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0110
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0074
32.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0114
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0073
34.	C	0.0000	0.0001	0.0002	0.0001	0.0000	0.0001	0.0000	0.0042	0.1006
35.	C	0.0000	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0001	0.0102
36.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0061
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0041
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0060
39.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0101
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0063
41.	H	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0017	0.0032
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0065
43.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0031
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0025
47.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0009	0.0070
48.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0019	0.0041
49.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0012	0.0057
50.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
52.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0008	0.0014
55.	C	0.0003	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0007	0.0005
56.	H	0.0002	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
57.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
59.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0017
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003

[illegible]

Atom		28	29	30	31	32	33	34	35	36
1.	B	0.0245	0.0276	0.0101	0.0003	0.0092	0.0002	0.0100	0.0018	0.0001
2.	C	0.0004	0.0004	0.0002	0.0000	0.0001	0.0000	0.0002	0.0005	0.0001
3.	C	0.0057	0.0034	0.0001	0.0001	0.0002	0.0000	0.0013	0.0013	0.0003
4.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0004	0.0000
5.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0004	0.0000
6.	C	0.0002	0.0003	0.0001	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0015	0.0010	0.0004	0.0001	0.0001	0.0000	0.0005	0.0011	0.0004
9.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0017	0.0005	0.0007	0.0000	0.0007	0.0000	0.0003	0.0000	0.0000
11.	H	0.0002	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
12.	H	0.0012	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	H	0.0003	0.0011	0.0001	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000
14.	C	0.0005	0.0003	0.0002	0.0000	0.0000	0.0000	0.0002	0.0003	0.0000
15.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
21.	H	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
22.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	N	0.0043	0.0074	0.0003	0.0000	0.0001	0.0000	0.0042	0.0001	0.0001
27.	C	1.3480	1.3641	0.0110	0.0074	0.0114	0.0073	0.1006	0.0102	0.0061
28.	C	0.0000	0.0113	1.4224	0.0064	0.0996	0.0003	0.0141	0.0086	0.0001
29.	C	0.0113	0.0000	0.1000	0.0003	1.3996	0.0063	0.0138	1.0154	0.0039
30.	C	1.4224	0.1000	0.0000	0.9281	0.0114	0.0079	1.3861	0.0013	0.0035
31.	H	0.0064	0.0003	0.9281	0.0000	0.0079	0.0002	0.0060	0.0004	0.0000
32.	C	0.0996	1.3996	0.0114	0.0079	0.0000	0.9284	1.4057	0.0084	0.0093
33.	H	0.0003	0.0063	0.0079	0.0002	0.9284	0.0000	0.0060	0.0021	0.0000
34.	C	0.0141	0.0138	1.3861	0.0060	1.4057	0.0060	0.0000	0.0076	0.0001
35.	C	0.0086	1.0154	0.0013	0.0004	0.0084	0.0021	0.0076	0.0000	0.9207
36.	H	0.0001	0.0039	0.0035	0.0000	0.0093	0.0000	0.0001	0.9207	0.0000
37.	H	0.0001	0.0040	0.0025	0.0000	0.0085	0.0001	0.0002	0.9181	0.0025
38.	H	0.0001	0.0033	0.0001	0.0000	0.0018	0.0002	0.0003	0.9352	0.0025
39.	C	1.0135	0.0085	0.0083	0.0021	0.0014	0.0004	0.0078	0.0005	0.0000
40.	H	0.0033	0.0002	0.0020	0.0002	0.0003	0.0000	0.0003	0.0002	0.0000
41.	H	0.0036	0.0001	0.0080	0.0001	0.0019	0.0000	0.0001	0.0000	0.0000
42.	H	0.0042	0.0001	0.0091	0.0000	0.0036	0.0000	0.0001	0.0000	0.0000
43.	C	0.0088	0.0081	0.0098	0.0021	0.0092	0.0021	1.0139	0.0004	0.0001
44.	H	0.0001	0.0003	0.0059	0.0001	0.0016	0.0002	0.0033	0.0001	0.0000
45.	H	0.0001	0.0001	0.0049	0.0000	0.0094	0.0000	0.0040	0.0001	0.0000
46.	H	0.0001	0.0001	0.0039	0.0000	0.0092	0.0000	0.0038	0.0001	0.0000
47.	C	0.0043	0.0062	0.0002	0.0000	0.0001	0.0001	0.0016	0.0003	0.0002
48.	C	0.0007	0.0007	0.0002	0.0000	0.0002	0.0000	0.0003	0.0001	0.0000
49.	C	0.0007	0.0011	0.0001	0.0000	0.0002	0.0000	0.0003	0.0001	0.0000
50.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
51.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	C	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	C	0.0002	0.0003	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
55.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	C	0.0007	0.0005	0.0003	0.0000	0.0001	0.0000	0.0002	0.0005	0.0001
60.	H	0.0003	0.0003	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
61.	H	0.0002	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0002	0.0004
62.	H	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
63.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Atom		37	38	39	40	41	42	43	44	45

1.	B	0.0005	0.0001	0.0032	0.0002	0.0012	0.0004	0.0007	0.0000	0.0003
2.	C	0.0008	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0012	0.0002	0.0006	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000
4.	C	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
5.	C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0005	0.0004	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0001	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0003	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
22.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	N	0.0001	0.0000	0.0012	0.0001	0.0017	0.0001	0.0000	0.0000	0.0002
27.	C	0.0041	0.0060	0.0101	0.0063	0.0032	0.0065	0.0011	0.0001	0.0031
28.	C	0.0001	0.0001	1.0135	0.0033	0.0036	0.0042	0.0088	0.0001	0.0001
29.	C	0.0040	0.0033	0.0085	0.0002	0.0001	0.0001	0.0081	0.0003	0.0001
30.	C	0.0025	0.0001	0.0083	0.0020	0.0080	0.0091	0.0098	0.0059	0.0049
31.	H	0.0000	0.0000	0.0021	0.0002	0.0001	0.0000	0.0021	0.0001	0.0000
32.	C	0.0085	0.0018	0.0014	0.0003	0.0019	0.0036	0.0092	0.0016	0.0094
33.	H	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000	0.0021	0.0002	0.0000
34.	C	0.0002	0.0003	0.0078	0.0003	0.0001	0.0001	1.0139	0.0033	0.0040
35.	C	0.9181	0.9352	0.0005	0.0002	0.0000	0.0000	0.0004	0.0001	0.0001
36.	H	0.0025	0.0025	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
37.	H	0.0000	0.0027	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
38.	H	0.0027	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
39.	C	0.0000	0.0002	0.0000	0.9344	0.9243	0.9129	0.0005	0.0002	0.0000
40.	H	0.0000	0.0000	0.9344	0.0000	0.0025	0.0026	0.0001	0.0000	0.0000
41.	H	0.0000	0.0000	0.9243	0.0025	0.0000	0.0025	0.0001	0.0000	0.0000
42.	H	0.0000	0.0000	0.9129	0.0026	0.0025	0.0000	0.0001	0.0000	0.0000
43.	C	0.0001	0.0001	0.0005	0.0001	0.0001	0.0001	0.0000	0.9356	0.9226
44.	H	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.9356	0.0000	0.0024
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9226	0.0024	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9243	0.0023	0.0023
47.	C	0.0000	0.0000	0.0017	0.0003	0.0003	0.0007	0.0000	0.0000	0.0001
48.	C	0.0000	0.0000	0.0007	0.0003	0.0002	0.0002	0.0000	0.0000	0.0000
49.	C	0.0000	0.0000	0.0005	0.0003	0.0001	0.0001	0.0000	0.0000	0.0000
50.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	C	0.0000	0.0000	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	C	0.0000	0.0000	0.0002	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000
55.	C	0.0000	0.0000	0.0004	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0001	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	Atom	46	47	48	49	50	51	52	53	54
1.	B	0.0003	0.8768	0.0263	0.0250	0.0090	0.0002	0.0100	0.0004	0.0101
2.	C	0.0000	0.0053	0.0007	0.0004	0.0001	0.0000	0.0002	0.0000	0.0003
3.	C	0.0000	0.0083	0.0065	0.0046	0.0003	0.0000	0.0002	0.0001	0.0018
4.	C	0.0000	0.0004	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0001	0.0002	0.0002	0.0001	0.0000	0.0000	0.0000	0.0001
6.	C	0.0000	0.0006	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
7.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0073	0.0015	0.0019	0.0002	0.0000	0.0004	0.0001	0.0006

[illegible]

17.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0007	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	H	0.0003	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	H	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	N	0.0007	0.0001	0.0001	0.0003	0.0001	0.0000	0.0000	0.0001	0.0000
27.	C	0.0005	0.0001	0.0001	0.0000	0.0017	0.0004	0.0003	0.0005	0.0000
28.	C	0.0001	0.0000	0.0000	0.0000	0.0007	0.0003	0.0002	0.0002	0.0000
29.	C	0.0001	0.0000	0.0000	0.0000	0.0005	0.0003	0.0001	0.0002	0.0000
30.	C	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000	0.0002	0.0000
31.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0000	0.0002	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000	0.0002	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	C	0.0004	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	C	0.0096	0.0067	0.0036	0.0064	0.0101	0.0061	0.0033	0.0066	0.0011
48.	C	0.0084	0.0001	0.0002	0.0002	1.0129	0.0033	0.0034	0.0042	0.0080
49.	C	1.0153	0.0042	0.0040	0.0034	0.0088	0.0002	0.0001	0.0001	0.0089
50.	C	0.0086	0.0094	0.0083	0.0018	0.0014	0.0002	0.0020	0.0037	0.0099
51.	H	0.0021	0.0000	0.0001	0.0002	0.0004	0.0000	0.0000	0.0000	0.0021
52.	C	0.0012	0.0038	0.0020	0.0002	0.0082	0.0019	0.0082	0.0088	0.0087
53.	H	0.0004	0.0000	0.0000	0.0000	0.0021	0.0002	0.0001	0.0000	0.0021
54.	C	0.0077	0.0001	0.0002	0.0003	0.0080	0.0003	0.0001	0.0001	1.0137
55.	C	0.0000	0.9206	0.9173	0.9343	0.0005	0.0002	0.0000	0.0000	0.0005
56.	H	0.9206	0.0000	0.0024	0.0025	0.0000	0.0000	0.0000	0.0000	0.0001
57.	H	0.9173	0.0024	0.0000	0.0027	0.0000	0.0000	0.0000	0.0000	0.0001
58.	H	0.9343	0.0025	0.0027	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001
59.	C	0.0005	0.0000	0.0000	0.0002	0.0000	0.9344	0.9270	0.9143	0.0004
60.	H	0.0002	0.0000	0.0000	0.0000	0.9344	0.0000	0.0025	0.0026	0.0001
61.	H	0.0000	0.0000	0.0000	0.0000	0.9270	0.0025	0.0000	0.0025	0.0001
62.	H	0.0000	0.0000	0.0000	0.0000	0.9143	0.0026	0.0025	0.0000	0.0000
63.	C	0.0005	0.0001	0.0001	0.0001	0.0004	0.0001	0.0001	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.9224
65.	H	0.0002	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.9360
66.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.9249

	Atom	64	65	66
1.	B	0.0004	0.0000	0.0003
2.	C	0.0000	0.0000	0.0000
3.	C	0.0001	0.0000	0.0001
4.	C	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000
6.	C	0.0000	0.0000	0.0000
7.	H	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000
9.	H	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000
11.	H	0.0000	0.0000	0.0000
12.	H	0.0000	0.0000	0.0000
13.	H	0.0000	0.0000	0.0000
14.	C	0.0000	0.0000	0.0000
15.	H	0.0000	0.0000	0.0000
16.	C	0.0000	0.0000	0.0000
17.	H	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0000
19.	H	0.0000	0.0000	0.0000
20.	H	0.0000	0.0000	0.0000
21.	H	0.0000	0.0000	0.0000
22.	C	0.0000	0.0000	0.0000
23.	H	0.0000	0.0000	0.0000
24.	C	0.0000	0.0000	0.0000

25.	H	0.0000	0.0000	0.0000
26.	N	0.0000	0.0000	0.0000
27.	C	0.0000	0.0000	0.0000
28.	C	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	0.0000
30.	C	0.0000	0.0000	0.0000
31.	H	0.0000	0.0000	0.0000
32.	C	0.0000	0.0000	0.0000
33.	H	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000
36.	H	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000
39.	C	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000
43.	C	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000
47.	C	0.0031	0.0001	0.0026
48.	C	0.0001	0.0003	0.0002
49.	C	0.0001	0.0001	0.0001
50.	C	0.0050	0.0058	0.0040
51.	H	0.0000	0.0001	0.0000
52.	C	0.0092	0.0016	0.0090
53.	H	0.0000	0.0002	0.0000
54.	C	0.0040	0.0033	0.0038
55.	C	0.0000	0.0002	0.0000
56.	H	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000
59.	C	0.0001	0.0001	0.0001
60.	H	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000
63.	C	0.9224	0.9360	0.9249
64.	H	0.0000	0.0024	0.0024
65.	H	0.0024	0.0000	0.0023
66.	H	0.0024	0.0023	0.0000

(Occupancy)		Bond orbital / Coefficients / Hybrids			
		Lewis			
1.	(1.99906) CR (1) B 1	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
2.	(1.99884) CR (1) C 2	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
3.	(1.99865) CR (1) C 3	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
4.	(1.99886) CR (1) C 4	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
5.	(1.99900) CR (1) C 5	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
6.	(1.99898) CR (1) C 6	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
7.	(1.99903) CR (1) C 8	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
8.	(1.99913) CR (1) C 10	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
9.	(1.99903) CR (1) C 14	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
10.	(1.99904) CR (1) C 16	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000
11.	(1.99914) CR (1) C 18	s(100.00%)			
		1.0000	0.0000	0.0000	0.0000

12. (1.99910) CR (1) C 22	0.0000 0.0000 0.0000 0.0000 s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
13. (1.99909) CR (1) C 24	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
14. (1.99940) CR (1) N 26	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
15. (1.99854) CR (1) C 27	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
16. (1.99899) CR (1) C 28	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
17. (1.99898) CR (1) C 29	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
18. (1.99889) CR (1) C 30	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
19. (1.99889) CR (1) C 32	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
20. (1.99901) CR (1) C 34	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
21. (1.99915) CR (1) C 35	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
22. (1.99916) CR (1) C 39	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
23. (1.99915) CR (1) C 43	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
24. (1.99859) CR (1) C 47	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
25. (1.99897) CR (1) C 48	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
26. (1.99900) CR (1) C 49	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
27. (1.99890) CR (1) C 50	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
28. (1.99890) CR (1) C 52	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
29. (1.99902) CR (1) C 54	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
30. (1.99915) CR (1) C 55	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
31. (1.99916) CR (1) C 59	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
32. (1.99916) CR (1) C 63	s(100.00%) 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
33. (1.86136) LP (1) N 26	s(16.07%)p 5.22(83.93%) 0.0000 0.4009 -0.0003 -0.8373 0.0242 -0.0126 0.0029 -0.3705 0.0134
34. (1.95821) BD (1) B 1- C 3 (30.69%) 0.5540* B 1	s(33.07%)p 2.02(66.93%) 0.0000 0.5750 0.0070 0.6033 0.0087 -0.5268 -0.0098 -0.1660 -0.0069 (69.31%) 0.8325* C 3 s(35.88%)p 1.79(64.12%) 0.0000 0.5986 -0.0222 -0.5169 0.0386 0.5099 -0.0295 0.3338 -0.0139
35. (1.95588) BD (1) B 1- C 27 (31.31%) 0.5595* B 1	s(34.32%)p 1.91(65.68%) 0.0000 0.5858 0.0007 0.1329 0.0076

				0.7990	0.0103	-0.0236	0.0000	
	(68.69%)	0.8288*	C 27	s(34.52%)	p 1.90(65.48%)			
				0.0000	0.5871	-0.0224	-0.0835	0.0082
				-0.8032	0.0476	0.0207	-0.0019	
36.	(1.95589)	BD (1) B	1- C 47					
	(31.43%)	0.5606*	B 1	s(32.53%)	p 2.07(67.47%)			
				0.0000	0.5703	-0.0028	-0.7561	-0.0050
				-0.2882	-0.0011	0.1413	0.0040	
	(68.57%)	0.8281*	C 47	s(34.52%)	p 1.90(65.48%)			
				0.0000	0.5870	-0.0253	0.7478	-0.0469
				0.2972	-0.0181	-0.0684	0.0083	
37.	(1.96738)	BD (1) C	2- C 3					
	(50.60%)	0.7113*	C 2	s(34.15%)	p 1.93(65.85%)			
				0.0000	0.5844	-0.0032	-0.7678	0.0036
				0.0930	-0.0010	-0.2453	0.0093	
	(49.40%)	0.7029*	C 3	s(32.32%)	p 2.09(67.68%)			
				0.0000	0.5683	0.0142	0.7800	0.0147
				-0.0453	-0.0074	0.2569	0.0094	
38.	(1.97225)	BD (1) C	2- C 4					
	(50.65%)	0.7117*	C 2	s(33.54%)	p 1.98(66.46%)			
				0.0000	0.5791	0.0050	0.2695	-0.0060
				0.3680	0.0006	0.6757	0.0004	
	(49.35%)	0.7025*	C 4	s(35.53%)	p 1.81(64.47%)			
				0.0000	0.5960	-0.0005	-0.3031	-0.0116
				-0.3163	0.0102	-0.6727	0.0091	
39.	(1.96767)	BD (1) C	2- C 5					
	(50.29%)	0.7092*	C 2	s(32.30%)	p 2.10(67.70%)			
				0.0000	0.5683	0.0020	0.5134	0.0018
				-0.4752	0.0029	-0.4331	0.0045	
	(49.71%)	0.7051*	C 5	s(33.00%)	p 2.03(67.00%)			
				0.0000	0.5744	-0.0053	-0.5165	0.0021
				0.4622	-0.0075	0.4352	-0.0103	
40.	(1.53840)	BD (2) C	2- C 5					
	(50.16%)	0.7083*	C 2	s(0.00%)	p 1.00(100.00%)			
				0.0000	-0.0034	0.0023	-0.2724	-0.0092
				-0.7937	0.0002	0.5437	0.0081	
	(49.84%)	0.7060*	C 5	s(0.00%)	p 1.00(100.00%)			
				0.0000	-0.0041	0.0045	-0.2546	-0.0069
				-0.7960	0.0026	0.5490	0.0073	
41.	(1.96554)	BD (1) C	3- C 8					
	(50.99%)	0.7140*	C 3	s(31.67%)	p 2.16(68.33%)			
				0.0000	0.5624	0.0206	-0.2329	-0.0087
				-0.4889	-0.0228	-0.6234	-0.0289	
	(49.01%)	0.7001*	C 8	s(35.23%)	p 1.84(64.77%)			
				0.0000	0.5936	-0.0024	0.2397	-0.0094
				0.3989	-0.0010	0.6565	0.0022	
42.	(1.70103)	BD (2) C	3- C 8					
	(49.35%)	0.7025*	C 3	s(0.01%)	p 1.00(99.99%)			
				0.0000	-0.0071	-0.0010	0.2630	0.0064
				0.7054	0.0064	-0.6581	-0.0035	
	(50.65%)	0.7117*	C 8	s(0.04%)	p99.99(99.96%)			
				0.0000	0.0208	-0.0001	0.2222	-0.0015
				0.7853	-0.0156	-0.5771	0.0130	
43.	(1.97666)	BD (1) C	4- C 6					
	(50.23%)	0.7087*	C 4	s(36.39%)	p 1.75(63.61%)			
				0.0000	0.6032	0.0008	0.7517	0.0103
				-0.1041	0.0054	0.2448	0.0120	
	(49.77%)	0.7055*	C 6	s(34.64%)	p 1.89(65.36%)			
				0.0000	0.5886	-0.0025	-0.7703	-0.0028
				0.1018	0.0111	-0.2224	0.0156	
44.	(1.73556)	BD (2) C	4- C 6					
	(49.31%)	0.7022*	C 4	s(0.01%)	p 1.00(99.99%)			
				0.0000	0.0077	0.0017	0.2709	-0.0004
				0.8214	-0.0154	-0.5016	0.0058	
	(50.69%)	0.7119*	C 6	s(0.00%)	p 1.00(100.00%)			
				0.0000	0.0051	0.0005	0.2604	-0.0035
				0.8166	-0.0186	-0.5146	0.0116	
45.	(1.98186)	BD (1) C	4- N 26					
	(40.19%)	0.6339*	C 4	s(28.04%)	p 2.57(71.96%)			
				0.0000	0.5296	0.0043	-0.5188	-0.0203
				0.4627	0.0018	0.4857	-0.0056	
	(59.81%)	0.7734*	N 26	s(30.17%)	p 2.31(69.83%)			
				0.0000	0.5493	-0.0001	0.4901	-0.0016
				-0.4577	-0.0073	-0.4984	-0.0106	
46.	(1.97440)	BD (1) C	5- C 14					
	(51.20%)	0.7155*	C 5	s(33.62%)	p 1.97(66.38%)			
				0.0000	0.5798	0.0053	-0.2616	0.0130

	(48.80%)	0.6986*	C 14	s(33.41%)p 1.99(66.59%)	-0.3819 -0.0069 -0.6704 -0.0033 0.0000 0.5780 -0.0024 0.2750 0.0240 0.3957 -0.0103 0.6580 -0.0055	
47. (1.97443)	BD (1) C (51.25%)	5- C 16 0.7159*	C 5	s(33.33%)p 2.00(66.67%)	0.0000 0.5773 0.0012 0.7745 0.0076 -0.0824 -0.0115 0.2443 -0.0129	
	(48.75%)	0.6982*	C 16	s(33.32%)p 2.00(66.68%)	0.0000 0.5772 -0.0054 -0.7719 0.0082 0.0829 -0.0126 -0.2521 -0.0158	
48. (1.98034)	BD (1) C (60.41%)	6- H 7 0.7772*	C 6	s(31.36%)p 2.19(68.64%)	0.0000 0.5600 -0.0022 0.2724 0.0185 0.3504 0.0007 0.6993 0.0089	
	(39.59%)	0.6292*	H 7	s(100.00%) 1.0000 -0.0013		
49. (1.97376)	BD (1) C (50.47%)	6- C 22 0.7105*	C 6	s(33.86%)p 1.95(66.14%)	0.0000 0.5818 0.0077 0.5138 0.0321 -0.4468 0.0014 -0.4432 0.0190	
	(49.53%)	0.7037*	C 22	s(33.15%)p 2.02(66.85%)	0.0000 0.5758 0.0019 -0.5056 0.0190 0.4552 0.0085 0.4524 0.0231	
50. (1.98086)	BD (1) C (60.72%)	8- H 9 0.7792*	C 8	s(31.73%)p 2.15(68.27%)	0.0000 0.5633 -0.0043 -0.7896 -0.0132 0.0317 -0.0103 -0.2405 -0.0091	
	(39.28%)	0.6268*	H 9	s(100.00%) 1.0000 -0.0018		
51. (1.97776)	BD (1) C (50.02%)	8- C 24 0.7072*	C 8	s(32.90%)p 2.04(67.10%)	0.0000 0.5735 0.0085 0.5192 -0.0189 -0.4718 -0.0098 -0.4216 -0.0226	
	(49.98%)	0.7070*	C 24	s(32.95%)p 2.03(67.05%)	0.0000 0.5740 0.0003 -0.5302 -0.0310 0.4489 -0.0052 0.4319 -0.0182	
52. (1.99312)	BD (1) C (59.77%)	10- H 11 0.7731*	C 10	s(25.75%)p 2.88(74.25%)	0.0000 0.5074 -0.0050 0.7563 0.0034 0.0097 0.0255 0.4121 -0.0017	
	(40.23%)	0.6343*	H 11	s(100.00%) 1.0000 0.0038		
53. (1.98761)	BD (1) C (61.01%)	10- H 12 0.7811*	C 10	s(25.89%)p 2.86(74.11%)	0.0000 0.5088 0.0019 -0.5880 0.0103 0.4474 0.0114 0.4414 -0.0056	
	(38.99%)	0.6244*	H 12	s(100.00%) 1.0000 0.0005		
54. (1.98857)	BD (1) C (61.65%)	10- H 13 0.7852*	C 10	s(26.31%)p 2.80(73.69%)	0.0000 0.5129 -0.0003 0.0846 0.0026 0.3121 0.0133 -0.7950 0.0124	
	(38.35%)	0.6193*	H 13	s(100.00%) 1.0000 0.0002		
55. (1.97866)	BD (1) C (39.00%)	10- N 26 0.6245*	C 10	s(22.01%)p 3.54(77.99%)	0.0000 0.4691 0.0081 -0.2734 -0.0189 -0.8377 -0.0051 -0.0555 -0.0028	
	(61.00%)	0.7810*	N 26	s(27.04%)p 2.70(72.96%)	0.0000 0.5200 -0.0005 0.2211 -0.0169 0.8238 0.0231 0.0338 -0.0059	
56. (1.98142)	BD (1) C (60.39%)	14- H 15 0.7771*	C 14	s(31.38%)p 2.19(68.62%)	0.0000 0.5602 -0.0040 0.5338 0.0036 -0.4522 -0.0075 -0.4435 -0.0097	
	(39.61%)	0.6294*	H 15	s(100.00%) 1.0000 -0.0009		
57. (1.97811)	BD (1) C (50.32%)	14- C 24 0.7094*	C 14	s(35.08%)p 1.85(64.92%)	0.0000 0.5923 0.0078 -0.7681 -0.0062 0.0571 -0.0183 -0.2339 -0.0279	
	(49.68%)	0.7048*	C 24	s(34.85%)p 1.87(65.15%)	0.0000 0.5903 0.0045 0.7774 0.0179 -0.0393 -0.0208 0.2108 -0.0217	
58. (1.74648)	BD (2) C (50.09%)	14- C 24 0.7077*	C 14	s(0.01%)p99.99(99.99%)		

				0.0000	0.0118	0.0020	-0.2211	0.0023
				-0.7970	0.0193	0.5614	-0.0122	
	(49.91%)	0.7065*	C 24	s(0.00%)	p 1.00	(100.00%)		
				0.0000	0.0054	0.0014	-0.1996	0.0045
				-0.7942	0.0229	0.5732	-0.0152	
59.	(1.98166)	BD (1)	C 16- H 17					
	(60.40%)	0.7772*	C 16	s(31.49%)	p 2.18	(68.51%)		
				0.0000	0.5612	-0.0035	0.5194	0.0138
				-0.4567	-0.0052	-0.4545	-0.0013	
	(39.60%)	0.6293*	H 17	s(100.00%)				
				1.0000	-0.0009			
60.	(1.97768)	BD (1)	C 16- C 22					
	(50.14%)	0.7081*	C 16	s(35.04%)	p 1.85	(64.96%)		
				0.0000	0.5919	0.0099	0.2628	0.0377
				0.3607	-0.0078	0.6700	0.0068	
	(49.86%)	0.7061*	C 22	s(34.92%)	p 1.86	(65.08%)		
				0.0000	0.5909	0.0052	-0.2512	0.0248
				-0.3490	-0.0159	-0.6818	-0.0131	
61.	(1.74442)	BD (2)	C 16- C 22					
	(50.00%)	0.7071*	C 16	s(0.00%)	p 1.00	(100.00%)		
				0.0000	0.0067	0.0017	-0.2549	0.0049
				-0.8088	0.0194	0.5295	-0.0086	
	(50.00%)	0.7071*	C 22	s(0.00%)	p 1.00	(100.00%)		
				0.0000	0.0062	0.0000	-0.2617	0.0066
				-0.8137	0.0231	0.5183	-0.0117	
62.	(1.98965)	BD (1)	C 18- H 19					
	(61.16%)	0.7821*	C 18	s(26.02%)	p 2.84	(73.98%)		
				0.0000	0.5101	0.0000	-0.1608	-0.0022
				-0.8428	0.0044	-0.0587	0.0158	
	(38.84%)	0.6232*	H 19	s(100.00%)				
				1.0000	-0.0003			
63.	(1.98864)	BD (1)	C 18- H 20					
	(60.89%)	0.7803*	C 18	s(25.83%)	p 2.87	(74.17%)		
				0.0000	0.5082	0.0029	-0.6388	0.0026
				0.4006	-0.0113	0.4158	0.0072	
	(39.11%)	0.6254*	H 20	s(100.00%)				
				1.0000	0.0005			
64.	(1.99353)	BD (1)	C 18- H 21					
	(59.95%)	0.7743*	C 18	s(25.87%)	p 2.87	(74.13%)		
				0.0000	0.5086	-0.0065	0.7504	-0.0065
				0.1372	-0.0105	0.3985	0.0223	
	(40.05%)	0.6328*	H 21	s(100.00%)				
				1.0000	0.0045			
65.	(1.97949)	BD (1)	C 18- N 26					
	(39.47%)	0.6283*	C 18	s(22.24%)	p 3.50	(77.76%)		
				0.0000	0.4715	0.0079	0.0526	-0.0204
				0.3320	0.0032	-0.8149	-0.0085	
	(60.53%)	0.7780*	N 26	s(26.69%)	p 2.75	(73.31%)		
				0.0000	0.5166	0.0020	-0.0945	-0.0302
				-0.3331	-0.0078	0.7823	0.0117	
66.	(1.98242)	BD (1)	C 22- H 23					
	(60.49%)	0.7778*	C 22	s(31.82%)	p 2.14	(68.18%)		
				0.0000	0.5641	-0.0052	0.7827	0.0108
				-0.0901	-0.0015	0.2469	0.0034	
	(39.51%)	0.6286*	H 23	s(100.00%)				
				1.0000	-0.0005			
67.	(1.98270)	BD (1)	C 24- H 25					
	(60.41%)	0.7772*	C 24	s(32.09%)	p 2.12	(67.91%)		
				0.0000	0.5665	-0.0030	-0.2710	-0.0050
				-0.4069	-0.0041	-0.6634	-0.0070	
	(39.59%)	0.6292*	H 25	s(100.00%)				
				1.0000	-0.0007			
68.	(1.96692)	BD (1)	C 27- C 28					
	(50.66%)	0.7117*	C 27	s(32.38%)	p 2.09	(67.62%)		
				0.0000	0.5688	0.0145	-0.3571	-0.0028
				0.4686	0.0229	0.5731	0.0139	
	(49.34%)	0.7024*	C 28	s(35.34%)	p 1.83	(64.66%)		
				0.0000	0.5944	-0.0032	0.3142	-0.0074
				-0.4798	-0.0096	-0.5634	0.0096	
69.	(1.96691)	BD (1)	C 27- C 29					
	(50.61%)	0.7114*	C 27	s(32.94%)	p 2.04	(67.06%)		
				0.0000	0.5736	0.0181	0.4377	0.0080
				0.3592	0.0175	-0.5910	-0.0183	
	(49.39%)	0.7028*	C 29	s(35.49%)	p 1.82	(64.51%)		
				0.0000	0.5957	-0.0009	-0.3797	0.0052
				-0.3932	-0.0134	0.5882	-0.0100	
70.	(1.62824)	BD (2)	C 27- C 29					

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( 52.63%) 0.7255* C 27 s( 0.00%)p 1.00(100.00%)
0.0000 -0.0018 -0.0008 -0.8208 -0.0053
0.0698 0.0058 -0.5668 -0.0110
( 47.37%) 0.6883* C 29 s( 0.00%)p 1.00(100.00%)
0.0000 0.0005 0.0032 -0.8515 0.0081
0.0414 -0.0007 -0.5227 -0.0024
71. (1.97321) BD ( 1) C 28- C 30
( 50.18%) 0.7083* C 28 s( 33.99%)p 1.94( 66.01%)
0.0000 0.5830 0.0056 0.0853 -0.0128
0.8072 0.0157 -0.0246 0.0174
( 49.82%) 0.7059* C 30 s( 34.73%)p 1.88( 65.27%)
0.0000 0.5893 0.0010 -0.0583 -0.0135
-0.8045 0.0017 0.0370 0.0220
72. (1.67375) BD ( 2) C 28- C 30
( 46.52%) 0.6821* C 28 s( 0.01%)p99.99( 99.99%)
0.0000 0.0099 0.0039 -0.8507 0.0084
0.0669 0.0036 -0.5211 0.0013
( 53.48%) 0.7313* C 30 s( 0.01%)p 1.00( 99.99%)
0.0000 0.0077 0.0014 -0.8550 0.0200
0.0437 0.0003 -0.5163 0.0087
73. (1.98097) BD ( 1) C 28- C 39
( 50.43%) 0.7102* C 28 s( 30.63%)p 2.26( 69.37%)
0.0000 0.5534 -0.0018 -0.4124 -0.0009
-0.3367 0.0071 0.6405 -0.0039
( 49.57%) 0.7040* C 39 s( 25.37%)p 2.94( 74.63%)
0.0000 0.5037 -0.0026 0.4274 -0.0079
0.3268 0.0028 -0.6756 0.0146
74. (1.97325) BD ( 1) C 29- C 32
( 50.16%) 0.7083* C 29 s( 33.74%)p 1.96( 66.26%)
0.0000 0.5809 0.0040 0.0487 0.0106
0.8120 0.0113 -0.0142 -0.0186
( 49.84%) 0.7060* C 32 s( 34.58%)p 1.89( 65.42%)
0.0000 0.5880 0.0006 -0.0448 0.0145
-0.8067 -0.0040 0.0271 -0.0233
75. (1.98109) BD ( 1) C 29- C 35
( 50.49%) 0.7106* C 29 s( 30.74%)p 2.25( 69.26%)
0.0000 0.5544 -0.0018 0.3581 0.0003
-0.4288 0.0040 -0.6168 0.0034
( 49.51%) 0.7036* C 35 s( 25.44%)p 2.93( 74.56%)
0.0000 0.5043 -0.0023 -0.3798 0.0103
0.4141 0.0000 0.6555 -0.0129
76. (1.98090) BD ( 1) C 30- H 31
( 60.23%) 0.7761* C 30 s( 30.68%)p 2.26( 69.32%)
0.0000 0.5539 -0.0040 -0.3381 -0.0054
0.4585 0.0113 0.6070 0.0094
( 39.77%) 0.6306* H 31 s(100.00%)
1.0000 -0.0011
77. (1.97365) BD ( 1) C 30- C 34
( 49.86%) 0.7061* C 30 s( 34.44%)p 1.90( 65.56%)
0.0000 0.5868 0.0049 0.3884 -0.0048
0.3744 0.0332 -0.6027 0.0101
( 50.14%) 0.7081* C 34 s( 34.34%)p 1.91( 65.66%)
0.0000 0.5860 0.0042 -0.3972 -0.0068
-0.3440 0.0132 0.6166 0.0124
78. (1.98107) BD ( 1) C 32- H 33
( 60.22%) 0.7760* C 32 s( 30.77%)p 2.25( 69.23%)
0.0000 0.5547 -0.0031 0.4101 0.0065
0.3608 0.0091 -0.6275 -0.0085
( 39.78%) 0.6307* H 33 s(100.00%)
1.0000 -0.0012
79. (1.97424) BD ( 1) C 32- C 34
( 49.83%) 0.7059* C 32 s( 34.50%)p 1.90( 65.50%)
0.0000 0.5874 0.0041 -0.3417 0.0091
0.4665 0.0341 0.5650 -0.0127
( 50.17%) 0.7083* C 34 s( 34.53%)p 1.90( 65.47%)
0.0000 0.5876 0.0030 0.3481 0.0084
-0.4425 0.0089 -0.5809 -0.0129
80. (1.66488) BD ( 2) C 32- C 34
( 53.07%) 0.7285* C 32 s( 0.00%)p 1.00(100.00%)
0.0000 -0.0002 0.0010 0.8443 -0.0183
-0.0291 0.0020 0.5347 -0.0096
( 46.93%) 0.6851* C 34 s( 0.00%)p 1.00(100.00%)
0.0000 0.0038 -0.0011 0.8479 -0.0117
-0.0232 0.0011 0.5295 -0.0024
81. (1.98145) BD ( 1) C 34- C 43
( 50.34%) 0.7095* C 34 s( 31.13%)p 2.21( 68.87%)
0.0000 0.5579 -0.0064 0.0448 -0.0005

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				0.8277	-0.0041	-0.0394	0.0001	
	(49.66%)	0.7047*	C 43	s(25.71%)	p 2.89(74.29%)			
				0.0000	0.5070	-0.0045	-0.0406	0.0017
				-0.8595	0.0192	0.0463	-0.0025	
82.	(1.97804)	BD (1)	C 35- H 36					
	(61.29%)	0.7829*	C 35	s(24.46%)	p 3.09(75.54%)			
				0.0000	0.4946	0.0001	-0.6065	0.0059
				-0.3817	-0.0036	-0.4913	-0.0195	
	(38.71%)	0.6222*	H 36	s(100.00%)				
				1.0000	-0.0003			
83.	(1.97944)	BD (1)	C 35- H 37					
	(61.77%)	0.7860*	C 35	s(24.96%)	p 3.01(75.04%)			
				0.0000	0.4996	-0.0006	0.5382	0.0121
				-0.6042	-0.0002	0.3086	-0.0152	
	(38.23%)	0.6183*	H 37	s(100.00%)				
				1.0000	-0.0006			
84.	(1.98840)	BD (1)	C 35- H 38					
	(61.05%)	0.7813*	C 35	s(25.02%)	p 3.00(74.98%)			
				0.0000	0.5002	0.0029	0.4451	0.0054
				0.5636	-0.0131	-0.4834	-0.0099	
	(38.95%)	0.6241*	H 38	s(100.00%)				
				1.0000	-0.0009			
85.	(1.98728)	BD (1)	C 39- H 40					
	(60.99%)	0.7810*	C 39	s(24.83%)	p 3.03(75.17%)			
				0.0000	0.4983	0.0033	-0.0558	-0.0081
				0.5975	-0.0108	0.6255	0.0115	
	(39.01%)	0.6246*	H 40	s(100.00%)				
				1.0000	-0.0010			
86.	(1.98169)	BD (1)	C 39- H 41					
	(61.32%)	0.7830*	C 39	s(24.96%)	p 3.01(75.04%)			
				0.0000	0.4996	-0.0008	0.4197	-0.0067
				-0.6945	-0.0001	0.3025	0.0197	
	(38.68%)	0.6220*	H 41	s(100.00%)				
				1.0000	-0.0002			
87.	(1.97626)	BD (1)	C 39- H 42					
	(61.97%)	0.7872*	C 39	s(24.72%)	p 3.04(75.28%)			
				0.0000	0.4972	0.0001	-0.7988	-0.0106
				-0.2318	-0.0002	-0.2463	0.0147	
	(38.03%)	0.6167*	H 42	s(100.00%)				
				1.0000	-0.0003			
88.	(1.98926)	BD (1)	C 43- H 44					
	(61.19%)	0.7822*	C 43	s(24.92%)	p 3.01(75.08%)			
				0.0000	0.4992	0.0016	0.3777	-0.0022
				0.2370	0.0160	-0.7428	0.0029	
	(38.81%)	0.6230*	H 44	s(100.00%)				
				1.0000	-0.0011			
89.	(1.97978)	BD (1)	C 43- H 45					
	(61.37%)	0.7834*	C 43	s(24.55%)	p 3.07(75.45%)			
				0.0000	0.4955	0.0012	0.4639	0.0052
				0.3067	0.0155	0.6670	-0.0014	
	(38.63%)	0.6215*	H 45	s(100.00%)				
				1.0000	-0.0007			
90.	(1.98139)	BD (1)	C 43- H 46					
	(61.41%)	0.7837*	C 43	s(24.72%)	p 3.05(75.28%)			
				0.0000	0.4971	0.0010	-0.8003	-0.0001
				0.3332	0.0154	0.0337	-0.0056	
	(38.59%)	0.6212*	H 46	s(100.00%)				
				1.0000	-0.0007			
91.	(1.96577)	BD (1)	C 47- C 48					
	(50.67%)	0.7118*	C 47	s(32.52%)	p 2.07(67.48%)			
				0.0000	0.5700	0.0170	-0.6099	-0.0273
				0.3004	0.0016	-0.4600	-0.0146	
	(49.33%)	0.7024*	C 48	s(35.40%)	p 1.82(64.60%)			
				0.0000	0.5950	-0.0022	0.6142	0.0073
				-0.2470	0.0115	0.4554	-0.0104	
92.	(1.96725)	BD (1)	C 47- C 49					
	(50.67%)	0.7119*	C 47	s(32.81%)	p 2.05(67.19%)			
				0.0000	0.5724	0.0201	-0.1598	-0.0095
				-0.6093	-0.0157	0.5239	0.0172	
	(49.33%)	0.7023*	C 49	s(35.16%)	p 1.84(64.84%)			
				0.0000	0.5930	0.0007	0.1907	0.0113
				0.5776	-0.0024	-0.5275	0.0065	
93.	(1.62402)	BD (2)	C 47- C 49					
	(53.18%)	0.7293*	C 47	s(0.00%)	p 1.00(100.00%)			
				0.0000	-0.0037	-0.0011	0.2042	0.0050
				-0.6704	-0.0082	-0.7133	-0.0047	
	(46.82%)	0.6842*	C 49	s(0.01%)	p 1.00(99.99%)			

				0.0000	0.0076	-0.0025	0.2070	-0.0001
				-0.7002	0.0011	-0.6832	0.0004	
94.	(1.97292)	BD (1) C 48-	C 52					
	(50.26%)	0.7089*	C 48	s(34.06%)	p 1.94(65.94%)			
				0.0000	0.5836	0.0054	-0.7454	-0.0209
				-0.3125	0.0095	0.0731	-0.0163	
	(49.74%)	0.7053*	C 52	s(34.63%)	p 1.89(65.37%)			
				0.0000	0.5885	0.0016	0.7475	-0.0072
				0.2967	0.0142	-0.0799	-0.0169	
95.	(1.66330)	BD (2) C 48-	C 52					
	(46.70%)	0.6834*	C 48	s(0.00%)	p 1.00(100.00%)			
				0.0000	0.0024	0.0006	-0.2246	-0.0023
				0.6990	-0.0037	0.6789	-0.0030	
	(53.30%)	0.7301*	C 52	s(0.00%)	p 1.00(100.00%)			
				0.0000	0.0029	-0.0017	-0.2079	0.0014
				0.7016	-0.0150	0.6813	-0.0118	
96.	(1.98119)	BD (1) C 48-	C 59					
	(50.44%)	0.7102*	C 48	s(30.50%)	p 2.28(69.50%)			
				0.0000	0.5523	-0.0022	0.1275	-0.0059
				0.5937	-0.0055	-0.5711	0.0047	
	(49.56%)	0.7040*	C 59	s(25.30%)	p 2.95(74.70%)			
				0.0000	0.5030	-0.0014	-0.1033	-0.0052
				-0.6107	0.0074	0.6025	-0.0128	
97.	(1.97370)	BD (1) C 49-	C 50					
	(50.20%)	0.7085*	C 49	s(34.23%)	p 1.92(65.77%)			
				0.0000	0.5851	0.0042	-0.7551	-0.0030
				-0.2865	-0.0149	0.0713	0.0126	
	(49.80%)	0.7057*	C 50	s(34.48%)	p 1.90(65.52%)			
				0.0000	0.5872	0.0010	0.7524	0.0119
				0.2891	-0.0190	-0.0681	0.0207	
98.	(1.98097)	BD (1) C 49-	C 55					
	(50.24%)	0.7088*	C 49	s(30.58%)	p 2.27(69.42%)			
				0.0000	0.5529	-0.0036	0.5920	-0.0068
				-0.3066	-0.0010	0.4997	-0.0015	
	(49.76%)	0.7054*	C 55	s(25.60%)	p 2.91(74.40%)			
				0.0000	0.5060	-0.0027	-0.6014	0.0051
				0.3231	-0.0131	-0.5268	0.0115	
99.	(1.98092)	BD (1) C 50-	H 51					
	(60.18%)	0.7758*	C 50	s(30.94%)	p 2.23(69.06%)			
				0.0000	0.5562	-0.0024	-0.1540	-0.0036
				-0.5991	-0.0084	0.5549	0.0072	
	(39.82%)	0.6310*	H 51	s(100.00%)				
				1.0000	-0.0014			
100.	(1.97424)	BD (1) C 50-	C 54					
	(49.86%)	0.7061*	C 50	s(34.44%)	p 1.90(65.56%)			
				0.0000	0.5869	0.0029	-0.6073	-0.0268
				0.2802	-0.0192	-0.4549	0.0129	
	(50.14%)	0.7081*	C 54	s(34.49%)	p 1.90(65.51%)			
				0.0000	0.5873	0.0033	0.5856	-0.0037
				-0.3000	-0.0118	0.4710	0.0110	
101.	(1.65564)	BD (2) C 50-	C 54					
	(53.15%)	0.7291*	C 50	s(0.00%)	p 1.00(100.00%)			
				0.0000	0.0019	0.0007	0.2016	0.0000
				-0.6919	0.0123	-0.6930	0.0135	
	(46.85%)	0.6845*	C 54	s(0.00%)	p 1.00(100.00%)			
				0.0000	-0.0011	0.0013	0.2025	0.0010
				-0.6931	0.0068	-0.6918	0.0085	
102.	(1.98073)	BD (1) C 52-	H 53					
	(60.24%)	0.7761*	C 52	s(30.83%)	p 2.24(69.17%)			
				0.0000	0.5553	-0.0050	-0.6059	-0.0131
				0.2926	0.0031	-0.4886	-0.0074	
	(39.76%)	0.6306*	H 53	s(100.00%)				
				1.0000	-0.0011			
103.	(1.97397)	BD (1) C 52-	C 54					
	(49.82%)	0.7058*	C 52	s(34.41%)	p 1.91(65.59%)			
				0.0000	0.5866	0.0056	-0.1752	-0.0316
				-0.5777	-0.0029	0.5388	-0.0062	
	(50.18%)	0.7084*	C 54	s(34.51%)	p 1.90(65.49%)			
				0.0000	0.5874	0.0037	0.1455	-0.0189
				0.5826	0.0055	-0.5421	-0.0107	
104.	(1.98150)	BD (1) C 54-	C 63					
	(50.29%)	0.7092*	C 54	s(30.99%)	p 2.23(69.01%)			
				0.0000	0.5567	-0.0062	-0.7711	0.0052
				-0.2999	0.0034	0.0739	-0.0029	
	(49.71%)	0.7050*	C 63	s(25.65%)	p 2.90(74.35%)			
				0.0000	0.5064	-0.0033	0.7999	-0.0170
				0.3120	-0.0066	-0.0770	0.0014	

105.	(1.97699)	BD (1) C 55- H 56	(61.17%)	0.7821*	C 55	s(24.55%)p 3.07(75.45%)	0.0000	0.4955	0.0002	0.1846	0.0049
							0.5788	-0.0065	0.6206	0.0156	
			(38.83%)	0.6231*	H 56	s(100.00%)	1.0000	-0.0006			
106.	(1.97924)	BD (1) C 55- H 57	(61.80%)	0.7861*	C 55	s(24.95%)p 3.01(75.05%)	0.0000	0.4995	-0.0009	0.7194	0.0052
							-0.1762	-0.0159	-0.4489	0.0096	
			(38.20%)	0.6181*	H 57	s(100.00%)	1.0000	-0.0004			
107.	(1.98811)	BD (1) C 55- H 58	(61.10%)	0.7816*	C 55	s(24.79%)p 3.03(75.21%)	0.0000	0.4979	0.0033	-0.2944	0.0145
							-0.7277	-0.0042	0.3684	0.0063	
			(38.90%)	0.6237*	H 58	s(100.00%)	1.0000	-0.0009			
108.	(1.98783)	BD (1) C 59- H 60	(61.07%)	0.7815*	C 59	s(25.03%)p 3.00(74.97%)	0.0000	0.5003	0.0027	-0.6852	0.0081
							0.0063	0.0115	-0.5291	-0.0105	
			(38.93%)	0.6239*	H 60	s(100.00%)	1.0000	-0.0009			
109.	(1.98166)	BD (1) C 59- H 61	(61.14%)	0.7819*	C 59	s(24.78%)p 3.04(75.22%)	0.0000	0.4978	-0.0001	0.7169	-0.0044
							-0.1638	0.0088	-0.4592	-0.0190	
			(38.86%)	0.6234*	H 61	s(100.00%)	1.0000	-0.0008			
110.	(1.97709)	BD (1) C 59- H 62	(61.91%)	0.7868*	C 59	s(24.77%)p 3.04(75.23%)	0.0000	0.4977	-0.0008	0.0757	-0.0048
							0.7747	0.0124	0.3822	-0.0123	
			(38.09%)	0.6172*	H 62	s(100.00%)	1.0000	-0.0003			
111.	(1.97977)	BD (1) C 63- H 64	(61.41%)	0.7837*	C 63	s(24.67%)p 3.05(75.33%)	0.0000	0.4967	0.0012	-0.0114	-0.0144
							-0.8356	-0.0057	-0.2339	-0.0030	
			(38.59%)	0.6212*	H 64	s(100.00%)	1.0000	-0.0007			
112.	(1.98948)	BD (1) C 63- H 65	(61.17%)	0.7821*	C 63	s(24.90%)p 3.02(75.10%)	0.0000	0.4990	0.0010	-0.5396	-0.0133
							0.4469	-0.0084	-0.5096	0.0051	
			(38.83%)	0.6231*	H 65	s(100.00%)	1.0000	-0.0011			
113.	(1.98157)	BD (1) C 63- H 66	(61.37%)	0.7834*	C 63	s(24.67%)p 3.05(75.33%)	0.0000	0.4967	0.0007	-0.2621	-0.0162
							0.0684	-0.0012	0.8244	0.0009	
			(38.63%)	0.6215*	H 66	s(100.00%)	1.0000	-0.0008			
----- non-Lewis -----											
114.	(0.22843)	LV (1) B 1				s(0.10%)p99.99(99.90%)	0.0000	0.0294	-0.0105	0.2154	-0.0081
							-0.0286	0.0046	0.9752	-0.0266	
115.	(0.02694)	BD*(1) B 1- C 3	(69.31%)	0.8325*	B 1	s(33.07%)p 2.02(66.93%)	0.0000	0.5750	0.0070	0.6033	0.0087
							-0.5268	-0.0098	-0.1660	-0.0069	
			(30.69%)	-0.5540*	C 3	s(35.88%)p 1.79(64.12%)	0.0000	0.5986	-0.0222	-0.5169	0.0386
							0.5099	-0.0295	0.3338	-0.0139	
116.	(0.02827)	BD*(1) B 1- C 27	(68.69%)	0.8288*	B 1	s(34.32%)p 1.91(65.68%)	0.0000	0.5858	0.0007	0.1329	0.0076
							0.7990	0.0103	-0.0236	0.0000	
			(31.31%)	-0.5595*	C 27	s(34.52%)p 1.90(65.48%)	0.0000	0.5871	-0.0224	-0.0835	0.0082
							-0.8032	0.0476	0.0207	-0.0019	
117.	(0.02441)	BD*(1) B 1- C 47	(68.57%)	0.8281*	B 1	s(32.53%)p 2.07(67.47%)	0.0000	0.5703	-0.0028	-0.7561	-0.0050
							-0.2882	-0.0011	0.1413	0.0040	
			(31.43%)	-0.5606*	C 47	s(34.52%)p 1.90(65.48%)					

					0.0000	0.5870	-0.0253	0.7478	-0.0469
					0.2972	-0.0181	-0.0684	0.0083	
118.	(0.03346)	BD*(1) C	2- C 3						
	(49.40%)	0.7029*	C 2	s(34.15%)p 1.93(65.85%)					
				0.0000	0.5844	-0.0032	-0.7678	0.0036	
				0.0930	-0.0010	-0.2453	0.0093		
	(50.60%)	-0.7113*	C 3	s(32.32%)p 2.09(67.68%)					
				0.0000	0.5683	0.0142	0.7800	0.0147	
				-0.0453	-0.0074	0.2569	0.0094		
119.	(0.03552)	BD*(1) C	2- C 4						
	(49.35%)	0.7025*	C 2	s(33.54%)p 1.98(66.46%)					
				0.0000	-0.5791	-0.0050	-0.2695	0.0060	
				-0.3680	-0.0006	-0.6757	-0.0004		
	(50.65%)	-0.7117*	C 4	s(35.53%)p 1.81(64.47%)					
				0.0000	-0.5960	0.0005	0.3031	0.0116	
				0.3163	-0.0102	0.6727	-0.0091		
120.	(0.03117)	BD*(1) C	2- C 5						
	(49.71%)	0.7051*	C 2	s(32.30%)p 2.10(67.70%)					
				0.0000	-0.5683	-0.0020	-0.5134	-0.0018	
				0.4752	-0.0029	0.4331	-0.0045		
	(50.29%)	-0.7092*	C 5	s(33.00%)p 2.03(67.00%)					
				0.0000	-0.5744	0.0053	0.5165	-0.0021	
				-0.4622	0.0075	-0.4352	0.0103		
121.	(0.45287)	BD*(2) C	2- C 5						
	(49.84%)	0.7060*	C 2	s(0.00%)p 1.00(100.00%)					
				0.0000	0.0034	-0.0023	0.2724	0.0092	
				0.7937	-0.0002	-0.5437	-0.0081		
	(50.16%)	-0.7083*	C 5	s(0.00%)p 1.00(100.00%)					
				0.0000	0.0041	-0.0045	0.2546	0.0069	
				0.7960	-0.0026	-0.5490	-0.0073		
122.	(0.02145)	BD*(1) C	3- C 8						
	(49.01%)	0.7001*	C 3	s(31.67%)p 2.16(68.33%)					
				0.0000	-0.5624	-0.0206	0.2329	0.0087	
				0.4889	0.0228	0.6234	0.0289		
	(50.99%)	-0.7140*	C 8	s(35.23%)p 1.84(64.77%)					
				0.0000	-0.5936	0.0024	-0.2397	0.0094	
				-0.3989	0.0010	-0.6565	-0.0022		
123.	(0.25213)	BD*(2) C	3- C 8						
	(50.65%)	0.7117*	C 3	s(0.01%)p 1.00(99.99%)					
				0.0000	0.0071	0.0010	-0.2630	-0.0064	
				-0.7054	-0.0064	0.6581	0.0035		
	(49.35%)	-0.7025*	C 8	s(0.04%)p99.99(99.96%)					
				0.0000	-0.0208	0.0001	-0.2222	0.0015	
				-0.7853	0.0156	0.5771	-0.0130		
124.	(0.02986)	BD*(1) C	4- C 6						
	(49.77%)	0.7055*	C 4	s(36.39%)p 1.75(63.61%)					
				0.0000	0.6032	0.0008	0.7517	0.0103	
				-0.1041	0.0054	0.2448	0.0120		
	(50.23%)	-0.7087*	C 6	s(34.64%)p 1.89(65.36%)					
				0.0000	0.5886	-0.0025	-0.7703	-0.0028	
				0.1018	0.0111	-0.2224	0.0156		
125.	(0.28611)	BD*(2) C	4- C 6						
	(50.69%)	0.7119*	C 4	s(0.01%)p 1.00(99.99%)					
				0.0000	0.0077	0.0017	0.2709	-0.0004	
				0.8214	-0.0154	-0.5016	0.0058		
	(49.31%)	-0.7022*	C 6	s(0.00%)p 1.00(100.00%)					
				0.0000	0.0051	0.0005	0.2604	-0.0035	
				0.8166	-0.0186	-0.5146	0.0116		
126.	(0.02950)	BD*(1) C	4- N 26						
	(59.81%)	0.7734*	C 4	s(28.04%)p 2.57(71.96%)					
				0.0000	0.5296	0.0043	-0.5188	-0.0203	
				0.4627	0.0018	0.4857	-0.0056		
	(40.19%)	-0.6339*	N 26	s(30.17%)p 2.31(69.83%)					
				0.0000	0.5493	-0.0001	0.4901	-0.0016	
				-0.4577	-0.0073	-0.4984	-0.0106		
127.	(0.02331)	BD*(1) C	5- C 14						
	(48.80%)	0.6986*	C 5	s(33.62%)p 1.97(66.38%)					
				0.0000	-0.5798	-0.0053	0.2616	-0.0130	
				0.3819	0.0069	0.6704	0.0033		
	(51.20%)	-0.7155*	C 14	s(33.41%)p 1.99(66.59%)					
				0.0000	-0.5780	0.0024	-0.2750	-0.0240	
				-0.3957	0.0103	-0.6580	0.0055		
128.	(0.02357)	BD*(1) C	5- C 16						
	(48.75%)	0.6982*	C 5	s(33.33%)p 2.00(66.67%)					
				0.0000	-0.5773	-0.0012	-0.7745	-0.0076	
				0.0824	0.0115	-0.2443	0.0129		
	(51.25%)	-0.7159*	C 16	s(33.32%)p 2.00(66.68%)					

				0.0000	-0.5772	0.0054	0.7719	-0.0082
				-0.0829	0.0126	0.2521	0.0158	
129.	(0.01271)	BD*(1) C 6- H 7						
	(39.59%)	0.6292* C 6	s(31.36%)p 2.19(68.64%)					
			0.0000	-0.5600	0.0022	-0.2724	-0.0185	
	(60.41%)	-0.7772* H 7	s(100.00%)					
			-1.0000	0.0013				
130.	(0.01903)	BD*(1) C 6- C 22						
	(49.53%)	0.7037* C 6	s(33.86%)p 1.95(66.14%)					
			0.0000	0.5818	0.0077	0.5138	0.0321	
			-0.4468	0.0014	-0.4432	0.0190		
	(50.47%)	-0.7105* C 22	s(33.15%)p 2.02(66.85%)					
			0.0000	0.5758	0.0019	-0.5056	0.0190	
			0.4552	0.0085	0.4524	0.0231		
131.	(0.01245)	BD*(1) C 8- H 9						
	(39.28%)	0.6268* C 8	s(31.73%)p 2.15(68.27%)					
			0.0000	-0.5633	0.0043	0.7896	0.0132	
			-0.0317	0.0103	0.2405	0.0091		
	(60.72%)	-0.7792* H 9	s(100.00%)					
			-1.0000	0.0018				
132.	(0.02168)	BD*(1) C 8- C 24						
	(49.98%)	0.7070* C 8	s(32.90%)p 2.04(67.10%)					
			0.0000	-0.5735	-0.0085	-0.5192	0.0189	
			0.4718	0.0098	0.4216	0.0226		
	(50.02%)	-0.7072* C 24	s(32.95%)p 2.03(67.05%)					
			0.0000	-0.5740	-0.0003	0.5302	0.0310	
			-0.4489	0.0052	-0.4319	0.0182		
133.	(0.01718)	BD*(1) C 10- H 11						
	(40.23%)	0.6343* C 10	s(25.75%)p 2.88(74.25%)					
			0.0000	-0.5074	0.0050	-0.7563	-0.0034	
			-0.0097	-0.0255	-0.4121	0.0017		
	(59.77%)	-0.7731* H 11	s(100.00%)					
			-1.0000	-0.0038				
134.	(0.00950)	BD*(1) C 10- H 12						
	(38.99%)	0.6244* C 10	s(25.89%)p 2.86(74.11%)					
			0.0000	-0.5088	-0.0019	0.5880	-0.0103	
			-0.4474	-0.0114	-0.4414	0.0056		
	(61.01%)	-0.7811* H 12	s(100.00%)					
			-1.0000	-0.0005				
135.	(0.00814)	BD*(1) C 10- H 13						
	(38.35%)	0.6193* C 10	s(26.31%)p 2.80(73.69%)					
			0.0000	-0.5129	0.0003	-0.0846	-0.0026	
			-0.3121	-0.0133	0.7950	-0.0124		
	(61.65%)	-0.7852* H 13	s(100.00%)					
			-1.0000	-0.0002				
136.	(0.01302)	BD*(1) C 10- N 26						
	(61.00%)	0.7810* C 10	s(22.01%)p 3.54(77.99%)					
			0.0000	0.4691	0.0081	-0.2734	-0.0189	
			-0.8377	-0.0051	-0.0555	-0.0028		
	(39.00%)	-0.6245* N 26	s(27.04%)p 2.70(72.96%)					
			0.0000	0.5200	-0.0005	0.2211	-0.0169	
			0.8238	0.0231	0.0338	-0.0059		
137.	(0.01235)	BD*(1) C 14- H 15						
	(39.61%)	0.6294* C 14	s(31.38%)p 2.19(68.62%)					
			0.0000	-0.5602	0.0040	-0.5338	-0.0036	
			0.4522	0.0075	0.4435	0.0097		
	(60.39%)	-0.7771* H 15	s(100.00%)					
			-1.0000	0.0009				
138.	(0.01660)	BD*(1) C 14- C 24						
	(49.68%)	0.7048* C 14	s(35.08%)p 1.85(64.92%)					
			0.0000	-0.5923	-0.0078	0.7681	0.0062	
			-0.0571	0.0183	0.2339	0.0279		
	(50.32%)	-0.7094* C 24	s(34.85%)p 1.87(65.15%)					
			0.0000	-0.5903	-0.0045	-0.7774	-0.0179	
			0.0393	0.0208	-0.2108	0.0217		
139.	(0.24814)	BD*(2) C 14- C 24						
	(49.91%)	0.7065* C 14	s(0.01%)p99.99(99.99%)					
			0.0000	0.0118	0.0020	-0.2211	0.0023	
			-0.7970	0.0193	0.5614	-0.0122		
	(50.09%)	-0.7077* C 24	s(0.00%)p 1.00(100.00%)					
			0.0000	0.0054	0.0014	-0.1996	0.0045	
			-0.7942	0.0229	0.5732	-0.0152		
140.	(0.01211)	BD*(1) C 16- H 17						
	(39.60%)	0.6293* C 16	s(31.49%)p 2.18(68.51%)					
			0.0000	-0.5612	0.0035	-0.5194	-0.0138	
			0.4567	0.0052	0.4545	0.0013		

	(60.40%)	-0.7772*	H 17	s(100.00%)	-1.0000	0.0009			
141.	(0.01624)	BD*(1)	C 16-	C 22					
	(49.86%)	0.7061*	C 16	s(35.04%)p 1.85(64.96%)	0.0000	-0.5919	-0.0099	-0.2628	-0.0377
					-0.3607	0.0078	-0.6700	-0.0068	
	(50.14%)	-0.7081*	C 22	s(34.92%)p 1.86(65.08%)	0.0000	-0.5909	-0.0052	0.2512	-0.0248
					0.3490	0.0159	0.6818	0.0131	
142.	(0.26137)	BD*(2)	C 16-	C 22					
	(50.00%)	0.7071*	C 16	s(0.00%)p 1.00(100.00%)	0.0000	0.0067	0.0017	-0.2549	0.0049
					-0.8088	0.0194	0.5295	-0.0086	
	(50.00%)	-0.7071*	C 22	s(0.00%)p 1.00(100.00%)	0.0000	0.0062	0.0000	-0.2617	0.0066
					-0.8137	0.0231	0.5183	-0.0117	
143.	(0.00691)	BD*(1)	C 18-	H 19					
	(38.84%)	0.6232*	C 18	s(26.02%)p 2.84(73.98%)	0.0000	-0.5101	0.0000	0.1608	0.0022
					0.8428	-0.0044	0.0587	-0.0158	
	(61.16%)	-0.7821*	H 19	s(100.00%)	-1.0000	0.0003			
144.	(0.00942)	BD*(1)	C 18-	H 20					
	(39.11%)	0.6254*	C 18	s(25.83%)p 2.87(74.17%)	0.0000	-0.5082	-0.0029	0.6388	-0.0026
					-0.4006	0.0113	-0.4158	-0.0072	
	(60.89%)	-0.7803*	H 20	s(100.00%)	-1.0000	-0.0005			
145.	(0.01867)	BD*(1)	C 18-	H 21					
	(40.05%)	0.6328*	C 18	s(25.87%)p 2.87(74.13%)	0.0000	-0.5086	0.0065	-0.7504	0.0065
					-0.1372	0.0105	-0.3985	-0.0223	
	(59.95%)	-0.7743*	H 21	s(100.00%)	-1.0000	-0.0045			
146.	(0.01366)	BD*(1)	C 18-	N 26					
	(60.53%)	0.7780*	C 18	s(22.24%)p 3.50(77.76%)	0.0000	0.4715	0.0079	0.0526	-0.0204
					0.3320	0.0032	-0.8149	-0.0085	
	(39.47%)	-0.6283*	N 26	s(26.69%)p 2.75(73.31%)	0.0000	0.5166	0.0020	-0.0945	-0.0302
					-0.3331	-0.0078	0.7823	0.0117	
147.	(0.01210)	BD*(1)	C 22-	H 23					
	(39.51%)	0.6286*	C 22	s(31.82%)p 2.14(68.18%)	0.0000	-0.5641	0.0052	-0.7827	-0.0108
					0.0901	0.0015	-0.2469	-0.0034	
	(60.49%)	-0.7778*	H 23	s(100.00%)	-1.0000	0.0005			
148.	(0.01138)	BD*(1)	C 24-	H 25					
	(39.59%)	0.6292*	C 24	s(32.09%)p 2.12(67.91%)	0.0000	-0.5665	0.0030	0.2710	0.0050
					0.4069	0.0041	0.6634	0.0070	
	(60.41%)	-0.7772*	H 25	s(100.00%)	-1.0000	0.0007			
149.	(0.02976)	BD*(1)	C 27-	C 28					
	(49.34%)	0.7024*	C 27	s(32.38%)p 2.09(67.62%)	0.0000	-0.5688	-0.0145	0.3571	0.0028
					-0.4686	-0.0229	-0.5731	-0.0139	
	(50.66%)	-0.7117*	C 28	s(35.34%)p 1.83(64.66%)	0.0000	-0.5944	0.0032	-0.3142	0.0074
					0.4798	0.0096	0.5634	-0.0096	
150.	(0.03079)	BD*(1)	C 27-	C 29					
	(49.39%)	0.7028*	C 27	s(32.94%)p 2.04(67.06%)	0.0000	-0.5736	-0.0181	-0.4377	-0.0080
					-0.3592	-0.0175	0.5910	0.0183	
	(50.61%)	-0.7114*	C 29	s(35.49%)p 1.82(64.51%)	0.0000	-0.5957	0.0009	0.3797	-0.0052
					0.3932	0.0134	-0.5882	0.0100	
151.	(0.35685)	BD*(2)	C 27-	C 29					
	(47.37%)	0.6883*	C 27	s(0.00%)p 1.00(100.00%)	0.0000	0.0018	0.0008	0.8208	0.0053
					-0.0698	-0.0058	0.5668	0.0110	
	(52.63%)	-0.7255*	C 29	s(0.00%)p 1.00(100.00%)	0.0000	-0.0005	-0.0032	0.8515	-0.0081
					-0.0414	0.0007	0.5227	0.0024	
152.	(0.02415)	BD*(1)	C 28-	C 30					
	(49.82%)	0.7059*	C 28	s(33.99%)p 1.94(66.01%)	0.0000	-0.5830	-0.0056	-0.0853	0.0128

	(50.18%)	-0.7083*	C 30	s(34.73%)p 1.88(65.27%)	-0.8072 -0.0157 0.0246 -0.0174 0.0000 -0.5893 -0.0010 0.0583 0.0135 0.8045 -0.0017 -0.0370 -0.0220
153.	(0.32934)	BD*(2) C 28-	C 30	s(0.01%)p99.99(99.99%)	0.0000 0.0099 0.0039 -0.8507 0.0084 0.0669 0.0036 -0.5211 0.0013
	(46.52%)	-0.6821*	C 30	s(0.01%)p 1.00(99.99%)	0.0000 0.0077 0.0014 -0.8550 0.0200 0.0437 0.0003 -0.5163 0.0087
154.	(0.01721)	BD*(1) C 28-	C 39	s(30.63%)p 2.26(69.37%)	0.0000 0.5534 -0.0018 -0.4124 -0.0009 -0.3367 0.0071 0.6405 -0.0039
	(50.43%)	-0.7102*	C 39	s(25.37%)p 2.94(74.63%)	0.0000 0.5037 -0.0026 0.4274 -0.0079 0.3268 0.0028 -0.6756 0.0146
155.	(0.02417)	BD*(1) C 29-	C 32	s(33.74%)p 1.96(66.26%)	0.0000 -0.5809 -0.0040 -0.0487 -0.0106 -0.8120 -0.0113 0.0142 0.0186
	(50.16%)	-0.7083*	C 32	s(34.58%)p 1.89(65.42%)	0.0000 -0.5880 -0.0006 0.0448 -0.0145 0.8067 0.0040 -0.0271 0.0233
156.	(0.01726)	BD*(1) C 29-	C 35	s(30.74%)p 2.25(69.26%)	0.0000 0.5544 -0.0018 0.3581 0.0003 -0.4288 0.0040 -0.6168 0.0034
	(50.49%)	-0.7106*	C 35	s(25.44%)p 2.93(74.56%)	0.0000 0.5043 -0.0023 -0.3798 0.0103 0.4141 0.0000 0.6555 -0.0129
157.	(0.01321)	BD*(1) C 30-	H 31	s(30.68%)p 2.26(69.32%)	0.0000 -0.5539 0.0040 0.3381 0.0054 -0.4585 -0.0113 -0.6070 -0.0094
	(60.23%)	-0.7761*	H 31	s(100.00%)	-1.0000 0.0011
158.	(0.02466)	BD*(1) C 30-	C 34	s(34.44%)p 1.90(65.56%)	0.0000 0.5868 0.0049 0.3884 -0.0048 0.3744 0.0332 -0.6027 0.0101
	(49.86%)	-0.7061*	C 34	s(34.34%)p 1.91(65.66%)	0.0000 0.5860 0.0042 -0.3972 -0.0068 -0.3440 0.0132 0.6166 0.0124
159.	(0.01316)	BD*(1) C 32-	H 33	s(30.77%)p 2.25(69.23%)	0.0000 -0.5547 0.0031 -0.4101 -0.0065 -0.3608 -0.0091 0.6275 0.0085
	(60.22%)	-0.7760*	H 33	s(100.00%)	-1.0000 0.0012
160.	(0.02416)	BD*(1) C 32-	C 34	s(34.50%)p 1.90(65.50%)	0.0000 0.5874 0.0041 -0.3417 0.0091 0.4665 0.0341 0.5650 -0.0127
	(49.83%)	-0.7059*	C 34	s(34.53%)p 1.90(65.47%)	0.0000 0.5876 0.0030 0.3481 0.0084 -0.4425 0.0089 -0.5809 -0.0129
161.	(0.34968)	BD*(2) C 32-	C 34	s(0.00%)p 1.00(100.00%)	0.0000 0.0002 -0.0010 -0.8443 0.0183 0.0291 -0.0020 -0.5347 0.0096
	(53.07%)	-0.7285*	C 34	s(0.00%)p 1.00(100.00%)	0.0000 -0.0038 0.0011 -0.8479 0.0117 0.0232 -0.0011 -0.5295 0.0024
162.	(0.01822)	BD*(1) C 34-	C 43	s(31.13%)p 2.21(68.87%)	0.0000 0.5579 -0.0064 0.0448 -0.0005 0.8277 -0.0041 -0.0394 0.0001
	(50.34%)	-0.7095*	C 43	s(25.71%)p 2.89(74.29%)	0.0000 0.5070 -0.0045 -0.0406 0.0017 -0.8595 0.0192 0.0463 -0.0025
163.	(0.00948)	BD*(1) C 35-	H 36	s(24.46%)p 3.09(75.54%)	0.0000 -0.4946 -0.0001 0.6065 -0.0059 0.3817 0.0036 0.4913 0.0195
	(61.29%)	-0.7829*	H 36	s(100.00%)	

				-1.0000	0.0003				
164.	(0.00896)	BD*(1) C 35-	H 37	s(24.96%)p 3.01(75.04%)					
	(38.23%)	0.6183*	C 35	0.0000 -0.4996 0.0006 -0.5382 -0.0121					
				0.6042 0.0002 -0.3086 0.0152					
	(61.77%)	-0.7860*	H 37	s(100.00%)					
				-1.0000 0.0006					
165.	(0.00634)	BD*(1) C 35-	H 38	s(25.02%)p 3.00(74.98%)					
	(38.95%)	0.6241*	C 35	0.0000 -0.5002 -0.0029 -0.4451 -0.0054					
				-0.5636 0.0131 0.4834 0.0099					
	(61.05%)	-0.7813*	H 38	s(100.00%)					
				-1.0000 0.0009					
166.	(0.00666)	BD*(1) C 39-	H 40	s(24.83%)p 3.03(75.17%)					
	(39.01%)	0.6246*	C 39	0.0000 -0.4983 -0.0033 0.0558 0.0081					
				-0.5975 0.0108 -0.6255 -0.0115					
	(60.99%)	-0.7810*	H 40	s(100.00%)					
				-1.0000 0.0010					
167.	(0.00877)	BD*(1) C 39-	H 41	s(24.96%)p 3.01(75.04%)					
	(38.68%)	0.6220*	C 39	0.0000 -0.4996 0.0008 -0.4197 0.0067					
				0.6945 0.0001 -0.3025 -0.0197					
	(61.32%)	-0.7830*	H 41	s(100.00%)					
				-1.0000 0.0002					
168.	(0.00948)	BD*(1) C 39-	H 42	s(24.72%)p 3.04(75.28%)					
	(38.03%)	0.6167*	C 39	0.0000 -0.4972 -0.0001 0.7988 0.0106					
				0.2318 0.0002 0.2463 -0.0147					
	(61.97%)	-0.7872*	H 42	s(100.00%)					
				-1.0000 0.0003					
169.	(0.00546)	BD*(1) C 43-	H 44	s(24.92%)p 3.01(75.08%)					
	(38.81%)	0.6230*	C 43	0.0000 -0.4992 -0.0016 -0.3777 0.0022					
				-0.2370 -0.0160 0.7428 -0.0029					
	(61.19%)	-0.7822*	H 44	s(100.00%)					
				-1.0000 0.0011					
170.	(0.00840)	BD*(1) C 43-	H 45	s(24.55%)p 3.07(75.45%)					
	(38.63%)	0.6215*	C 43	0.0000 -0.4955 -0.0012 -0.4639 -0.0052					
				-0.3067 -0.0155 -0.6670 0.0014					
	(61.37%)	-0.7834*	H 45	s(100.00%)					
				-1.0000 0.0007					
171.	(0.00774)	BD*(1) C 43-	H 46	s(24.72%)p 3.05(75.28%)					
	(38.59%)	0.6212*	C 43	0.0000 -0.4971 -0.0010 0.8003 0.0001					
				-0.3332 -0.0154 -0.0337 0.0056					
	(61.41%)	-0.7837*	H 46	s(100.00%)					
				-1.0000 0.0007					
172.	(0.02995)	BD*(1) C 47-	C 48	s(32.52%)p 2.07(67.48%)					
	(49.33%)	0.7024*	C 47	0.0000 -0.5700 -0.0170 0.6099 0.0273					
				-0.3004 -0.0016 0.4600 0.0146					
	(50.67%)	-0.7118*	C 48	s(35.40%)p 1.82(64.60%)					
				0.0000 -0.5950 0.0022 -0.6142 -0.0073					
				0.2470 -0.0115 -0.4554 0.0104					
173.	(0.03011)	BD*(1) C 47-	C 49	s(32.81%)p 2.05(67.19%)					
	(49.33%)	0.7023*	C 47	0.0000 -0.5724 -0.0201 0.1598 0.0095					
				0.6093 0.0157 -0.5239 -0.0172					
	(50.67%)	-0.7119*	C 49	s(35.16%)p 1.84(64.84%)					
				0.0000 -0.5930 -0.0007 -0.					

176. (0.34253) BD*(2) C 48- C 52
 (53.30%) 0.7301* C 48 s(0.00%)p 1.00(100.00%)
 0.0000 -0.0024 -0.0006 0.2246 0.0023
 -0.6990 0.0037 -0.6789 0.0030
 (46.70%) -0.6834* C 52 s(0.00%)p 1.00(100.00%)
 0.0000 -0.0029 0.0017 0.2079 -0.0014
 -0.7016 0.0150 -0.6813 0.0118

177. (0.01735) BD*(1) C 48- C 59
 (49.56%) 0.7040* C 48 s(30.50%)p 2.28(69.50%)
 0.0000 0.5523 -0.0022 0.1275 -0.0059
 0.5937 -0.0055 -0.5711 0.0047
 (50.44%) -0.7102* C 59 s(25.30%)p 2.95(74.70%)
 0.0000 0.5030 -0.0014 -0.1033 -0.0052
 -0.6107 0.0074 0.6025 -0.0128

178. (0.02422) BD*(1) C 49- C 50
 (49.80%) 0.7057* C 49 s(34.23%)p 1.92(65.77%)
 0.0000 -0.5851 -0.0042 0.7551 0.0030
 0.2865 0.0149 -0.0713 -0.0126
 (50.20%) -0.7085* C 50 s(34.48%)p 1.90(65.52%)
 0.0000 -0.5872 -0.0010 -0.7524 -0.0119
 -0.2891 0.0190 0.0681 -0.0207

179. (0.01759) BD*(1) C 49- C 55
 (49.76%) 0.7054* C 49 s(30.58%)p 2.27(69.42%)
 0.0000 0.5529 -0.0036 0.5920 -0.0068
 -0.3066 -0.0010 0.4997 -0.0015
 (50.24%) -0.7088* C 55 s(25.60%)p 2.91(74.40%)
 0.0000 0.5060 -0.0027 -0.6014 0.0051
 0.3231 -0.0131 -0.5268 0.0115

180. (0.01295) BD*(1) C 50- H 51
 (39.82%) 0.6310* C 50 s(30.94%)p 2.23(69.06%)
 0.0000 -0.5562 0.0024 0.1540 0.0036
 0.5991 0.0084 -0.5549 -0.0072
 (60.18%) -0.7758* H 51 s(100.00%)
 -1.0000 0.0014

181. (0.02448) BD*(1) C 50- C 54
 (50.14%) 0.7081* C 50 s(34.44%)p 1.90(65.56%)
 0.0000 0.5869 0.0029 -0.6073 -0.0268
 0.2802 -0.0192 -0.4549 0.0129
 (49.86%) -0.7061* C 54 s(34.49%)p 1.90(65.51%)
 0.0000 0.5873 0.0033 0.5856 -0.0037
 -0.3000 -0.0118 0.4710 0.0110

182. (0.35606) BD*(2) C 50- C 54
 (46.85%) 0.6845* C 50 s(0.00%)p 1.00(100.00%)
 0.0000 0.0019 0.0007 0.2016 0.0000
 -0.6919 0.0123 -0.6930 0.0135
 (53.15%) -0.7291* C 54 s(0.00%)p 1.00(100.00%)
 0.0000 -0.0011 0.0013 0.2025 0.0010
 -0.6931 0.0068 -0.6918 0.0085

183. (0.01319) BD*(1) C 52- H 53
 (39.76%) 0.6306* C 52 s(30.83%)p 2.24(69.17%)
 0.0000 -0.5553 0.0050 0.6059 0.0131
 -0.2926 -0.0031 0.4886 0.0074
 (60.24%) -0.7761* H 53 s(100.00%)
 -1.0000 0.0011

184. (0.02380) BD*(1) C 52- C 54
 (50.18%) 0.7084* C 52 s(34.41%)p 1.91(65.59%)
 0.0000 0.5866 0.0056 -0.1752 -0.0316
 -0.5777 -0.0029 0.5388 -0.0062
 (49.82%) -0.7058* C 54 s(34.51%)p 1.90(65.49%)
 0.0000 0.5874 0.0037 0.1455 -0.0189
 0.5826 0.0055 -0.5421 -0.0107

185. (0.01803) BD*(1) C 54- C 63
 (49.71%) 0.7050* C 54 s(30.99%)p 2.23(69.01%)
 0.0000 0.5567 -0.0062 -0.7711 0.0052
 -0.2999 0.0034 0.0739 -0.0029
 (50.29%) -0.7092* C 63 s(25.65%)p 2.90(74.35%)
 0.0000 0.5064 -0.0033 0.7999 -0.0170
 0.3120 -0.0066 -0.0770 0.0014

186. (0.00964) BD*(1) C 55- H 56
 (38.83%) 0.6231* C 55 s(24.55%)p 3.07(75.45%)
 0.0000 -0.4955 -0.0002 -0.1846 -0.0049
 -0.5788 0.0065 -0.6206 -0.0156
 (61.17%) -0.7821* H 56 s(100.00%)
 -1.0000 0.0006

187. (0.00920) BD*(1) C 55- H 57
 (38.20%) 0.6181* C 55 s(24.95%)p 3.01(75.05%)
 0.0000 -0.4995 0.0009 -0.7194 -0.0052

				0.1762	0.0159	0.4489	-0.0096	
	(61.80%)	-0.7861*	H 57	s(100.00%)				
				-1.0000	0.0004			
188.	(0.00656)	BD*(1) C 55-	H 58					
	(38.90%)	0.6237*	C 55	s(24.79%)p 3.03(75.21%)				
				0.0000	-0.4979	-0.0033	0.2944	-0.0145
				0.7277	0.0042	-0.3684	-0.0063	
	(61.10%)	-0.7816*	H 58	s(100.00%)				
				-1.0000	0.0009			
189.	(0.00644)	BD*(1) C 59-	H 60					
	(38.93%)	0.6239*	C 59	s(25.03%)p 3.00(74.97%)				
				0.0000	-0.5003	-0.0027	0.6852	-0.0081
				-0.0063	-0.0115	0.5291	0.0105	
	(61.07%)	-0.7815*	H 60	s(100.00%)				
				-1.0000	0.0009			
190.	(0.00769)	BD*(1) C 59-	H 61					
	(38.86%)	0.6234*	C 59	s(24.78%)p 3.04(75.22%)				
				0.0000	-0.4978	0.0001	-0.7169	0.0044
				0.1638	-0.0088	0.4592	0.0190	
	(61.14%)	-0.7819*	H 61	s(100.00%)				
				-1.0000	0.0008			
191.	(0.00939)	BD*(1) C 59-	H 62					
	(38.09%)	0.6172*	C 59	s(24.77%)p 3.04(75.23%)				
				0.0000	-0.4977	0.0008	-0.0757	0.0048
				-0.7747	-0.0124	-0.3822	0.0123	
	(61.91%)	-0.7868*	H 62	s(100.00%)				
				-1.0000	0.0003			
192.	(0.00825)	BD*(1) C 63-	H 64					
	(38.59%)	0.6212*	C 63	s(24.67%)p 3.05(75.33%)				
				0.0000	-0.4967	-0.0012	0.0114	0.0144
				0.8356	0.0057	0.2339	0.0030	
	(61.41%)	-0.7837*	H 64	s(100.00%)				
				-1.0000	0.0007			
193.	(0.00545)	BD*(1) C 63-	H 65					
	(38.83%)	0.6231*	C 63	s(24.90%)p 3.02(75.10%)				
				0.0000	-0.4990	-0.0010	0.5396	0.0133
				-0.4469	0.0084	0.5096	-0.0051	
	(61.17%)	-0.7821*	H 65	s(100.00%)				
				-1.0000	0.0011			
194.	(0.00771)	BD*(1) C 63-	H 66					
	(38.63%)	0.6215*	C 63	s(24.67%)p 3.05(75.33%)				
				0.0000	-0.4967	-0.0007	0.2621	0.0162
				-0.0684	0.0012	-0.8244	-0.0009	
	(61.37%)	-0.7834*	H 66	s(100.00%)				
				-1.0000	0.0008			
195.	(0.00518)	RY (1) B 1		s(0.08%)p99.99(99.92%)				
				0.0000	0.0064	0.0281	0.0101	-0.9678
				-0.0002	0.2171	-0.0078	0.1231	
196.	(0.00449)	RY (2) B 1		s(0.33%)p99.99(99.67%)				
				0.0000	0.0013	0.0576	0.0002	-0.2016
				0.0136	-0.9709	0.0070	0.1148	
197.	(0.00290)	RY (3) B 1		s(2.72%)p35.74(97.28%)				
				0.0000	-0.0020	0.1650	-0.0123	-0.1363
				0.0050	-0.0771	-0.0227	-0.9734	
198.	(0.00176)	RY (4) B 1		s(96.85%)p 0.03(3.15%)				
				0.0000	-0.0025	0.9841	-0.0025	0.0621
				0.0005	0.0637	0.0156	0.1527	
199.	(0.00548)	RY (1) C 2		s(2.45%)p39.81(97.55%)				
				0.0000	0.0000	0.1565	0.0012	0.9469
				-0.0043	-0.2787	0.0093	0.0342	
200.	(0.00501)	RY (2) C 2		s(1.57%)p62.73(98.43%)				
				0.0000	0.0067	0.1251	-0.0045	-0.1765
				-0.0056	-0.6217	-0.0024	-0.7527	
201.	(0.00066)	RY (3) C 2		s(40.92%)p 1.44(59.08%)				
				0.0000	-0.0053	0.6396	0.0020	-0.2626
				0.0055	-0.4655	-0.0062	0.5523	
202.	(0.00059)	RY (4) C 2		s(55.07%)p 0.82(44.93%)				
				0.0000	0.0005	0.7421	-0.0069	0.0565
				-0.0012	0.5648	-0.0023	-0.3564	
203.	(0.00433)	RY (1) C 3		s(0.98%)p99.99(99.02%)				
				0.0000	-0.0434	0.0890	0.0247	0.3124
				-0.0031	-0.5750	0.0084	-0.7492	
204.	(0.00338)	RY (2) C 3		s(0.48%)p99.99(99.52%)				
				0.0000	0.0155	0.0678	0.0022	-0.9409
				0.0291	-0.0884	0.0235	-0.3172	
205.	(0.00097)	RY (3) C 3		s(2.10%)p46.53(97.90%)				
				0.0000	-0.0144	0.1443	-0.0018	-0.1111

206.	(0.00060)	RY	(4)	C	3	0.0047 -0.7935 -0.0076 0.5804 s(96.55%)p 0.04(3.45%) 0.0000 -0.0015 0.9826 -0.0200 0.0538 0.0207 0.1747 0.0150 0.0046
207.	(0.00509)	RY	(1)	C	4	s(0.35%)p99.99(99.65%) 0.0000 0.0108 0.0584 -0.0236 0.9640 0.0044 -0.1723 0.0014 0.1922
208.	(0.00440)	RY	(2)	C	4	s(1.83%)p53.50(98.17%) 0.0000 -0.0147 0.1347 -0.0050 -0.0843 0.0086 0.5142 0.0057 0.8426
209.	(0.00279)	RY	(3)	C	4	s(0.17%)p99.99(99.83%) 0.0000 -0.0010 0.0412 0.0034 0.2447 0.0136 0.8346 -0.0071 -0.4915
210.	(0.00137)	RY	(4)	C	4	s(97.67%)p 0.02(2.33%) 0.0000 -0.0011 0.9883 0.0029 -0.0556 -0.0055 -0.0946 -0.0023 -0.1057
211.	(0.00514)	RY	(1)	C	5	s(0.59%)p99.99(99.41%) 0.0000 0.0103 0.0762 0.0019 -0.9564 -0.0004 0.1144 -0.0094 -0.2573
212.	(0.00436)	RY	(2)	C	5	s(0.66%)p99.99(99.34%) 0.0000 0.0227 0.0783 0.0072 -0.1504 0.0086 0.5406 -0.0001 0.8236
213.	(0.00052)	RY	(3)	C	5	s(95.48%)p 0.05(4.52%) 0.0000 -0.0035 0.9771 -0.0017 0.0406 0.0079 -0.2029 0.0035 0.0477
214.	(0.00038)	RY	(4)	C	5	s(3.32%)p29.15(96.68%) 0.0000 0.0010 0.1821 -0.0007 0.2464 -0.0013 0.8082 0.0022 -0.5028
215.	(0.00371)	RY	(1)	C	6	s(0.15%)p99.99(99.85%) 0.0000 0.0358 -0.0145 0.0085 -0.4557 -0.0058 -0.3702 -0.0064 -0.8085
216.	(0.00237)	RY	(2)	C	6	s(6.31%)p14.84(93.69%) 0.0000 0.0121 0.2509 0.0215 -0.8418 -0.0046 0.3702 0.0031 0.3012
217.	(0.00082)	RY	(3)	C	6	s(2.74%)p35.44(97.26%) 0.0000 0.0000 0.1657 0.0057 0.2276 0.0178 0.8158 -0.0110 -0.5047
218.	(0.00074)	RY	(4)	C	6	s(90.93%)p 0.10(9.07%) 0.0000 -0.0046 0.9536 -0.0122 0.1748 0.0023 -0.2448 0.0059 -0.0040
219.	(0.00163)	RY	(1)	H	7	s(100.00%) 0.0013 1.0000
220.	(0.00474)	RY	(1)	C	8	s(0.18%)p99.99(99.82%) 0.0000 -0.0270 0.0320 -0.0024 -0.9103 0.0129 0.1064 0.0061 -0.3976
221.	(0.00158)	RY	(2)	C	8	s(1.37%)p72.01(98.63%) 0.0000 0.0143 0.1162 -0.0001 -0.2282 -0.0082 0.6591 -0.0121 0.7068
222.	(0.00081)	RY	(3)	C	8	s(4.92%)p19.33(95.08%) 0.0000 0.0071 0.2217 -0.0011 0.3438 0.0183 0.7032 -0.0084 -0.5812
223.	(0.00040)	RY	(4)	C	8	s(93.63%)p 0.07(6.37%) 0.0000 -0.0035 0.9676 -0.0071 -0.0212 0.0018 -0.2437 0.0073 0.0616
224.	(0.00179)	RY	(1)	H	9	s(100.00%) 0.0018 1.0000
225.	(0.00236)	RY	(1)	C	10	s(11.38%)p 7.79(88.62%) 0.0000 0.0069 0.3373 0.0049 -0.0645 0.0054 -0.3777 0.0139 0.8597
226.	(0.00208)	RY	(2)	C	10	s(11.85%)p 7.44(88.15%) 0.0000 0.0115 0.3441 0.0096 0.7427 -0.0059 -0.4923 -0.0044 -0.2956
227.	(0.00084)	RY	(3)	C	10	s(24.94%)p 3.01(75.06%) 0.0000 0.0081 0.4993 0.0123 -0.6536 0.0238 -0.3875 0.0006 -0.4155
228.	(0.00014)	RY	(4)	C	10	s(51.88%)p 0.93(48.12%) 0.0000 -0.0172 0.7201 -0.0055 0.1287 -0.0078 0.6811 -0.0029 0.0267
229.	(0.00338)	RY	(1)	H	11	s(100.00%) -0.0038 1.0000
230.	(0.00163)	RY	(1)	H	12	s(100.00%) -0.0005 1.0000
231.	(0.00142)	RY	(1)	H	13	s(100.00%) -0.0002 1.0000
232.	(0.00436)	RY	(1)	C	14	s(0.95%)p99.99(99.05%) 0.0000 -0.0294 0.0929 -0.0011 0.7763 -0.0092 -0.5013 -0.0072 -0.3695

233. (0.00229) RY (2) C 14	s(1.06%)p92.95(98.94%) 0.0000 0.0189 0.1014 -0.0203 0.5606 -0.0053 0.3328 -0.0136 0.7508
234. (0.00071) RY (3) C 14	s(0.25%)p99.99(99.75%) 0.0000 0.0003 0.0495 -0.0033 -0.2622 -0.0177 -0.7965 0.0135 0.5421
235. (0.00038) RY (4) C 14	s(97.86%)p 0.02(2.14%) 0.0000 -0.0002 0.9892 0.0117 -0.1171 0.0026 0.0529 0.0019 -0.0692
236. (0.00167) RY (1) H 15	s(100.00%) 0.0009 1.0000
237. (0.00423) RY (1) C 16	s(0.51%)p99.99(99.49%) 0.0000 -0.0324 0.0636 0.0028 0.5917 -0.0076 -0.5762 -0.0036 -0.5591
238. (0.00237) RY (2) C 16	s(0.16%)p99.99(99.84%) 0.0000 0.0203 0.0348 0.0165 -0.7700 0.0048 -0.2031 0.0196 -0.6029
239. (0.00072) RY (3) C 16	s(2.26%)p43.29(97.74%) 0.0000 0.0001 0.1503 -0.0073 -0.2337 -0.0178 -0.7744 0.0086 0.5680
240. (0.00036) RY (4) C 16	s(97.20%)p 0.03(2.80%) 0.0000 0.0006 0.9859 -0.0042 0.0244 -0.0004 0.1623 -0.0124 -0.0294
241. (0.00153) RY (1) H 17	s(100.00%) 0.0009 1.0000
242. (0.00213) RY (1) C 18	s(6.06%)p15.49(93.94%) 0.0000 0.0051 0.2462 0.0021 0.0799 0.0093 0.9572 0.0097 0.1288
243. (0.00174) RY (2) C 18	s(21.53%)p 3.64(78.47%) 0.0000 0.0157 0.4637 0.0121 0.7798 -0.0028 -0.1307 -0.0026 -0.3992
244. (0.00057) RY (3) C 18	s(14.64%)p 5.83(85.36%) 0.0000 0.0057 0.3825 0.0048 -0.5849 -0.0108 0.0462 0.0252 -0.7132
245. (0.00005) RY (4) C 18	s(57.82%)p 0.73(42.18%)
246. (0.00122) RY (1) H 19	s(100.00%) 0.0003 1.0000
247. (0.00142) RY (1) H 20	s(100.00%) -0.0005 1.0000
248. (0.00371) RY (1) H 21	s(100.00%) -0.0045 1.0000
249. (0.00435) RY (1) C 22	s(0.11%)p99.99(99.89%) 0.0000 0.0329 0.0031 -0.0087 -0.9452 0.0024 0.0959 -0.0002 -0.3101
250. (0.00219) RY (2) C 22	s(0.05%)p99.99(99.95%) 0.0000 -0.0035 0.0220 -0.0041 0.2150 0.0164 -0.5303 0.0261 -0.8192
251. (0.00073) RY (3) C 22	s(0.19%)p99.99(99.81%) 0.0000 -0.0003 0.0437 -0.0070 -0.2431 -0.0210 -0.8405 0.0149 0.4816
252. (0.00028) RY (4) C 22	s(99.75%)p 0.00(0.25%) 0.0000 -0.0012 0.9988 0.0067 0.0087 0.0010 0.0482 0.0028 -0.0020
253. (0.00133) RY (1) H 23	s(100.00%) 0.0005 1.0000
254. (0.00429) RY (1) C 24	s(0.15%)p99.99(99.85%) 0.0000 0.0339 -0.0188 -0.0011 0.3678 0.0089 0.4943 0.0099 0.7866
255. (0.00260) RY (2) C 24	s(0.22%)p99.99(99.78%) 0.0000 0.0026 0.0467 0.0340 -0.9185 -0.0110 0.3137 -0.0027 0.2336
256. (0.00065) RY (3) C 24	s(0.20%)p99.99(99.80%) 0.0000 0.0001 0.0445 -0.0085 -0.1293 -0.0211 -0.8095 0.0162 0.5703
257. (0.00036) RY (4) C 24	s(99.55%)p 0.00(0.45%) 0.0000 -0.0005 0.9977 -0.0051 0.0556 0.0016 0.0308 -0.0043 -0.0214
258. (0.00129) RY (1) H 25	s(100.00%) 0.0007 1.0000
259. (0.00429) RY (1) N 26	s(5.06%)p18.75(94.94%) 0.0000 -0.0113 0.2247 -0.0279 -0.8155 -0.0037 -0.0431 -0.0220 -0.5303
260. (0.00096) RY (2) N 26	s(1.34%)p73.87(98.66%) 0.0000 -0.0110 0.1150 0.0025 -0.3670 -0.0173 0.7379 -0.0152 0.5541
261. (0.00084) RY (3) N 26	s(0.15%)p99.99(99.85%) 0.0000 -0.0040 0.0391 0.0038 -0.3700

262.	(0.00016)	RY	(4)	N	26	0.0181 -0.6712 -0.0198 0.6406 s(93.47%)p 0.07(6.53%) 0.0000 0.0035 0.9668 0.0061 0.2482 0.0032 -0.0506 0.0059 0.0314
263.	(0.00518)	RY	(1)	C	27	s(2.12%)p46.24(97.88%) 0.0000 -0.0512 0.1362 0.0086 -0.0123 0.0163 0.9891 -0.0004 0.0072
264.	(0.00248)	RY	(2)	C	27	s(0.60%)p99.99(99.40%) 0.0000 0.0034 0.0772 0.0025 0.0930 -0.0029 -0.0166 -0.0243 0.9922
265.	(0.00191)	RY	(3)	C	27	s(8.12%)p11.31(91.88%) 0.0000 -0.0081 0.2849 -0.0100 0.9515 -0.0042 -0.0268 0.0065 -0.1116
266.	(0.00061)	RY	(4)	C	27	s(89.33%)p 0.12(10.67%) 0.0000 0.0038 0.9451 -0.0041 -0.2926 -0.0339 -0.1326 0.0026 -0.0484
267.	(0.00497)	RY	(1)	C	28	s(0.18%)p99.99(99.82%) 0.0000 0.0123 0.0404 0.0123 0.4662 0.0032 0.4827 -0.0101 -0.7400
268.	(0.00351)	RY	(2)	C	28	s(0.30%)p99.99(99.70%) 0.0000 0.0151 0.0530 -0.0020 0.2345 0.0188 -0.8749 0.0031 -0.4197
269.	(0.00183)	RY	(3)	C	28	s(6.06%)p15.49(93.94%) 0.0000 0.0029 0.2462 0.0064 0.8182 -0.0023 -0.0149 0.0056 0.5192
270.	(0.00052)	RY	(4)	C	28	s(93.49%)p 0.07(6.51%) 0.0000 -0.0025 0.9669 0.0012 -0.2407 -0.0077 0.0314 0.0004 -0.0784
271.	(0.00497)	RY	(1)	C	29	s(0.61%)p99.99(99.39%) 0.0000 0.0136 0.0771 -0.0118 -0.3772 0.0039 0.5827 0.0101 0.7154
272.	(0.00337)	RY	(2)	C	29	s(0.24%)p99.99(99.76%) 0.0000 0.0109 0.0475 0.0007 -0.3135 0.0184 -0.8115 -0.0055 0.4903
273.	(0.00144)	RY	(3)	C	29	s(0.65%)p99.99(99.35%) 0.0000 -0.0011 0.0804 0.0048 0.8709 0.0004 -0.0399 0.0042 0.4831
274.	(0.00044)	RY	(4)	C	29	s(98.53%)p 0.01(1.47%) 0.0000 -0.0023 0.9926 0.0033 -0.0263 -0.0058 -0.0033 0.0003 -0.1181
275.	(0.00438)	RY	(1)	C	30	s(1.52%)p64.68(98.48%) 0.0000 -0.0383 0.1173 -0.0069 -0.3887 -0.0012 0.6338 0.0074 0.6571
276.	(0.00229)	RY	(2)	C	30	s(0.07%)p99.99(99.93%) 0.0000 -0.0028 0.0255 -0.0055 0.3384 -0.0200 0.7668 0.0119 -0.5443
277.	(0.00069)	RY	(3)	C	30	s(1.98%)p49.49(98.02%) 0.0000 0.0010 0.1407 -0.0182 -0.8418 0.0017 -0.0026 -0.0108 -0.5206
278.	(0.00044)	RY	(4)	C	30	s(96.58%)p 0.04(3.42%) 0.0000 0.0032 0.9827 0.0016 0.1582 0.0012 -0.0953 0.0065 0.0102
279.	(0.00180)	RY	(1)	H	31	s(100.00%) 0.0011 1.0000
280.	(0.00428)	RY	(1)	C	32	s(1.41%)p70.03(98.59%) 0.0000 -0.0383 0.1123 0.0064 0.4608 -0.0017 0.4973 -0.0095 -0.7254
281.	(0.00229)	RY	(2)	C	32	s(0.02%)p99.99(99.98%) 0.0000 0.0042 0.0134 -0.0042 0.2289 0.0249 -0.8648 0.0110 -0.4458
282.	(0.00077)	RY	(3)	C	32	s(0.02%)p99.99(99.98%) 0.0000 0.0007 0.0143 -0.0171 -0.8560 0.0004 0.0390 -0.0117 -0.5149
283.	(0.00048)	RY	(4)	C	32	s(98.70%)p 0.01(1.30%) 0.0000 0.0032 0.9935 0.0014 -0.0428 -0.0004 -0.0452 -0.0037 0.0955
284.	(0.00180)	RY	(1)	H	33	s(100.00%) 0.0012 1.0000
285.	(0.00512)	RY	(1)	C	34	s(2.11%)p46.38(97.89%) 0.0000 0.0104 0.1449 -0.0016 -0.0617 -0.0106 -0.9871 0.0030 -0.0238
286.	(0.00333)	RY	(2)	C	34	s(0.00%)p 1.00(100.00%) 0.0000 -0.0004 0.0036 -0.0079 0.4831 0.0020 -0.0085 0.0195 -0.8753
287.	(0.00148)	RY	(3)	C	34	s(0.03%)p99.99(99.97%) 0.0000 -0.0003 0.0161 -0.0092 -0.8730 0.0004 0.0685 -0.0069 -0.4825

288.	(0.00036)	RY	(4)	C	34	s(97.87%)p 0.02(2.13%) 0.0000 -0.0022 0.9893 0.0023 0.0215 0.0097 0.1434 -0.0009 0.0145
289.	(0.00201)	RY	(1)	C	35	s(1.27%)p77.77(98.73%) 0.0000 -0.0012 0.1127 0.0038 0.2287 0.0070 0.9488 -0.0082 -0.1861
290.	(0.00061)	RY	(2)	C	35	s(19.72%)p 4.07(80.28%) 0.0000 0.0307 0.4430 -0.0022 -0.5123 -0.0044 0.2092 0.0013 0.7047
291.	(0.00026)	RY	(3)	C	35	s(0.09%)p99.99(99.91%) 0.0000 0.0027 0.0293 -0.0040 0.8031 -0.0021 -0.0814 -0.0040 0.5895
292.	(0.00012)	RY	(4)	C	35	s(79.04%)p 0.27(20.96%) 0.0000 -0.0153 0.8889 -0.0013 0.1999 0.0002 -0.2218 0.0040 -0.3471
293.	(0.00144)	RY	(1)	H	36	s(100.00%) 0.0003 1.0000
294.	(0.00165)	RY	(1)	H	37	s(100.00%) 0.0006 1.0000
295.	(0.00140)	RY	(1)	H	38	s(100.00%) 0.0009 1.0000
296.	(0.00177)	RY	(1)	C	39	s(1.08%)p91.45(98.92%) 0.0000 -0.0008 0.1040 -0.0019 -0.0363 0.0059 0.9838 0.0082 0.1413
297.	(0.00063)	RY	(2)	C	39	s(19.73%)p 4.07(80.27%) 0.0000 0.0311 0.4431 0.0013 0.3593 -0.0046 0.0838 -0.0015 -0.8164
298.	(0.00033)	RY	(3)	C	39	s(5.02%)p18.91(94.98%) 0.0000 -0.0068 0.2240 0.0036 -0.9303 -0.0023 -0.0164 -0.0003 -0.2898
299.	(0.00011)	RY	(4)	C	39	s(74.29%)p 0.35(25.71%) 0.0000 -0.0141 0.8618 0.0006 0.0615 0.0004 -0.1575 -0.0043 0.4781
300.	(0.00142)	RY	(1)	H	40	s(100.00%) 0.0010 1.0000
301.	(0.00174)	RY	(1)	H	41	s(100.00%) 0.0002 1.0000
302.	(0.00134)	RY	(1)	H	42	s(100.00%) 0.0003 1.0000
303.	(0.00219)	RY	(1)	C	43	s(0.05%)p99.99(99.95%) 0.0000 -0.0013 0.0219 0.0033 0.5563 0.0003 -0.0795 -0.0057 -0.8268
304.	(0.00053)	RY	(2)	C	43	s(11.48%)p 7.71(88.52%) 0.0000 0.0315 0.3374 -0.0001 -0.0929 -0.0044 -0.9355 0.0006 0.0364
305.	(0.00028)	RY	(3)	C	43	s(0.04%)p99.99(99.96%) 0.0000 0.0017 0.0192 -0.0041 0.8257 -0.0002 -0.0532 -0.0023 0.5612
306.	(0.00002)	RY	(4)	C	43	s(88.54%)p 0.13(11.46%)
307.	(0.00132)	RY	(1)	H	44	s(100.00%) 0.0011 1.0000
308.	(0.00141)	RY	(1)	H	45	s(100.00%) 0.0007 1.0000
309.	(0.00140)	RY	(1)	H	46	s(100.00%) 0.0007 1.0000
310.	(0.00470)	RY	(1)	C	47	s(1.21%)p81.34(98.79%) 0.0000 -0.0524 0.0970 -0.0159 -0.9585 -0.0147 -0.2610 0.0055 0.0222
311.	(0.00227)	RY	(2)	C	47	s(2.51%)p38.91(97.49%) 0.0000 -0.0075 0.1581 -0.0082 0.2321 0.0199 -0.7414 -0.0152 0.6088
312.	(0.00139)	RY	(3)	C	47	s(3.04%)p31.90(96.96%) 0.0000 -0.0008 0.1743 0.0034 -0.1328 0.0006 0.6166 -0.0128 0.7560
313.	(0.00059)	RY	(4)	C	47	s(93.39%)p 0.07(6.61%) 0.0000 0.0001 0.9664 0.0362 0.0816 0.0125 0.0361 -0.0012 -0.2381
314.	(0.00498)	RY	(1)	C	48	s(0.53%)p99.99(99.47%) 0.0000 0.0132 0.0718 -0.0003 -0.2007 -0.0138 -0.7125 0.0124 0.6681
315.	(0.00352)	RY	(2)	C	48	s(0.04%)p99.99(99.96%) 0.0000 0.0144 -0.0141 -0.0211 0.9471 -0.0020 0.0304 -0.0003 0.3181
316.	(0.00139)	RY	(3)	C	48	s(0.50%)p99.99(99.50%) 0.0000 0.0003 0.0709 0.0003 0.2491 -0.0022 -0.6935 -0.0036 -0.6723
317.	(0.00043)	RY	(4)	C	48	s(98.96%)p 0.01(1.04%)

		0.0000	-0.0014	0.9948	0.0056	0.0102
		0.0031	0.1013	-0.0017	0.0043	
318.	(0.00544) RY (1) C 49	s(0.99%)p99.99(99.01%)				
		0.0000	0.0096	0.0988	-0.0072	-0.7888
		0.0067	0.3326	-0.0090	-0.5070	
319.	(0.00314) RY (2) C 49	s(0.28%)p99.99(99.72%)				
		0.0000	0.0112	0.0517	-0.0111	0.5909
		-0.0071	0.6381	0.0046	-0.4905	
320.	(0.00150) RY (3) C 49	s(1.65%)p59.72(98.35%)				
		0.0000	-0.0006	0.1283	0.0017	0.1663
		0.0001	-0.6938	-0.0016	-0.6889	
321.	(0.00043) RY (4) C 49	s(97.11%)p 0.03(2.89%)				
		0.0000	-0.0024	0.9854	0.0068	0.0264
		-0.0024	0.0236	0.0011	0.1662	
322.	(0.00432) RY (1) C 50	s(1.97%)p49.80(98.03%)				
		0.0000	-0.0374	0.1352	0.0014	-0.2540
		-0.0083	-0.7053	0.0088	0.6467	
323.	(0.00270) RY (2) C 50	s(0.00%)p 1.00(100.00%)				
		0.0000	0.0013	0.0039	-0.0273	0.9443
		0.0025	-0.0411	-0.0048	0.3254	
324.	(0.00070) RY (3) C 50	s(1.31%)p75.25(98.69%)				
		0.0000	0.0010	0.1145	-0.0018	-0.2000
		0.0123	0.7069	0.0129	0.6684	
325.	(0.00046) RY (4) C 50	s(96.86%)p 0.03(3.14%)				
		0.0000	0.0040	0.9842	0.0007	0.0545
		-0.0024	0.0149	0.0006	-0.1680	
326.	(0.00178) RY (1) H 51	s(100.00%)				
		0.0014	1.0000			
327.	(0.00437) RY (1) C 52	s(0.84%)p99.99(99.16%)				
		0.0000	-0.0353	0.0847	-0.0015	-0.7374
		0.0047	0.3471	-0.0057	-0.5721	
328.	(0.00186) RY (2) C 52	s(0.01%)p 1.00(99.99%)				
		0.0000	0.0062	0.0066	-0.0148	0.6399
		-0.0114	0.6264	0.0120	-0.4444	
329.	(0.00074) RY (3) C 52	s(0.19%)p99.99(99.81%)				
		0.0000	-0.0002	0.0431	0.0037	0.2074
		-0.0132	-0.6976	-0.0127	-0.6842	
330.	(0.00041) RY (4) C 52	s(99.09%)p 0.01(0.91%)				
		0.0000	0.0015	0.9954	-0.0035	0.0496
		0.0056	-0.0035	-0.0032	0.0812	
331.	(0.00180) RY (1) H 53	s(100.00%)				
		0.0011	1.0000			
332.	(0.00514) RY (1) C 54	s(1.91%)p51.37(98.09%)				
		0.0000	0.0104	0.1378	0.0088	0.9621
		0.0116	0.2331	-0.0048	0.0268	
333.	(0.00340) RY (2) C 54	s(0.71%)p99.99(99.29%)				
		0.0000	-0.0015	0.0840	0.0093	-0.1557
		-0.0132	0.6756	0.0137	-0.7154	
334.	(0.00149) RY (3) C 54	s(0.07%)p99.99(99.93%)				
		0.0000	0.0003	0.0264	-0.0029	-0.1906
		0.0070	0.6908	0.0072	0.6969	
335.	(0.00035) RY (4) C 54	s(97.32%)p 0.03(2.68%)				
		0.0000	-0.0020	0.9865	-0.0095	-0.1159
		-0.0028	-0.1086	0.0012	0.0385	
336.	(0.00216) RY (1) C 55	s(0.92%)p99.99(99.08%)				
		0.0000	-0.0043	0.0957	-0.0044	-0.7877
		-0.0079	-0.5657	0.0067	0.2239	
337.	(0.00068) RY (2) C 55	s(18.42%)p 4.43(81.58%)				
		0.0000	0.0292	0.4282	0.0011	-0.5028
		0.0020	0.5876	-0.0038	-0.4666	
338.	(0.00024) RY (3) C 55	s(2.50%)p39.02(97.50%)				
		0.0000	-0.0073	0.1579	0.0006	-0.0883
		-0.0046	0.4877	-0.0057	0.8540	
339.	(0.00010) RY (4) C 55	s(78.27%)p 0.28(21.73%)				
340.	(0.00167) RY (1) H 56	s(100.00%)				
		0.0006	1.0000			
341.	(0.00133) RY (1) H 57	s(100.00%)				
		0.0004	1.0000			
342.	(0.00144) RY (1) H 58	s(100.00%)				
		0.0009	1.0000			
343.	(0.00193) RY (1) C 59	s(0.62%)p99.99(99.38%)				
		0.0000	-0.0018	0.0790	-0.0091	-0.9652
		0.0012	-0.2204	-0.0068	-0.1162	
344.	(0.00057) RY (2) C 59	s(21.50%)p 3.65(78.50%)				
		0.0000	0.0301	0.4627	0.0050	0.0695
		0.0009	-0.5167	-0.0001	0.7163	
345.	(0.00022) RY (3) C 59	s(0.21%)p99.99(99.79%)				

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0.0000 -0.0012 0.0463 0.0024 -0.2440
-0.0036 0.7885 -0.0020 0.5627
346. (0.00011) RY ( 4) C 59 s( 77.77%)p 0.29( 22.23%)
0.0000 -0.0158 0.8818 0.0001 0.0627
-0.0007 0.2495 0.0037 -0.3950
347. (0.00146) RY ( 1) H 60 s(100.00%)
0.0009 1.0000
348. (0.00131) RY ( 1) H 61 s(100.00%)
0.0008 1.0000
349. (0.00146) RY ( 1) H 62 s(100.00%)
0.0003 1.0000
350. (0.00219) RY ( 1) C 63 s( 0.13%)p99.99( 99.87%)
0.0000 0.0029 0.0356 0.0019 0.3619
-0.0043 -0.5920 0.0047 0.7192
351. (0.00053) RY ( 2) C 63 s( 10.83%)p 8.23( 89.17%)
0.0000 0.0303 0.3277 0.0026 0.8703
0.0022 0.3048 -0.0002 -0.2034
352. (0.00025) RY ( 3) C 63 s( 0.00%)p 1.00(100.00%)
0.0000 0.0034 0.0044 0.0012 -0.1063
-0.0027 0.7409 -0.0032 0.6632
353. (0.00002) RY ( 4) C 63 s( 89.14%)p 0.12( 10.86%)
354. (0.00143) RY ( 1) H 64 s(100.00%)
0.0007 1.0000
355. (0.00135) RY ( 1) H 65 s(100.00%)
0.0011 1.0000
356. (0.00140) RY ( 1) H 66 s(100.00%)
0.0008 1.0000

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SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
1. CR (1) B 1	118. BD*(1) C 2- C 3	1.19	7.17	0.083
1. CR (1) B 1	149. BD*(1) C 27- C 28	0.64	7.21	0.061
1. CR (1) B 1	150. BD*(1) C 27- C 29	0.82	7.22	0.069
1. CR (1) B 1	172. BD*(1) C 47- C 48	0.66	7.21	0.061
1. CR (1) B 1	173. BD*(1) C 47- C 49	0.78	7.22	0.067
2. CR (1) C 2	115. BD*(1) B 1- C 3	1.07	10.51	0.095
2. CR (1) C 2	124. BD*(1) C 4- C 6	0.75	10.63	0.080
2. CR (1) C 2	126. BD*(1) C 4- N 26	0.67	10.42	0.075
2. CR (1) C 2	127. BD*(1) C 5- C 14	0.64	10.60	0.073
2. CR (1) C 2	128. BD*(1) C 5- C 16	0.65	10.58	0.074
2. CR (1) C 2	204. RY (2) C 3	1.54	11.17	0.117
2. CR (1) C 2	208. RY (2) C 4	1.44	11.16	0.113
2. CR (1) C 2	210. RY (4) C 4	0.70	11.16	0.079
2. CR (1) C 2	211. RY (1) C 5	0.65	11.24	0.076
2. CR (1) C 2	212. RY (2) C 5	1.35	11.24	0.110
3. CR (1) C 3	115. BD*(1) B 1- C 3	1.34	10.47	0.106
3. CR (1) C 3	119. BD*(1) C 2- C 4	0.85	10.56	0.084
3. CR (1) C 3	120. BD*(1) C 2- C 5	0.70	10.55	0.077
3. CR (1) C 3	131. BD*(1) C 8- H 9	0.54	10.75	0.068
3. CR (1) C 3	132. BD*(1) C 8- C 24	0.78	10.56	0.081
3. CR (1) C 3	195. RY (1) B 1	2.78	10.81	0.155
3. CR (1) C 3	196. RY (2) B 1	0.93	10.77	0.089
3. CR (1) C 3	199. RY (1) C 2	1.39	11.22	0.112
3. CR (1) C 3	221. RY (2) C 8	1.22	10.85	0.103
4. CR (1) C 4	118. BD*(1) C 2- C 3	0.91	10.61	0.088
4. CR (1) C 4	119. BD*(1) C 2- C 4	0.56	10.63	0.069
4. CR (1) C 4	120. BD*(1) C 2- C 5	0.67	10.62	0.075
4. CR (1) C 4	124. BD*(1) C 4- C 6	0.63	10.67	0.073
4. CR (1) C 4	129. BD*(1) C 6- H 7	0.59	10.79	0.071
4. CR (1) C 4	130. BD*(1) C 6- C 22	0.72	10.65	0.078
4. CR (1) C 4	136. BD*(1) C 10- N 26	0.50	10.41	0.065
4. CR (1) C 4	146. BD*(1) C 18- N 26	0.50	10.41	0.065
4. CR (1) C 4	200. RY (2) C 2	1.67	11.29	0.122
4. CR (1) C 4	216. RY (2) C 6	1.31	10.85	0.106
4. CR (1) C 4	260. RY (2) N 26	0.76	11.10	0.082
5. CR (1) C 5	118. BD*(1) C 2- C 3	0.73	10.58	0.079
5. CR (1) C 5	119. BD*(1) C 2- C 4	0.68	10.60	0.076
5. CR (1) C 5	137. BD*(1) C 14- H 15	0.51	10.77	0.066
5. CR (1) C 5	138. BD*(1) C 14- C 24	0.62	10.68	0.073
5. CR (1) C 5	141. BD*(1) C 16- C 22	0.60	10.68	0.071
5. CR (1) C 5	199. RY (1) C 2	1.34	11.26	0.110

5. CR (1) C 5	200. RY (2) C 2	0.93	11.26	0.091
5. CR (1) C 5	233. RY (2) C 14	1.46	10.79	0.112
5. CR (1) C 5	238. RY (2) C 16	1.17	10.76	0.100
6. CR (1) C 6	119. BD* (1) C 2- C 4	1.02	10.57	0.093
6. CR (1) C 6	124. BD* (1) C 4- C 6	0.51	10.61	0.065
6. CR (1) C 6	126. BD* (1) C 4- N 26	0.69	10.40	0.076
6. CR (1) C 6	141. BD* (1) C 16- C 22	0.64	10.65	0.074
6. CR (1) C 6	147. BD* (1) C 22- H 23	0.52	10.74	0.067
6. CR (1) C 6	207. RY (1) C 4	3.12	11.05	0.166
6. CR (1) C 6	219. RY (1) H 7	0.79	10.54	0.081
6. CR (1) C 6	250. RY (2) C 22	1.30	10.70	0.105
7. CR (1) C 8	115. BD* (1) B 1- C 3	1.28	10.48	0.103
7. CR (1) C 8	118. BD* (1) C 2- C 3	0.82	10.55	0.083
7. CR (1) C 8	122. BD* (1) C 3- C 8	0.50	10.61	0.065
7. CR (1) C 8	138. BD* (1) C 14- C 24	0.60	10.65	0.071
7. CR (1) C 8	148. BD* (1) C 24- H 25	0.51	10.75	0.066
7. CR (1) C 8	203. RY (1) C 3	1.81	11.17	0.127
7. CR (1) C 8	204. RY (2) C 3	0.74	11.15	0.081
7. CR (1) C 8	224. RY (1) H 9	0.83	10.59	0.084
7. CR (1) C 8	255. RY (2) C 24	1.44	10.70	0.111
8. CR (1) C 10	229. RY (1) H 11	0.64	10.66	0.074
8. CR (1) C 10	230. RY (1) H 12	0.76	10.70	0.080
8. CR (1) C 10	231. RY (1) H 13	0.86	10.75	0.086
9. CR (1) C 14	120. BD* (1) C 2- C 5	0.83	10.56	0.083
9. CR (1) C 14	128. BD* (1) C 5- C 16	0.75	10.56	0.080
9. CR (1) C 14	132. BD* (1) C 8- C 24	0.73	10.58	0.079
9. CR (1) C 14	148. BD* (1) C 24- H 25	0.63	10.75	0.073
9. CR (1) C 14	212. RY (2) C 5	1.50	11.22	0.116
9. CR (1) C 14	213. RY (3) C 5	0.57	11.06	0.071
9. CR (1) C 14	236. RY (1) H 15	0.75	10.49	0.079
9. CR (1) C 14	255. RY (2) C 24	1.47	10.70	0.112
9. CR (1) C 14	257. RY (4) C 24	0.56	11.03	0.070
10. CR (1) C 16	120. BD* (1) C 2- C 5	0.79	10.56	0.081
10. CR (1) C 16	127. BD* (1) C 5- C 14	0.73	10.58	0.078
10. CR (1) C 16	130. BD* (1) C 6- C 22	0.77	10.59	0.081
10. CR (1) C 16	147. BD* (1) C 22- H 23	0.63	10.74	0.074
10. CR (1) C 16	211. RY (1) C 5	1.94	11.22	0.132
10. CR (1) C 16	213. RY (3) C 5	0.58	11.06	0.071
10. CR (1) C 16	241. RY (1) H 17	0.75	10.49	0.079
10. CR (1) C 16	250. RY (2) C 22	1.55	10.70	0.115
11. CR (1) C 18	246. RY (1) H 19	0.76	10.69	0.081
11. CR (1) C 18	247. RY (1) H 20	0.72	10.66	0.078
11. CR (1) C 18	248. RY (1) H 21	0.67	10.66	0.075
11. CR (1) C 18	261. RY (3) N 26	0.74	11.09	0.081
12. CR (1) C 22	124. BD* (1) C 4- C 6	0.77	10.62	0.081
12. CR (1) C 22	128. BD* (1) C 5- C 16	0.85	10.57	0.085
12. CR (1) C 22	129. BD* (1) C 6- H 7	0.56	10.74	0.069
12. CR (1) C 22	140. BD* (1) C 16- H 17	0.64	10.74	0.074
12. CR (1) C 22	216. RY (2) C 6	0.99	10.80	0.092
12. CR (1) C 22	218. RY (4) C 6	0.87	11.05	0.087
12. CR (1) C 22	238. RY (2) C 16	1.49	10.73	0.113
12. CR (1) C 22	240. RY (4) C 16	0.62	11.08	0.074
12. CR (1) C 22	253. RY (1) H 23	0.75	10.49	0.079
13. CR (1) C 24	122. BD* (1) C 3- C 8	0.76	10.61	0.080
13. CR (1) C 24	127. BD* (1) C 5- C 14	0.86	10.58	0.085
13. CR (1) C 24	137. BD* (1) C 14- H 15	0.65	10.74	0.074
13. CR (1) C 24	221. RY (2) C 8	1.15	10.87	0.100
13. CR (1) C 24	223. RY (4) C 8	0.52	11.05	0.068
13. CR (1) C 24	232. RY (1) C 14	0.52	11.12	0.068
13. CR (1) C 24	233. RY (2) C 14	1.02	10.76	0.094
13. CR (1) C 24	235. RY (4) C 14	0.79	11.06	0.083
13. CR (1) C 24	258. RY (1) H 25	0.79	10.49	0.081
14. CR (1) N 26	124. BD* (1) C 4- C 6	0.51	14.77	0.077
14. CR (1) N 26	207. RY (1) C 4	0.80	15.20	0.098
14. CR (1) N 26	208. RY (2) C 4	1.45	15.29	0.133
14. CR (1) N 26	227. RY (3) C 10	0.65	15.08	0.088
14. CR (1) N 26	244. RY (3) C 18	0.66	14.90	0.089
15. CR (1) C 27	116. BD* (1) B 1- C 27	1.18	10.46	0.099
15. CR (1) C 27	152. BD* (1) C 28- C 30	0.68	10.58	0.076
15. CR (1) C 27	154. BD* (1) C 28- C 39	0.79	10.41	0.081
15. CR (1) C 27	155. BD* (1) C 29- C 32	0.67	10.58	0.075
15. CR (1) C 27	156. BD* (1) C 29- C 35	0.84	10.41	0.083
15. CR (1) C 27	196. RY (2) B 1	3.60	10.75	0.176
15. CR (1) C 27	268. RY (2) C 28	2.00	10.94	0.132
15. CR (1) C 27	272. RY (2) C 29	1.97	10.93	0.131
16. CR (1) C 28	116. BD* (1) B 1- C 27	1.22	10.51	0.101
16. CR (1) C 28	149. BD* (1) C 27- C 28	0.59	10.61	0.070

16. CR (1) C 28	150. BD* (1) C 27- C 29	0.69	10.62	0.076
16. CR (1) C 28	157. BD* (1) C 30- H 31	0.58	10.76	0.070
16. CR (1) C 28	158. BD* (1) C 30- C 34	0.82	10.65	0.083
16. CR (1) C 28	263. RY (1) C 27	0.88	11.27	0.089
16. CR (1) C 28	264. RY (2) C 27	0.93	11.04	0.090
16. CR (1) C 28	276. RY (2) C 30	1.09	10.81	0.097
16. CR (1) C 28	297. RY (2) C 39	0.65	10.89	0.075
17. CR (1) C 29	116. BD* (1) B 1- C 27	1.23	10.51	0.102
17. CR (1) C 29	149. BD* (1) C 27- C 28	0.68	10.61	0.076
17. CR (1) C 29	150. BD* (1) C 27- C 29	0.58	10.62	0.070
17. CR (1) C 29	159. BD* (1) C 32- H 33	0.57	10.76	0.070
17. CR (1) C 29	160. BD* (1) C 32- C 34	0.82	10.65	0.083
17. CR (1) C 29	263. RY (1) C 27	0.53	11.27	0.069
17. CR (1) C 29	264. RY (2) C 27	0.90	11.04	0.089
17. CR (1) C 29	265. RY (3) C 27	0.89	11.07	0.088
17. CR (1) C 29	281. RY (2) C 32	1.26	10.81	0.104
17. CR (1) C 29	290. RY (2) C 35	0.70	10.85	0.078
18. CR (1) C 30	149. BD* (1) C 27- C 28	0.89	10.57	0.087
18. CR (1) C 30	154. BD* (1) C 28- C 39	0.63	10.41	0.072
18. CR (1) C 30	160. BD* (1) C 32- C 34	0.72	10.61	0.078
18. CR (1) C 30	162. BD* (1) C 34- C 43	0.79	10.41	0.081
18. CR (1) C 30	267. RY (1) C 28	0.71	11.21	0.080
18. CR (1) C 30	268. RY (2) C 28	1.94	10.94	0.130
18. CR (1) C 30	270. RY (4) C 28	0.50	11.10	0.067
18. CR (1) C 30	279. RY (1) H 31	0.67	10.50	0.075
18. CR (1) C 30	285. RY (1) C 34	0.59	11.18	0.072
18. CR (1) C 30	286. RY (2) C 34	2.13	10.90	0.136
19. CR (1) C 32	150. BD* (1) C 27- C 29	0.90	10.57	0.087
19. CR (1) C 32	156. BD* (1) C 29- C 35	0.59	10.42	0.070
19. CR (1) C 32	158. BD* (1) C 30- C 34	0.74	10.60	0.079
19. CR (1) C 32	162. BD* (1) C 34- C 43	0.79	10.41	0.081
19. CR (1) C 32	271. RY (1) C 29	0.72	11.21	0.080
19. CR (1) C 32	272. RY (2) C 29	1.91	10.94	0.129
19. CR (1) C 32	284. RY (1) H 33	0.69	10.51	0.076
19. CR (1) C 32	285. RY (1) C 34	0.88	11.18	0.089
19. CR (1) C 32	286. RY (2) C 34	1.89	10.90	0.128
20. CR (1) C 34	152. BD* (1) C 28- C 30	0.80	10.64	0.082
20. CR (1) C 34	155. BD* (1) C 29- C 32	0.81	10.63	0.083
20. CR (1) C 34	157. BD* (1) C 30- H 31	0.62	10.76	0.073
20. CR (1) C 34	158. BD* (1) C 30- C 34	0.52	10.65	0.066
20. CR (1) C 34	159. BD* (1) C 32- H 33	0.63	10.76	0.073
20. CR (1) C 34	160. BD* (1) C 32- C 34	0.55	10.66	0.068
20. CR (1) C 34	276. RY (2) C 30	1.58	10.81	0.117
20. CR (1) C 34	281. RY (2) C 32	1.58	10.81	0.117
20. CR (1) C 34	304. RY (2) C 43	0.75	10.69	0.080
21. CR (1) C 35	150. BD* (1) C 27- C 29	0.68	10.56	0.075
21. CR (1) C 35	271. RY (1) C 29	1.37	11.20	0.110
21. CR (1) C 35	293. RY (1) H 36	0.73	10.69	0.079
21. CR (1) C 35	294. RY (1) H 37	0.88	10.77	0.087
21. CR (1) C 35	295. RY (1) H 38	0.67	10.60	0.075
22. CR (1) C 39	149. BD* (1) C 27- C 28	0.63	10.55	0.073
22. CR (1) C 39	267. RY (1) C 28	1.41	11.20	0.112
22. CR (1) C 39	300. RY (1) H 40	0.65	10.60	0.074
22. CR (1) C 39	301. RY (1) H 41	0.81	10.84	0.084
22. CR (1) C 39	302. RY (1) H 42	0.82	10.67	0.084
23. CR (1) C 43	158. BD* (1) C 30- C 34	0.53	10.60	0.067
23. CR (1) C 43	160. BD* (1) C 32- C 34	0.51	10.61	0.066
23. CR (1) C 43	285. RY (1) C 34	1.31	11.18	0.108
23. CR (1) C 43	307. RY (1) H 44	0.70	10.60	0.077
23. CR (1) C 43	308. RY (1) H 45	0.71	10.58	0.078
23. CR (1) C 43	309. RY (1) H 46	0.72	10.59	0.078
24. CR (1) C 47	117. BD* (1) B 1- C 47	1.12	10.45	0.096
24. CR (1) C 47	175. BD* (1) C 48- C 52	0.67	10.59	0.075
24. CR (1) C 47	177. BD* (1) C 48- C 59	0.81	10.41	0.082
24. CR (1) C 47	178. BD* (1) C 49- C 50	0.71	10.59	0.077
24. CR (1) C 47	179. BD* (1) C 49- C 55	0.74	10.41	0.079
24. CR (1) C 47	195. RY (1) B 1	2.53	10.79	0.147
24. CR (1) C 47	196. RY (2) B 1	1.12	10.75	0.098
24. CR (1) C 47	315. RY (2) C 48	1.85	10.93	0.127
24. CR (1) C 47	319. RY (2) C 49	2.06	10.94	0.134
25. CR (1) C 48	117. BD* (1) B 1- C 47	1.24	10.50	0.102
25. CR (1) C 48	172. BD* (1) C 47- C 48	0.57	10.62	0.069
25. CR (1) C 48	173. BD* (1) C 47- C 49	0.66	10.62	0.075
25. CR (1) C 48	183. BD* (1) C 52- H 53	0.58	10.76	0.071
25. CR (1) C 48	184. BD* (1) C 52- C 54	0.83	10.65	0.084
25. CR (1) C 48	310. RY (1) C 47	0.96	11.25	0.093
25. CR (1) C 48	311. RY (2) C 47	0.97	11.11	0.093

25. CR (1) C 48	313. RY (4) C 47	0.56	11.32	0.071
25. CR (1) C 48	328. RY (2) C 52	1.24	10.82	0.103
25. CR (1) C 48	344. RY (2) C 59	0.70	10.88	0.078
26. CR (1) C 49	117. BD* (1) B 1- C 47	1.20	10.50	0.100
26. CR (1) C 49	172. BD* (1) C 47- C 48	0.69	10.62	0.076
26. CR (1) C 49	173. BD* (1) C 47- C 49	0.60	10.62	0.071
26. CR (1) C 49	180. BD* (1) C 50- H 51	0.58	10.77	0.070
26. CR (1) C 49	181. BD* (1) C 50- C 54	0.78	10.65	0.081
26. CR (1) C 49	311. RY (2) C 47	1.84	11.11	0.128
26. CR (1) C 49	323. RY (2) C 50	1.24	10.79	0.103
26. CR (1) C 49	337. RY (2) C 55	0.66	10.86	0.075
27. CR (1) C 50	173. BD* (1) C 47- C 49	0.91	10.57	0.088
27. CR (1) C 50	179. BD* (1) C 49- C 55	0.64	10.42	0.073
27. CR (1) C 50	184. BD* (1) C 52- C 54	0.72	10.61	0.078
27. CR (1) C 50	185. BD* (1) C 54- C 63	0.78	10.41	0.081
27. CR (1) C 50	318. RY (1) C 49	0.85	11.20	0.087
27. CR (1) C 50	319. RY (2) C 49	1.73	10.94	0.123
27. CR (1) C 50	326. RY (1) H 51	0.71	10.49	0.077
27. CR (1) C 50	332. RY (1) C 54	1.20	11.18	0.104
27. CR (1) C 50	333. RY (2) C 54	1.47	10.90	0.113
28. CR (1) C 52	172. BD* (1) C 47- C 48	0.91	10.57	0.088
28. CR (1) C 52	177. BD* (1) C 48- C 59	0.61	10.41	0.071
28. CR (1) C 52	181. BD* (1) C 50- C 54	0.74	10.60	0.079
28. CR (1) C 52	185. BD* (1) C 54- C 63	0.78	10.41	0.080
28. CR (1) C 52	314. RY (1) C 48	0.63	11.21	0.075
28. CR (1) C 52	315. RY (2) C 48	2.19	10.93	0.138
28. CR (1) C 52	331. RY (1) H 53	0.69	10.51	0.076
28. CR (1) C 52	333. RY (2) C 54	2.53	10.90	0.148
29. CR (1) C 54	175. BD* (1) C 48- C 52	0.81	10.64	0.083
29. CR (1) C 54	178. BD* (1) C 49- C 50	0.77	10.64	0.081
29. CR (1) C 54	180. BD* (1) C 50- H 51	0.63	10.77	0.073
29. CR (1) C 54	181. BD* (1) C 50- C 54	0.52	10.65	0.067
29. CR (1) C 54	183. BD* (1) C 52- H 53	0.62	10.76	0.073
29. CR (1) C 54	184. BD* (1) C 52- C 54	0.52	10.65	0.067
29. CR (1) C 54	323. RY (2) C 50	1.54	10.79	0.115
29. CR (1) C 54	328. RY (2) C 52	1.42	10.82	0.111
29. CR (1) C 54	351. RY (2) C 63	0.76	10.69	0.080
30. CR (1) C 55	173. BD* (1) C 47- C 49	0.59	10.56	0.071
30. CR (1) C 55	318. RY (1) C 49	1.34	11.19	0.109
30. CR (1) C 55	340. RY (1) H 56	0.77	10.75	0.081
30. CR (1) C 55	341. RY (1) H 57	0.85	10.74	0.085
30. CR (1) C 55	342. RY (1) H 58	0.67	10.59	0.075
31. CR (1) C 59	172. BD* (1) C 47- C 48	0.64	10.56	0.073
31. CR (1) C 59	314. RY (1) C 48	1.33	11.20	0.109
31. CR (1) C 59	347. RY (1) H 60	0.66	10.60	0.075
31. CR (1) C 59	348. RY (1) H 61	0.73	10.75	0.079
31. CR (1) C 59	349. RY (1) H 62	0.83	10.68	0.084
32. CR (1) C 63	181. BD* (1) C 50- C 54	0.51	10.60	0.066
32. CR (1) C 63	184. BD* (1) C 52- C 54	0.52	10.61	0.066
32. CR (1) C 63	332. RY (1) C 54	1.26	11.18	0.106
32. CR (1) C 63	354. RY (1) H 64	0.72	10.58	0.078
32. CR (1) C 63	355. RY (1) H 65	0.69	10.60	0.077
32. CR (1) C 63	356. RY (1) H 66	0.71	10.59	0.077
33. LP (1) N 26	114. LV (1) B 1	8.31	0.31	0.045
33. LP (1) N 26	115. BD* (1) B 1- C 3	0.62	0.74	0.019
33. LP (1) N 26	119. BD* (1) C 2- C 4	3.09	0.83	0.045
33. LP (1) N 26	124. BD* (1) C 4- C 6	7.68	0.87	0.073
33. LP (1) N 26	133. BD* (1) C 10- H 11	5.40	0.90	0.062
33. LP (1) N 26	134. BD* (1) C 10- H 12	1.13	0.92	0.029
33. LP (1) N 26	135. BD* (1) C 10- H 13	0.61	0.93	0.021
33. LP (1) N 26	144. BD* (1) C 18- H 20	1.50	0.91	0.033
33. LP (1) N 26	145. BD* (1) C 18- H 21	5.49	0.90	0.063
33. LP (1) N 26	208. RY (2) C 4	0.70	1.40	0.028
34. BD (1) B 1- C 3	118. BD* (1) C 2- C 3	4.42	1.06	0.061
34. BD (1) B 1- C 3	120. BD* (1) C 2- C 5	3.60	1.06	0.055
34. BD (1) B 1- C 3	122. BD* (1) C 3- C 8	3.53	1.11	0.056
34. BD (1) B 1- C 3	132. BD* (1) C 8- C 24	4.55	1.08	0.063
34. BD (1) B 1- C 3	149. BD* (1) C 27- C 28	1.41	1.10	0.035
34. BD (1) B 1- C 3	172. BD* (1) C 47- C 48	1.22	1.10	0.033
34. BD (1) B 1- C 3	174. BD* (2) C 47- C 49	1.08	0.57	0.022
34. BD (1) B 1- C 3	200. RY (2) C 2	2.09	1.73	0.054
34. BD (1) B 1- C 3	220. RY (1) C 8	1.22	1.63	0.040
35. BD (1) B 1- C 27	122. BD* (1) C 3- C 8	0.82	1.10	0.027
35. BD (1) B 1- C 27	123. BD* (2) C 3- C 8	1.61	0.55	0.027
35. BD (1) B 1- C 27	149. BD* (1) C 27- C 28	4.16	1.09	0.060
35. BD (1) B 1- C 27	150. BD* (1) C 27- C 29	4.34	1.09	0.061
35. BD (1) B 1- C 27	152. BD* (1) C 28- C 30	3.70	1.11	0.057

35. BD (1) B 1- C 27	155. BD* (1) C 29- C 32	3.47	1.11	0.055
35. BD (1) B 1- C 27	173. BD* (1) C 47- C 49	1.52	1.09	0.036
35. BD (1) B 1- C 27	174. BD* (2) C 47- C 49	0.70	0.56	0.018
35. BD (1) B 1- C 27	267. RY (1) C 28	1.71	1.73	0.048
35. BD (1) B 1- C 27	271. RY (1) C 29	1.81	1.73	0.050
36. BD (1) B 1- C 47	118. BD* (1) C 2- C 3	2.31	1.04	0.044
36. BD (1) B 1- C 47	123. BD* (2) C 3- C 8	0.73	0.55	0.018
36. BD (1) B 1- C 47	150. BD* (1) C 27- C 29	1.57	1.09	0.037
36. BD (1) B 1- C 47	151. BD* (2) C 27- C 29	1.01	0.56	0.021
36. BD (1) B 1- C 47	172. BD* (1) C 47- C 48	4.05	1.09	0.059
36. BD (1) B 1- C 47	173. BD* (1) C 47- C 49	4.16	1.09	0.060
36. BD (1) B 1- C 47	175. BD* (1) C 48- C 52	3.67	1.11	0.057
36. BD (1) B 1- C 47	178. BD* (1) C 49- C 50	3.73	1.11	0.057
36. BD (1) B 1- C 47	314. RY (1) C 48	1.78	1.73	0.050
36. BD (1) B 1- C 47	318. RY (1) C 49	2.04	1.72	0.053
37. BD (1) C 2- C 3	115. BD* (1) B 1- C 3	5.78	1.13	0.072
37. BD (1) C 2- C 3	119. BD* (1) C 2- C 4	4.06	1.22	0.063
37. BD (1) C 2- C 3	120. BD* (1) C 2- C 5	3.85	1.20	0.061
37. BD (1) C 2- C 3	122. BD* (1) C 3- C 8	2.93	1.25	0.054
37. BD (1) C 2- C 3	124. BD* (1) C 4- C 6	1.94	1.26	0.044
37. BD (1) C 2- C 3	128. BD* (1) C 5- C 16	2.28	1.21	0.047
37. BD (1) C 2- C 3	131. BD* (1) C 8- H 9	1.99	1.40	0.047
37. BD (1) C 2- C 3	196. RY (2) B 1	0.64	1.42	0.027
37. BD (1) C 2- C 3	207. RY (1) C 4	0.55	1.69	0.027
37. BD (1) C 2- C 3	208. RY (2) C 4	0.64	1.78	0.030
37. BD (1) C 2- C 3	211. RY (1) C 5	0.53	1.86	0.028
38. BD (1) C 2- C 4	118. BD* (1) C 2- C 3	4.55	1.22	0.066
38. BD (1) C 2- C 4	120. BD* (1) C 2- C 5	3.11	1.22	0.055
38. BD (1) C 2- C 4	122. BD* (1) C 3- C 8	1.37	1.27	0.037
38. BD (1) C 2- C 4	124. BD* (1) C 4- C 6	4.06	1.28	0.064
38. BD (1) C 2- C 4	126. BD* (1) C 4- N 26	1.13	1.06	0.031
38. BD (1) C 2- C 4	127. BD* (1) C 5- C 14	2.29	1.24	0.048
38. BD (1) C 2- C 4	129. BD* (1) C 6- H 7	1.82	1.40	0.045
38. BD (1) C 2- C 4	136. BD* (1) C 10- N 26	0.90	1.02	0.027
38. BD (1) C 2- C 4	146. BD* (1) C 18- N 26	1.05	1.01	0.029
38. BD (1) C 2- C 4	203. RY (1) C 3	0.92	1.83	0.037
38. BD (1) C 2- C 4	211. RY (1) C 5	1.29	1.88	0.044
38. BD (1) C 2- C 4	259. RY (1) N 26	0.70	1.83	0.032
39. BD (1) C 2- C 5	115. BD* (1) B 1- C 3	2.47	1.13	0.047
39. BD (1) C 2- C 5	118. BD* (1) C 2- C 3	3.69	1.21	0.060
39. BD (1) C 2- C 5	119. BD* (1) C 2- C 4	3.22	1.22	0.056
39. BD (1) C 2- C 5	126. BD* (1) C 4- N 26	3.61	1.05	0.055
39. BD (1) C 2- C 5	127. BD* (1) C 5- C 14	3.00	1.22	0.054
39. BD (1) C 2- C 5	128. BD* (1) C 5- C 16	3.27	1.21	0.056
39. BD (1) C 2- C 5	137. BD* (1) C 14- H 15	1.67	1.39	0.043
39. BD (1) C 2- C 5	140. BD* (1) C 16- H 17	1.57	1.39	0.042
39. BD (1) C 2- C 5	203. RY (1) C 3	1.06	1.82	0.039
39. BD (1) C 2- C 5	207. RY (1) C 4	1.45	1.69	0.044
39. BD (1) C 2- C 5	232. RY (1) C 14	0.62	1.77	0.029
40. BD (2) C 2- C 5	123. BD* (2) C 3- C 8	17.31	0.28	0.062
40. BD (2) C 2- C 5	125. BD* (2) C 4- C 6	21.03	0.26	0.067
40. BD (2) C 2- C 5	139. BD* (2) C 14- C 24	18.71	0.27	0.064
40. BD (2) C 2- C 5	142. BD* (2) C 16- C 22	18.68	0.27	0.064
40. BD (2) C 2- C 5	205. RY (3) C 3	0.79	1.10	0.026
40. BD (2) C 2- C 5	209. RY (3) C 4	0.89	0.98	0.026
40. BD (2) C 2- C 5	234. RY (3) C 14	1.48	0.86	0.032
40. BD (2) C 2- C 5	239. RY (3) C 16	1.40	0.86	0.031
41. BD (1) C 3- C 8	114. LV (1) B 1	2.64	0.71	0.039
41. BD (1) C 3- C 8	115. BD* (1) B 1- C 3	5.36	1.15	0.070
41. BD (1) C 3- C 8	116. BD* (1) B 1- C 27	0.84	1.15	0.028
41. BD (1) C 3- C 8	118. BD* (1) C 2- C 3	3.33	1.22	0.057
41. BD (1) C 3- C 8	119. BD* (1) C 2- C 4	3.36	1.23	0.057
41. BD (1) C 3- C 8	131. BD* (1) C 8- H 9	3.57	1.42	0.064
41. BD (1) C 3- C 8	132. BD* (1) C 8- C 24	3.00	1.24	0.054
41. BD (1) C 3- C 8	148. BD* (1) C 24- H 25	1.57	1.41	0.042
41. BD (1) C 3- C 8	195. RY (1) B 1	1.27	1.49	0.039
41. BD (1) C 3- C 8	200. RY (2) C 2	1.13	1.89	0.041
41. BD (1) C 3- C 8	254. RY (1) C 24	0.86	1.80	0.035
41. BD (1) C 3- C 8	255. RY (2) C 24	1.18	1.36	0.036
42. BD (2) C 3- C 8	114. LV (1) B 1	11.67	0.27	0.050
42. BD (2) C 3- C 8	116. BD* (1) B 1- C 27	2.68	0.71	0.039
42. BD (2) C 3- C 8	117. BD* (1) B 1- C 47	1.43	0.70	0.028
42. BD (2) C 3- C 8	121. BD* (2) C 2- C 5	17.46	0.27	0.062
42. BD (2) C 3- C 8	139. BD* (2) C 14- C 24	19.01	0.28	0.065
42. BD (2) C 3- C 8	201. RY (3) C 2	0.52	1.16	0.022
42. BD (2) C 3- C 8	256. RY (3) C 24	1.39	0.87	0.031
43. BD (1) C 4- C 6	118. BD* (1) C 2- C 3	2.92	1.25	0.054

43. BD (1) C 4- C 6	119. BD* (1) C 2- C 4	4.61	1.26	0.068
43. BD (1) C 4- C 6	126. BD* (1) C 4- N 26	0.86	1.09	0.027
43. BD (1) C 4- C 6	129. BD* (1) C 6- H 7	3.66	1.43	0.064
43. BD (1) C 4- C 6	130. BD* (1) C 6- C 22	3.56	1.28	0.060
43. BD (1) C 4- C 6	147. BD* (1) C 22- H 23	1.67	1.43	0.044
43. BD (1) C 4- C 6	199. RY (1) C 2	1.39	1.92	0.046
43. BD (1) C 4- C 6	249. RY (1) C 22	0.79	1.83	0.034
43. BD (1) C 4- C 6	250. RY (2) C 22	0.96	1.39	0.033
43. BD (1) C 4- C 6	259. RY (1) N 26	0.52	1.86	0.028
44. BD (2) C 4- C 6	121. BD* (2) C 2- C 5	17.13	0.29	0.063
44. BD (2) C 4- C 6	134. BD* (1) C 10- H 12	0.73	0.91	0.023
44. BD (2) C 4- C 6	136. BD* (1) C 10- N 26	1.70	0.60	0.029
44. BD (2) C 4- C 6	142. BD* (2) C 16- C 22	18.80	0.30	0.067
44. BD (2) C 4- C 6	144. BD* (1) C 18- H 20	0.70	0.90	0.022
44. BD (2) C 4- C 6	146. BD* (1) C 18- N 26	1.64	0.59	0.028
44. BD (2) C 4- C 6	201. RY (3) C 2	0.58	1.18	0.023
44. BD (2) C 4- C 6	251. RY (3) C 22	1.49	0.88	0.032
45. BD (1) C 4- N 26	119. BD* (1) C 2- C 4	1.85	1.29	0.044
45. BD (1) C 4- N 26	120. BD* (1) C 2- C 5	2.05	1.28	0.046
45. BD (1) C 4- N 26	124. BD* (1) C 4- C 6	1.68	1.33	0.042
45. BD (1) C 4- N 26	130. BD* (1) C 6- C 22	1.86	1.31	0.044
45. BD (1) C 4- N 26	134. BD* (1) C 10- H 12	1.13	1.38	0.035
45. BD (1) C 4- N 26	144. BD* (1) C 18- H 20	1.06	1.37	0.034
45. BD (1) C 4- N 26	199. RY (1) C 2	1.38	1.95	0.046
45. BD (1) C 4- N 26	226. RY (2) C 10	0.94	1.56	0.034
45. BD (1) C 4- N 26	243. RY (2) C 18	0.60	1.61	0.028
46. BD (1) C 5- C 14	119. BD* (1) C 2- C 4	2.48	1.23	0.049
46. BD (1) C 5- C 14	120. BD* (1) C 2- C 5	3.34	1.22	0.057
46. BD (1) C 5- C 14	128. BD* (1) C 5- C 16	3.00	1.22	0.054
46. BD (1) C 5- C 14	137. BD* (1) C 14- H 15	2.86	1.40	0.056
46. BD (1) C 5- C 14	138. BD* (1) C 14- C 24	3.56	1.31	0.061
46. BD (1) C 5- C 14	141. BD* (1) C 16- C 22	1.71	1.31	0.042
46. BD (1) C 5- C 14	148. BD* (1) C 24- H 25	2.22	1.41	0.050
46. BD (1) C 5- C 14	199. RY (1) C 2	1.02	1.89	0.039
46. BD (1) C 5- C 14	237. RY (1) C 16	0.74	1.80	0.032
46. BD (1) C 5- C 14	254. RY (1) C 24	0.76	1.80	0.033
46. BD (1) C 5- C 14	255. RY (2) C 24	1.34	1.36	0.038
47. BD (1) C 5- C 16	118. BD* (1) C 2- C 3	2.68	1.21	0.051
47. BD (1) C 5- C 16	120. BD* (1) C 2- C 5	3.48	1.22	0.058
47. BD (1) C 5- C 16	127. BD* (1) C 5- C 14	3.00	1.23	0.054
47. BD (1) C 5- C 16	138. BD* (1) C 14- C 24	1.76	1.31	0.043
47. BD (1) C 5- C 16	140. BD* (1) C 16- H 17	2.96	1.39	0.057
47. BD (1) C 5- C 16	141. BD* (1) C 16- C 22	3.39	1.31	0.059
47. BD (1) C 5- C 16	147. BD* (1) C 22- H 23	2.31	1.40	0.051
47. BD (1) C 5- C 16	200. RY (2) C 2	0.78	1.89	0.034
47. BD (1) C 5- C 16	232. RY (1) C 14	0.79	1.77	0.033
47. BD (1) C 5- C 16	249. RY (1) C 22	0.72	1.80	0.032
47. BD (1) C 5- C 16	250. RY (2) C 22	1.21	1.36	0.036
48. BD (1) C 6- H 7	119. BD* (1) C 2- C 4	4.83	1.14	0.066
48. BD (1) C 6- H 7	124. BD* (1) C 4- C 6	2.31	1.18	0.047
48. BD (1) C 6- H 7	130. BD* (1) C 6- C 22	1.36	1.15	0.035
48. BD (1) C 6- H 7	141. BD* (1) C 16- C 22	3.00	1.22	0.054
48. BD (1) C 6- H 7	207. RY (1) C 4	0.58	1.61	0.027
48. BD (1) C 6- H 7	208. RY (2) C 4	0.69	1.70	0.031
48. BD (1) C 6- H 7	249. RY (1) C 22	0.72	1.71	0.031
49. BD (1) C 6- C 22	124. BD* (1) C 4- C 6	3.99	1.27	0.064
49. BD (1) C 6- C 22	126. BD* (1) C 4- N 26	4.29	1.06	0.060
49. BD (1) C 6- C 22	129. BD* (1) C 6- H 7	3.13	1.40	0.059
49. BD (1) C 6- C 22	140. BD* (1) C 16- H 17	2.49	1.40	0.053
49. BD (1) C 6- C 22	141. BD* (1) C 16- C 22	3.17	1.31	0.058
49. BD (1) C 6- C 22	147. BD* (1) C 22- H 23	2.88	1.40	0.057
49. BD (1) C 6- C 22	208. RY (2) C 4	2.37	1.80	0.058
49. BD (1) C 6- C 22	237. RY (1) C 16	0.73	1.80	0.032
49. BD (1) C 6- C 22	238. RY (2) C 16	1.42	1.39	0.040
50. BD (1) C 8- H 9	114. LV (1) B 1	0.65	0.60	0.018
50. BD (1) C 8- H 9	118. BD* (1) C 2- C 3	4.13	1.10	0.060
50. BD (1) C 8- H 9	122. BD* (1) C 3- C 8	2.23	1.16	0.045
50. BD (1) C 8- H 9	132. BD* (1) C 8- C 24	1.20	1.12	0.033
50. BD (1) C 8- H 9	138. BD* (1) C 14- C 24	2.98	1.20	0.053
50. BD (1) C 8- H 9	203. RY (1) C 3	0.84	1.72	0.034
50. BD (1) C 8- H 9	254. RY (1) C 24	0.66	1.69	0.030
51. BD (1) C 8- C 24	115. BD* (1) B 1- C 3	2.56	1.13	0.048
51. BD (1) C 8- C 24	122. BD* (1) C 3- C 8	3.23	1.25	0.057
51. BD (1) C 8- C 24	131. BD* (1) C 8- H 9	2.73	1.41	0.055
51. BD (1) C 8- C 24	137. BD* (1) C 14- H 15	2.57	1.38	0.053
51. BD (1) C 8- C 24	138. BD* (1) C 14- C 24	3.19	1.30	0.057
51. BD (1) C 8- C 24	148. BD* (1) C 24- H 25	2.61	1.40	0.054

51. BD (1) C 8- C 24	204. RY (2) C 3	2.36	1.80	0.058
51. BD (1) C 8- C 24	233. RY (2) C 14	1.43	1.40	0.040
52. BD (1) C 10- H 11	134. BD* (1) C 10- H 12	1.51	1.20	0.038
52. BD (1) C 10- H 11	135. BD* (1) C 10- H 13	1.58	1.21	0.039
53. BD (1) C 10- H 12	126. BD* (1) C 4- N 26	3.02	0.93	0.047
53. BD (1) C 10- H 12	133. BD* (1) C 10- H 11	1.35	1.17	0.036
53. BD (1) C 10- H 12	135. BD* (1) C 10- H 13	1.82	1.20	0.042
54. BD (1) C 10- H 13	133. BD* (1) C 10- H 11	1.48	1.17	0.037
54. BD (1) C 10- H 13	134. BD* (1) C 10- H 12	1.96	1.19	0.043
54. BD (1) C 10- H 13	146. BD* (1) C 18- N 26	2.89	0.87	0.045
55. BD (1) C 10- N 26	119. BD* (1) C 2- C 4	1.40	1.24	0.037
55. BD (1) C 10- N 26	125. BD* (2) C 4- C 6	2.80	0.71	0.040
55. BD (1) C 10- N 26	126. BD* (1) C 4- N 26	0.60	1.06	0.023
55. BD (1) C 10- N 26	133. BD* (1) C 10- H 11	0.62	1.31	0.025
55. BD (1) C 10- N 26	134. BD* (1) C 10- H 12	0.93	1.32	0.031
55. BD (1) C 10- N 26	135. BD* (1) C 10- H 13	0.90	1.34	0.031
55. BD (1) C 10- N 26	143. BD* (1) C 18- H 19	1.46	1.32	0.039
55. BD (1) C 10- N 26	207. RY (1) C 4	0.61	1.71	0.029
55. BD (1) C 10- N 26	209. RY (3) C 4	0.91	1.43	0.032
55. BD (1) C 10- N 26	242. RY (1) C 18	0.85	1.42	0.031
56. BD (1) C 14- H 15	120. BD* (1) C 2- C 5	4.14	1.12	0.061
56. BD (1) C 14- H 15	127. BD* (1) C 5- C 14	1.53	1.13	0.037
56. BD (1) C 14- H 15	132. BD* (1) C 8- C 24	3.94	1.13	0.060
56. BD (1) C 14- H 15	138. BD* (1) C 14- C 24	2.07	1.21	0.045
56. BD (1) C 14- H 15	211. RY (1) C 5	1.23	1.77	0.042
56. BD (1) C 14- H 15	254. RY (1) C 24	0.67	1.70	0.030
57. BD (1) C 14- C 24	127. BD* (1) C 5- C 14	3.56	1.26	0.060
57. BD (1) C 14- C 24	128. BD* (1) C 5- C 16	2.94	1.25	0.054
57. BD (1) C 14- C 24	131. BD* (1) C 8- H 9	1.72	1.45	0.045
57. BD (1) C 14- C 24	132. BD* (1) C 8- C 24	3.01	1.26	0.055
57. BD (1) C 14- C 24	137. BD* (1) C 14- H 15	3.78	1.42	0.065
57. BD (1) C 14- C 24	148. BD* (1) C 24- H 25	3.51	1.44	0.063
57. BD (1) C 14- C 24	211. RY (1) C 5	1.49	1.90	0.048
57. BD (1) C 14- C 24	212. RY (2) C 5	1.17	1.91	0.042
57. BD (1) C 14- C 24	220. RY (1) C 8	0.97	1.81	0.037
57. BD (1) C 14- C 24	221. RY (2) C 8	0.75	1.55	0.030
58. BD (2) C 14- C 24	121. BD* (2) C 2- C 5	18.54	0.29	0.065
58. BD (2) C 14- C 24	123. BD* (2) C 3- C 8	16.74	0.30	0.063
58. BD (2) C 14- C 24	214. RY (4) C 5	0.72	0.98	0.024
58. BD (2) C 14- C 24	222. RY (3) C 8	1.12	0.97	0.030
59. BD (1) C 16- H 17	120. BD* (1) C 2- C 5	4.05	1.12	0.060
59. BD (1) C 16- H 17	128. BD* (1) C 5- C 16	1.57	1.12	0.038
59. BD (1) C 16- H 17	130. BD* (1) C 6- C 22	3.91	1.15	0.060
59. BD (1) C 16- H 17	141. BD* (1) C 16- C 22	1.96	1.21	0.044
59. BD (1) C 16- H 17	212. RY (2) C 5	0.90	1.78	0.036
59. BD (1) C 16- H 17	249. RY (1) C 22	0.72	1.70	0.031
60. BD (1) C 16- C 22	127. BD* (1) C 5- C 14	2.76	1.26	0.053
60. BD (1) C 16- C 22	128. BD* (1) C 5- C 16	3.44	1.25	0.059
60. BD (1) C 16- C 22	129. BD* (1) C 6- H 7	1.99	1.43	0.048
60. BD (1) C 16- C 22	130. BD* (1) C 6- C 22	3.07	1.28	0.056
60. BD (1) C 16- C 22	140. BD* (1) C 16- H 17	3.61	1.43	0.064
60. BD (1) C 16- C 22	147. BD* (1) C 22- H 23	3.68	1.43	0.065
60. BD (1) C 16- C 22	212. RY (2) C 5	2.51	1.91	0.062
60. BD (1) C 16- C 22	215. RY (1) C 6	1.15	1.83	0.041
60. BD (1) C 16- C 22	216. RY (2) C 6	0.76	1.48	0.030
61. BD (2) C 16- C 22	121. BD* (2) C 2- C 5	18.04	0.29	0.065
61. BD (2) C 16- C 22	125. BD* (2) C 4- C 6	18.30	0.29	0.065
61. BD (2) C 16- C 22	214. RY (4) C 5	0.72	0.98	0.024
61. BD (2) C 16- C 22	217. RY (3) C 6	1.34	0.92	0.031
62. BD (1) C 18- H 19	136. BD* (1) C 10- N 26	2.75	0.89	0.044
62. BD (1) C 18- H 19	144. BD* (1) C 18- H 20	1.80	1.19	0.041
62. BD (1) C 18- H 19	145. BD* (1) C 18- H 21	1.41	1.18	0.036
63. BD (1) C 18- H 20	126. BD* (1) C 4- N 26	2.95	0.94	0.047
63. BD (1) C 18- H 20	143. BD* (1) C 18- H 19	1.64	1.19	0.039
63. BD (1) C 18- H 20	145. BD* (1) C 18- H 21	1.38	1.18	0.036
64. BD (1) C 18- H 21	143. BD* (1) C 18- H 19	1.55	1.20	0.039
64. BD (1) C 18- H 21	144. BD* (1) C 18- H 20	1.50	1.19	0.038
65. BD (1) C 18- N 26	119. BD* (1) C 2- C 4	1.60	1.24	0.040
65. BD (1) C 18- N 26	125. BD* (2) C 4- C 6	2.69	0.71	0.039
65. BD (1) C 18- N 26	126. BD* (1) C 4- N 26	0.58	1.07	0.022
65. BD (1) C 18- N 26	135. BD* (1) C 10- H 13	1.46	1.34	0.039
65. BD (1) C 18- N 26	143. BD* (1) C 18- H 19	0.87	1.32	0.030
65. BD (1) C 18- N 26	144. BD* (1) C 18- H 20	1.01	1.32	0.032
65. BD (1) C 18- N 26	145. BD* (1) C 18- H 21	0.68	1.30	0.027
65. BD (1) C 18- N 26	207. RY (1) C 4	0.60	1.71	0.029
65. BD (1) C 18- N 26	209. RY (3) C 4	0.77	1.43	0.030
65. BD (1) C 18- N 26	225. RY (1) C 10	0.91	1.47	0.033

66. BD (1) C 22- H 23	124. BD* (1) C 4- C 6	3.48	1.17	0.057
66. BD (1) C 22- H 23	128. BD* (1) C 5- C 16	4.18	1.12	0.061
66. BD (1) C 22- H 23	130. BD* (1) C 6- C 22	1.40	1.15	0.036
66. BD (1) C 22- H 23	141. BD* (1) C 16- C 22	2.06	1.22	0.045
66. BD (1) C 22- H 23	215. RY (1) C 6	0.65	1.70	0.030
66. BD (1) C 22- H 23	237. RY (1) C 16	0.66	1.70	0.030
67. BD (1) C 24- H 25	122. BD* (1) C 3- C 8	3.26	1.17	0.055
67. BD (1) C 24- H 25	127. BD* (1) C 5- C 14	4.18	1.13	0.061
67. BD (1) C 24- H 25	132. BD* (1) C 8- C 24	1.24	1.14	0.034
67. BD (1) C 24- H 25	138. BD* (1) C 14- C 24	2.00	1.21	0.044
67. BD (1) C 24- H 25	220. RY (1) C 8	0.69	1.69	0.030
67. BD (1) C 24- H 25	232. RY (1) C 14	0.58	1.68	0.028
68. BD (1) C 27- C 28	115. BD* (1) B 1- C 3	0.72	1.13	0.025
68. BD (1) C 27- C 28	116. BD* (1) B 1- C 27	6.05	1.13	0.074
68. BD (1) C 27- C 28	150. BD* (1) C 27- C 29	3.57	1.24	0.059
68. BD (1) C 27- C 28	152. BD* (1) C 28- C 30	3.74	1.26	0.061
68. BD (1) C 27- C 28	154. BD* (1) C 28- C 39	1.48	1.08	0.036
68. BD (1) C 27- C 28	156. BD* (1) C 29- C 35	3.40	1.09	0.054
68. BD (1) C 27- C 28	157. BD* (1) C 30- H 31	1.76	1.38	0.044
68. BD (1) C 27- C 28	196. RY (2) B 1	0.54	1.42	0.025
68. BD (1) C 27- C 28	272. RY (2) C 29	1.10	1.61	0.037
68. BD (1) C 27- C 28	276. RY (2) C 30	0.64	1.43	0.027
69. BD (1) C 27- C 29	114. LV (1) B 1	0.53	0.69	0.017
69. BD (1) C 27- C 29	116. BD* (1) B 1- C 27	6.18	1.13	0.075
69. BD (1) C 27- C 29	149. BD* (1) C 27- C 28	3.62	1.24	0.060
69. BD (1) C 27- C 29	154. BD* (1) C 28- C 39	3.22	1.08	0.053
69. BD (1) C 27- C 29	155. BD* (1) C 29- C 32	3.70	1.26	0.061
69. BD (1) C 27- C 29	156. BD* (1) C 29- C 35	1.61	1.09	0.037
69. BD (1) C 27- C 29	159. BD* (1) C 32- H 33	1.71	1.39	0.044
69. BD (1) C 27- C 29	268. RY (2) C 28	1.06	1.61	0.037
69. BD (1) C 27- C 29	280. RY (1) C 32	0.51	1.79	0.027
69. BD (1) C 27- C 29	281. RY (2) C 32	0.64	1.44	0.027
70. BD (2) C 27- C 29	114. LV (1) B 1	12.93	0.25	0.051
70. BD (2) C 27- C 29	115. BD* (1) B 1- C 3	1.47	0.69	0.028
70. BD (2) C 27- C 29	117. BD* (1) B 1- C 47	2.17	0.68	0.034
70. BD (2) C 27- C 29	151. BD* (2) C 27- C 29	0.55	0.28	0.011
70. BD (2) C 27- C 29	153. BD* (2) C 28- C 30	23.33	0.27	0.071
70. BD (2) C 27- C 29	161. BD* (2) C 32- C 34	18.78	0.27	0.064
70. BD (2) C 27- C 29	163. BD* (1) C 35- H 36	2.11	0.86	0.038
70. BD (2) C 27- C 29	164. BD* (1) C 35- H 37	1.40	0.88	0.031
70. BD (2) C 27- C 29	269. RY (3) C 28	0.75	1.04	0.025
70. BD (2) C 27- C 29	282. RY (3) C 32	1.62	0.87	0.033
71. BD (1) C 28- C 30	116. BD* (1) B 1- C 27	2.97	1.14	0.052
71. BD (1) C 28- C 30	149. BD* (1) C 27- C 28	3.99	1.25	0.063
71. BD (1) C 28- C 30	154. BD* (1) C 28- C 39	1.21	1.09	0.032
71. BD (1) C 28- C 30	157. BD* (1) C 30- H 31	3.88	1.39	0.066
71. BD (1) C 28- C 30	158. BD* (1) C 30- C 34	4.42	1.28	0.067
71. BD (1) C 28- C 30	162. BD* (1) C 34- C 43	3.28	1.09	0.053
71. BD (1) C 28- C 30	263. RY (1) C 27	0.87	1.91	0.036
71. BD (1) C 28- C 30	285. RY (1) C 34	1.18	1.86	0.042
71. BD (1) C 28- C 30	286. RY (2) C 34	1.49	1.57	0.043
72. BD (2) C 28- C 30	151. BD* (2) C 27- C 29	16.23	0.29	0.061
72. BD (2) C 28- C 30	161. BD* (2) C 32- C 34	24.85	0.28	0.075
72. BD (2) C 28- C 30	167. BD* (1) C 39- H 41	1.63	0.89	0.034
72. BD (2) C 28- C 30	168. BD* (1) C 39- H 42	2.61	0.89	0.043
72. BD (2) C 28- C 30	287. RY (3) C 34	0.86	0.93	0.025
73. BD (1) C 28- C 39	149. BD* (1) C 27- C 28	2.09	1.16	0.044
73. BD (1) C 28- C 39	150. BD* (1) C 27- C 29	2.76	1.17	0.051
73. BD (1) C 28- C 39	152. BD* (1) C 28- C 30	1.69	1.18	0.040
73. BD (1) C 28- C 39	158. BD* (1) C 30- C 34	2.94	1.20	0.053
73. BD (1) C 28- C 39	166. BD* (1) C 39- H 40	1.99	1.23	0.044
73. BD (1) C 28- C 39	167. BD* (1) C 39- H 41	2.09	1.24	0.045
73. BD (1) C 28- C 39	168. BD* (1) C 39- H 42	2.14	1.24	0.046
73. BD (1) C 28- C 39	263. RY (1) C 27	1.09	1.82	0.040
73. BD (1) C 28- C 39	275. RY (1) C 30	0.67	1.70	0.030
74. BD (1) C 29- C 32	116. BD* (1) B 1- C 27	3.06	1.14	0.053
74. BD (1) C 29- C 32	150. BD* (1) C 27- C 29	3.99	1.25	0.063
74. BD (1) C 29- C 32	156. BD* (1) C 29- C 35	1.25	1.09	0.033
74. BD (1) C 29- C 32	159. BD* (1) C 32- H 33	3.79	1.39	0.065
74. BD (1) C 29- C 32	160. BD* (1) C 32- C 34	4.46	1.29	0.068
74. BD (1) C 29- C 32	162. BD* (1) C 34- C 43	3.26	1.09	0.053
74. BD (1) C 29- C 32	263. RY (1) C 27	1.18	1.90	0.042
74. BD (1) C 29- C 32	285. RY (1) C 34	0.87	1.86	0.036
74. BD (1) C 29- C 32	286. RY (2) C 34	1.83	1.57	0.048
74. BD (1) C 29- C 32	289. RY (1) C 35	0.53	1.40	0.024
75. BD (1) C 29- C 35	149. BD* (1) C 27- C 28	2.70	1.17	0.050
75. BD (1) C 29- C 35	150. BD* (1) C 27- C 29	2.20	1.17	0.045

75. BD (1) C 29- C 35	155. BD* (1) C 29- C 32	1.74	1.18	0.041
75. BD (1) C 29- C 35	160. BD* (1) C 32- C 34	3.03	1.21	0.054
75. BD (1) C 29- C 35	163. BD* (1) C 35- H 36	2.00	1.23	0.044
75. BD (1) C 29- C 35	164. BD* (1) C 35- H 37	2.19	1.25	0.047
75. BD (1) C 29- C 35	165. BD* (1) C 35- H 38	1.95	1.23	0.044
75. BD (1) C 29- C 35	263. RY (1) C 27	1.07	1.83	0.039
75. BD (1) C 29- C 35	280. RY (1) C 32	0.69	1.71	0.031
76. BD (1) C 30- H 31	149. BD* (1) C 27- C 28	4.09	1.13	0.061
76. BD (1) C 30- H 31	152. BD* (1) C 28- C 30	2.17	1.16	0.045
76. BD (1) C 30- H 31	158. BD* (1) C 30- C 34	1.89	1.17	0.042
76. BD (1) C 30- H 31	160. BD* (1) C 32- C 34	3.66	1.18	0.059
76. BD (1) C 30- H 31	267. RY (1) C 28	1.04	1.78	0.038
76. BD (1) C 30- H 31	285. RY (1) C 34	1.29	1.75	0.042
77. BD (1) C 30- C 34	152. BD* (1) C 28- C 30	4.25	1.28	0.066
77. BD (1) C 30- C 34	154. BD* (1) C 28- C 39	2.58	1.10	0.048
77. BD (1) C 30- C 34	157. BD* (1) C 30- H 31	3.56	1.40	0.063
77. BD (1) C 30- C 34	159. BD* (1) C 32- H 33	2.28	1.40	0.051
77. BD (1) C 30- C 34	160. BD* (1) C 32- C 34	3.49	1.30	0.060
77. BD (1) C 30- C 34	162. BD* (1) C 34- C 43	1.55	1.10	0.037
77. BD (1) C 30- C 34	169. BD* (1) C 43- H 44	0.52	1.31	0.023
77. BD (1) C 30- C 34	267. RY (1) C 28	1.04	1.90	0.040
77. BD (1) C 30- C 34	268. RY (2) C 28	2.16	1.63	0.053
77. BD (1) C 30- C 34	280. RY (1) C 32	0.66	1.80	0.031
77. BD (1) C 30- C 34	281. RY (2) C 32	0.61	1.45	0.026
77. BD (1) C 30- C 34	303. RY (1) C 43	0.60	1.31	0.025
78. BD (1) C 32- H 33	150. BD* (1) C 27- C 29	4.08	1.14	0.061
78. BD (1) C 32- H 33	155. BD* (1) C 29- C 32	2.13	1.15	0.044
78. BD (1) C 32- H 33	158. BD* (1) C 30- C 34	3.67	1.17	0.058
78. BD (1) C 32- H 33	160. BD* (1) C 32- C 34	1.96	1.18	0.043
78. BD (1) C 32- H 33	271. RY (1) C 29	1.07	1.78	0.039
78. BD (1) C 32- H 33	285. RY (1) C 34	1.36	1.75	0.043
79. BD (1) C 32- C 34	155. BD* (1) C 29- C 32	4.32	1.27	0.066
79. BD (1) C 32- C 34	156. BD* (1) C 29- C 35	2.42	1.10	0.046
79. BD (1) C 32- C 34	157. BD* (1) C 30- H 31	2.31	1.40	0.051
79. BD (1) C 32- C 34	158. BD* (1) C 30- C 34	3.53	1.29	0.060
79. BD (1) C 32- C 34	159. BD* (1) C 32- H 33	3.62	1.41	0.064
79. BD (1) C 32- C 34	162. BD* (1) C 34- C 43	1.63	1.10	0.038
79. BD (1) C 32- C 34	271. RY (1) C 29	1.05	1.90	0.040
79. BD (1) C 32- C 34	272. RY (2) C 29	2.00	1.63	0.051
79. BD (1) C 32- C 34	275. RY (1) C 30	0.64	1.80	0.030
79. BD (1) C 32- C 34	303. RY (1) C 43	0.51	1.31	0.023
80. BD (2) C 32- C 34	151. BD* (2) C 27- C 29	23.11	0.29	0.073
80. BD (2) C 32- C 34	153. BD* (2) C 28- C 30	17.78	0.28	0.063
80. BD (2) C 32- C 34	170. BD* (1) C 43- H 45	2.61	0.87	0.043
80. BD (2) C 32- C 34	171. BD* (1) C 43- H 46	2.20	0.87	0.039
80. BD (2) C 32- C 34	273. RY (3) C 29	0.85	0.99	0.026
80. BD (2) C 32- C 34	277. RY (3) C 30	1.48	0.89	0.032
81. BD (1) C 34- C 43	152. BD* (1) C 28- C 30	2.70	1.20	0.051
81. BD (1) C 34- C 43	155. BD* (1) C 29- C 32	2.76	1.19	0.051
81. BD (1) C 34- C 43	158. BD* (1) C 30- C 34	2.02	1.21	0.044
81. BD (1) C 34- C 43	160. BD* (1) C 32- C 34	2.13	1.22	0.045
81. BD (1) C 34- C 43	169. BD* (1) C 43- H 44	1.85	1.23	0.043
81. BD (1) C 34- C 43	170. BD* (1) C 43- H 45	2.02	1.23	0.045
81. BD (1) C 34- C 43	171. BD* (1) C 43- H 46	1.93	1.23	0.043
81. BD (1) C 34- C 43	275. RY (1) C 30	0.72	1.72	0.031
81. BD (1) C 34- C 43	280. RY (1) C 32	0.68	1.72	0.030
82. BD (1) C 35- H 36	151. BD* (2) C 27- C 29	4.00	0.58	0.043
82. BD (1) C 35- H 36	155. BD* (1) C 29- C 32	1.10	1.13	0.031
82. BD (1) C 35- H 36	156. BD* (1) C 29- C 35	1.09	0.95	0.029
82. BD (1) C 35- H 36	164. BD* (1) C 35- H 37	1.45	1.19	0.037
82. BD (1) C 35- H 36	165. BD* (1) C 35- H 38	1.46	1.18	0.037
82. BD (1) C 35- H 36	273. RY (3) C 29	0.74	1.28	0.028
83. BD (1) C 35- H 37	151. BD* (2) C 27- C 29	2.96	0.58	0.037
83. BD (1) C 35- H 37	155. BD* (1) C 29- C 32	1.83	1.12	0.040
83. BD (1) C 35- H 37	156. BD* (1) C 29- C 35	1.17	0.95	0.030
83. BD (1) C 35- H 37	163. BD* (1) C 35- H 36	1.49	1.17	0.037
83. BD (1) C 35- H 37	165. BD* (1) C 35- H 38	1.64	1.17	0.039
84. BD (1) C 35- H 38	150. BD* (1) C 27- C 29	4.34	1.11	0.062
84. BD (1) C 35- H 38	156. BD* (1) C 29- C 35	1.10	0.96	0.029
84. BD (1) C 35- H 38	163. BD* (1) C 35- H 36	1.60	1.17	0.039
84. BD (1) C 35- H 38	164. BD* (1) C 35- H 37	1.75	1.19	0.041
85. BD (1) C 39- H 40	149. BD* (1) C 27- C 28	3.97	1.11	0.059
85. BD (1) C 39- H 40	154. BD* (1) C 28- C 39	1.09	0.95	0.029
85. BD (1) C 39- H 40	167. BD* (1) C 39- H 41	1.71	1.19	0.040
85. BD (1) C 39- H 40	168. BD* (1) C 39- H 42	1.65	1.18	0.039
86. BD (1) C 39- H 41	114. LV (1) B 1	0.84	0.56	0.019
86. BD (1) C 39- H 41	152. BD* (1) C 28- C 30	2.24	1.13	0.045

86. BD (1) C 39- H 41	153. BD* (2) C 28- C 30	2.39	0.58	0.033
86. BD (1) C 39- H 41	154. BD* (1) C 28- C 39	1.15	0.95	0.029
86. BD (1) C 39- H 41	166. BD* (1) C 39- H 40	1.58	1.17	0.038
86. BD (1) C 39- H 41	168. BD* (1) C 39- H 42	1.55	1.18	0.038
87. BD (1) C 39- H 42	152. BD* (1) C 28- C 30	0.79	1.12	0.027
87. BD (1) C 39- H 42	153. BD* (2) C 28- C 30	4.31	0.57	0.044
87. BD (1) C 39- H 42	154. BD* (1) C 28- C 39	1.15	0.95	0.029
87. BD (1) C 39- H 42	166. BD* (1) C 39- H 40	1.55	1.17	0.038
87. BD (1) C 39- H 42	167. BD* (1) C 39- H 41	1.49	1.18	0.038
87. BD (1) C 39- H 42	269. RY (3) C 28	0.73	1.34	0.028
88. BD (1) C 43- H 44	158. BD* (1) C 30- C 34	3.99	1.15	0.060
88. BD (1) C 43- H 44	162. BD* (1) C 34- C 43	1.06	0.96	0.028
88. BD (1) C 43- H 44	170. BD* (1) C 43- H 45	1.52	1.17	0.038
88. BD (1) C 43- H 44	171. BD* (1) C 43- H 46	1.52	1.17	0.038
89. BD (1) C 43- H 45	160. BD* (1) C 32- C 34	1.52	1.16	0.037
89. BD (1) C 43- H 45	161. BD* (2) C 32- C 34	3.86	0.59	0.043
89. BD (1) C 43- H 45	162. BD* (1) C 34- C 43	1.07	0.96	0.029
89. BD (1) C 43- H 45	169. BD* (1) C 43- H 44	1.41	1.17	0.036
89. BD (1) C 43- H 45	171. BD* (1) C 43- H 46	1.32	1.17	0.035
89. BD (1) C 43- H 45	287. RY (3) C 34	0.72	1.24	0.027
90. BD (1) C 43- H 46	160. BD* (1) C 32- C 34	2.01	1.16	0.043
90. BD (1) C 43- H 46	161. BD* (2) C 32- C 34	3.40	0.59	0.040
90. BD (1) C 43- H 46	162. BD* (1) C 34- C 43	1.10	0.96	0.029
90. BD (1) C 43- H 46	169. BD* (1) C 43- H 44	1.45	1.17	0.037
90. BD (1) C 43- H 46	170. BD* (1) C 43- H 45	1.35	1.17	0.036
90. BD (1) C 43- H 46	287. RY (3) C 34	0.56	1.24	0.024
91. BD (1) C 47- C 48	114. LV (1) B 1	1.35	0.69	0.027
91. BD (1) C 47- C 48	117. BD* (1) B 1- C 47	5.90	1.12	0.073
91. BD (1) C 47- C 48	173. BD* (1) C 47- C 49	3.52	1.25	0.059
91. BD (1) C 47- C 48	175. BD* (1) C 48- C 52	3.83	1.27	0.062
91. BD (1) C 47- C 48	177. BD* (1) C 48- C 59	1.49	1.08	0.036
91. BD (1) C 47- C 48	179. BD* (1) C 49- C 55	3.17	1.09	0.052
91. BD (1) C 47- C 48	183. BD* (1) C 52- H 53	1.74	1.39	0.044
91. BD (1) C 47- C 48	196. RY (2) B 1	0.68	1.42	0.028
91. BD (1) C 47- C 48	318. RY (1) C 49	0.53	1.87	0.028
91. BD (1) C 47- C 48	319. RY (2) C 49	1.00	1.62	0.036
91. BD (1) C 47- C 48	327. RY (1) C 52	0.57	1.80	0.029
92. BD (1) C 47- C 49	117. BD* (1) B 1- C 47	5.71	1.12	0.071
92. BD (1) C 47- C 49	172. BD* (1) C 47- C 48	3.66	1.24	0.060
92. BD (1) C 47- C 49	177. BD* (1) C 48- C 59	3.42	1.08	0.054
92. BD (1) C 47- C 49	178. BD* (1) C 49- C 50	3.63	1.26	0.060
92. BD (1) C 47- C 49	179. BD* (1) C 49- C 55	1.49	1.09	0.036
92. BD (1) C 47- C 49	180. BD* (1) C 50- H 51	1.71	1.39	0.044
92. BD (1) C 47- C 49	195. RY (1) B 1	0.79	1.47	0.030
92. BD (1) C 47- C 49	314. RY (1) C 48	0.51	1.89	0.028
92. BD (1) C 47- C 49	315. RY (2) C 48	1.12	1.60	0.038
92. BD (1) C 47- C 49	322. RY (1) C 50	0.56	1.79	0.028
92. BD (1) C 47- C 49	323. RY (2) C 50	0.73	1.42	0.029
93. BD (2) C 47- C 49	114. LV (1) B 1	9.80	0.25	0.044
93. BD (2) C 47- C 49	115. BD* (1) B 1- C 3	2.25	0.69	0.035
93. BD (2) C 47- C 49	116. BD* (1) B 1- C 27	2.14	0.69	0.034
93. BD (2) C 47- C 49	174. BD* (2) C 47- C 49	0.50	0.27	0.011
93. BD (2) C 47- C 49	176. BD* (2) C 48- C 52	24.16	0.27	0.072
93. BD (2) C 47- C 49	182. BD* (2) C 50- C 54	18.56	0.27	0.063
93. BD (2) C 47- C 49	186. BD* (1) C 55- H 56	2.31	0.86	0.040
93. BD (2) C 47- C 49	187. BD* (1) C 55- H 57	1.22	0.88	0.029
93. BD (2) C 47- C 49	316. RY (3) C 48	0.95	0.95	0.027
93. BD (2) C 47- C 49	324. RY (3) C 50	1.56	0.87	0.033
94. BD (1) C 48- C 52	117. BD* (1) B 1- C 47	2.95	1.13	0.052
94. BD (1) C 48- C 52	172. BD* (1) C 47- C 48	4.21	1.25	0.065
94. BD (1) C 48- C 52	177. BD* (1) C 48- C 59	1.18	1.09	0.032
94. BD (1) C 48- C 52	183. BD* (1) C 52- H 53	3.91	1.40	0.066
94. BD (1) C 48- C 52	184. BD* (1) C 52- C 54	4.19	1.29	0.066
94. BD (1) C 48- C 52	185. BD* (1) C 54- C 63	3.25	1.09	0.053
94. BD (1) C 48- C 52	310. RY (1) C 47	0.83	1.88	0.035
94. BD (1) C 48- C 52	311. RY (2) C 47	0.56	1.74	0.028
94. BD (1) C 48- C 52	332. RY (1) C 54	1.58	1.86	0.048
94. BD (1) C 48- C 52	333. RY (2) C 54	1.45	1.58	0.043
94. BD (1) C 48- C 52	343. RY (1) C 59	0.53	1.42	0.025
95. BD (2) C 48- C 52	174. BD* (2) C 47- C 49	16.62	0.29	0.062
95. BD (2) C 48- C 52	182. BD* (2) C 50- C 54	24.93	0.28	0.075
95. BD (2) C 48- C 52	190. BD* (1) C 59- H 61	1.74	0.88	0.035
95. BD (2) C 48- C 52	191. BD* (1) C 59- H 62	2.67	0.89	0.043
95. BD (2) C 48- C 52	312. RY (3) C 47	0.73	1.12	0.026
95. BD (2) C 48- C 52	334. RY (3) C 54	0.93	0.93	0.026
96. BD (1) C 48- C 59	172. BD* (1) C 47- C 48	2.05	1.16	0.044
96. BD (1) C 48- C 59	173. BD* (1) C 47- C 49	2.67	1.17	0.050

96. BD (1) C 48- C 59	175. BD* (1) C 48- C 52	1.64	1.19	0.039
96. BD (1) C 48- C 59	184. BD* (1) C 52- C 54	3.01	1.20	0.054
96. BD (1) C 48- C 59	189. BD* (1) C 59- H 60	1.94	1.23	0.044
96. BD (1) C 48- C 59	190. BD* (1) C 59- H 61	1.99	1.23	0.044
96. BD (1) C 48- C 59	191. BD* (1) C 59- H 62	2.10	1.24	0.046
96. BD (1) C 48- C 59	310. RY (1) C 47	0.97	1.80	0.037
96. BD (1) C 48- C 59	327. RY (1) C 52	0.83	1.72	0.034
97. BD (1) C 49- C 50	117. BD* (1) B 1- C 47	2.88	1.13	0.051
97. BD (1) C 49- C 50	173. BD* (1) C 47- C 49	3.82	1.25	0.062
97. BD (1) C 49- C 50	179. BD* (1) C 49- C 55	1.34	1.10	0.034
97. BD (1) C 49- C 50	180. BD* (1) C 50- H 51	3.64	1.40	0.064
97. BD (1) C 49- C 50	181. BD* (1) C 50- C 54	4.46	1.28	0.067
97. BD (1) C 49- C 50	185. BD* (1) C 54- C 63	3.27	1.09	0.053
97. BD (1) C 49- C 50	310. RY (1) C 47	1.12	1.88	0.041
97. BD (1) C 49- C 50	332. RY (1) C 54	0.61	1.86	0.030
97. BD (1) C 49- C 50	333. RY (2) C 54	1.87	1.58	0.049
97. BD (1) C 49- C 50	336. RY (1) C 55	0.52	1.41	0.024
98. BD (1) C 49- C 55	172. BD* (1) C 47- C 48	2.82	1.17	0.051
98. BD (1) C 49- C 55	173. BD* (1) C 47- C 49	2.12	1.17	0.045
98. BD (1) C 49- C 55	178. BD* (1) C 49- C 50	1.78	1.19	0.041
98. BD (1) C 49- C 55	181. BD* (1) C 50- C 54	2.83	1.20	0.052
98. BD (1) C 49- C 55	186. BD* (1) C 55- H 56	2.08	1.23	0.045
98. BD (1) C 49- C 55	187. BD* (1) C 55- H 57	2.28	1.24	0.047
98. BD (1) C 49- C 55	188. BD* (1) C 55- H 58	2.06	1.23	0.045
98. BD (1) C 49- C 55	310. RY (1) C 47	1.03	1.80	0.038
98. BD (1) C 49- C 55	322. RY (1) C 50	0.65	1.71	0.030
99. BD (1) C 50- H 51	173. BD* (1) C 47- C 49	4.11	1.14	0.061
99. BD (1) C 50- H 51	178. BD* (1) C 49- C 50	2.05	1.16	0.044
99. BD (1) C 50- H 51	181. BD* (1) C 50- C 54	1.95	1.17	0.043
99. BD (1) C 50- H 51	184. BD* (1) C 52- C 54	3.71	1.17	0.059
99. BD (1) C 50- H 51	318. RY (1) C 49	1.17	1.77	0.041
99. BD (1) C 50- H 51	332. RY (1) C 54	1.39	1.75	0.044
100. BD (1) C 50- C 54	178. BD* (1) C 49- C 50	4.26	1.28	0.066
100. BD (1) C 50- C 54	179. BD* (1) C 49- C 55	2.64	1.11	0.048
100. BD (1) C 50- C 54	180. BD* (1) C 50- H 51	3.55	1.41	0.063
100. BD (1) C 50- C 54	183. BD* (1) C 52- H 53	2.22	1.40	0.050
100. BD (1) C 50- C 54	184. BD* (1) C 52- C 54	3.48	1.29	0.060
100. BD (1) C 50- C 54	185. BD* (1) C 54- C 63	1.55	1.10	0.037
100. BD (1) C 50- C 54	193. BD* (1) C 63- H 65	0.53	1.31	0.024
100. BD (1) C 50- C 54	318. RY (1) C 49	0.93	1.89	0.037
100. BD (1) C 50- C 54	319. RY (2) C 49	1.92	1.63	0.050
100. BD (1) C 50- C 54	327. RY (1) C 52	0.53	1.81	0.028
100. BD (1) C 50- C 54	328. RY (2) C 52	0.56	1.46	0.026
100. BD (1) C 50- C 54	350. RY (1) C 63	0.61	1.31	0.025
101. BD (2) C 50- C 54	174. BD* (2) C 47- C 49	23.89	0.29	0.074
101. BD (2) C 50- C 54	176. BD* (2) C 48- C 52	17.71	0.28	0.063
101. BD (2) C 50- C 54	192. BD* (1) C 63- H 64	1.74	0.87	0.035
101. BD (2) C 50- C 54	194. BD* (1) C 63- H 66	1.35	0.87	0.031
101. BD (2) C 50- C 54	320. RY (3) C 49	0.85	0.96	0.026
101. BD (2) C 50- C 54	329. RY (3) C 52	1.62	0.88	0.034
102. BD (1) C 52- H 53	172. BD* (1) C 47- C 48	4.13	1.14	0.061
102. BD (1) C 52- H 53	175. BD* (1) C 48- C 52	2.18	1.16	0.045
102. BD (1) C 52- H 53	181. BD* (1) C 50- C 54	3.68	1.17	0.059
102. BD (1) C 52- H 53	184. BD* (1) C 52- C 54	1.94	1.17	0.043
102. BD (1) C 52- H 53	314. RY (1) C 48	1.04	1.78	0.038
102. BD (1) C 52- H 53	332. RY (1) C 54	1.21	1.75	0.041
103. BD (1) C 52- C 54	175. BD* (1) C 48- C 52	4.13	1.28	0.065
103. BD (1) C 52- C 54	177. BD* (1) C 48- C 59	2.58	1.10	0.048
103. BD (1) C 52- C 54	180. BD* (1) C 50- H 51	2.29	1.41	0.051
103. BD (1) C 52- C 54	181. BD* (1) C 50- C 54	3.58	1.29	0.061
103. BD (1) C 52- C 54	183. BD* (1) C 52- H 53	3.66	1.40	0.064
103. BD (1) C 52- C 54	185. BD* (1) C 54- C 63	1.45	1.09	0.036
103. BD (1) C 52- C 54	314. RY (1) C 48	1.16	1.90	0.042
103. BD (1) C 52- C 54	315. RY (2) C 48	2.21	1.62	0.053
103. BD (1) C 52- C 54	322. RY (1) C 50	0.63	1.80	0.030
103. BD (1) C 52- C 54	323. RY (2) C 50	0.54	1.43	0.025
103. BD (1) C 52- C 54	350. RY (1) C 63	0.51	1.31	0.023
104. BD (1) C 54- C 63	175. BD* (1) C 48- C 52	2.68	1.20	0.051
104. BD (1) C 54- C 63	178. BD* (1) C 49- C 50	2.77	1.19	0.051
104. BD (1) C 54- C 63	181. BD* (1) C 50- C 54	2.05	1.21	0.044
104. BD (1) C 54- C 63	184. BD* (1) C 52- C 54	1.88	1.21	0.043
104. BD (1) C 54- C 63	192. BD* (1) C 63- H 64	1.95	1.23	0.044
104. BD (1) C 54- C 63	193. BD* (1) C 63- H 65	1.87	1.23	0.043
104. BD (1) C 54- C 63	194. BD* (1) C 63- H 66	1.94	1.23	0.044
104. BD (1) C 54- C 63	322. RY (1) C 50	0.72	1.72	0.031
104. BD (1) C 54- C 63	327. RY (1) C 52	0.71	1.73	0.031
105. BD (1) C 55- H 56	174. BD* (2) C 47- C 49	4.45	0.59	0.046

105. BD (1) C 55- H 56	178. BD* (1) C 49- C 50	0.86	1.13	0.028
105. BD (1) C 55- H 56	179. BD* (1) C 49- C 55	1.16	0.96	0.030
105. BD (1) C 55- H 56	187. BD* (1) C 55- H 57	1.43	1.19	0.037
105. BD (1) C 55- H 56	188. BD* (1) C 55- H 58	1.48	1.18	0.037
105. BD (1) C 55- H 56	320. RY (3) C 49	0.76	1.25	0.028
106. BD (1) C 55- H 57	174. BD* (2) C 47- C 49	2.33	0.58	0.033
106. BD (1) C 55- H 57	178. BD* (1) C 49- C 50	2.28	1.13	0.045
106. BD (1) C 55- H 57	179. BD* (1) C 49- C 55	1.25	0.96	0.031
106. BD (1) C 55- H 57	186. BD* (1) C 55- H 56	1.44	1.17	0.037
106. BD (1) C 55- H 57	188. BD* (1) C 55- H 58	1.64	1.17	0.039
107. BD (1) C 55- H 58	173. BD* (1) C 47- C 49	4.01	1.12	0.060
107. BD (1) C 55- H 58	179. BD* (1) C 49- C 55	1.15	0.96	0.030
107. BD (1) C 55- H 58	186. BD* (1) C 55- H 56	1.63	1.17	0.039
107. BD (1) C 55- H 58	187. BD* (1) C 55- H 57	1.75	1.19	0.041
108. BD (1) C 59- H 60	172. BD* (1) C 47- C 48	4.09	1.11	0.060
108. BD (1) C 59- H 60	177. BD* (1) C 48- C 59	1.07	0.95	0.028
108. BD (1) C 59- H 60	190. BD* (1) C 59- H 61	1.69	1.18	0.040
108. BD (1) C 59- H 60	191. BD* (1) C 59- H 62	1.63	1.18	0.039
109. BD (1) C 59- H 61	114. LV (1) B 1	0.85	0.56	0.020
109. BD (1) C 59- H 61	175. BD* (1) C 48- C 52	2.09	1.13	0.043
109. BD (1) C 59- H 61	176. BD* (2) C 48- C 52	2.57	0.58	0.034
109. BD (1) C 59- H 61	177. BD* (1) C 48- C 59	1.04	0.95	0.028
109. BD (1) C 59- H 61	189. BD* (1) C 59- H 60	1.54	1.18	0.038
109. BD (1) C 59- H 61	191. BD* (1) C 59- H 62	1.51	1.18	0.038
110. BD (1) C 59- H 62	175. BD* (1) C 48- C 52	0.84	1.13	0.027
110. BD (1) C 59- H 62	176. BD* (2) C 48- C 52	4.23	0.57	0.044
110. BD (1) C 59- H 62	177. BD* (1) C 48- C 59	1.12	0.95	0.029
110. BD (1) C 59- H 62	189. BD* (1) C 59- H 60	1.52	1.17	0.038
110. BD (1) C 59- H 62	190. BD* (1) C 59- H 61	1.42	1.17	0.036
110. BD (1) C 59- H 62	316. RY (3) C 48	0.77	1.26	0.028
111. BD (1) C 63- H 64	182. BD* (2) C 50- C 54	3.63	0.59	0.041
111. BD (1) C 63- H 64	184. BD* (1) C 52- C 54	1.49	1.16	0.037
111. BD (1) C 63- H 64	185. BD* (1) C 54- C 63	1.08	0.96	0.029
111. BD (1) C 63- H 64	193. BD* (1) C 63- H 65	1.42	1.17	0.036
111. BD (1) C 63- H 64	194. BD* (1) C 63- H 66	1.33	1.17	0.035
111. BD (1) C 63- H 64	334. RY (3) C 54	0.69	1.23	0.026
112. BD (1) C 63- H 65	181. BD* (1) C 50- C 54	3.91	1.15	0.060
112. BD (1) C 63- H 65	185. BD* (1) C 54- C 63	1.04	0.96	0.028
112. BD (1) C 63- H 65	192. BD* (1) C 63- H 64	1.52	1.17	0.038
112. BD (1) C 63- H 65	194. BD* (1) C 63- H 66	1.52	1.17	0.038
112. BD (1) C 63- H 65	333. RY (2) C 54	0.56	1.45	0.026
113. BD (1) C 63- H 66	182. BD* (2) C 50- C 54	2.92	0.59	0.037
113. BD (1) C 63- H 66	184. BD* (1) C 52- C 54	1.99	1.16	0.043
113. BD (1) C 63- H 66	185. BD* (1) C 54- C 63	1.07	0.96	0.029
113. BD (1) C 63- H 66	192. BD* (1) C 63- H 64	1.35	1.17	0.036
113. BD (1) C 63- H 66	193. BD* (1) C 63- H 65	1.45	1.17	0.037
113. BD (1) C 63- H 66	334. RY (3) C 54	0.60	1.23	0.024